The Simulation Experiment Description Markup Language

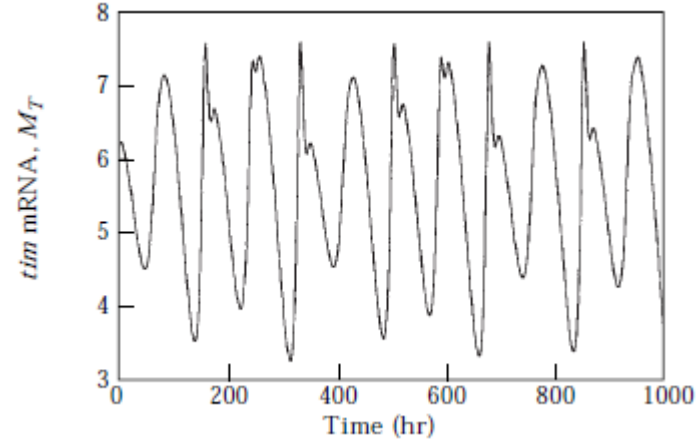
Frank T. Bergmann
HARMONY, NY

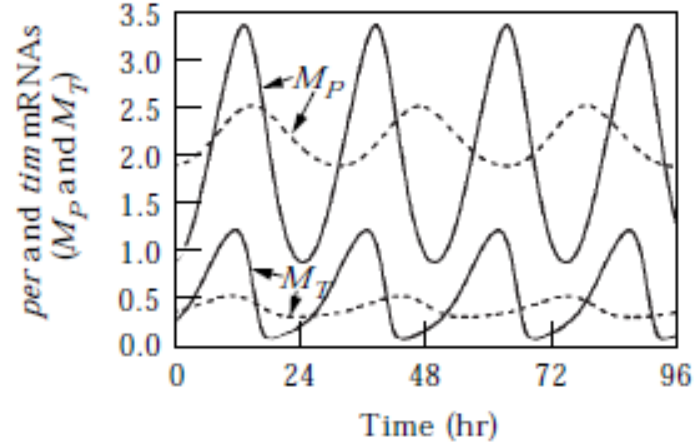
MOTIVATION

Motivation

Chaos and Birhythmicity in a Model for Circadian Oscillations of the PER and TIM Proteins in *Drosophila*

JEAN-CHRISTOPHE LELOUP AND ALBERT GOLDBETER*

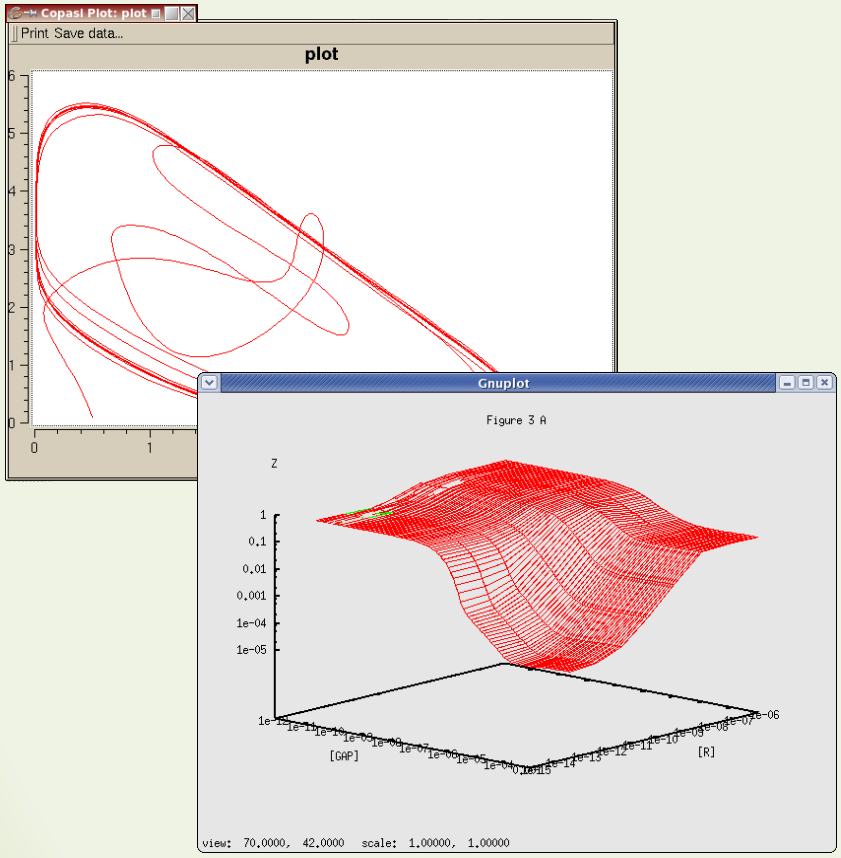




J. theor. Biol. (1999) **198**, 445-459
Article No. jtbi.1999.0924, available online at http://www.idealibrary.com

Motivation

BM 22



BM 86

- Changes in model parameterization
- Use of a number of different models in one experiment
- Choice of correct simulation algorithm
- Post-processing of the result data, e.g. normalization, logarithmic scale …

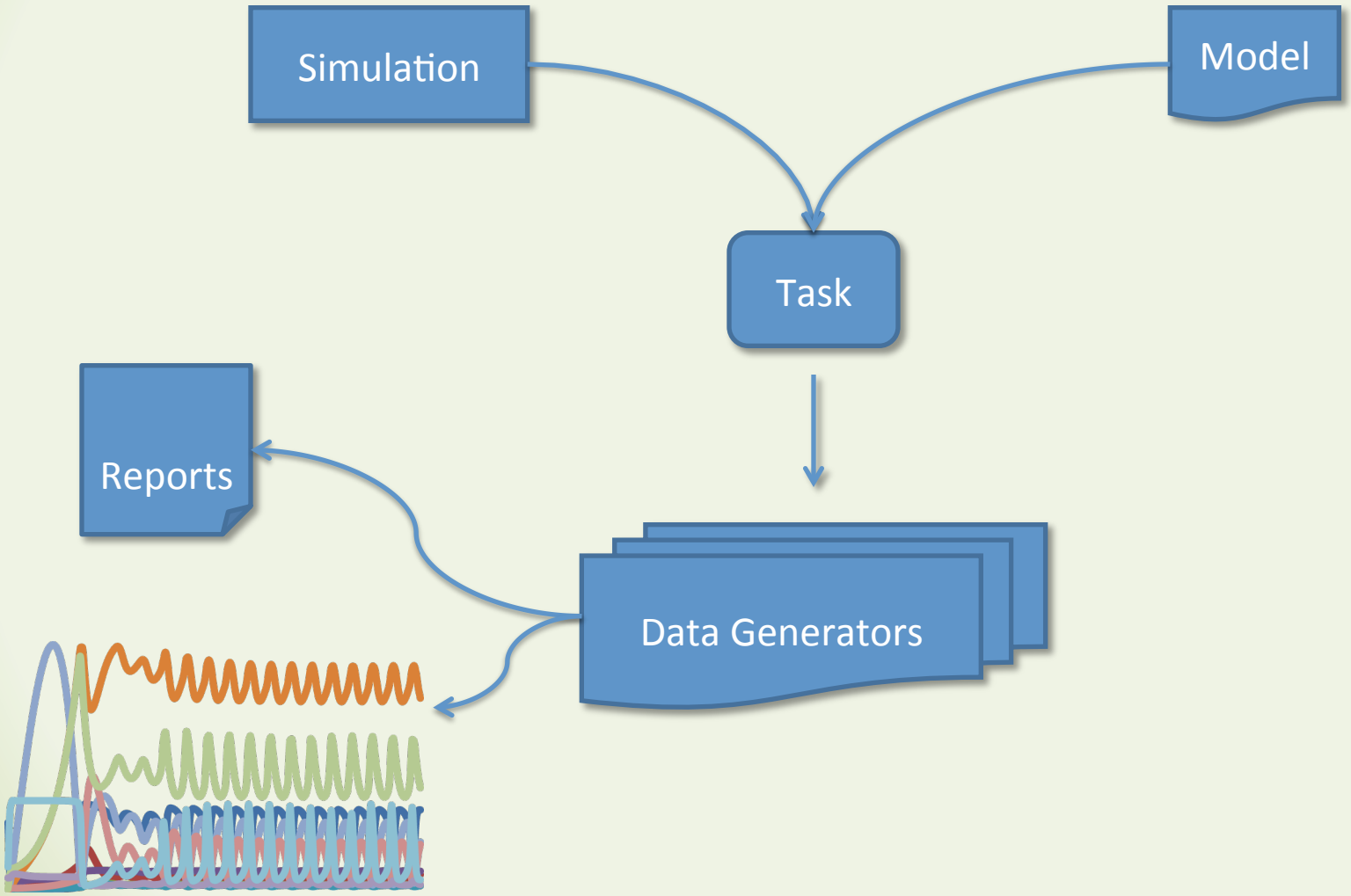
HOW DOES SED-ML HELP?

Repeatable simulation experiments

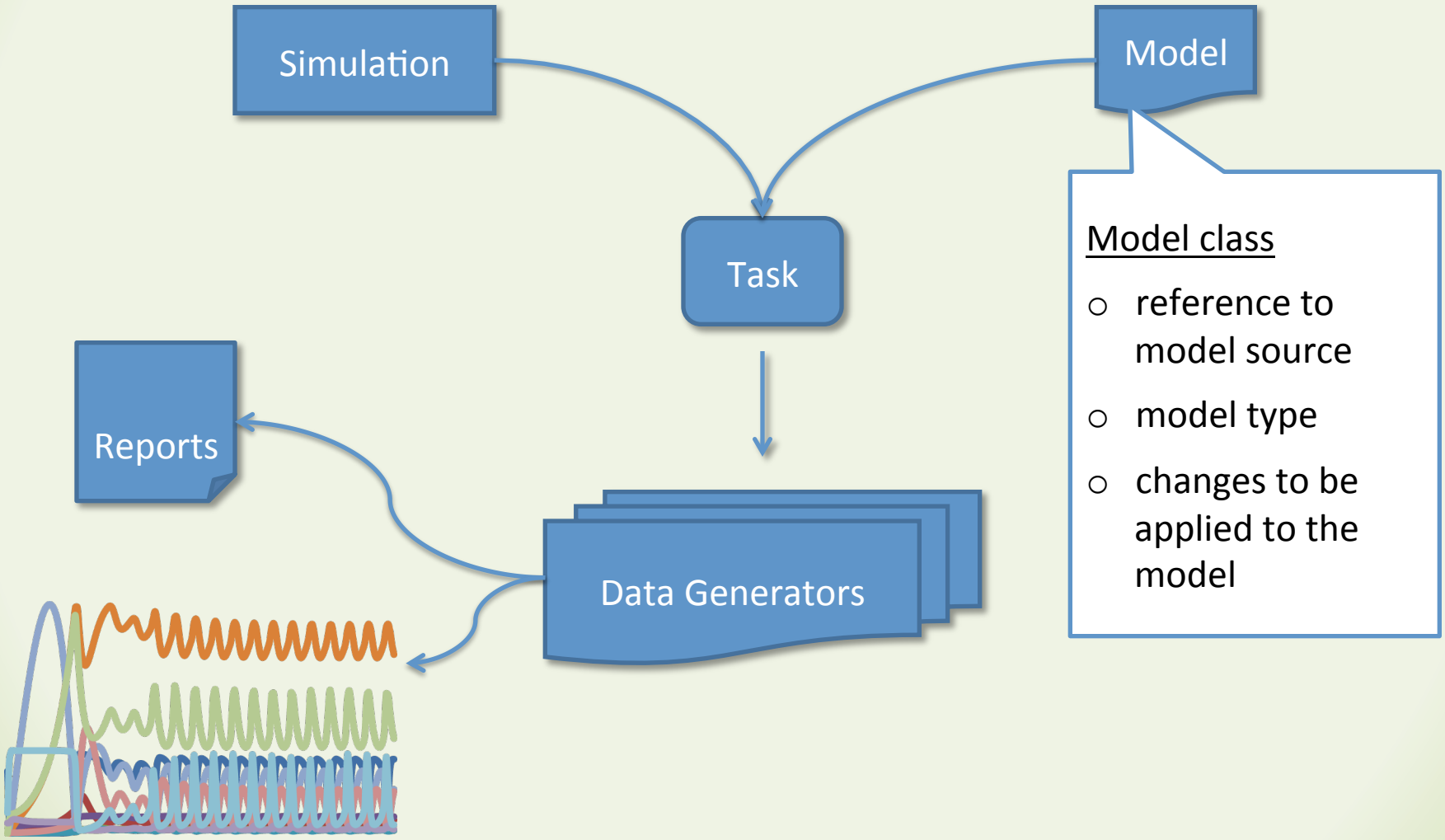
Simulation Experiment Description – Markup Language (SED-ML):

Is a language that aims to standardize the exchange of simulation experiments, independently from the model description language and the simulation tool.

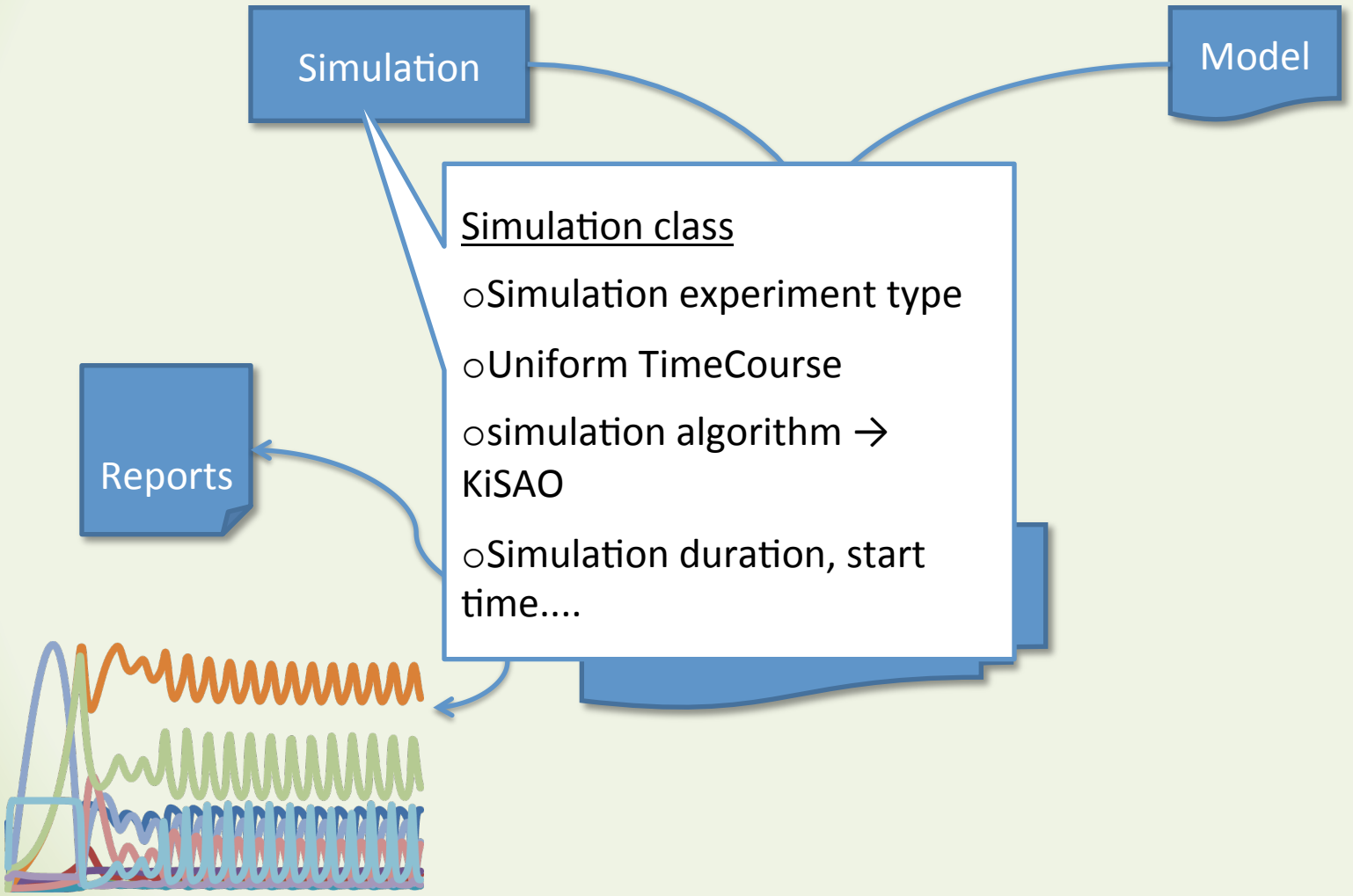
Repeatable simulation experiments



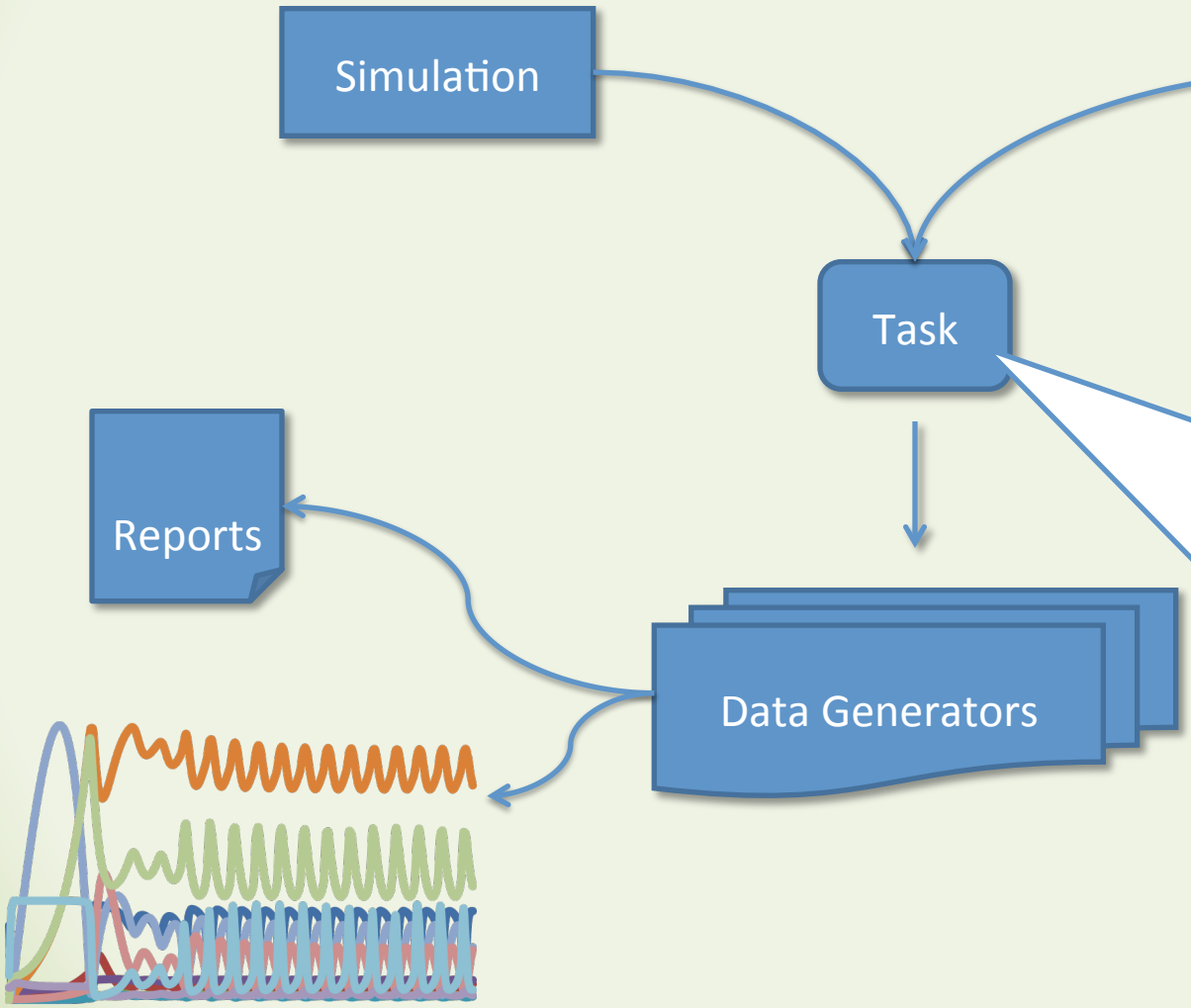
Repeatable simulation experiments



Repeatable simulation experiments



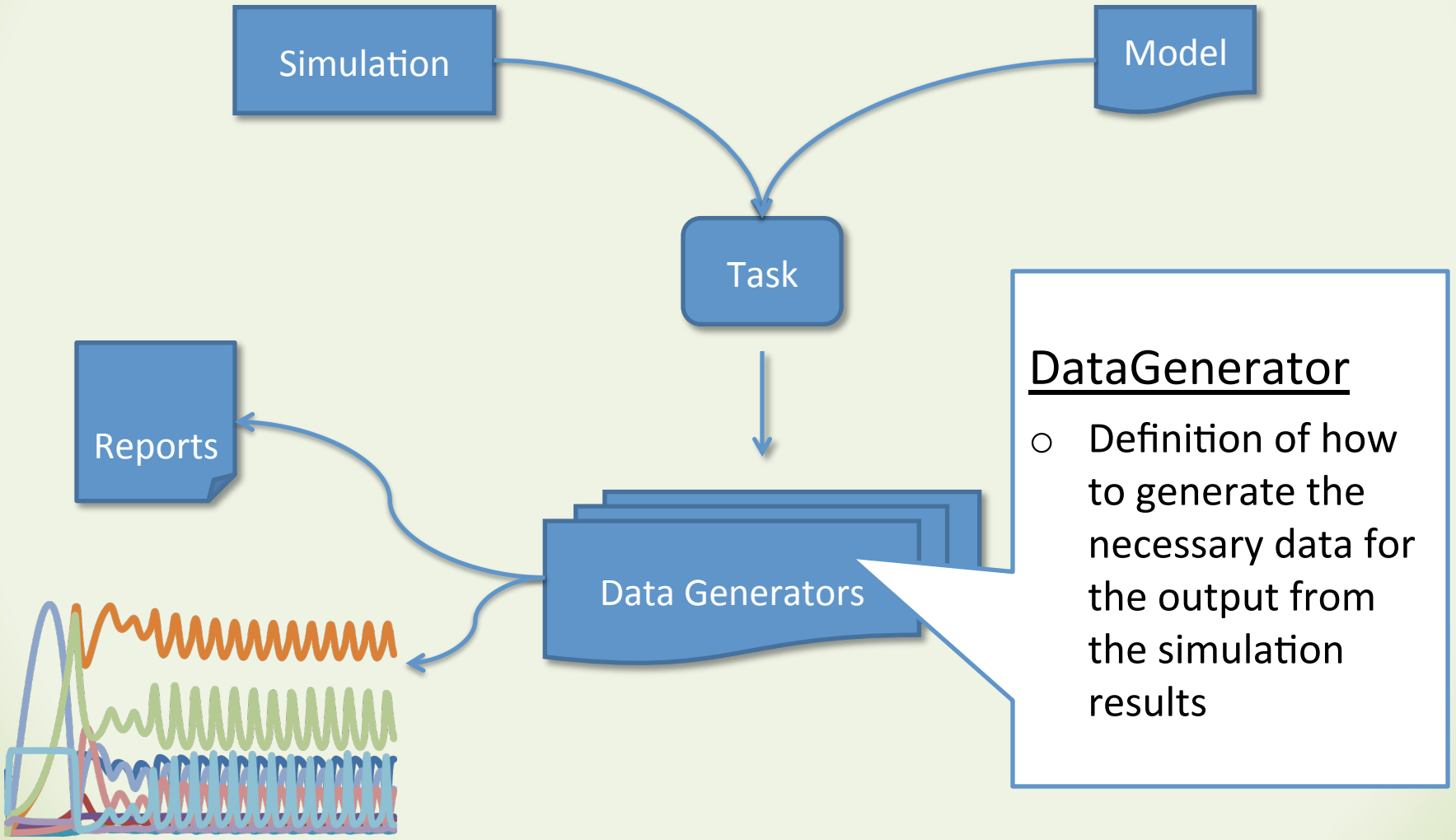
Repeatable simulation experiments



Task class

- Connector of one Model object and one Simulation object

Repeatable simulation experiments



SED-ML Main Concepts

- No storage of simulation results
  - SBRML
- No description of the layout of the output curves

SED-ML L1 V1 Released!

- final version available from

  http://sed-ml.org

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

March 25, 2011

Editors

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

To get subscribed to the mailing list, please write to the same address
sed-ml-discuss@lists.sourceforge.net.

To contact the authors of the SED-ML specification, please write to
sed-ml-editors@lists.sourceforge.net

SED-ML

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Written by libSedML v1.1.4092.21172 see http://libsedml.sf.net -->
- <sedML xmlns="http://www.biomodels.net/sed-ml">
  - <listOfSimulations>
    - <uniformTimeCourse numberOfPoints="1000" outputEndTime="380" outputStartTime="0" initialTime="0" id="simulation1">
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    </listOfSimulations>
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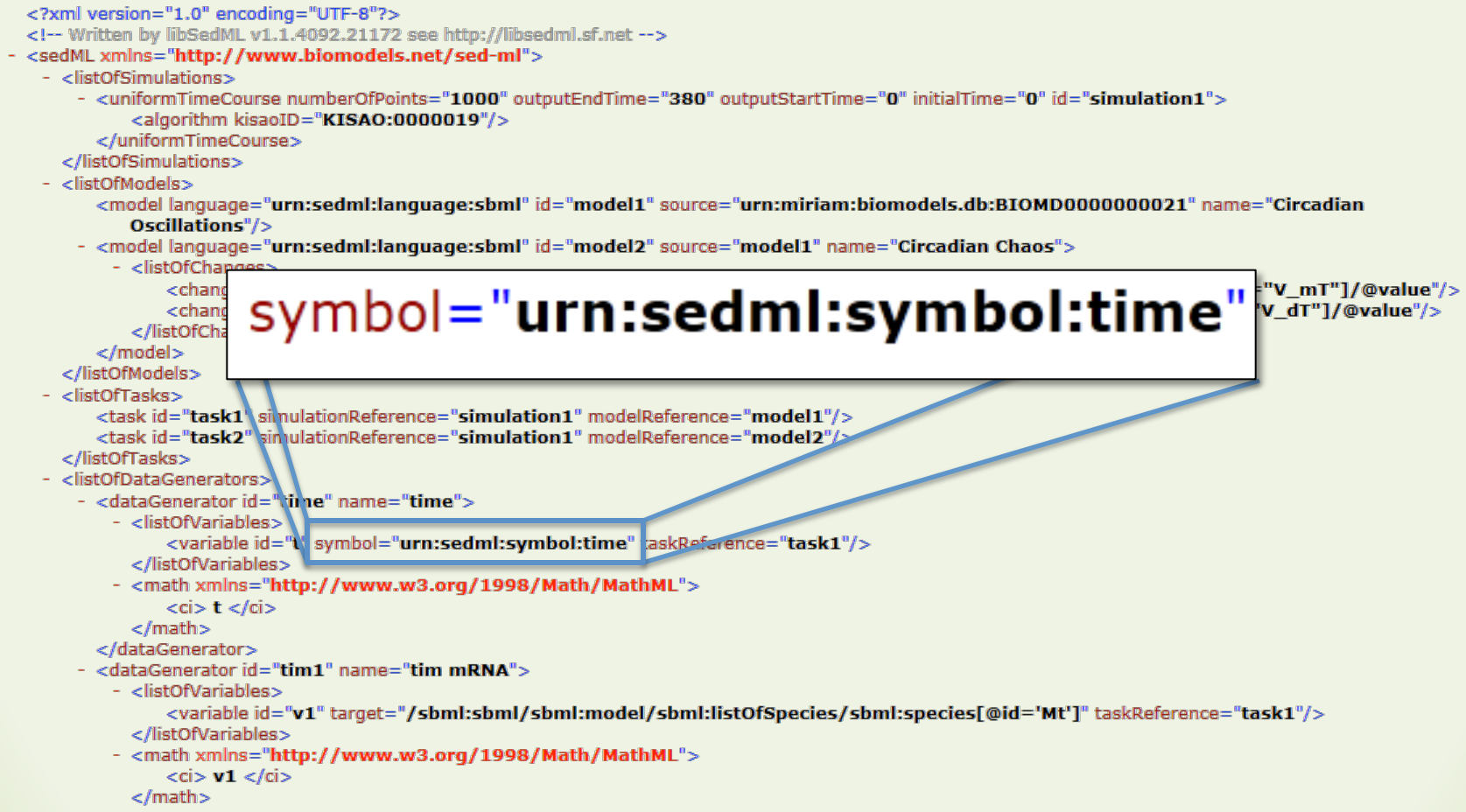
SED-ML

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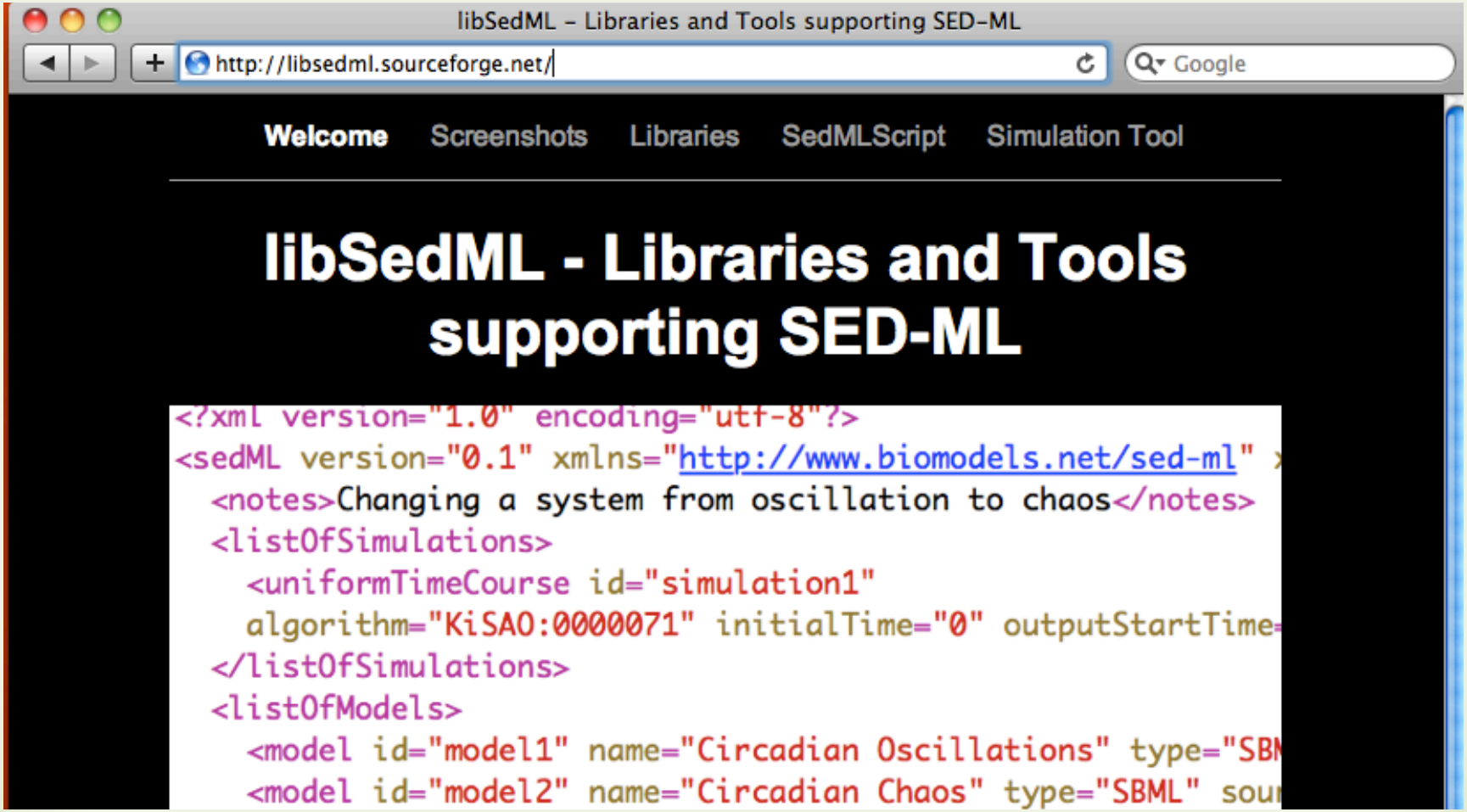
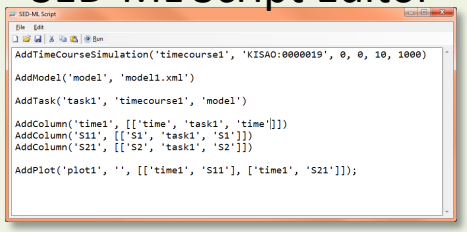
IMPLEMENTATION

http://libsedml.sf.net



Implementation

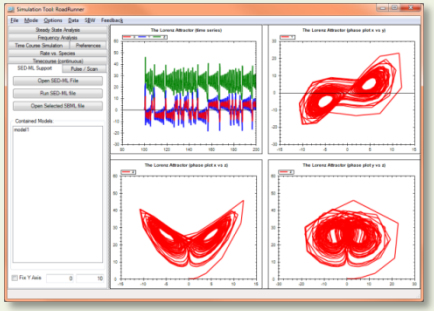
SED-ML Script Editor



libSedMLScript

libSedML

libSedMLRunner



Simulation Tool

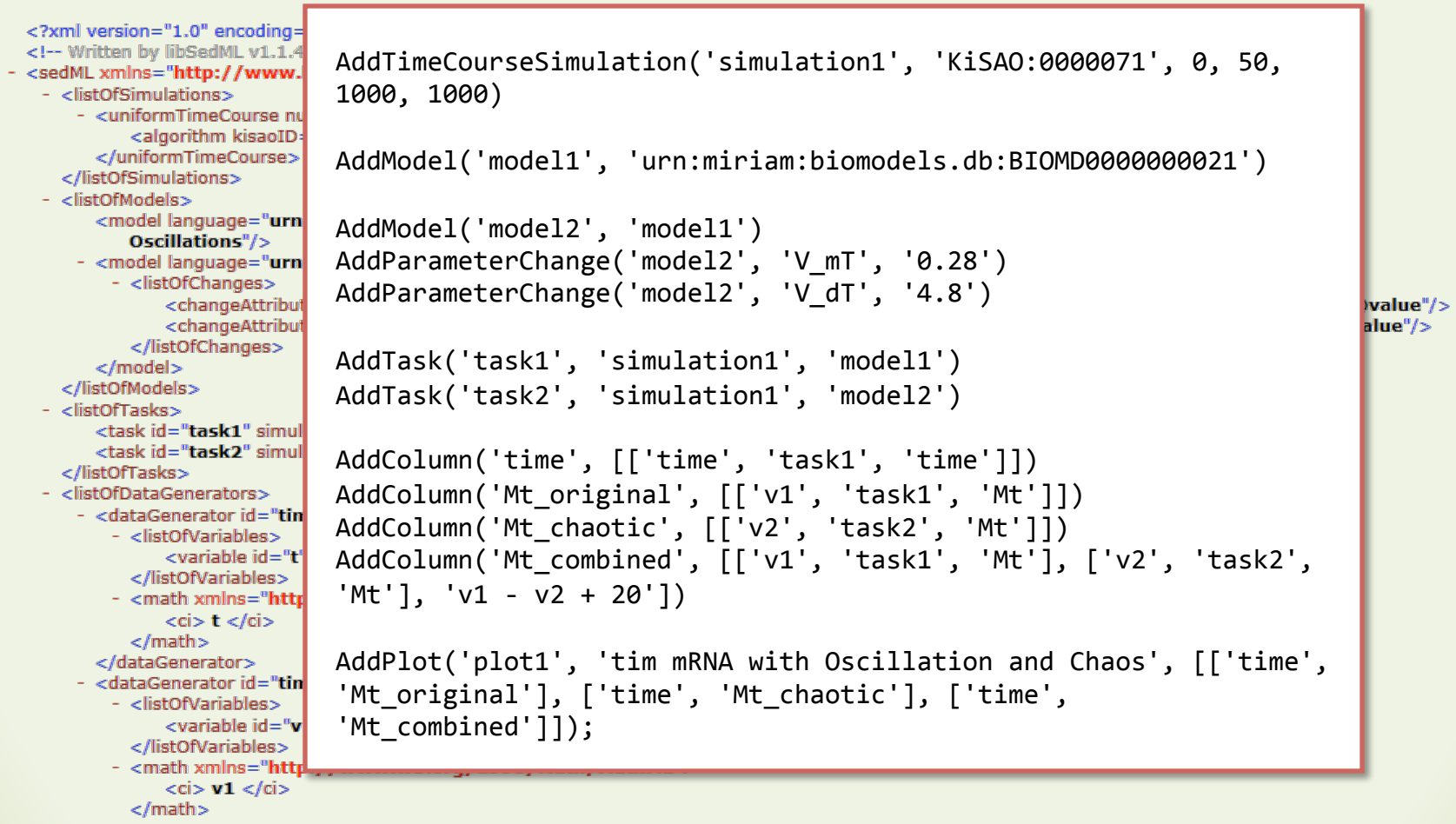
RoadRunner

JSim

iBioSim

http://libsedml.sf.net

Implementation



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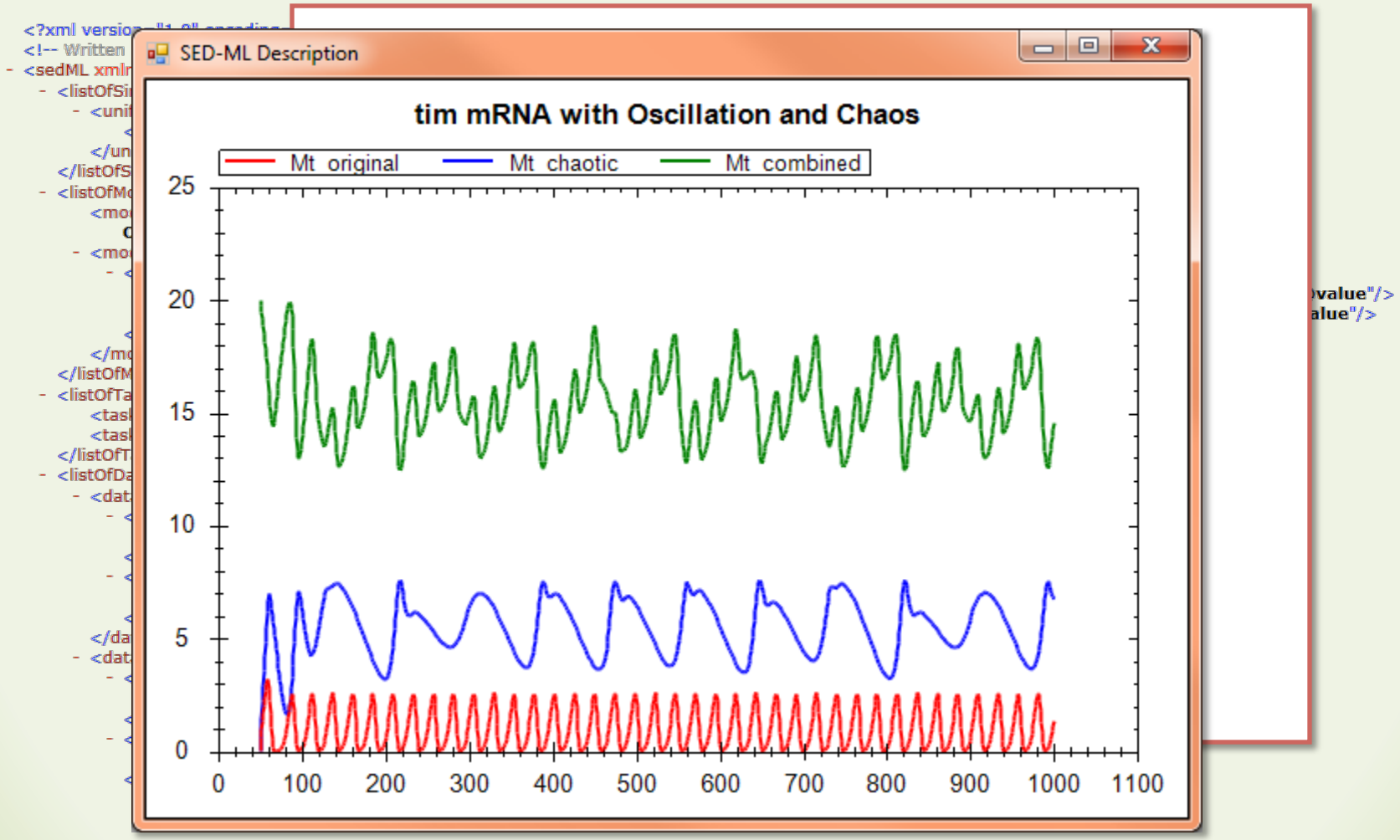
Implementation



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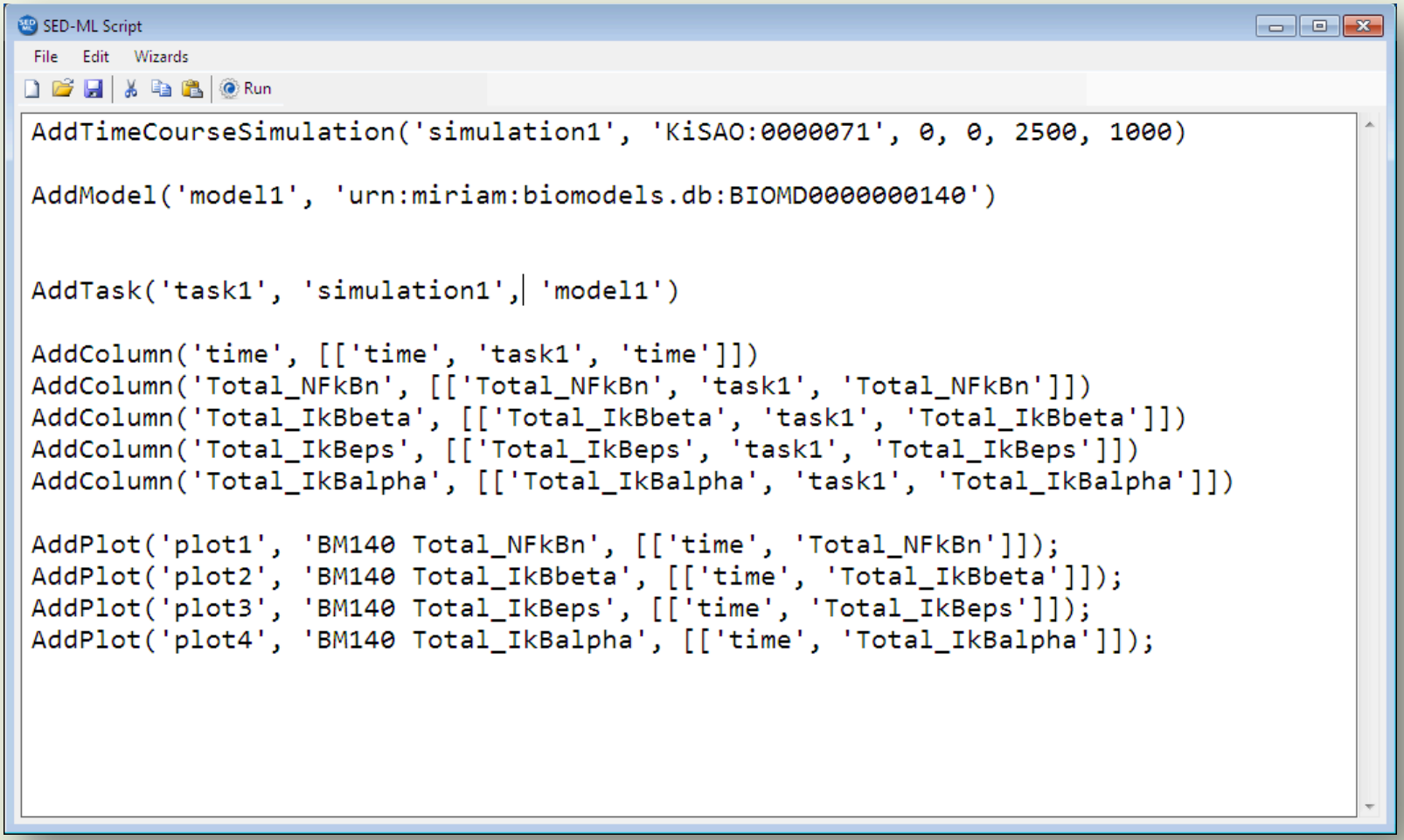
SED-ML script editor



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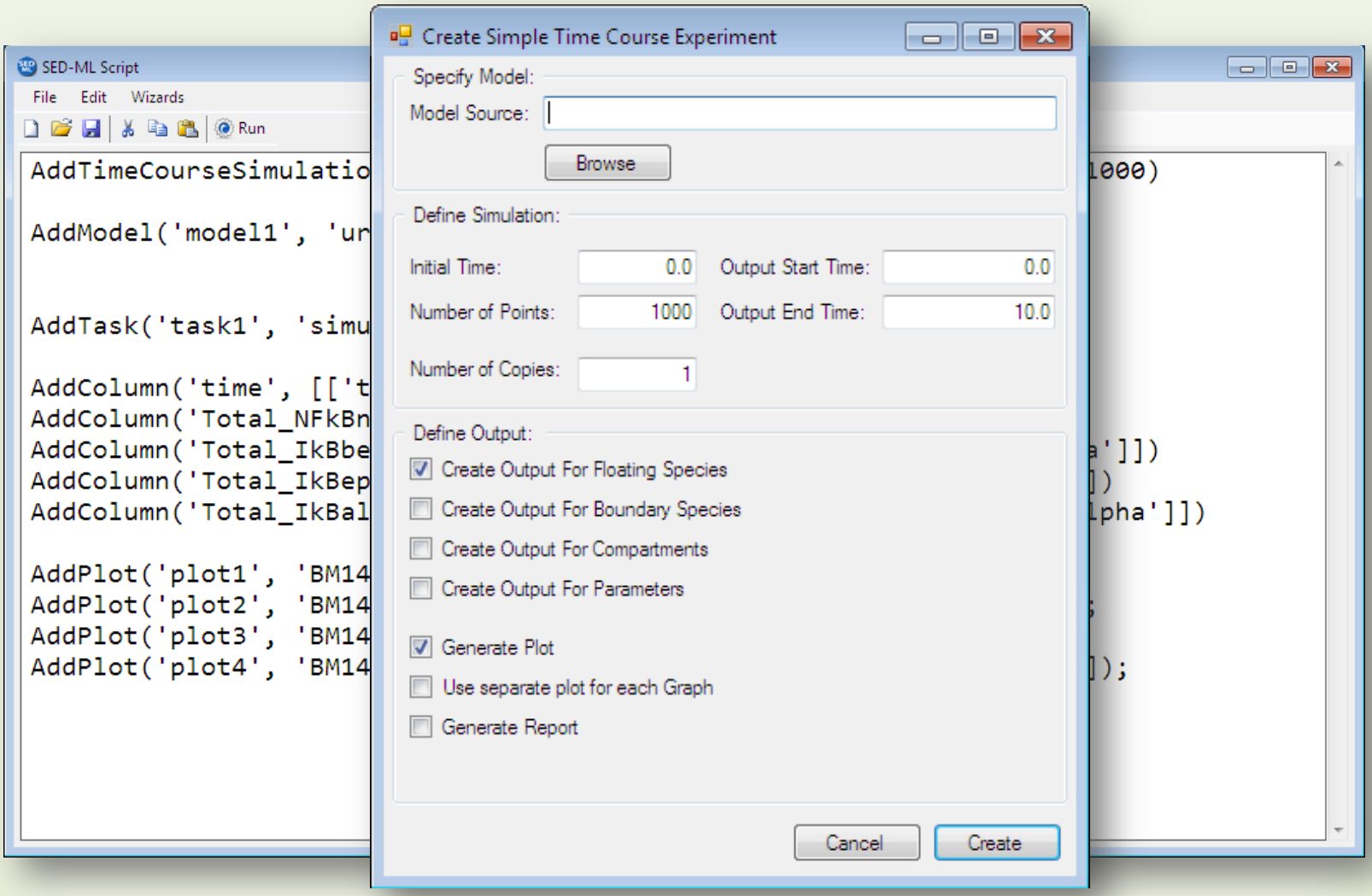

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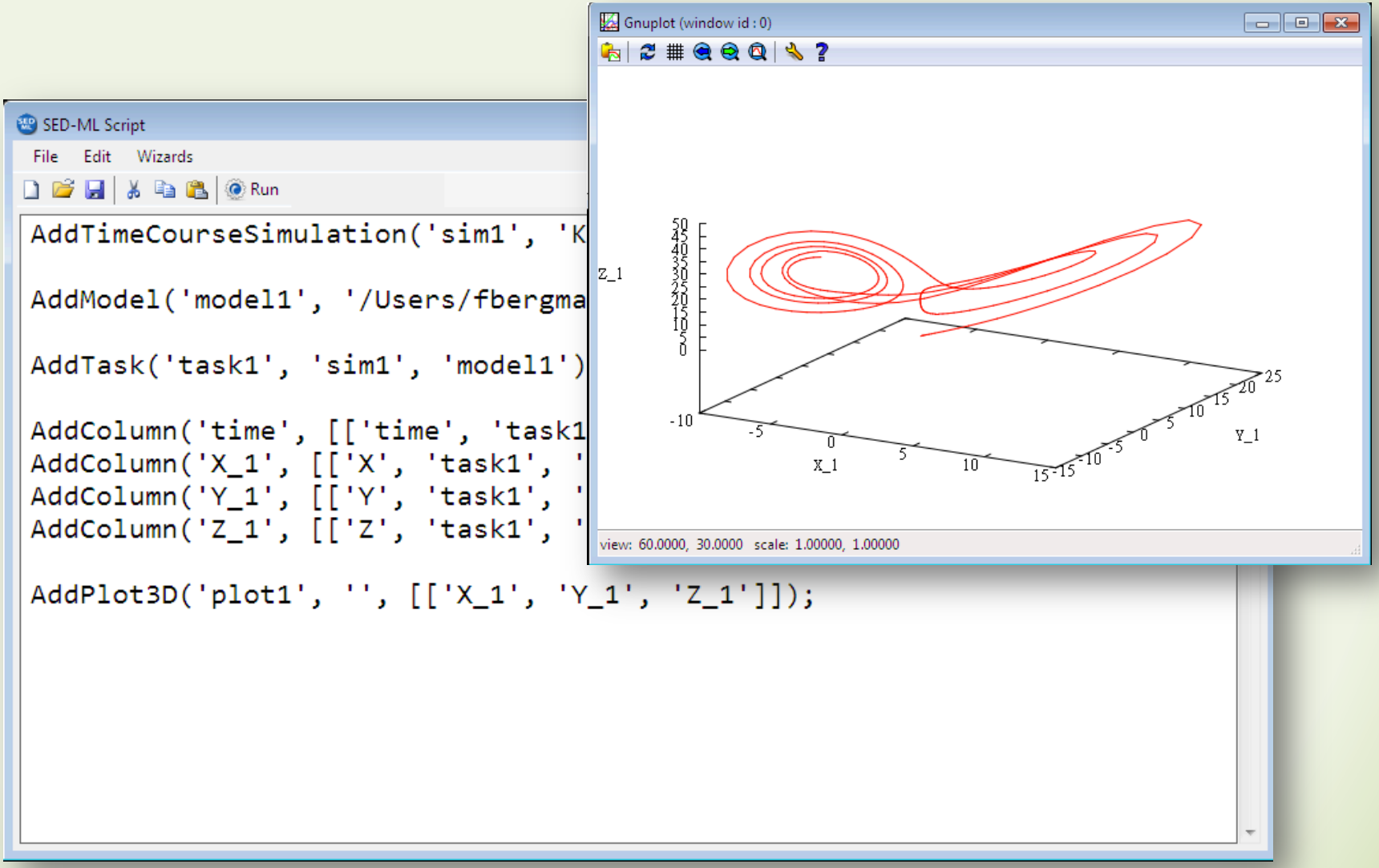
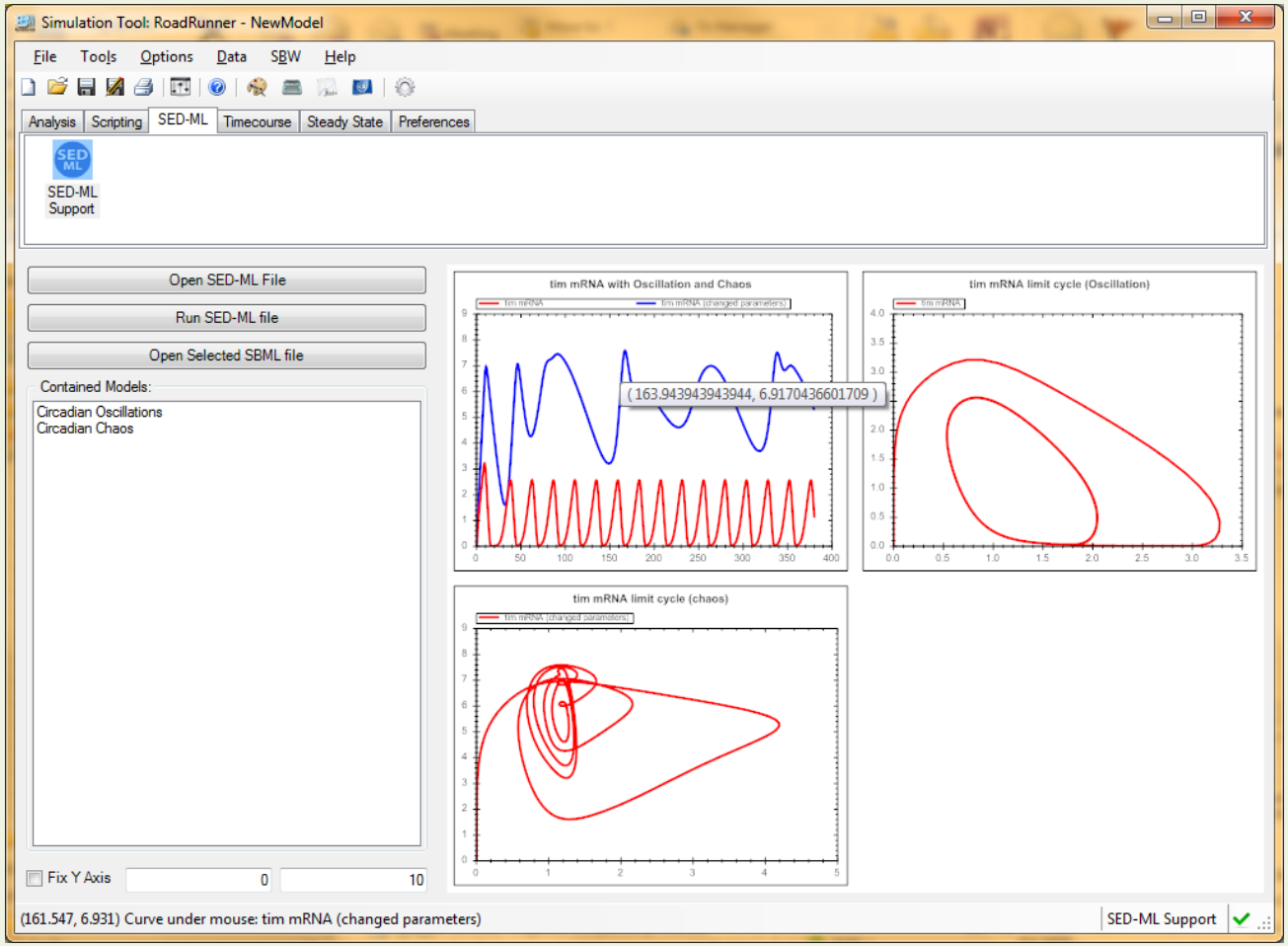


http://libsedml.sf.net

Available in SBW!

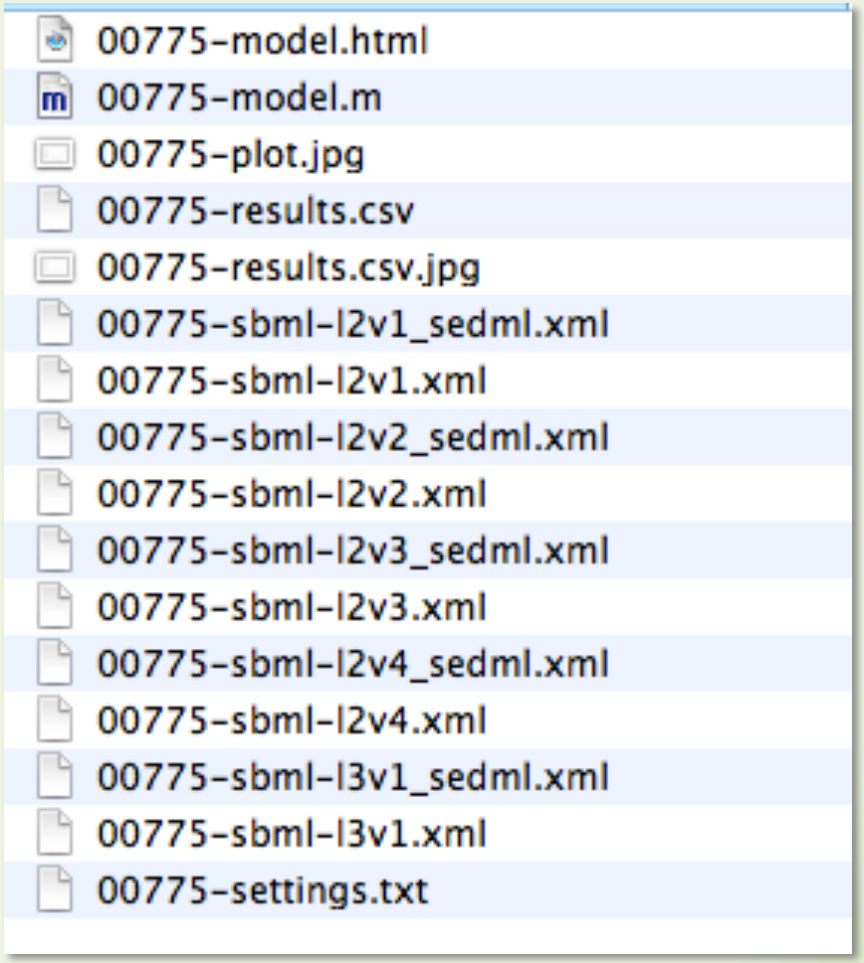


http://sys-bio.org

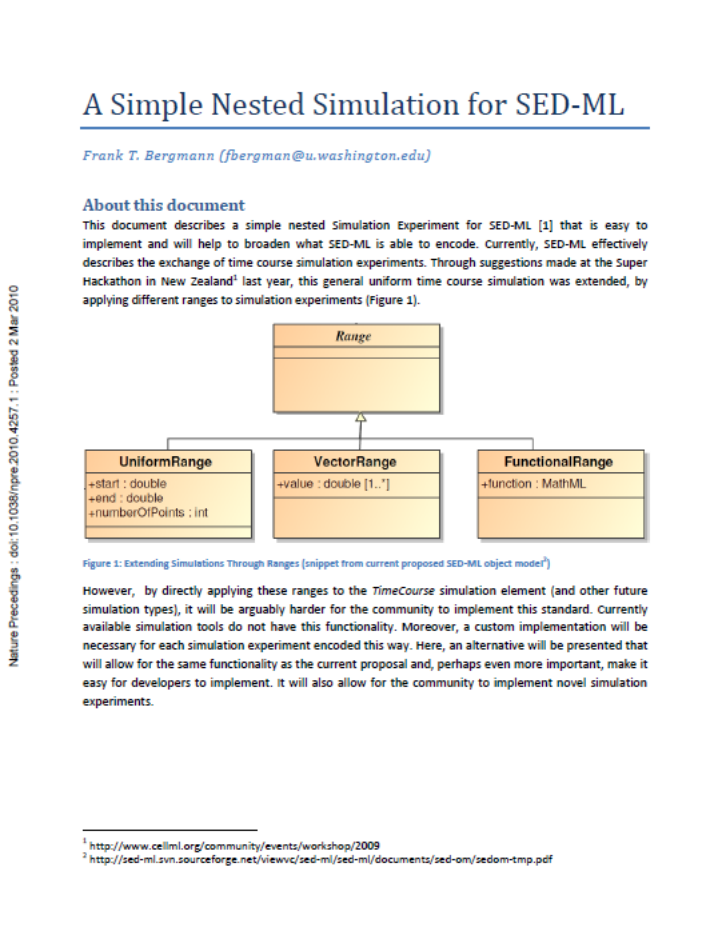
SBML Test Suite

- Next release of the SBML Test Suite will come with SED-ML models for all test cases:

- That's 4872 SED-ML models!



Outlook



Nature Precedings : doi:10.1038/npre.2010.4257.1 : Posted 2 Mar 2010

A Simple Nested Simulation for SED-ML

Frank T. Bergmann (fbergman@u.washington.edu)

About this document

This document describes a simple nested Simulation Experiment for SED-ML [1] that is easy to implement and will help to broaden what SED-ML is able to encode. Currently, SED-ML effectively describes the exchange of time course simulation experiments. Through suggestions made at the Super Hackathon in New Zealand[1] last year, this general uniform time course simulation was extended, by applying different ranges to simulation experiments (Figure 1).

Figure 1: Extending Simulations Through Ranges (snippet from current proposed SED-ML object model[2])

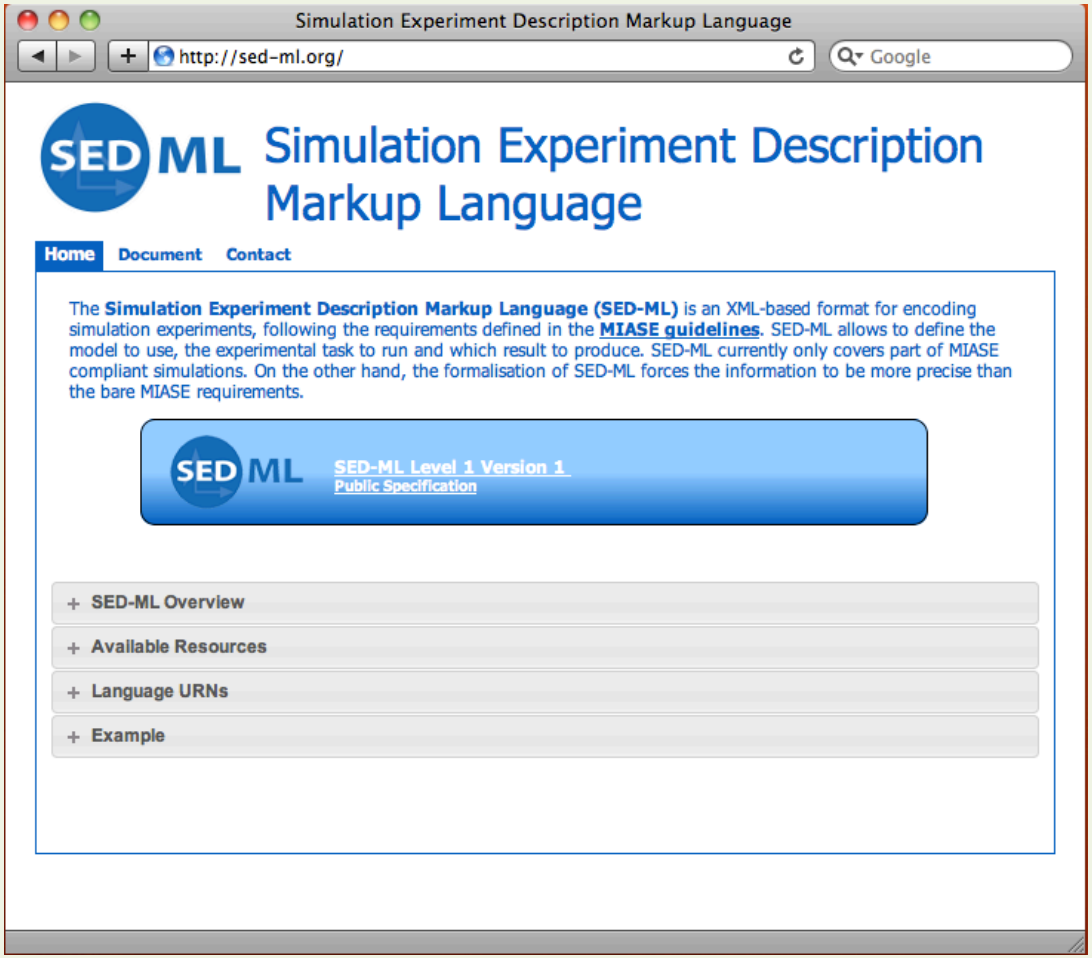
However, by directly applying these ranges to the *TimeCourse* simulation element (and other future simulation types), it will be arguably harder for the community to implement this standard. Currently available simulation tools do not have this functionality. Moreover, a custom implementation will be necessary for each simulation experiment encoded this way. Here, an alternative will be presented that will allow for the same functionality as the current proposal and, perhaps even more important, make it easy for developers to implement. It will also allow for the community to implement novel simulation experiments.

[1] http://www.cellml.org/community/events/workshop/2009
[2] http://sed-ml.svn.sourceforge.net/viewvc/sed-ml/sed-ml/documents/sed-om/sedom-tmp.pdf

- Nested Tasks
- More Simulation Experiments
- Advanced Post processing

http://dx.doi.org/10.1038/npre.2010.4257.1

More Information



http://sed-ml.org

Acknowledgments

Nicolas Le Novére, Richard Adams
Dagmar Waltemath

Mike Hucka
Ion Moraru
Sven Sahle
David Nickerson
Henning Schmidt
Fedor Kolpakov

http://sed-ml.org