

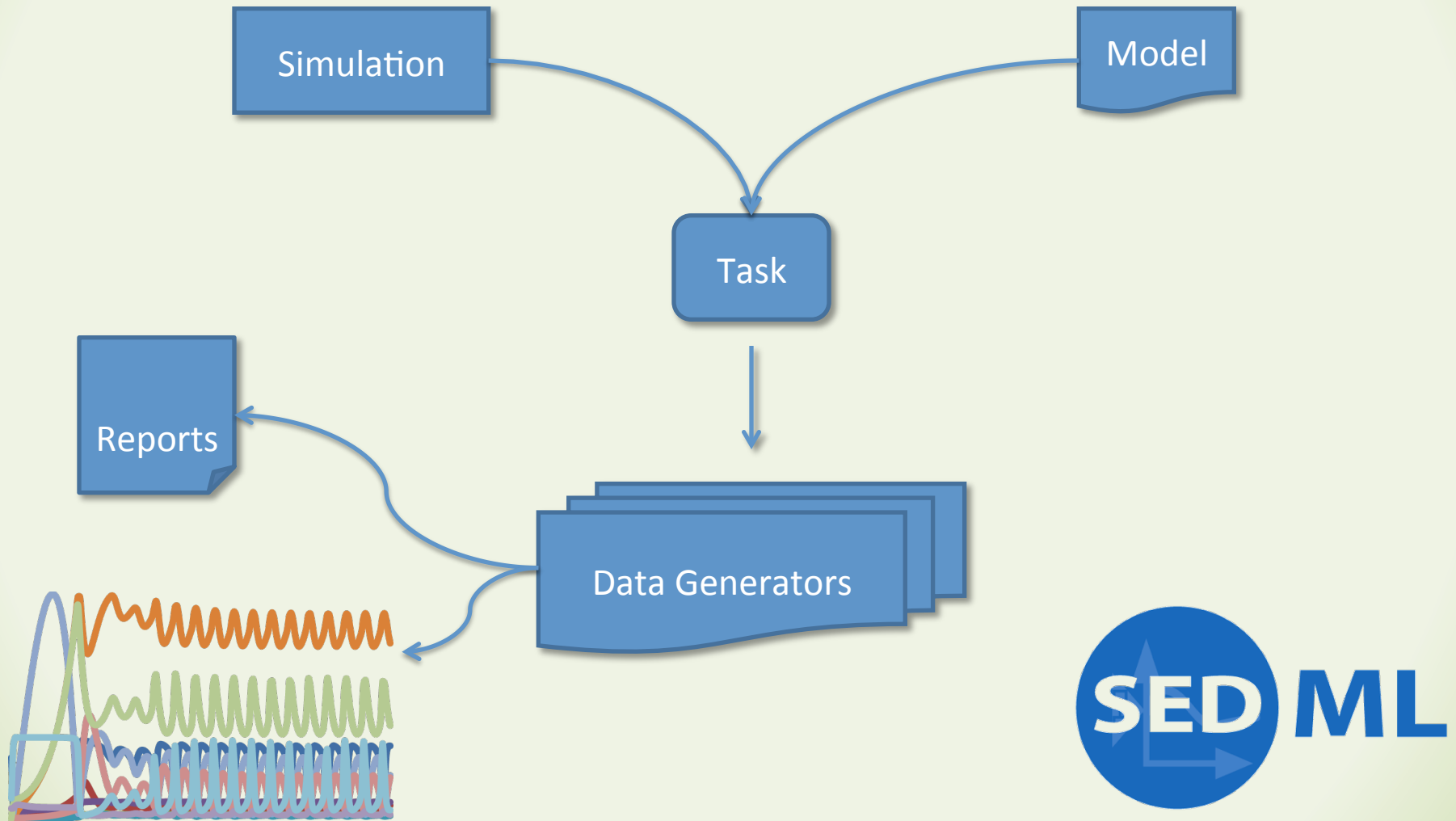
LibSedML

<http://libsedml.sf.net>

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HARMONY 2012, Maastricht, NL

Repeatable simulation experiments



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']]);
```



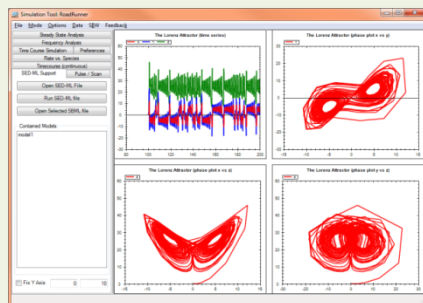
libSedMLScript



libSedML



libSedMLRunner



Simulation Tool



JSim

iBioSim

RoadRunner

<http://libsedml.sf.net>

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:BIOMD0000000021" />
    <model id="model2"
      source="urn:miriam:biomodels.db:BIOMD0000000021" />
    <listOfChanges>
      <changeAttribute type="parameter"
        [@id='V_mT'] />
      <changeAttribute type="parameter"
        [@id='V_dT'] />
    </listOfChanges>
  </model>
</listOfModels>
  <listOfTasks>
    <task id="task1" name="task1" />
    <task id="task2" name="task2" />
  </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: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']]);
```

MathML">

libSedML

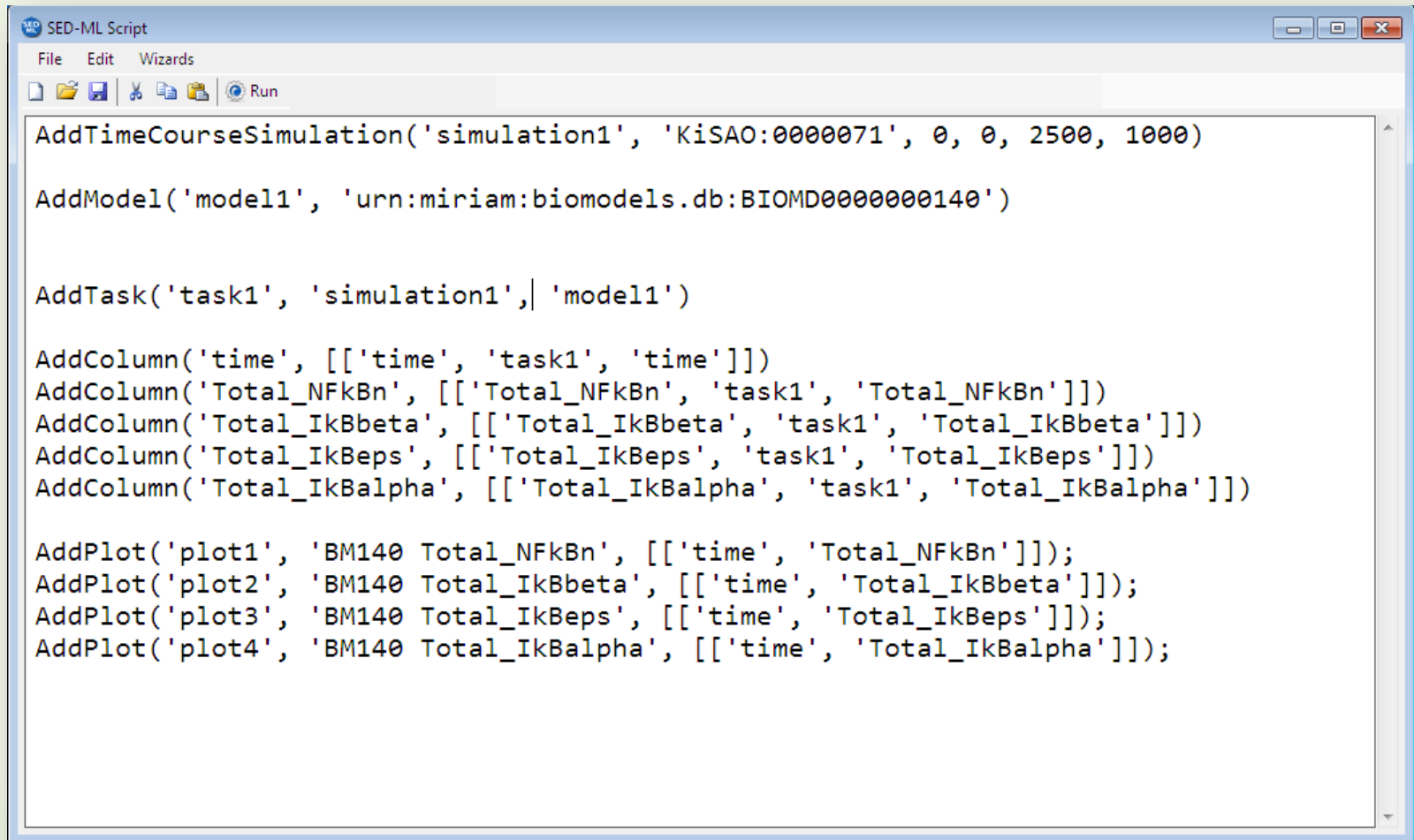


<http://libsedml.sf.net>

Features

- LibSedML
 - Read, Create, Write, Manipulate
 - Validate, Archive
 - Resolve models from FS, Web + Miriam URN
 - Applies changes to models
- Supported Model Description languages:
 - SBML + CellML

SED-ML script editor



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

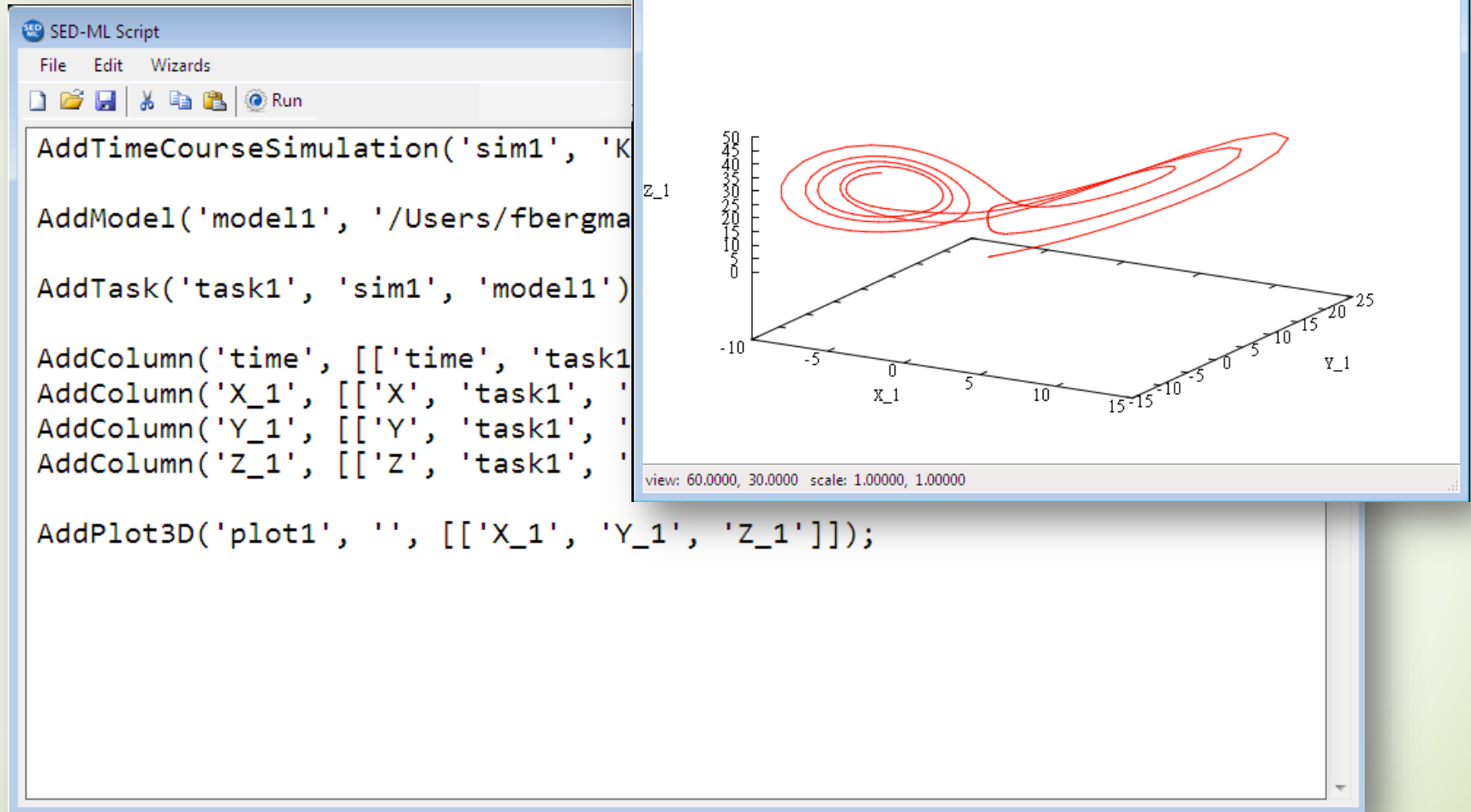
AddModel('model1', 'urn:miriam:biomodels.db:BIOMD0000000140')

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

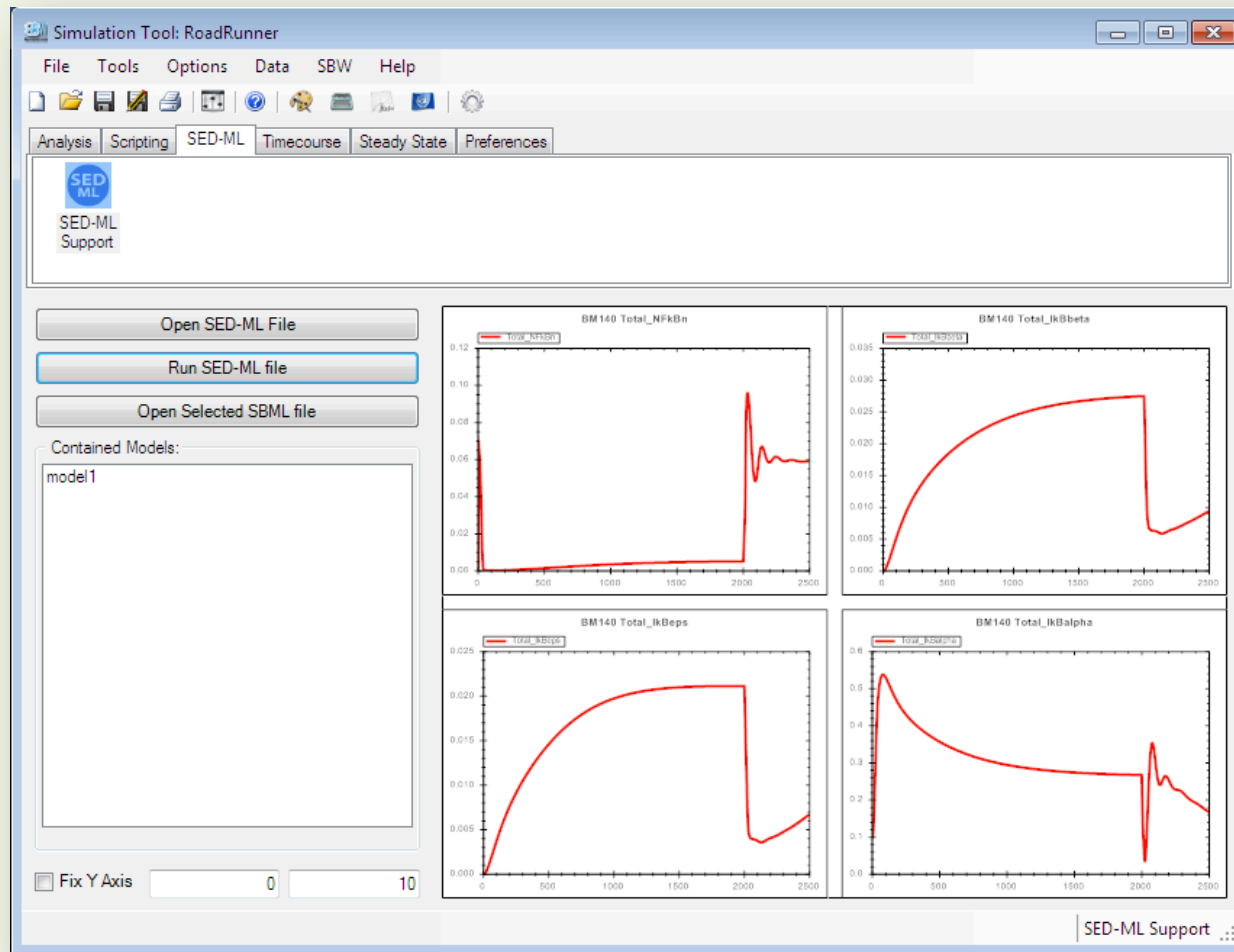
AddColumn('time', [['time', 'task1', 'time']])
AddColumn('Total_NFkBn', [['Total_NFkBn', 'task1', 'Total_NFkBn']])
AddColumn('Total_IkBbeta', [['Total_IkBbeta', 'task1', 'Total_IkBbeta']])
AddColumn('Total_IkBeps', [['Total_IkBeps', 'task1', 'Total_IkBeps']])
AddColumn('Total_IkBalpha', [['Total_IkBalpha',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

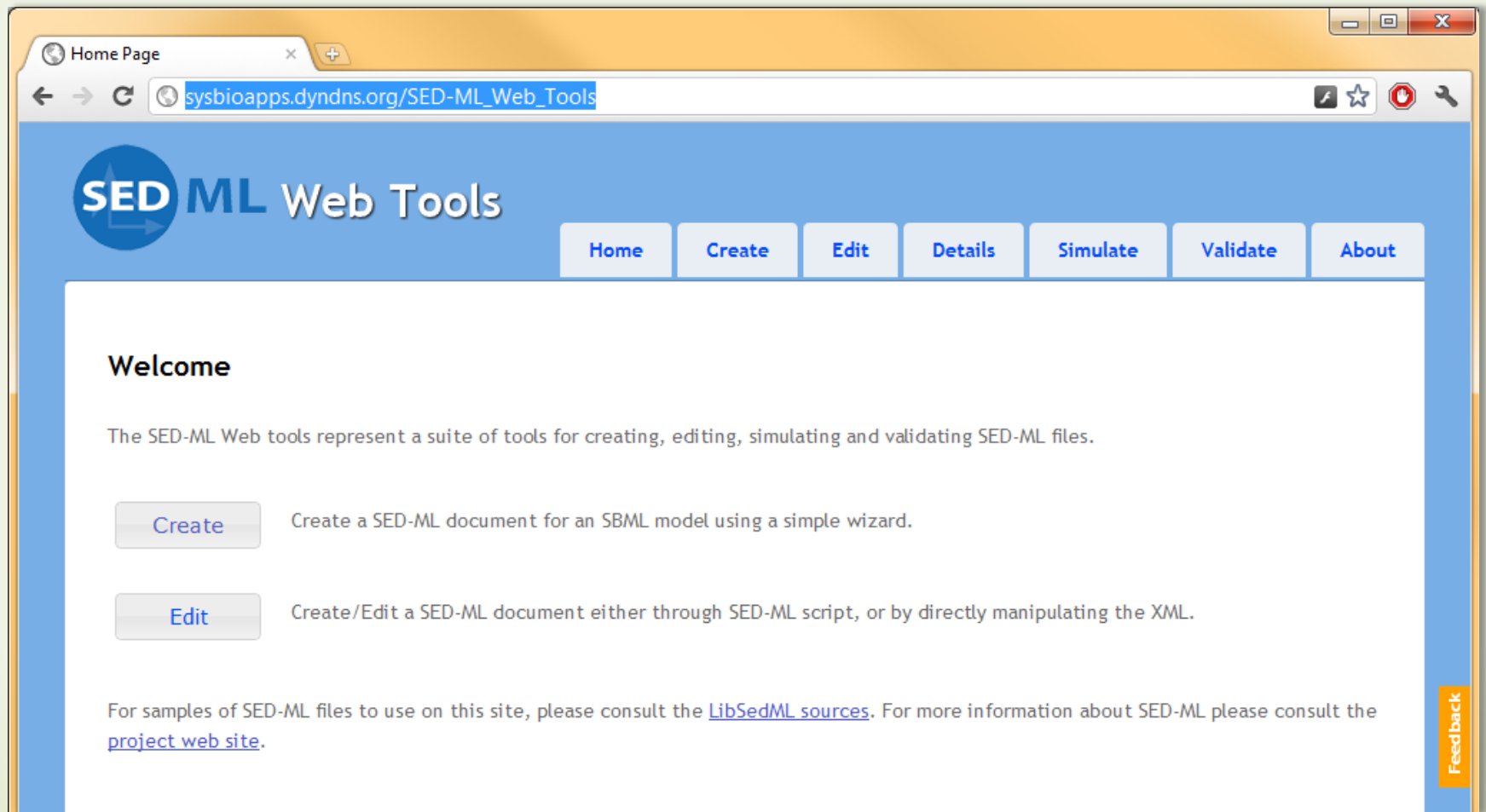
SED-ML script editor



SBW Simulation Tool



SED-ML Web Tools



http://sysbioapps.dyndns.org/SED-ML_Web_Tools

HARMONY 2012

- Tuesday 11am:
 - Troubleshooting session: ROOM 123
- Wednesday 11am:
 - Nested Simulations, ROOM 147

