The Simulation Experiment Description Markup Language

Frank T. Bergmann & Dagmar Waltemath

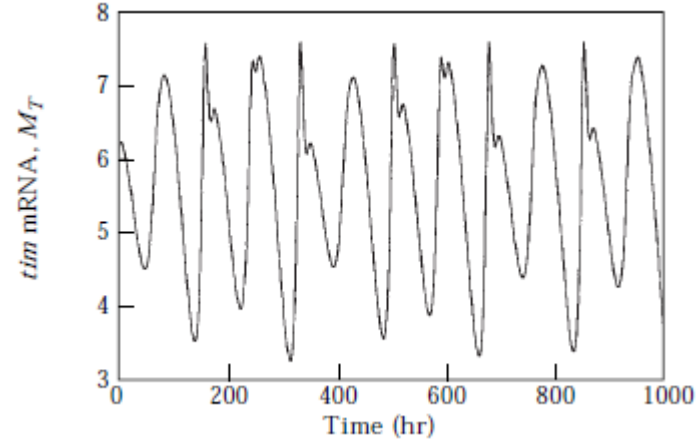
SBML & BioModels Hackathon, Seattle 2010

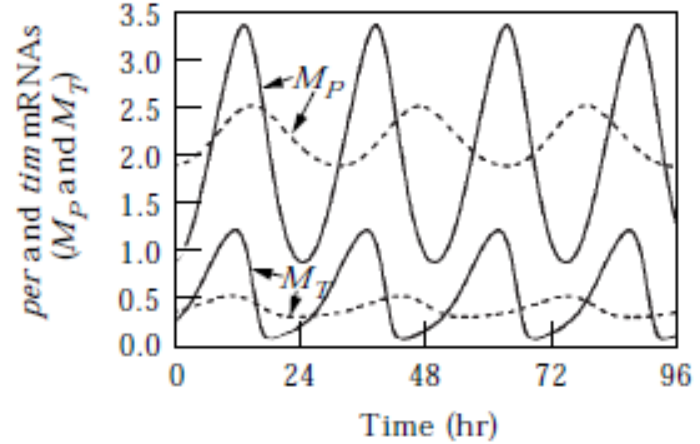
MOTIVATION

Motivation

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

JEAN-CHRISTOPHE LELOUP AND ALBERT GOLDBETER*

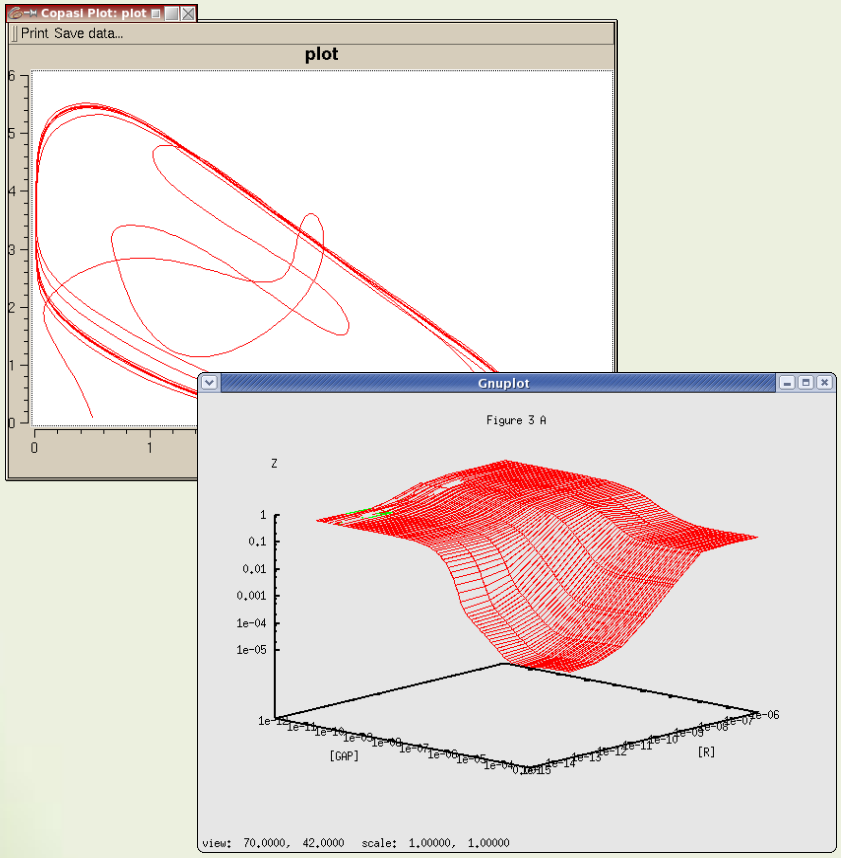




J. theor. Biol. (1999) **198**, 445-459
Article No. jtbi.1999.0924, available online at http://www.idealibrary.com

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 …

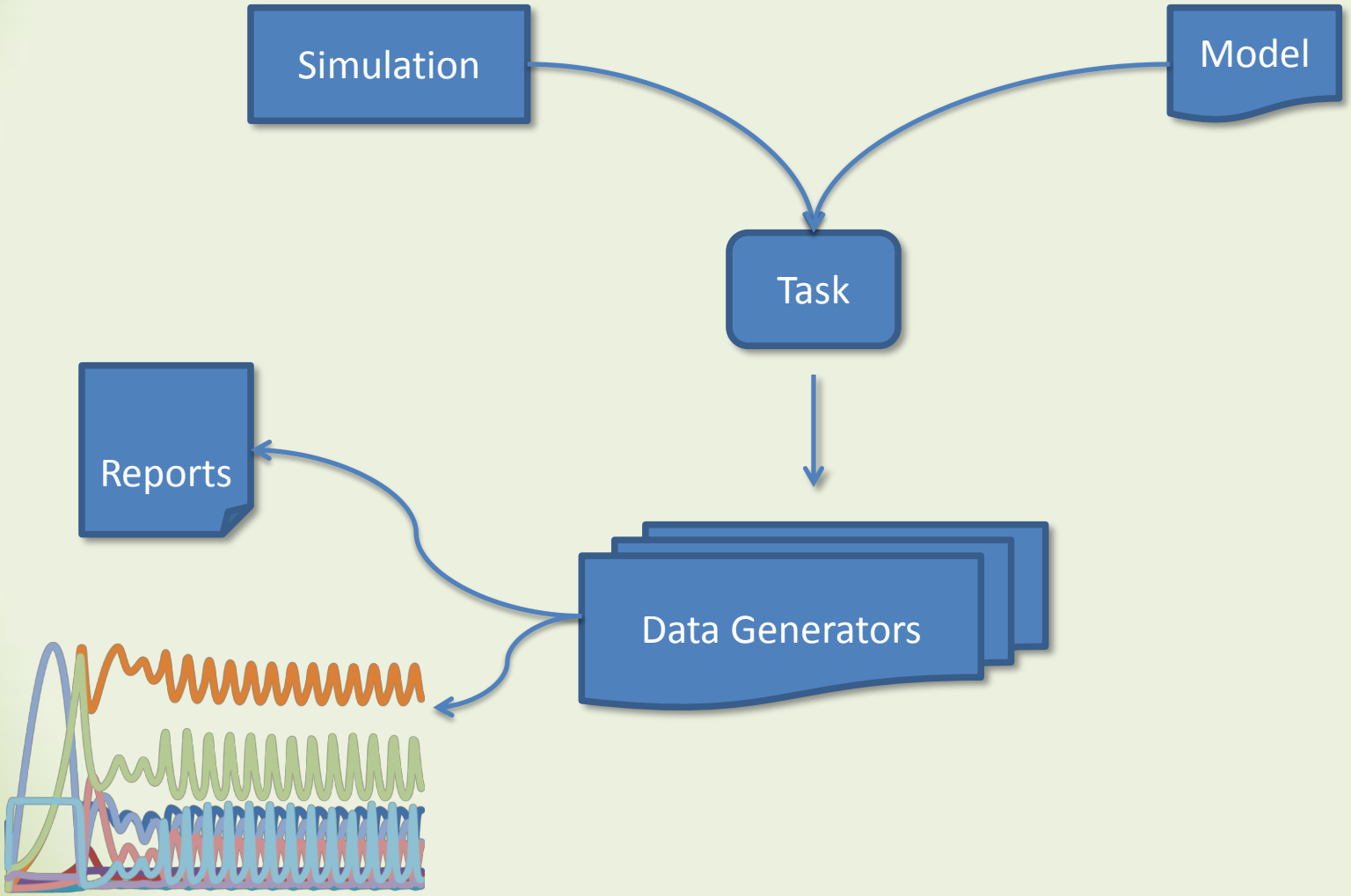
HOW DOES SED-ML HELP?

Repeatable simulation experiments

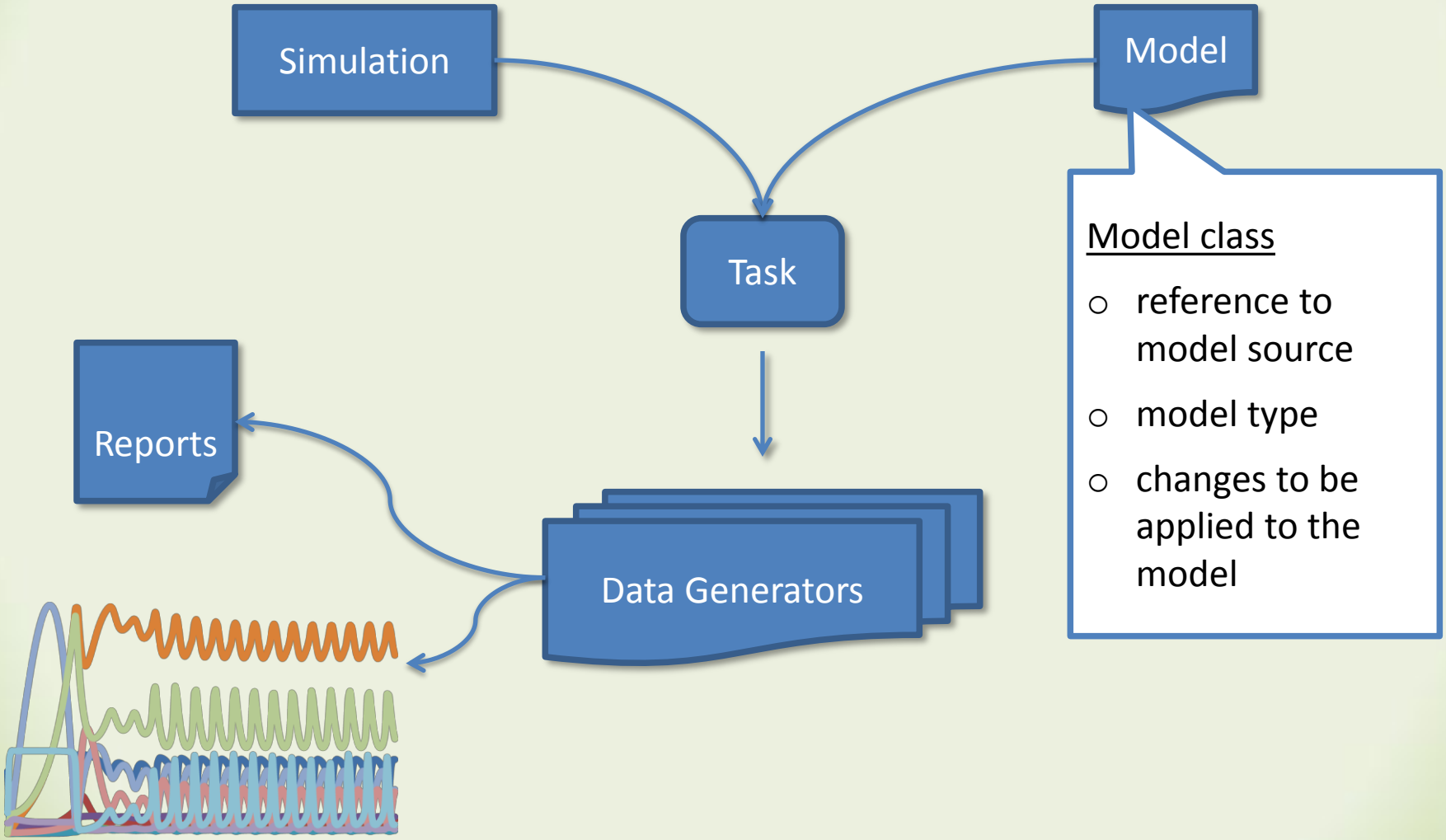
Simulation Experiment Description – Markup Language (SED-ML):

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

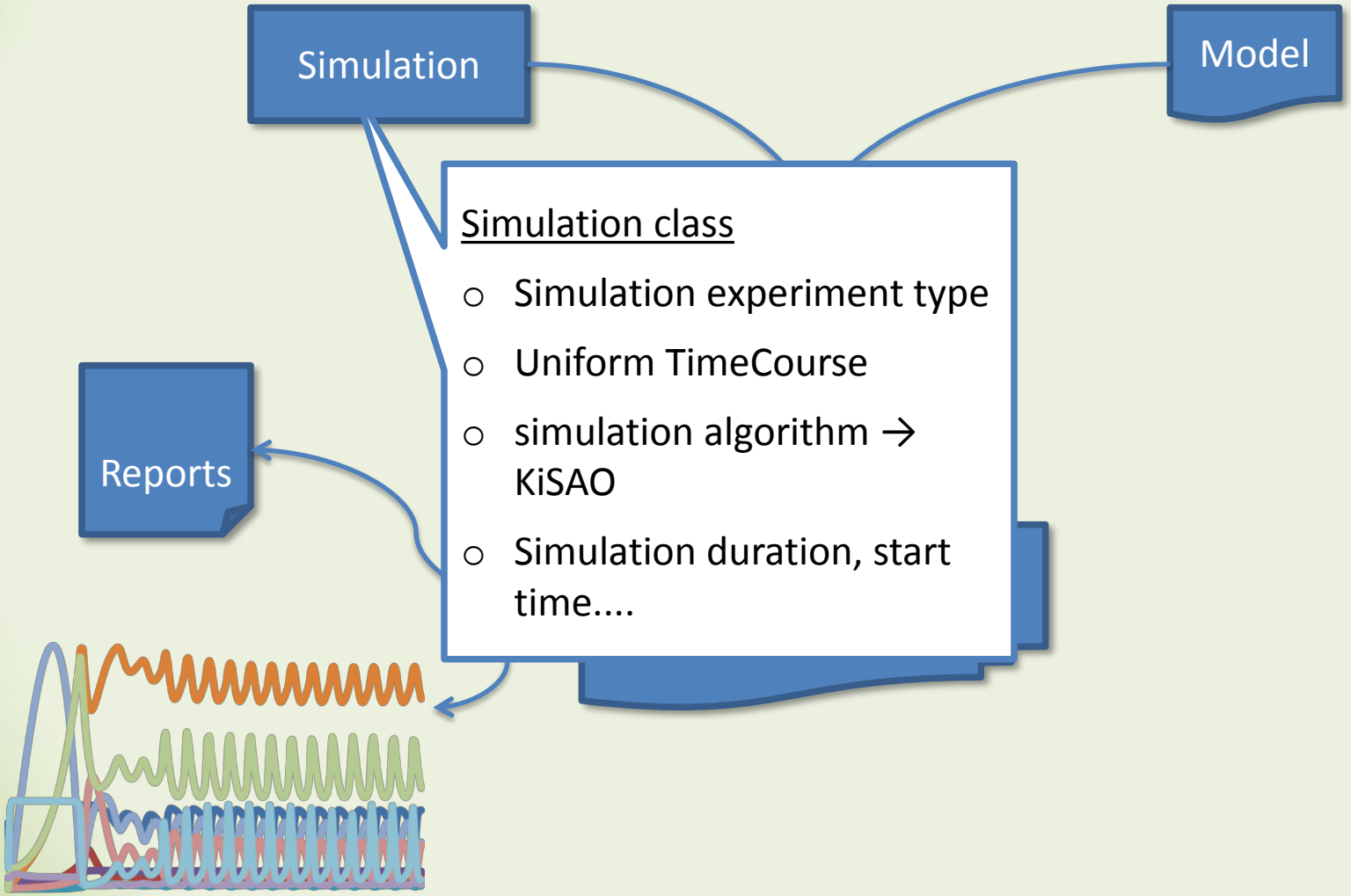
Repeatable simulation experiments



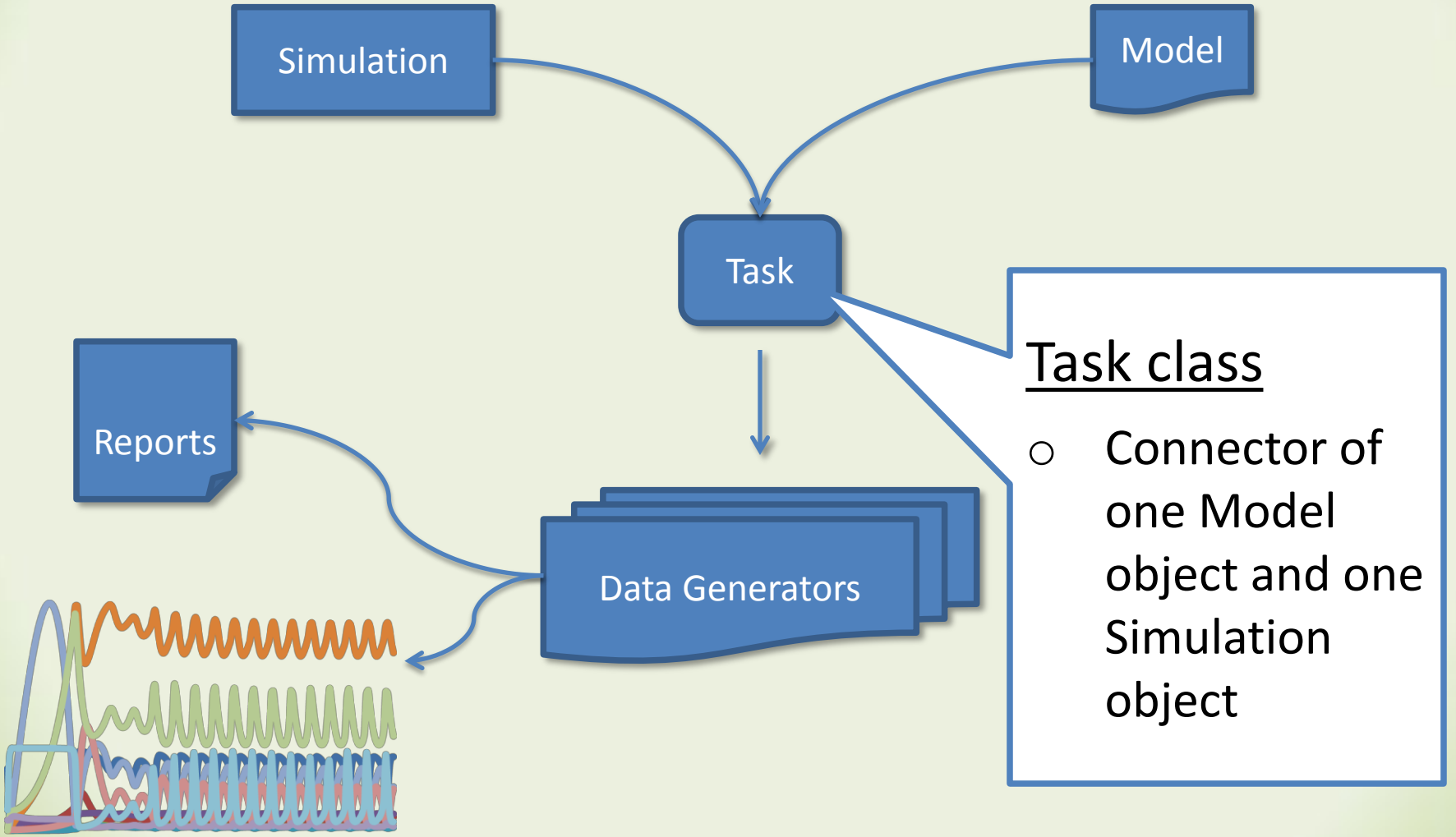
Repeatable simulation experiments



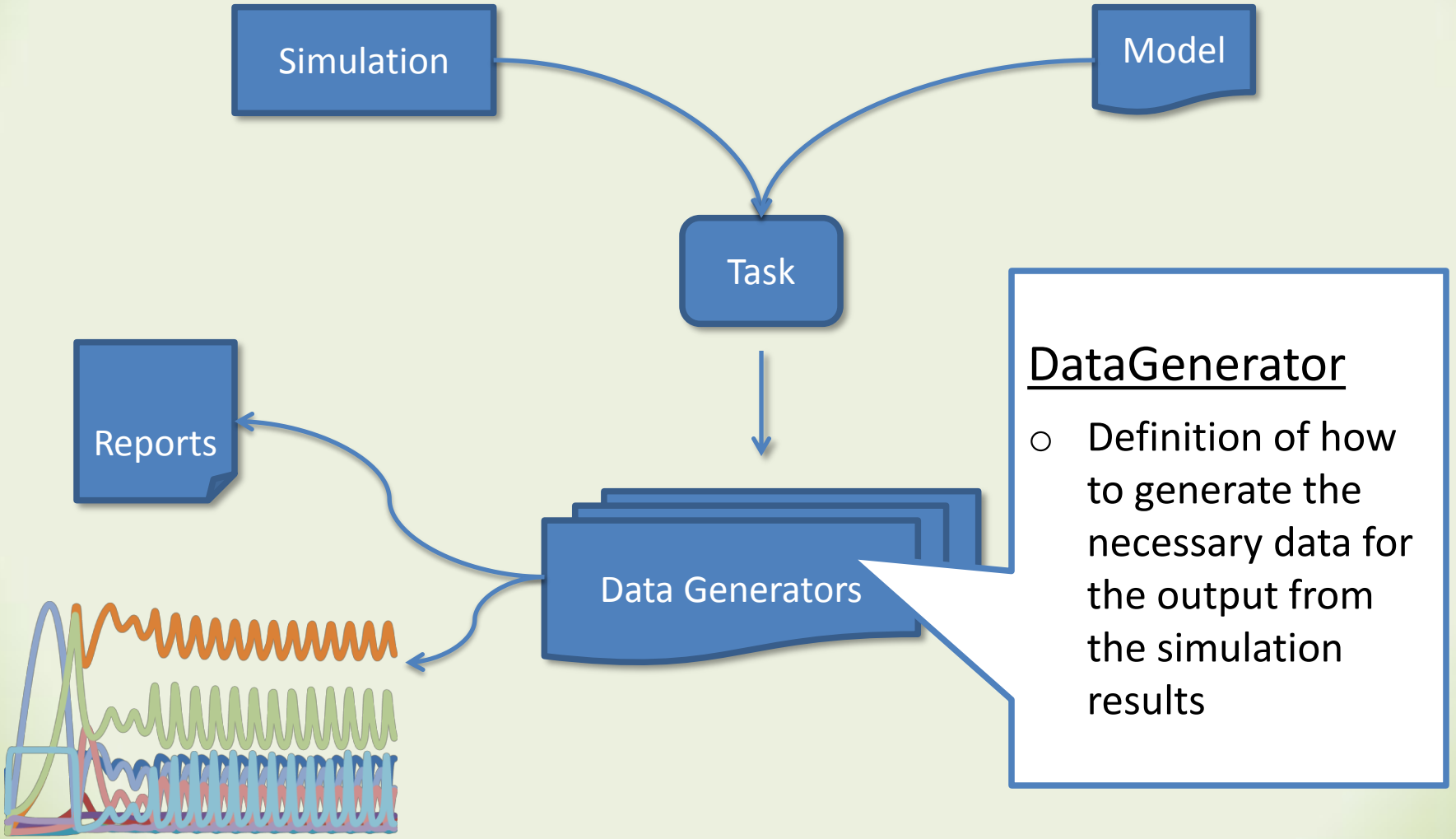
Repeatable simulation experiments



Repeatable simulation experiments



Repeatable simulation experiments



SED-ML Main Concepts

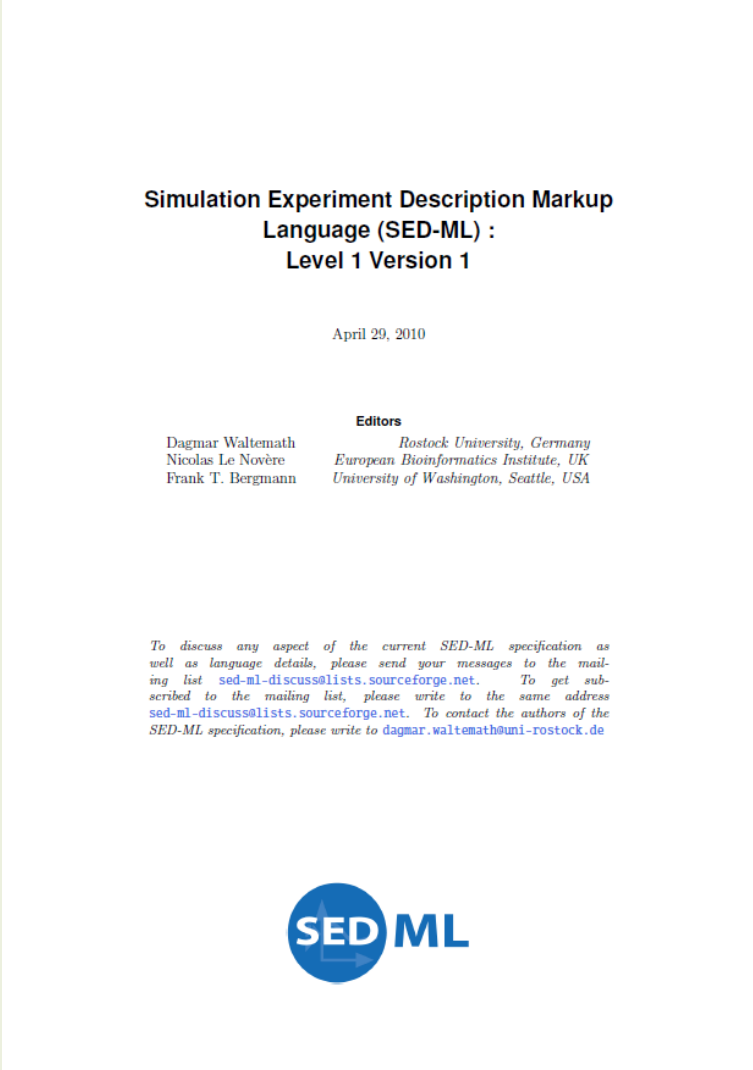
- No description of the simulation results
  - SBRML
- No description of the layout of the output curves

SED-ML

```
<?xml version="1.0" encoding="utf-8" ?>
<sedML version="0.1" xmlns="http://www.biomodels.net/sed-ml" xmlns:math="http://www.w3.org/1998/Math/MathML">
  <notes>Changing a system from oscillation to chaos</notes>
  <listOfSimulations>
    <uniformTimeCourse id="simulation1" algorithm="KiSAO:0000071" initialTime="0" outputStartTime="50"
      outputEndTime="1000" numberOfPoints="1000" />
  </listOfSimulations>
  <listOfModels>
    <model id="model1" name="Circadian Oscillations" type="SBML"
      source="urn:miriam:biomodels.db:BIOMD0000000021" />
    <model id="model2" name="Circadian Chaos" type="SBML" source="model1">
      <listOfChanges>
        <changeAttribute target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
          [@id='V_mT']/@value" newValue="0.28" />
        <changeAttribute target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
          [@id='V_dT']/@value" newValue="4.8" />
      </listOfChanges>
    </model>
  </listOfModels>
  <listOfTasks>
    <task id="task1" name="Baseline" modelReference="model1" simulationReference="simulation1" />
    <task id="task2" name="Modified parameters" modelReference="model2" simulationReference="simulation1" />
  </listOfTasks>
  <listOfDataGenerators>
    <dataGenerator id="time" name="Time">
      <listOfVariables>
        <variable id="time" taskReference="task1" target="time" />
      </listOfVariables>
      <listOfParameters />
```

SED-ML L1 V1

- SED-ML Spec is on the way
- preliminary version available from Source forge
- Feel free to read, bug report and start implementing :-)



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

April 29, 2010

Editors

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Nicolas Le Novère — *European Bioinformatics Institute, UK*
Frank T. Bergmann — *University of Washington, Seattle, USA*

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* dagmar.waltemath@uni-rostock.de

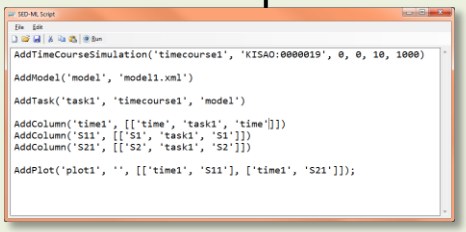
SED ML

http://sourceforge.net/projects/sed-ml/

IMPLEMENTATION

Implementation

SED-ML Script Editor



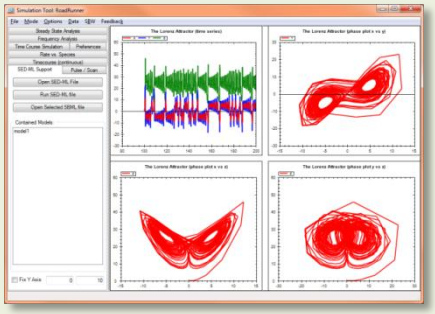
libSedMLScript

libSedML

libSedMLRunner

Other SBW enabled Simulators

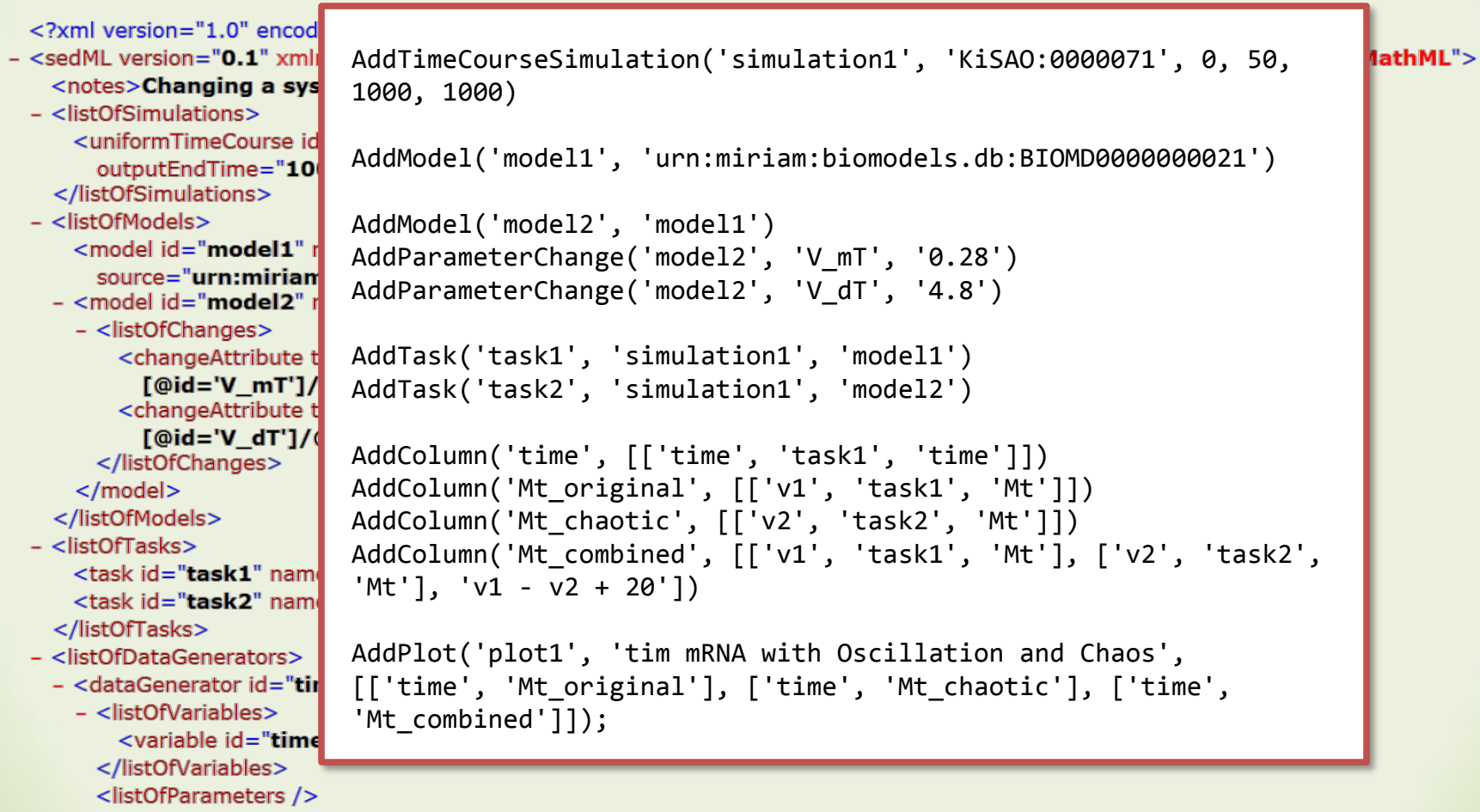
RoadRunner



Simulation Tool

http://libsedml.sf.net

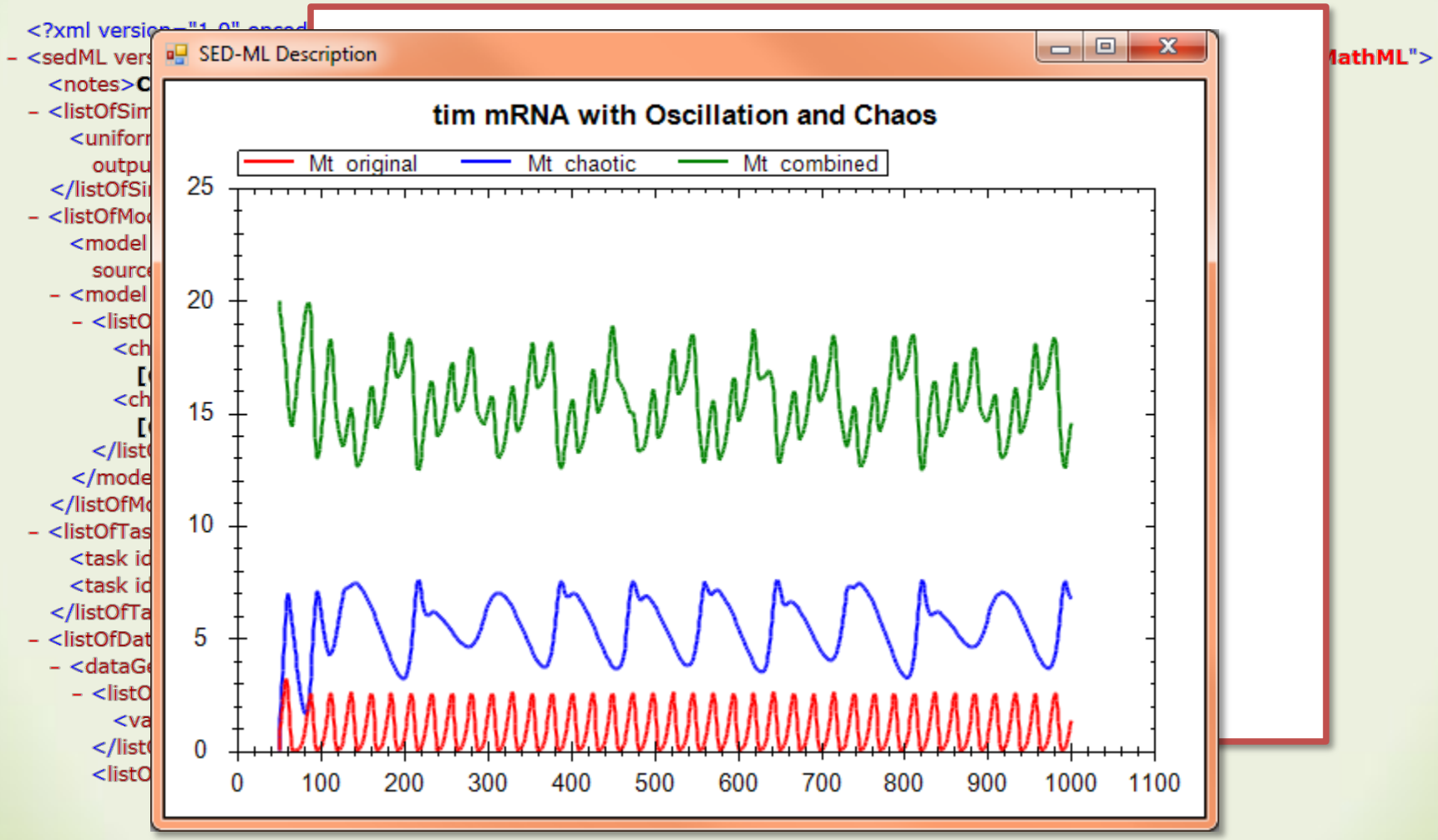
Implementation




```
AddTimeCourseSimulation('simulation1', 'KiSAO:0000071', 0, 50,
1000, 1000)

AddModel('model1', 'urn:miriam:biomodels.db:BIOMD0000000021')

AddModel('model2', 'model1')
AddParameterChange('model2', 'V_mT', '0.28')
AddParameterChange('model2', 'V_dT', '4.8')

AddTask('task1', 'simulation1', 'model1')
AddTask('task2', 'simulation1', 'model2')

AddColumn('time', [['time', 'task1', 'time']])
AddColumn('Mt_original', [['v1', 'task1', 'Mt']])
AddColumn('Mt_chaotic', [['v2', 'task2', 'Mt']])
AddColumn('Mt_combined', [['v1', 'task1', 'Mt'], ['v2', 'task2',
'Mt'], 'v1 - v2 + 20'])

AddPlot('plot1', 'tim mRNA with Oscillation and Chaos',
[['time', 'Mt_original'], ['time', 'Mt_chaotic'], ['time',
'Mt_combined']]);
```

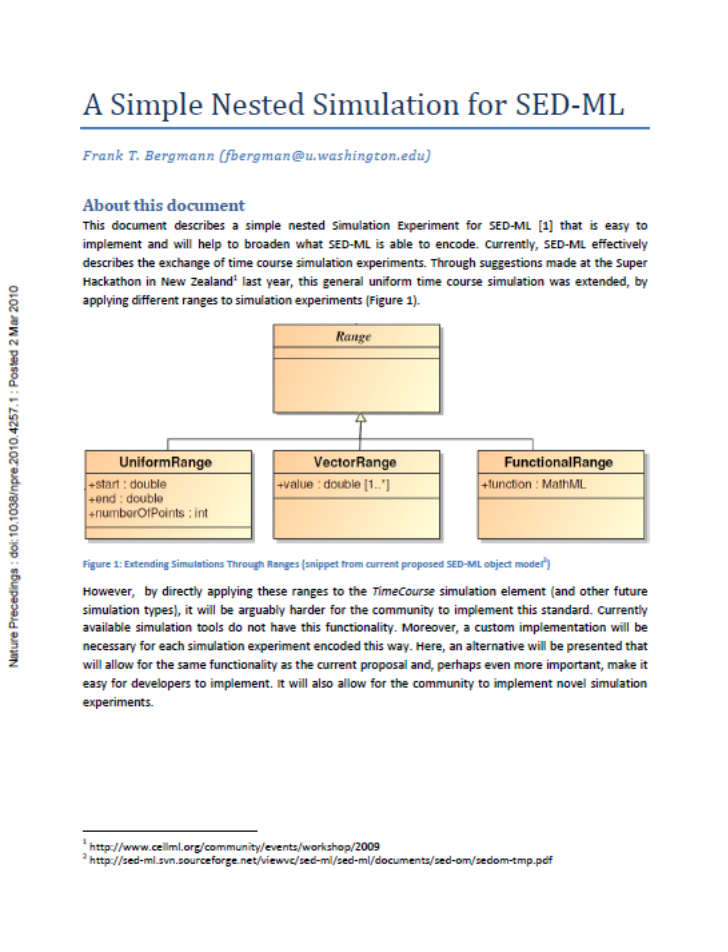
http://libsedml.sf.net

Implementation



http://libsedml.sf.net

Outlook



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

A Simple Nested Simulation for SED-ML

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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

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http://biomodels.net/sed-ml