

# The Simulation Experiment Description Markup Language

Frank T. Bergmann

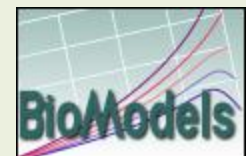
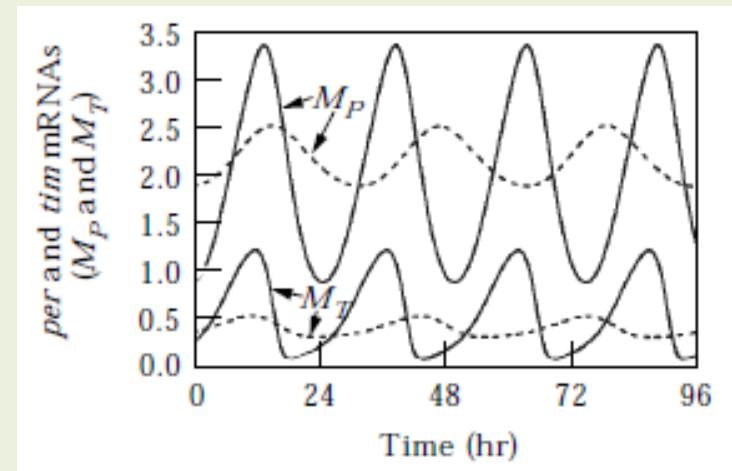
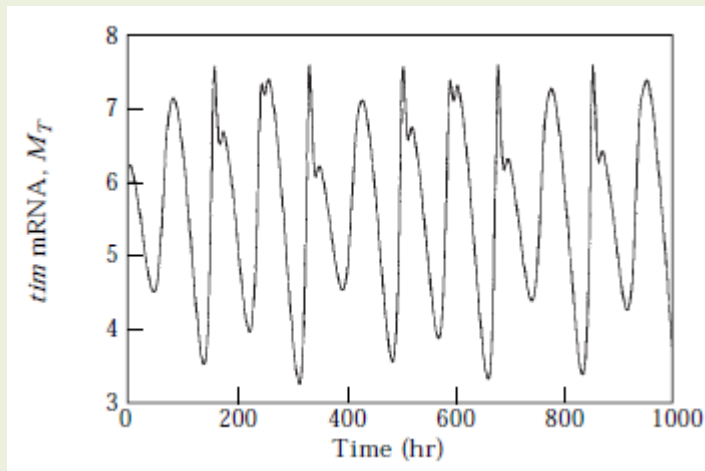
COMBINE 2010, Edinburgh, UK

# 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\*

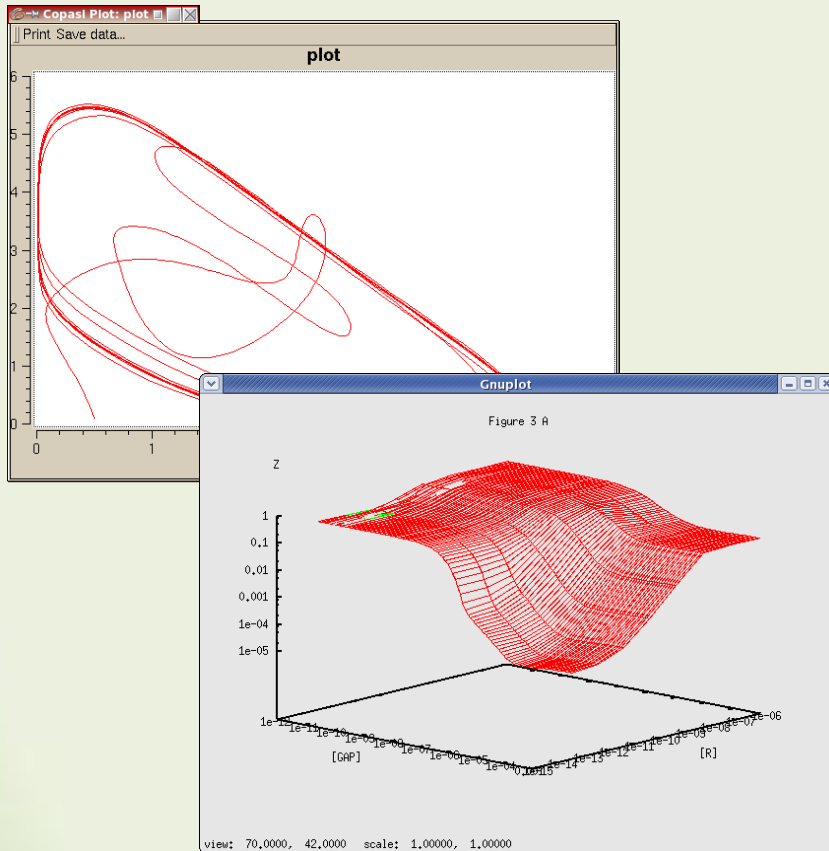


*J. theor. Biol.* (1999) **198**, 445-459

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 ...

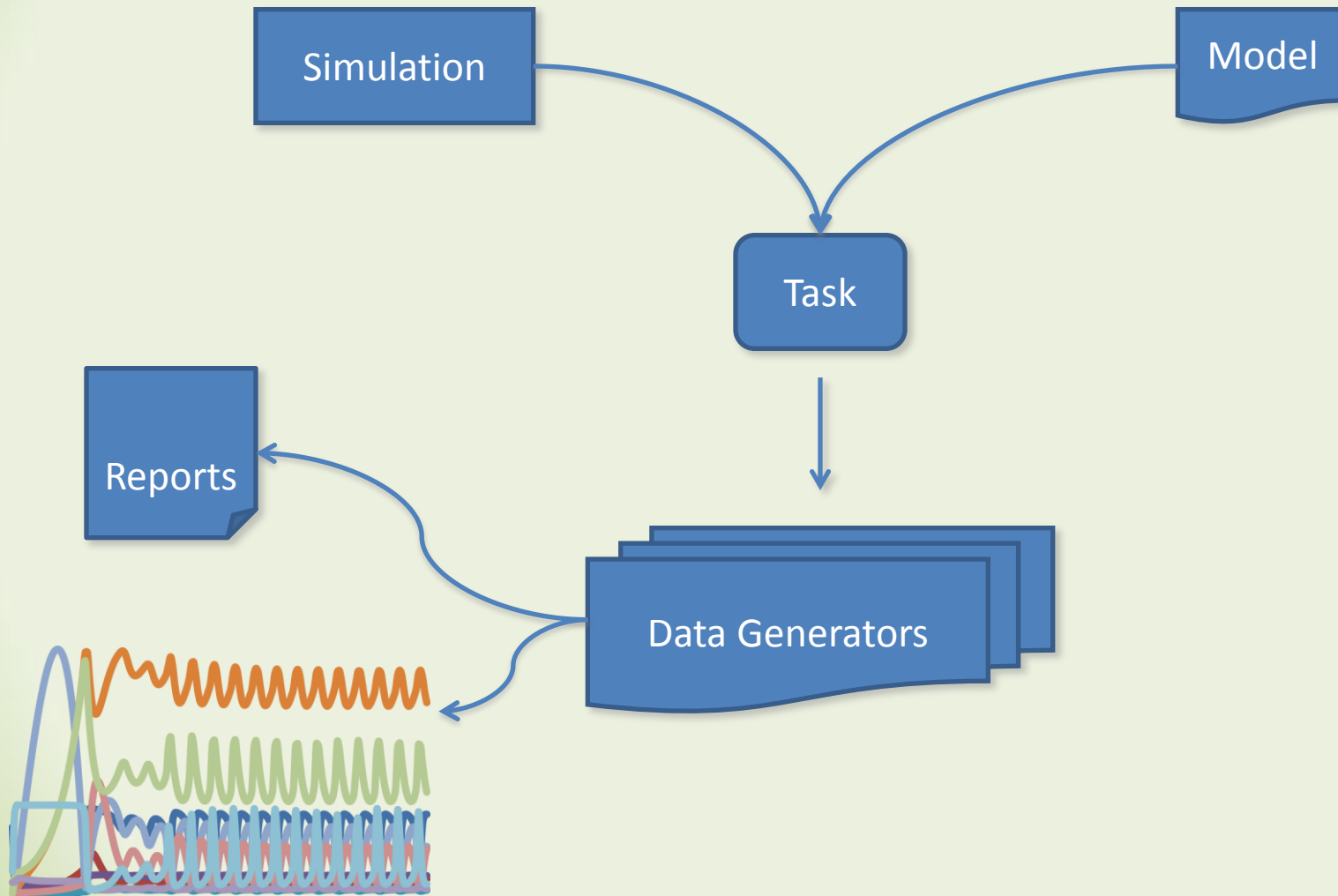
**HOW DOES SED-ML HELP?**

# Repeatable simulation experiments

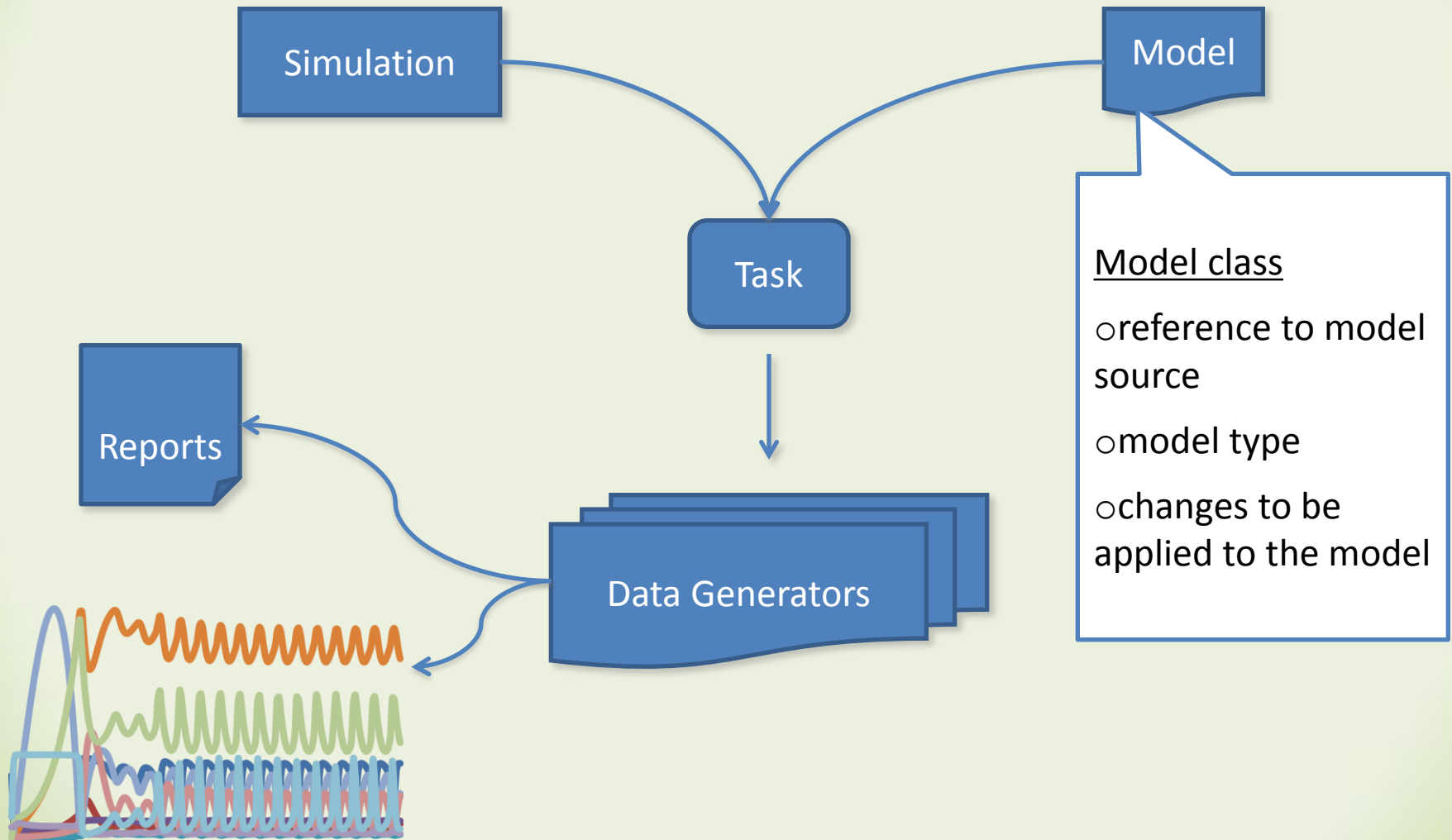
## Simulation Experiment Description – Markup Language (SED-ML):

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

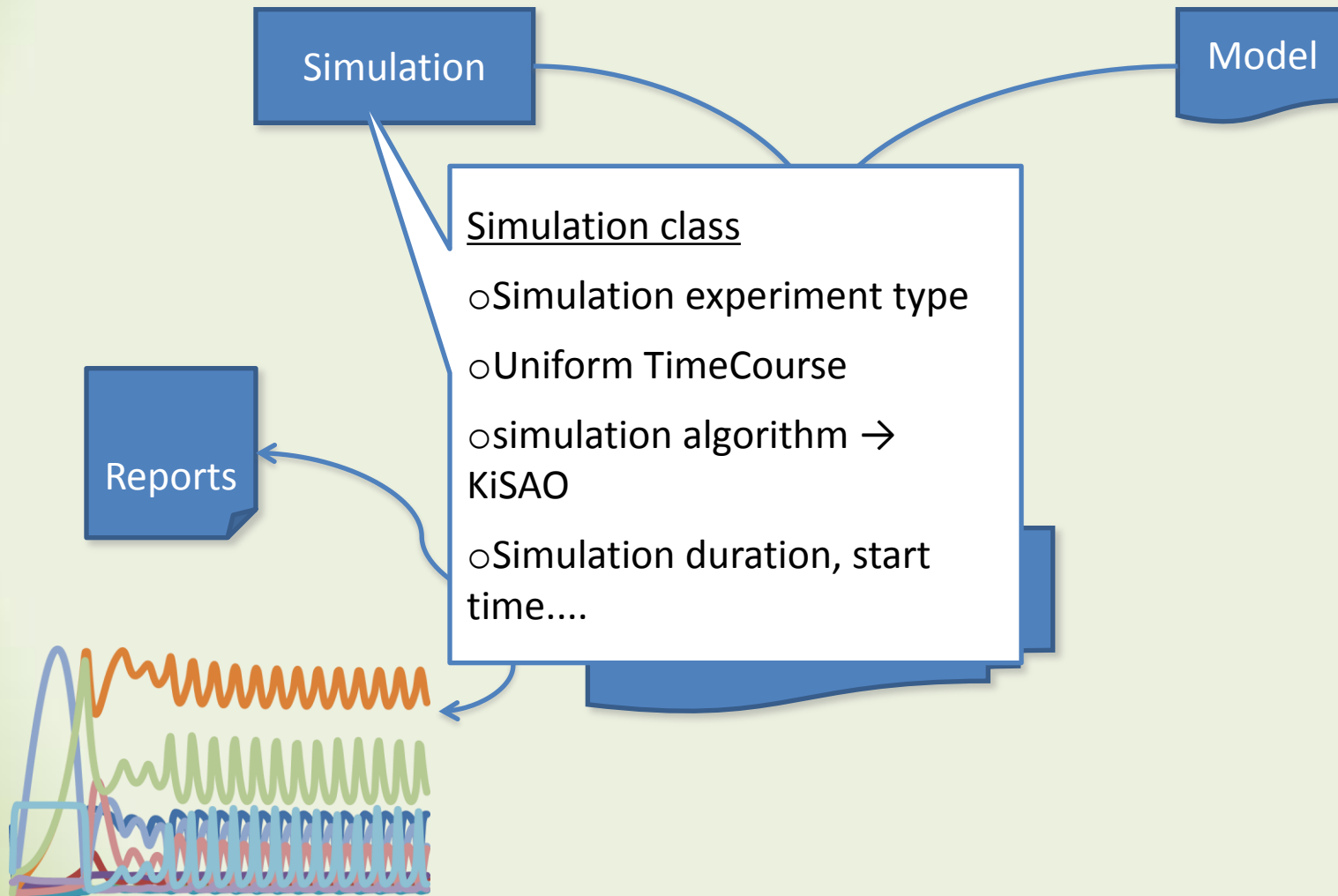


# Repeatable simulation experiments

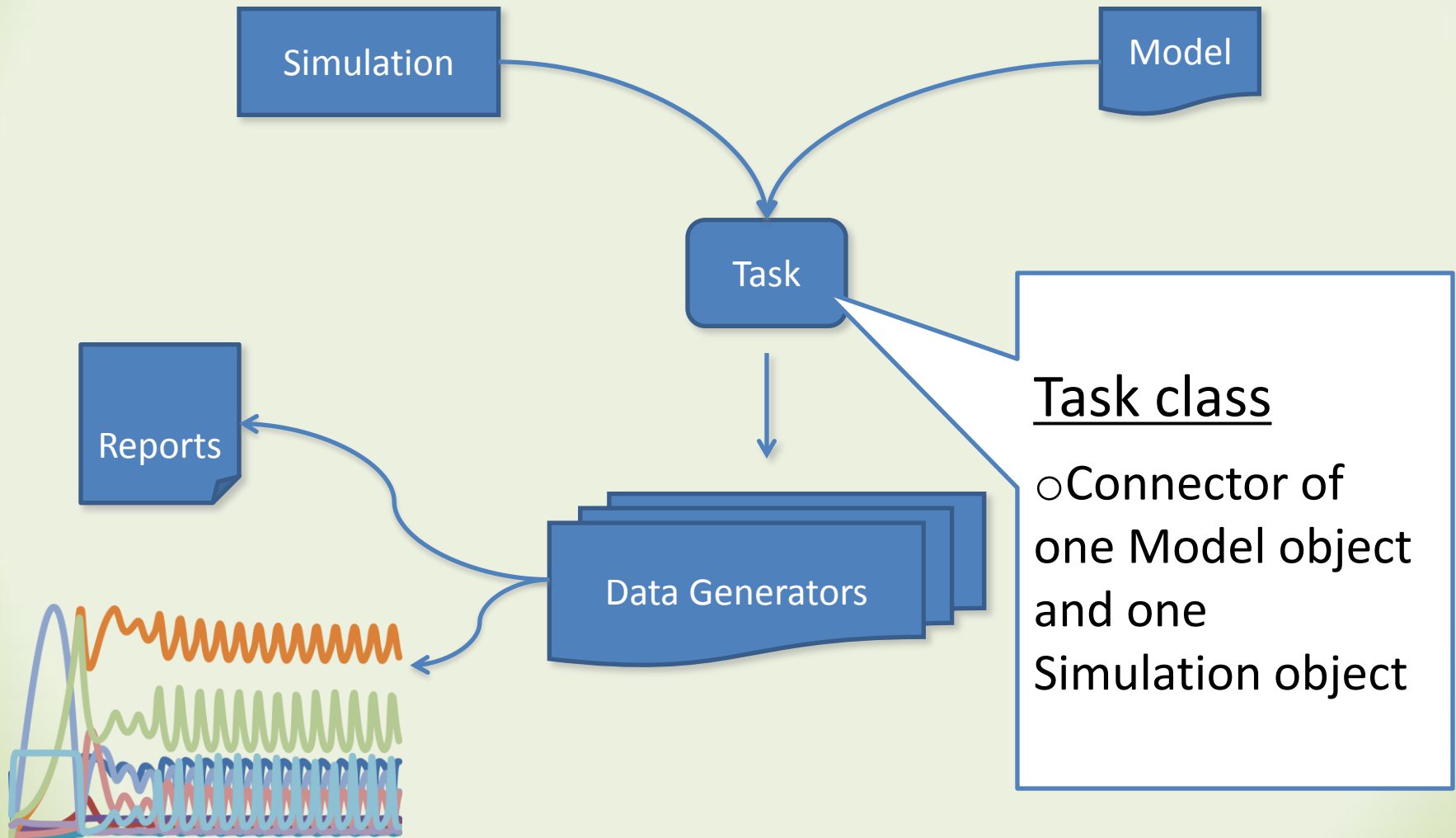




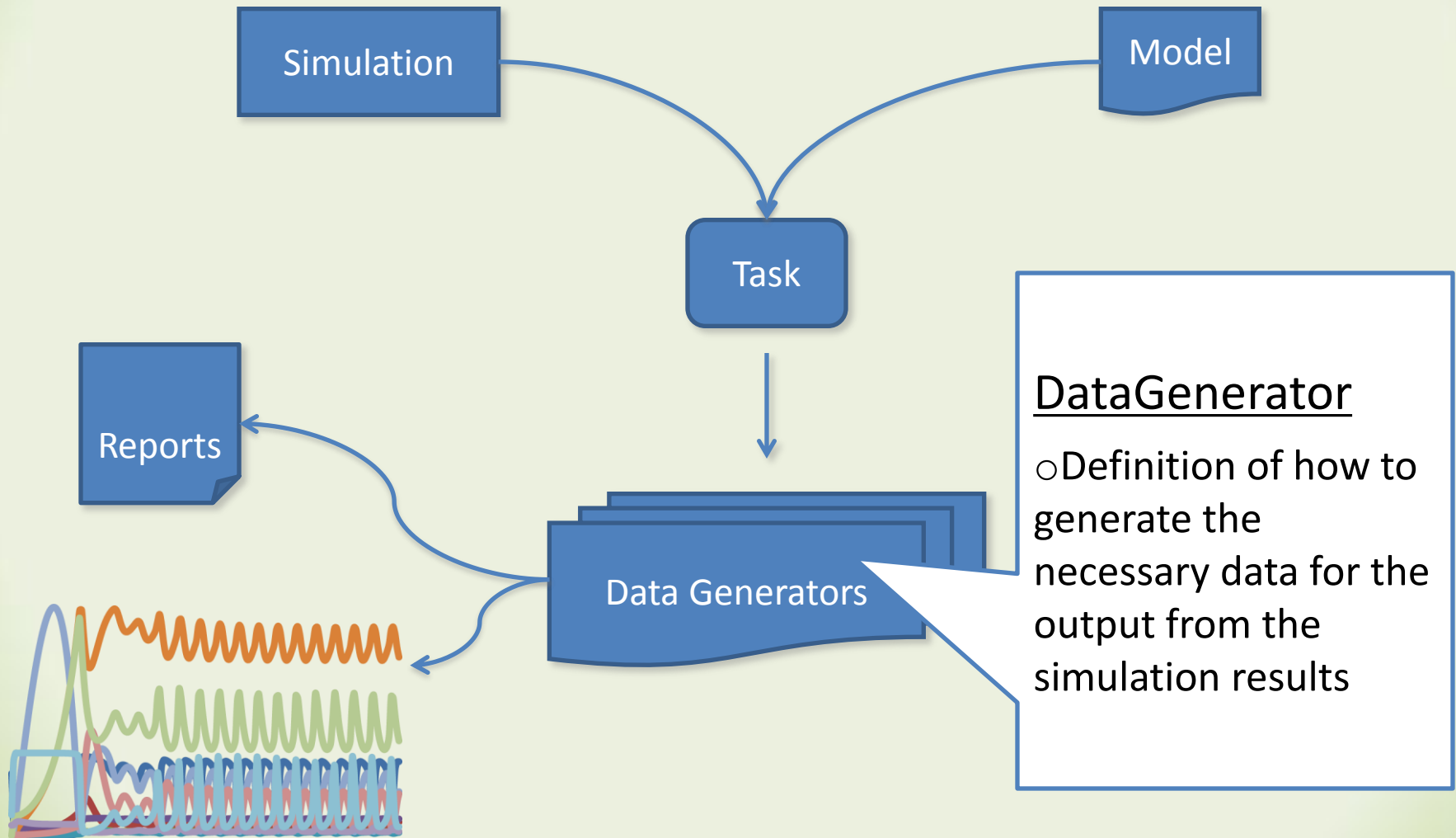
# Repeatable simulation experiments



# 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>
    </dataGenerator>
  </listOfDataGenerators>
  <listOfParameters />
</sedML>
```

# SED-ML L1 V1

- Spec Release Candidate 1
- available from Source forge

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

October 6, 2010

**Editors**

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

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

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)



<http://sourceforge.net/projects/sed-ml/files>

# This Session

- Update on available software implementations
  - LibSedML (.net implementation)
  - jlisedml (java implementation)

# **IMPLEMENTATION**



# libsedml



# libsedml

## SED-ML Script Editor

```
SED-ML Script Editor
AddTimeCourseSimulation('timecourse1', 'KISAO:0000019', 0, 0, 10, 1000)
AddModel('model', 'model1.xml')
AddTask('task1', 'timecourse1', 'model')
AddColumn('time1', [['time', 'task1', 'time']])
AddColumn('S11', [['S1', 'task1', 'S1']])
AddColumn('S21', [['S2', 'task1', 'S2']])
AddPlot('plot1', '', [['time1', 'S11'], ['time1', 'S21']]);
```



libSedMLScript



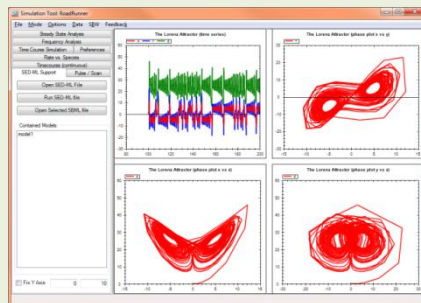
libSedML



libSedMLRunner



Other SBW enabled  
Simulators  
RoadRunner



## Simulation Tool

<http://libsedml.sf.net>

# libsedml

## SED-ML Script Editor

```
SED-ML Script Editor
AddTimeCourseSimulation('timecourse1', 'KISAO:0000019', 0, 0, 10, 1000)
AddModel('model1', 'model1.xml')
AddTask('task1', 'timecourse1', 'model1')
AddColumn('time1', [['time', 'task1', 'time']])
AddColumn('S11', [['S1', 'task1', 'S1']])
AddColumn('S21', [['S2', 'task1', 'S2']])
AddPlot('plot1', '', [['time1', 'S11'], ['time1', 'S21']]);
```



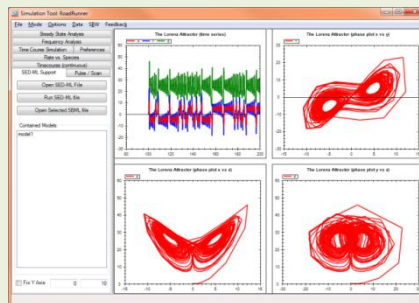
libSedMLScript



libSedML



libSedMLRunner



Simulation Tool



*JSim*

*iBioSim*

# Libsedml script

```
<?xml version="1.0" encoding="UTF-8" ?>
<sedML version="0.1" xmlns="http://sed-ml.org/sedML#">
  <notes>Changing a system</notes>
  <listOfSimulations>
    <uniformTimeCourse id="simulation1"
      outputEndTime="1000" />
  </listOfSimulations>
  <listOfModels>
    <model id="model1"
      source="urn:miriam:biomodels.db:K1SAO:0000071" />
    <model id="model2"
      source="urn:miriam:biomodels.db:BIOMD000000021" />
    <listOfChanges>
      <changeAttribute type="parameter"
        [@id='V_mT'] />
      <changeAttribute type="parameter"
        [@id='V_dT'] />
    </listOfChanges>
  </listOfModels>
  <listOfTasks>
    <task id="task1" name="AddTask" />
    <task id="task2" name="AddTask" />
  </listOfTasks>
  <listOfDataGenerators>
    <dataGenerator id="tim"
      <listOfVariables>
        <variable id="time" />
      </listOfVariables>
    </listOfDataGenerators>
  </listOfParameters />
</sedML>
```

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

```
AddModel('model1', 'urn:miriam:biomodels.db:BIOMD000000021')
```

```
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']])
```

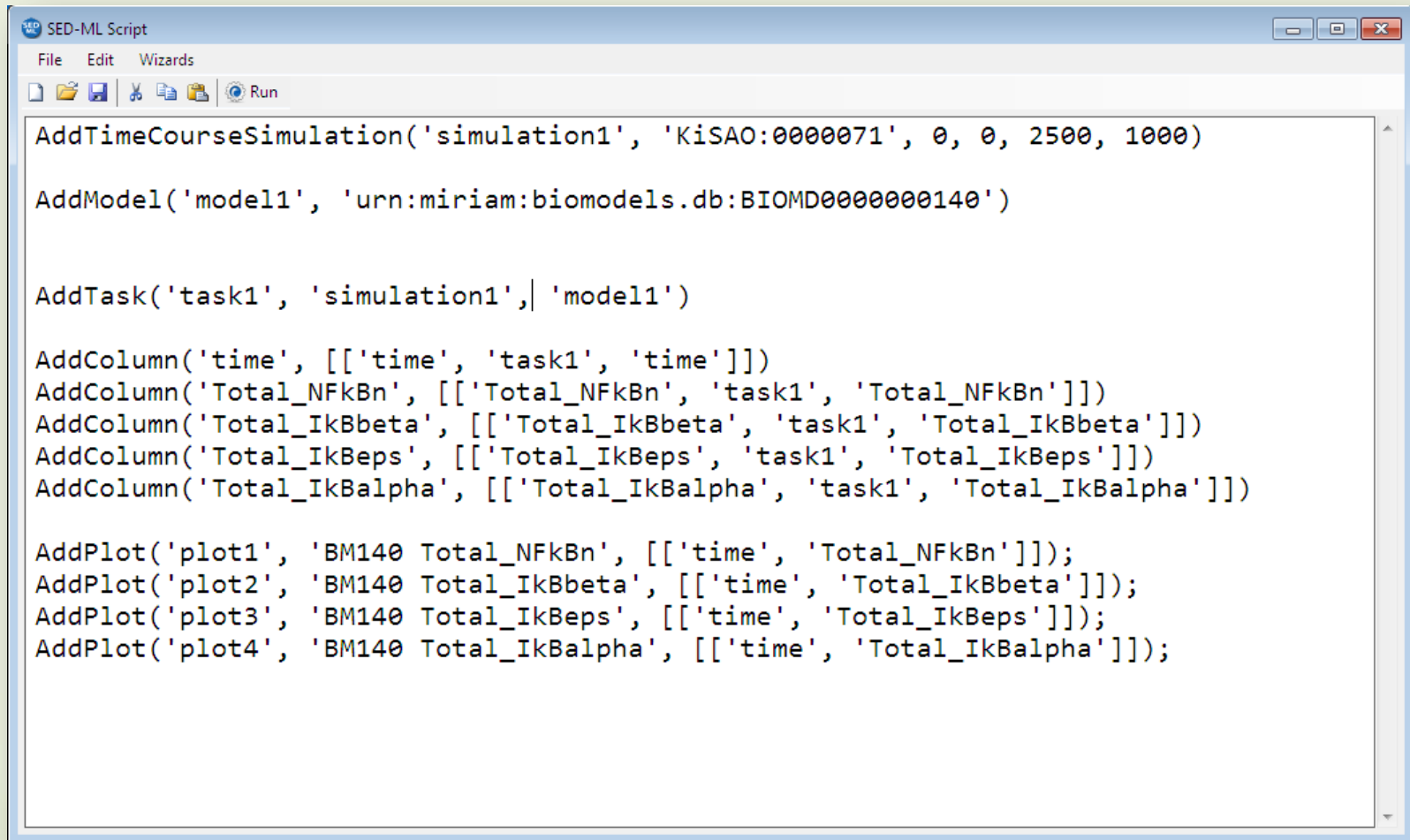
```
AddColumn('Mt_combined', [['v1', 'task1', 'Mt'], ['v2', 'task2',
'Mt'], 'v1 - v2 + 20'])
```

```
AddPlot('plot1', 'tim mRNA with Oscillation and Chaos',
```

```
[[ 'time', 'Mt_original'], [ 'time', 'Mt_chaotic'], [ 'time',
'Mt_combined']]);
```

MathML">

# SED-ML script editor



```
SED-ML Script
File Edit Wizards
AddTimeCourseSimulation('simulation1', 'KISA0:0000071', 0, 0, 2500, 1000)

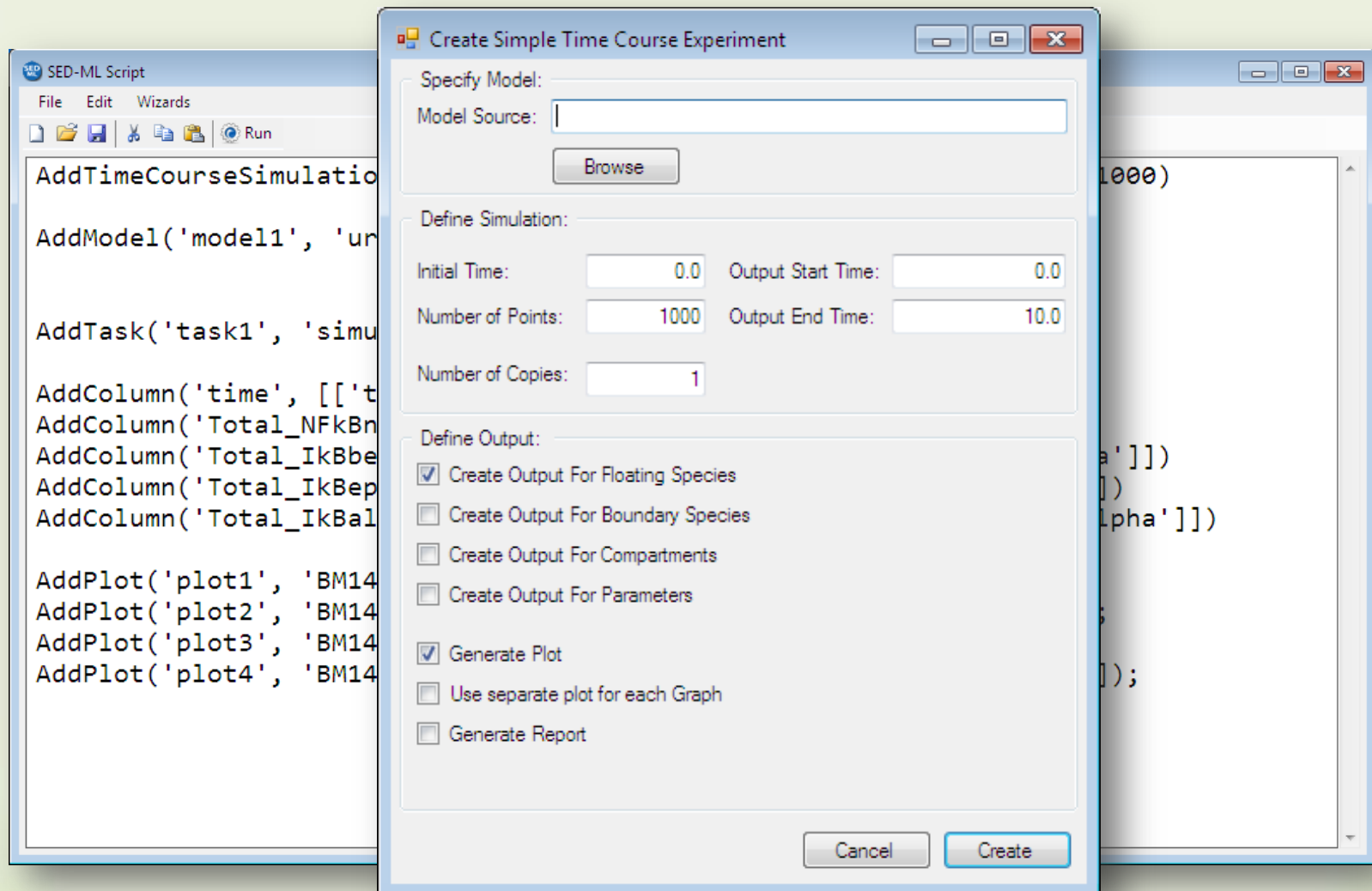
AddModel('model1', 'urn:miriam:biomodels.db:BIOMD0000000140')

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

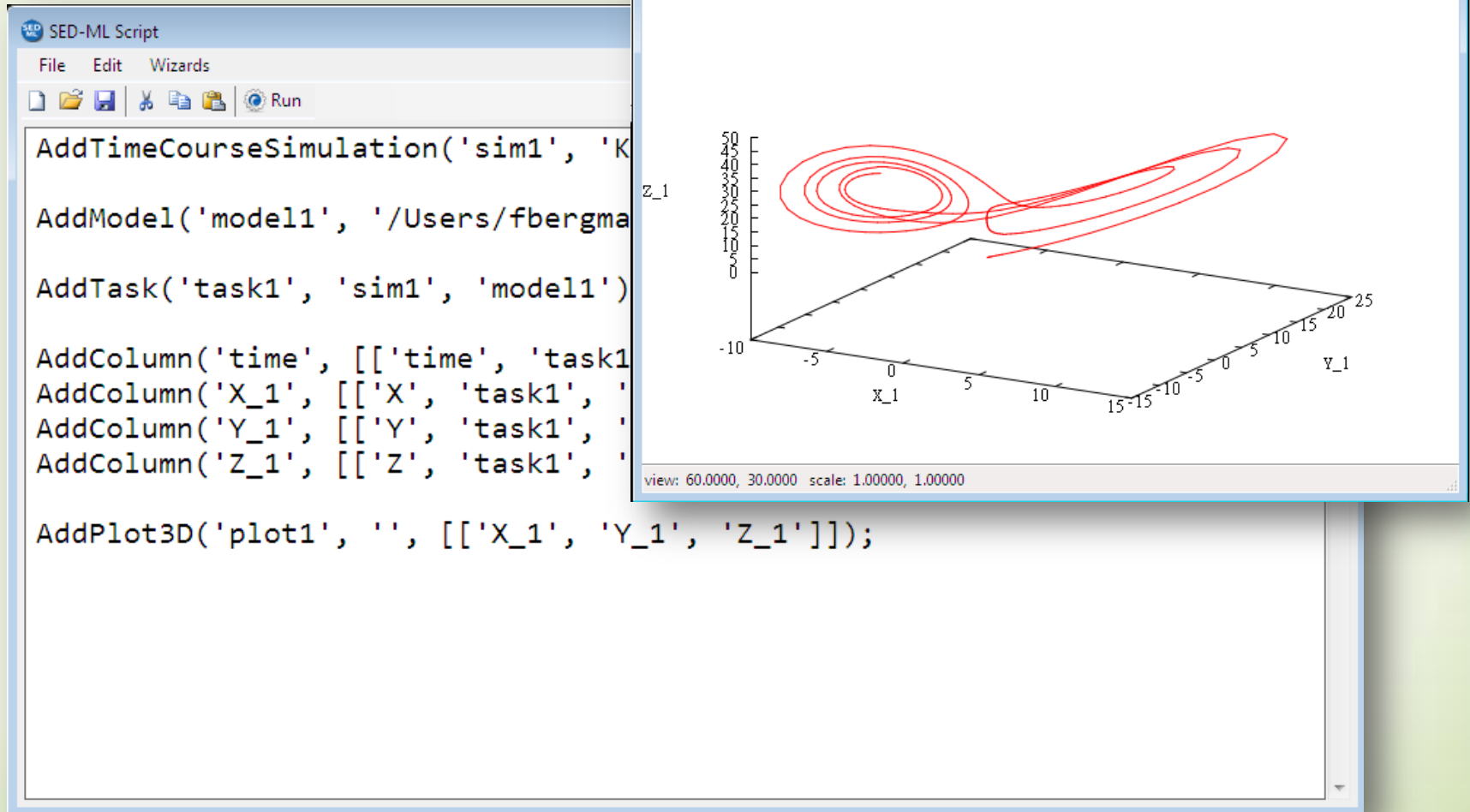
AddColumn('time', [['time', 'task1', 'time']])
AddColumn('Total_NFkBn', [['Total_NFkBn', 'task1', 'Total_NFkBn']])
AddColumn('Total_IkBbeta', [['Total_IkBbeta', 'task1', 'Total_IkBbeta']])
AddColumn('Total_IkBeps', [['Total_IkBeps', 'task1', 'Total_IkBeps']])
AddColumn('Total_IkBalpha', [['Total_IkBalpha', 'task1', 'Total_IkBalpha']])

AddPlot('plot1', 'BM140 Total_NFkBn', [['time', 'Total_NFkBn']]);
AddPlot('plot2', 'BM140 Total_IkBbeta', [['time', 'Total_IkBbeta']]);
AddPlot('plot3', 'BM140 Total_IkBeps', [['time', 'Total_IkBeps']]);
AddPlot('plot4', 'BM140 Total_IkBalpha', [['time', 'Total_IkBalpha']]);
```

# SED-ML script editor

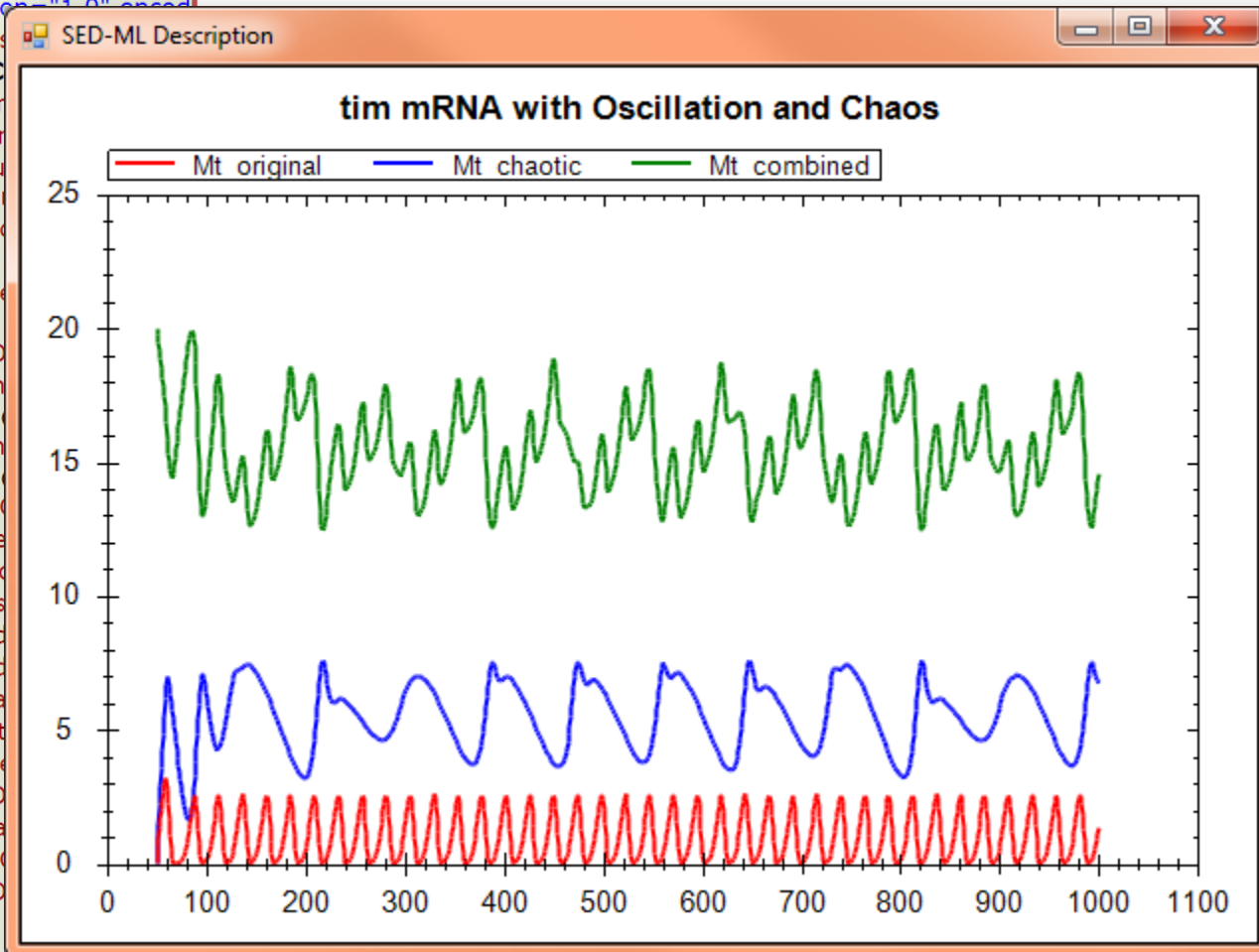


# SED-ML script editor



# Libsedml - runner

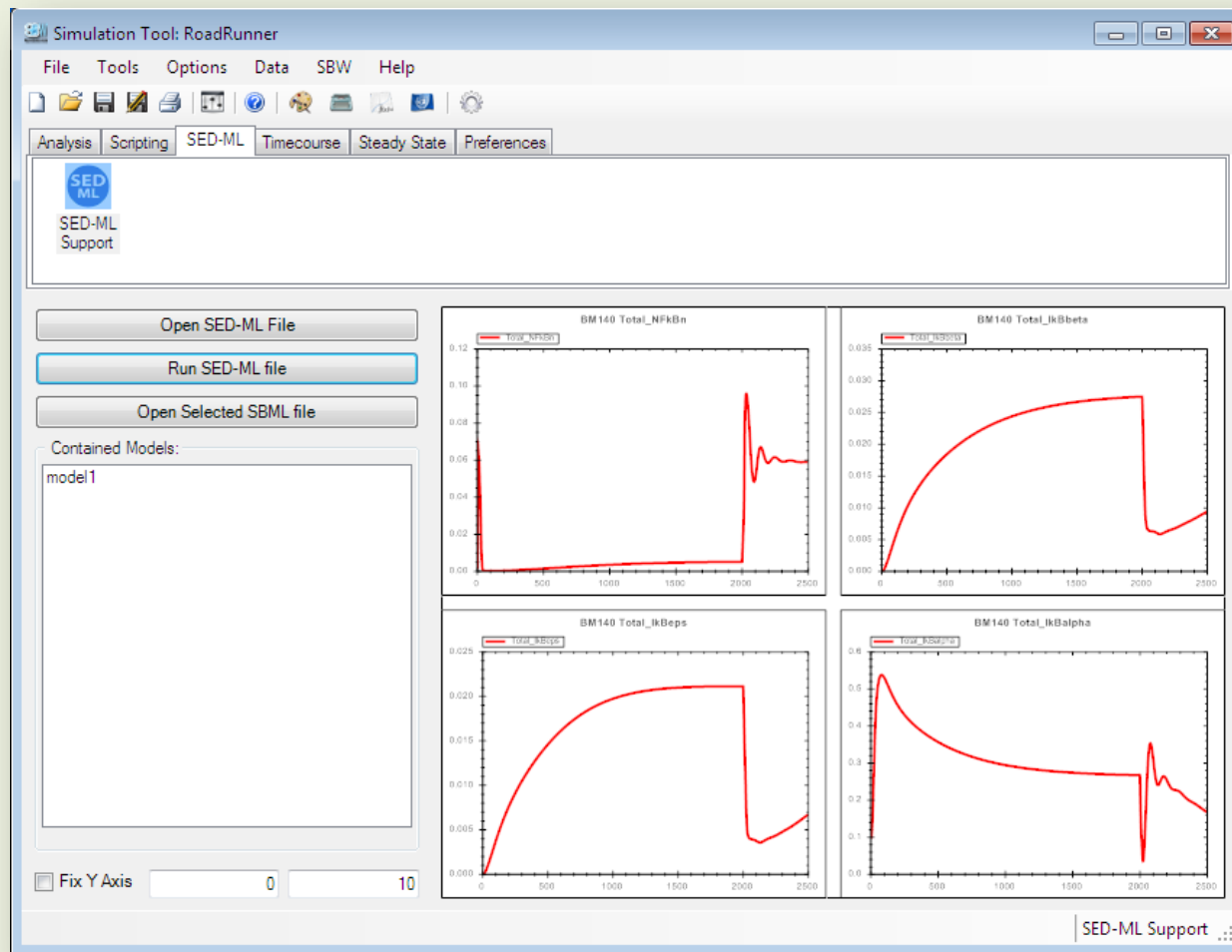
```
<?xml version="1.0" encoding="UTF-8" ?>
<sedML version="1.0" >
  <notes>
    <listOfSimulations>
      <uniformRandomGenerator>
        <output>
          </listOfSimulations>
        </listOfSimulations>
      </listOfSimulations>
    </notes>
    <listOfModels>
      <model>
        <source>
          <model>
            <listOfParameters>
              <parameter>
                <name>
                  <value>
                </value>
              </parameter>
            </listOfParameters>
          </model>
        </source>
      </model>
    </listOfModels>
    <listOfTasks>
      <task id="1">
        <task id="1">
          </listOfTasks>
        </task id="1">
      </listOfTasks>
    </listOfTasks>
    <listOfDataGenerators>
      <dataGenerator>
        <listOfDataGenerators>
          <dataGenerator>
            <value>
          </value>
        </listOfDataGenerators>
      </dataGenerator>
    </listOfDataGenerators>
  </sedML>
```



MathML">



# Simulation Tool



# Outlook

- Research how to encode more simulation experiments
- Add Advanced Post processing
- Performance improvements

# Acknowledgements

Nicolas Le Novère

Sven Sahle

Henning Schmidt

Mike Hucka

Ion Moraru

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Richard Adams

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