



libSedML Updates and SED-ML Web Tools

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LIBSEDML UPDATE

LibSedML

SED-ML Script Editor

```
lib SED-ML Script
File Edit View Help
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



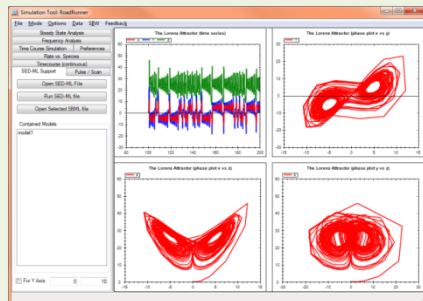
libSedML



libSedMLRunner



Other SBW enabled
Simulators
RoadRunner



Simulation Tool

What is new - LibSedML

- Clear separation of model specific code
 - **Introduction of** `IModelingLanguage` interface for
 - Resolving the native identifier for a SED-ML Variable
 - Constructing the XPath expression for SED-ML Variables
 - Ensuring that SED-ML Variables point to the right things
 - Implementation of SBML and CellML Language
 - Introduction of a Language Store concept, where all supported languages will be registered.
- Adding of Validation Routines

What is new - LibSedML

- Adding AutoCorrect options:
 - Fix time symbol
 - Add missing Ids
 - Check for duplicated Variables
 - Fix the language element
 - Fix the KISAO id

What is new - LibSedMLScript

- Follows the separation from LibSedML and now also supports the modification of CellML experiments
- Finally documented the supported language elements are:

<http://dx.doi.org/10.1038/npre.2011.6105.1>

Nature Precedings : doi:10.1038/npre.2011.6105.1 : Posted 11 Jul 2011

SED-ML Script Language

Editing / Creating SED-ML descriptions

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7/9/2011

This document describes a human readable alternative to writing SED-ML descriptions.

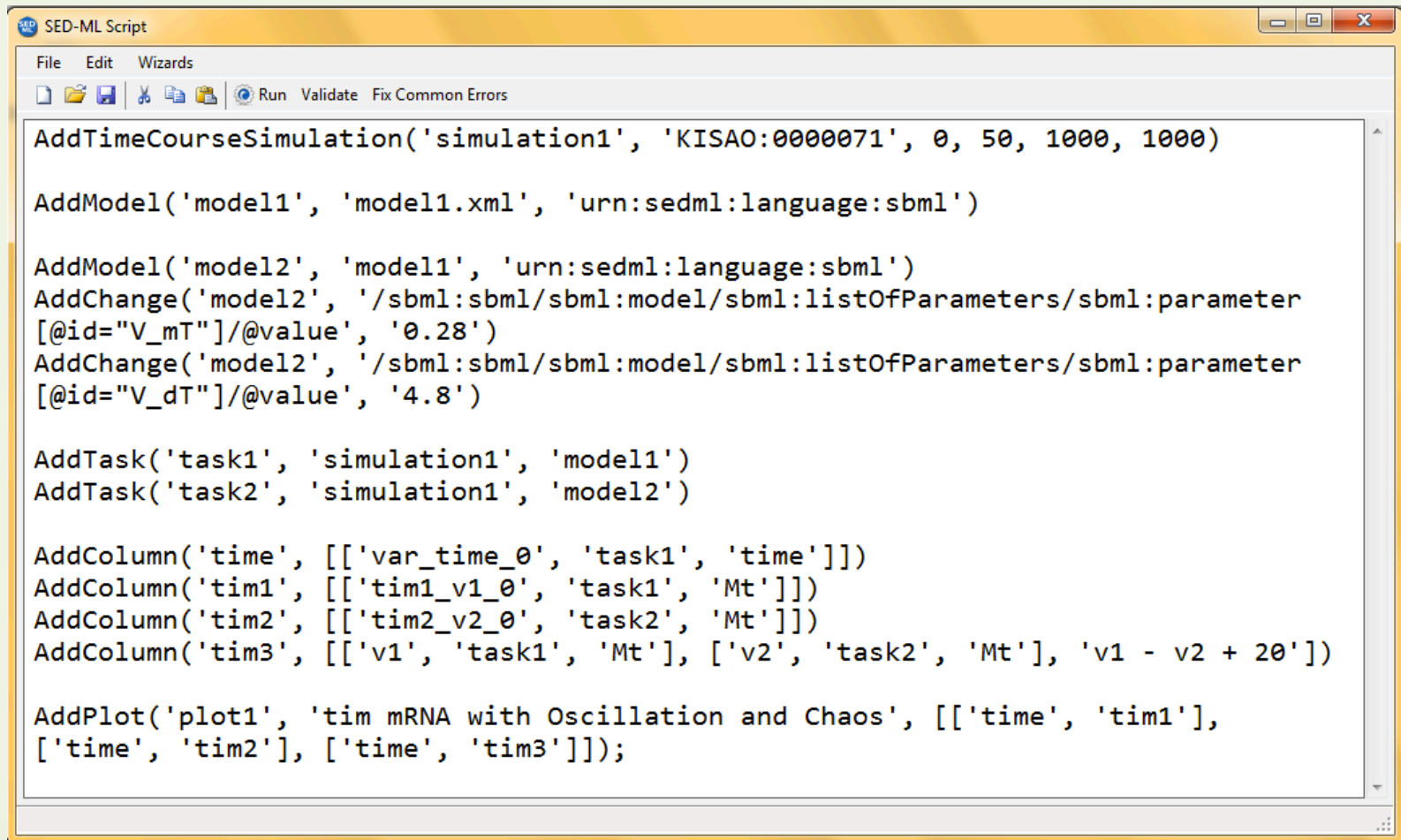
What is new - LibSedMLRunner

- Similar to LibSedML clear abstraction of supported simulators
- Based on binaries from David Nickerson:
 - Simulation Support for CellML models

<http://sf.net/projects/libsedml/files>

SED-ML SCRIPT EDITOR 1.6

SED-ML Script Editor



```
SED-ML Script
File Edit Wizards
AddTimeCourseSimulation('simulation1', 'KISA0:0000071', 0, 50, 1000, 1000)

AddModel('model1', 'model1.xml', 'urn:sedml:language:sbml')

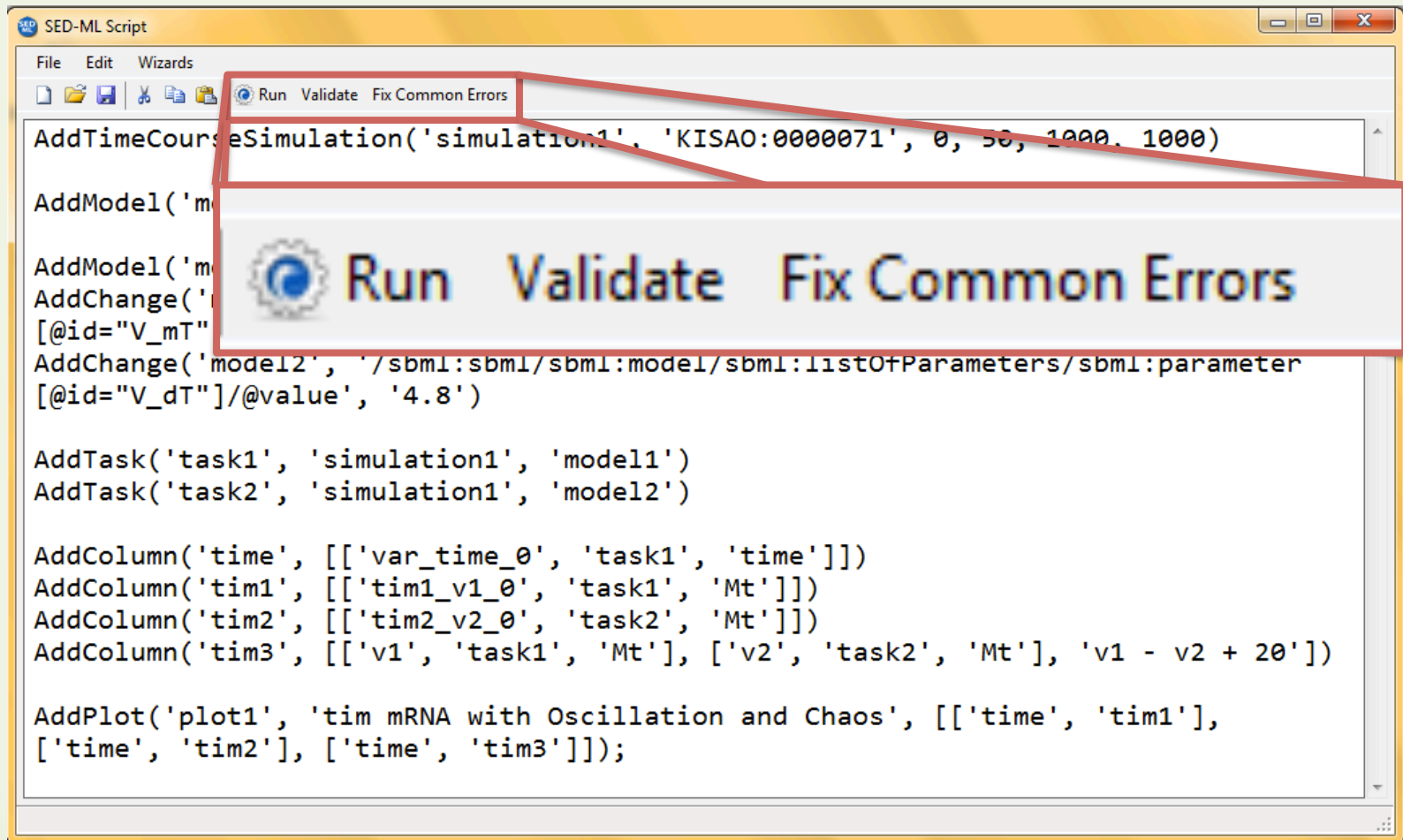
AddModel('model2', 'model1', 'urn:sedml:language:sbml')
AddChange('model2', '/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
[@id="V_mT"]/@value', '0.28')
AddChange('model2', '/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
[@id="V_dT"]/@value', '4.8')

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

AddColumn('time', [['var_time_0', 'task1', 'time']])
AddColumn('tim1', [['tim1_v1_0', 'task1', 'Mt']])
AddColumn('tim2', [['tim2_v2_0', 'task2', 'Mt']])
AddColumn('tim3', [['v1', 'task1', 'Mt'], ['v2', 'task2', 'Mt'], 'v1 - v2 + 20'])

AddPlot('plot1', 'tim mRNA with Oscillation and Chaos', [['time', 'tim1'],
['time', 'tim2'], ['time', 'tim3']]);
```

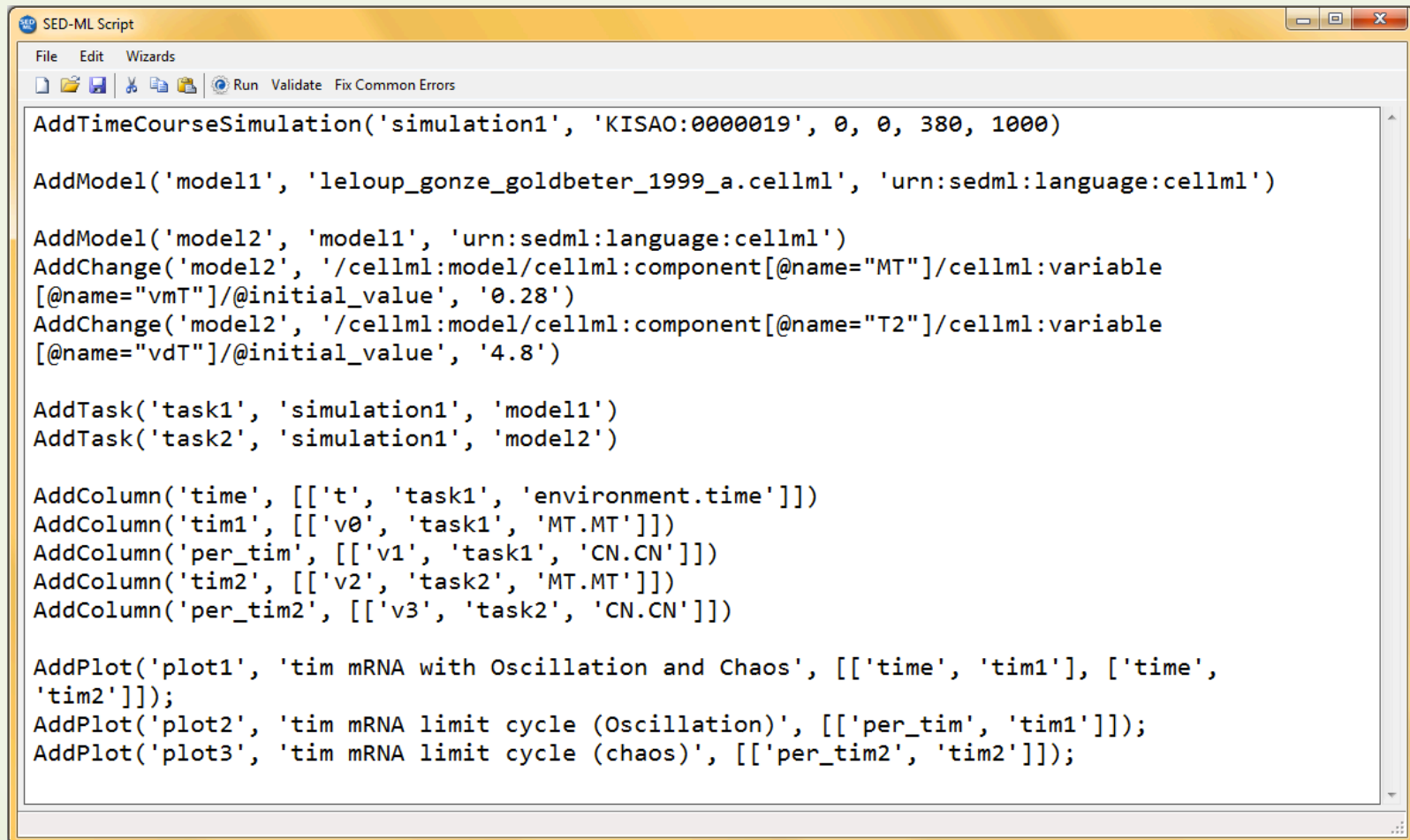
SED-ML Script Editor



SED-ML Script Editor - Validation



SED-ML Script Editor - CellML



```
SED-ML Script
File Edit Wizards
AddTimeCourseSimulation('simulation1', 'KISAO:0000019', 0, 0, 380, 1000)

AddModel('model1', 'leloup_gonze_goldebeter_1999_a.cellml', 'urn:sedml:language:cellml')

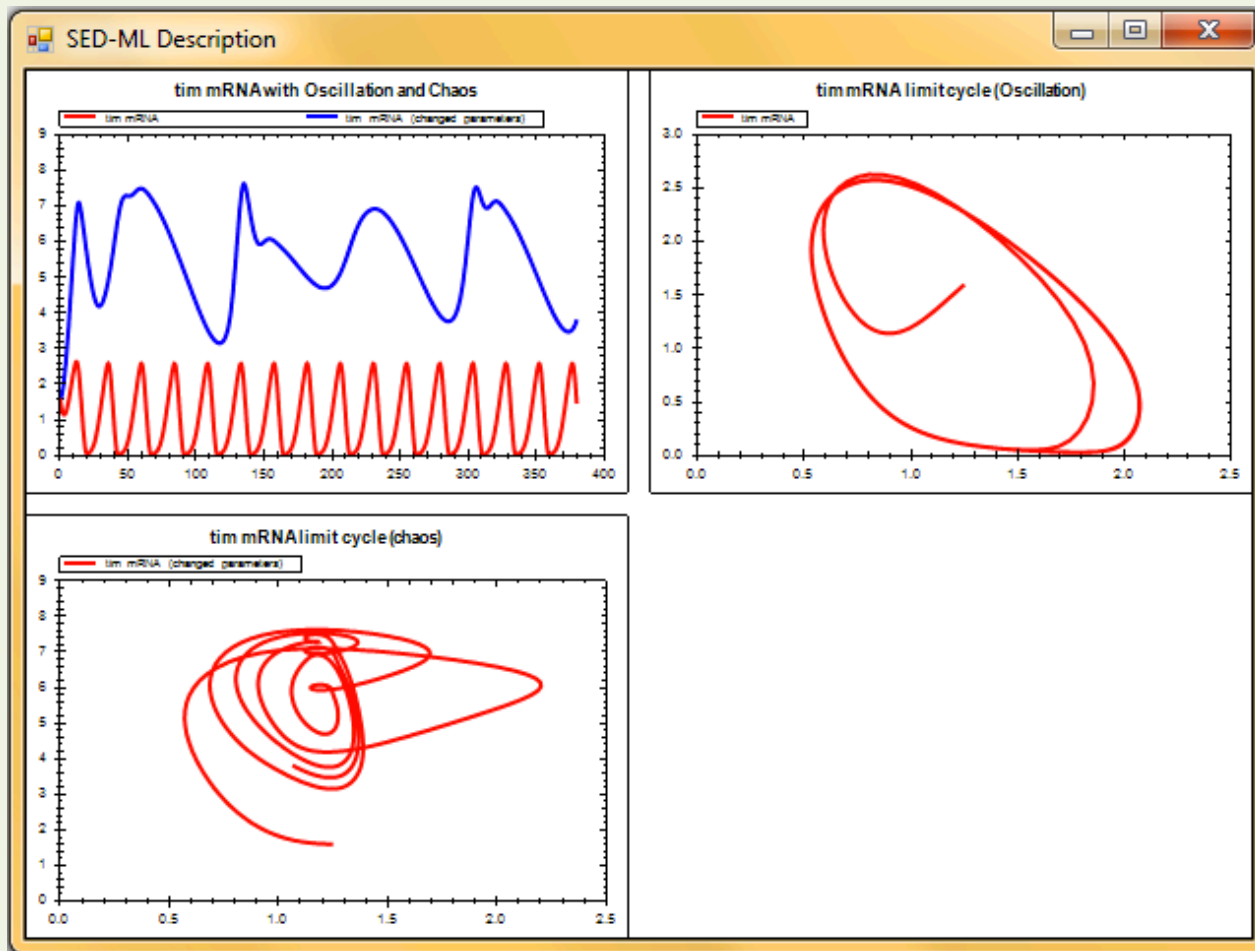
AddModel('model2', 'model1', 'urn:sedml:language:cellml')
AddChange('model2', '/cellml:model/cellml:component[@name="MT"]/cellml:variable
[@name="vmT"]/@initial_value', '0.28')
AddChange('model2', '/cellml:model/cellml:component[@name="T2"]/cellml:variable
[@name="vdT"]/@initial_value', '4.8')

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

AddColumn('time', [['t', 'task1', 'environment.time']])
AddColumn('tim1', [['v0', 'task1', 'MT.MT']])
AddColumn('per_tim', [['v1', 'task1', 'CN.CN']])
AddColumn('tim2', [['v2', 'task2', 'MT.MT']])
AddColumn('per_tim2', [['v3', 'task2', 'CN.CN']])

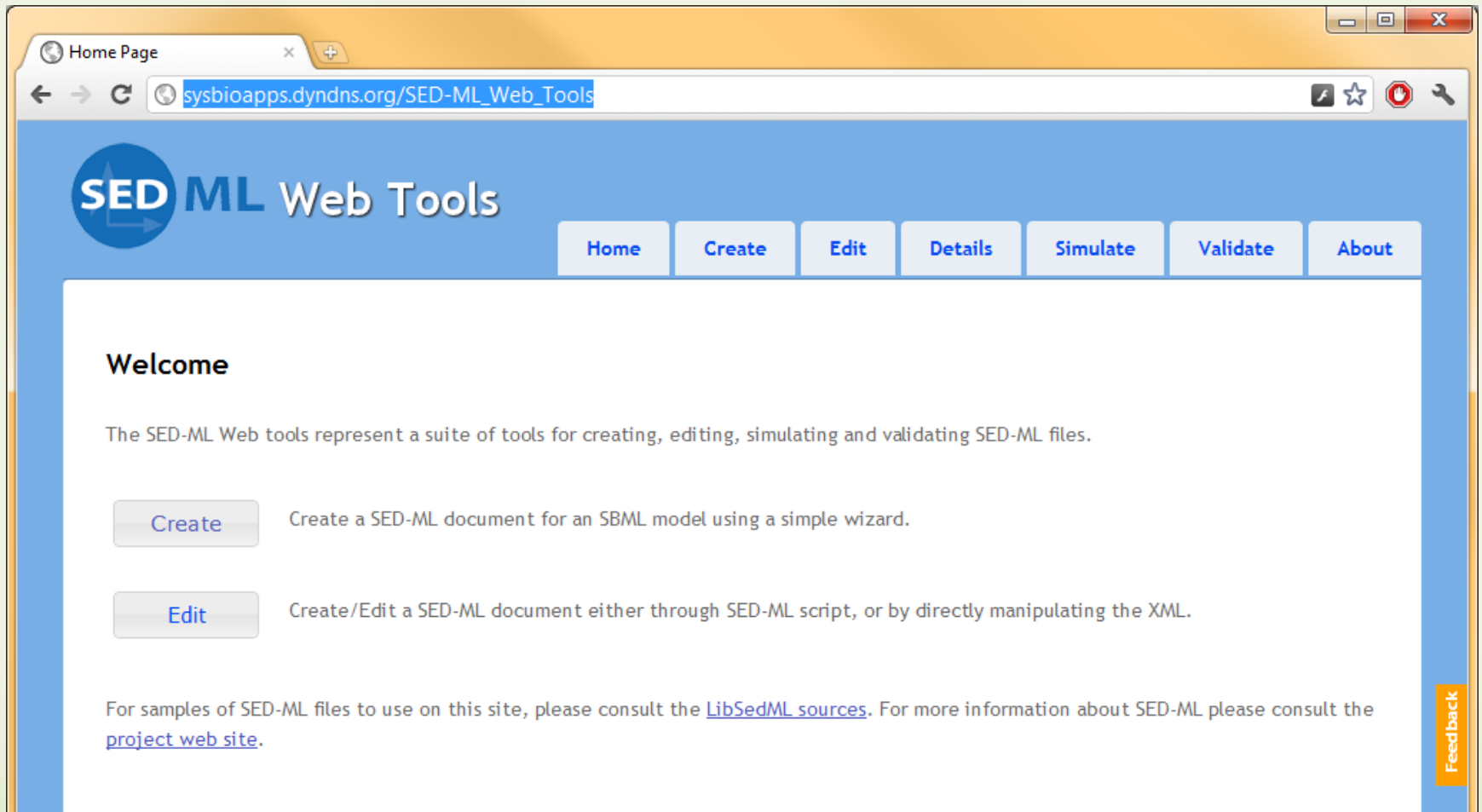
AddPlot('plot1', 'tim mRNA with Oscillation and Chaos', [['time', 'tim1'], ['time',
'tim2']]);
AddPlot('plot2', 'tim mRNA limit cycle (Oscillation)', [['per_tim', 'tim1']]);
AddPlot('plot3', 'tim mRNA limit cycle (chaos)', [['per_tim2', 'tim2']]);
```

SED-ML Script Editor - CellML



SED-ML WEB TOOLS

SED-ML Web Tools



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

SED-ML Web Tools - Create

Create

sysbioapps.dyndns.org/SED-ML_Web_Tools/Home/Create?Length=4

SED ML Web Tools

Home Create Edit Details Simulate Validate About

Create SED-ML Descriptions

This first version allows creating SED-ML description for an SBML model. Simply upload the SBML model (or refer to one by miriam URN, or web site) and select the output options you would like to generate.

Define Model

FromFile: Browse

FromURL:

Define Simulation

Initial Time

Start Time

End Time

Number of Points

Define Output

- ☒ Create Output For Floating Species
- ☐ Create Output For Boundary Species
- ☐ Create Output For Compartments
- ☐ Create Output For Global Parameters
- ☒ Generate Plots
- ☐ Use separate plots for each trace
- ☐ Generate Report

Feedback

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

SED-ML Web Tools - Edit

Add Model

Edit Script

Edit SED-ML

Edit Script

Edit the document using the [SED-ML Script language](#)

```
AddTimeCourseSimulation('sim1', 'KISAO:0000019', 0, 0, 100, 1000)

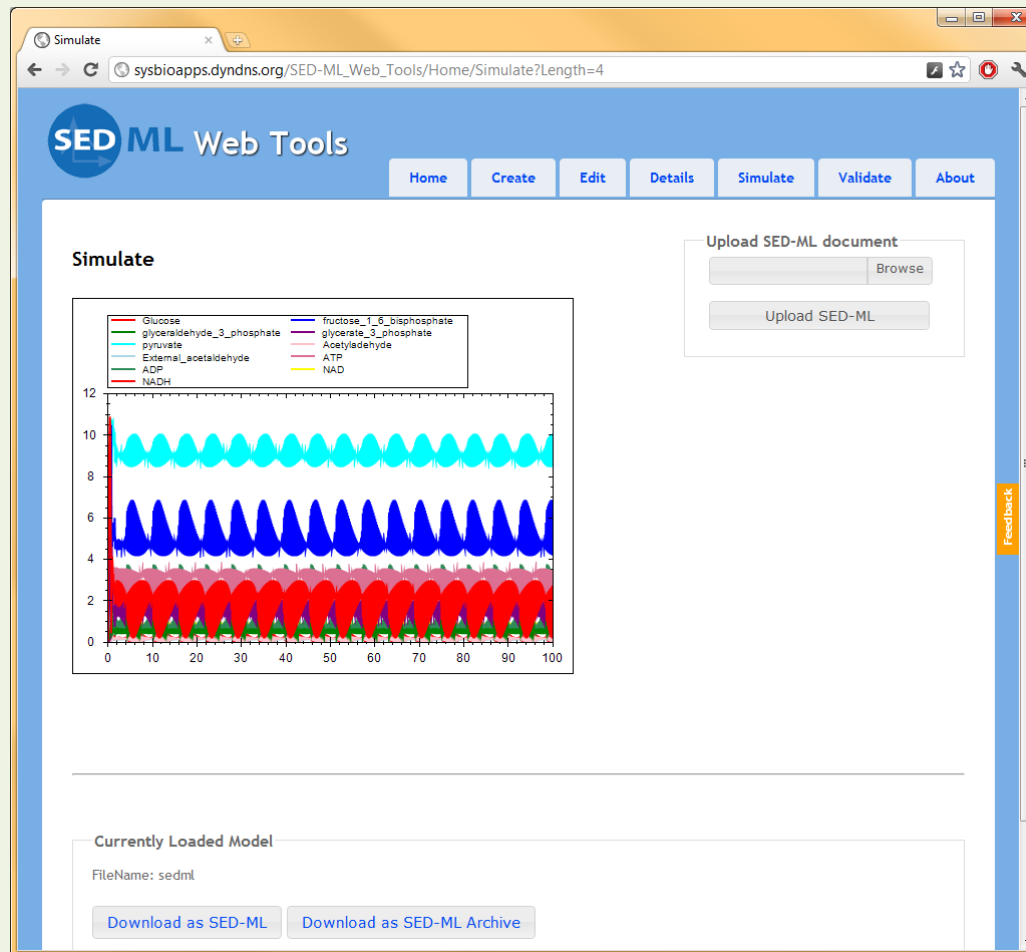
AddModel('model1', 'model1.xml', 'urn:sedml:language:sbml')

AddTask('task1', 'sim1', 'model1')

AddColumn('time', [['var_time_0', 'task1', 'time']])
AddColumn('Glucose_1', [['Glucose', 'task1', 'Glucose']])
AddColumn('fructose_1_6_bisphosphate_1', [['fructose_1_6_bisphosphate', 'task1',
'fructose_1_6_bisphosphate']])
AddColumn('glyceraldehyde_3_phosphate_1', [['glyceraldehyde_3_phosphate', 'task1',
'glyceraldehyde_3_phosphate']])
AddColumn('glycerate_3_phosphate_1', [['glycerate_3_phosphate', 'task1', 'glycerate_3_phosphate']])
AddColumn('pyruvate_1', [['pyruvate', 'task1', 'pyruvate']])
AddColumn('Acetyladehyde_1', [['Acetyladehyde', 'task1', 'Acetyladehyde']])
AddColumn('External_acetaldehyde_1', [['External_acetaldehyde', 'task1', 'External_acetaldehyde']])
AddColumn('ATP_1', [['ATP', 'task1', 'ATP']])
AddColumn('ADP_1', [['ADP', 'task1', 'ADP']])
AddColumn('NAD_1', [['NAD', 'task1', 'NAD']])
```

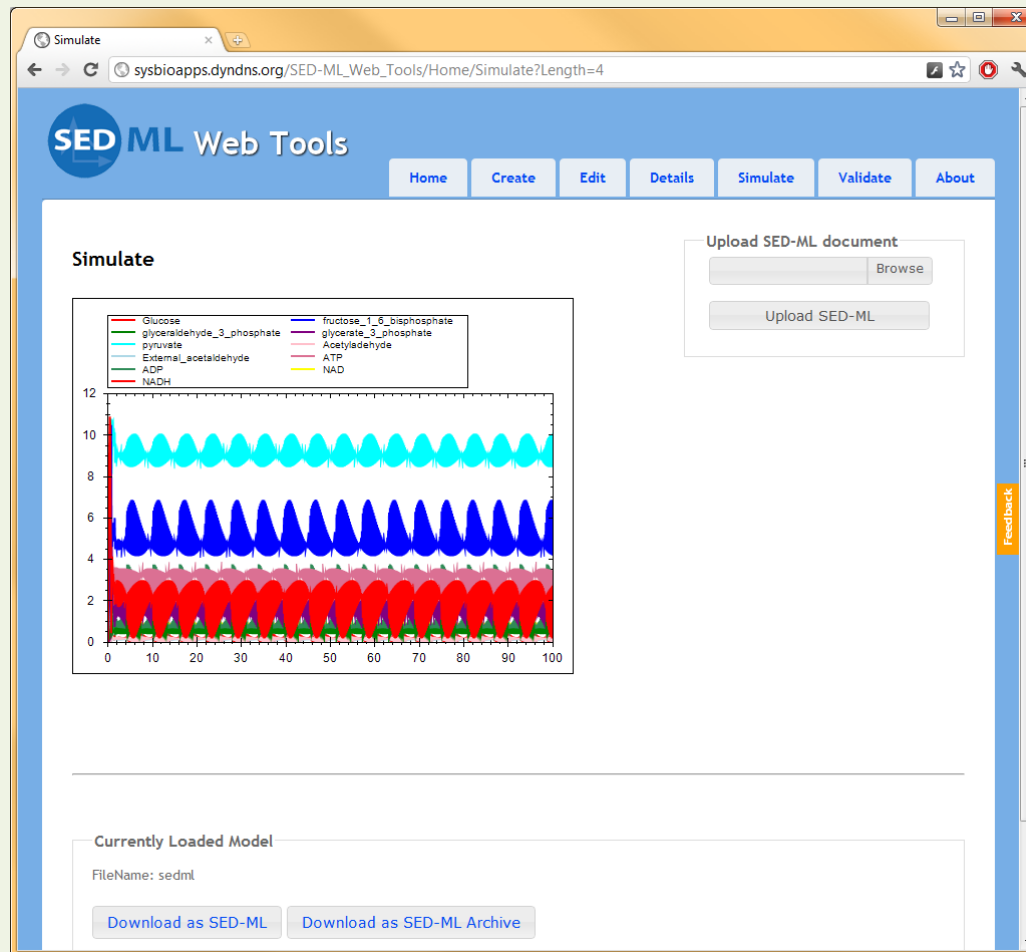
Save changes

SED-ML Web Tools - Simulate



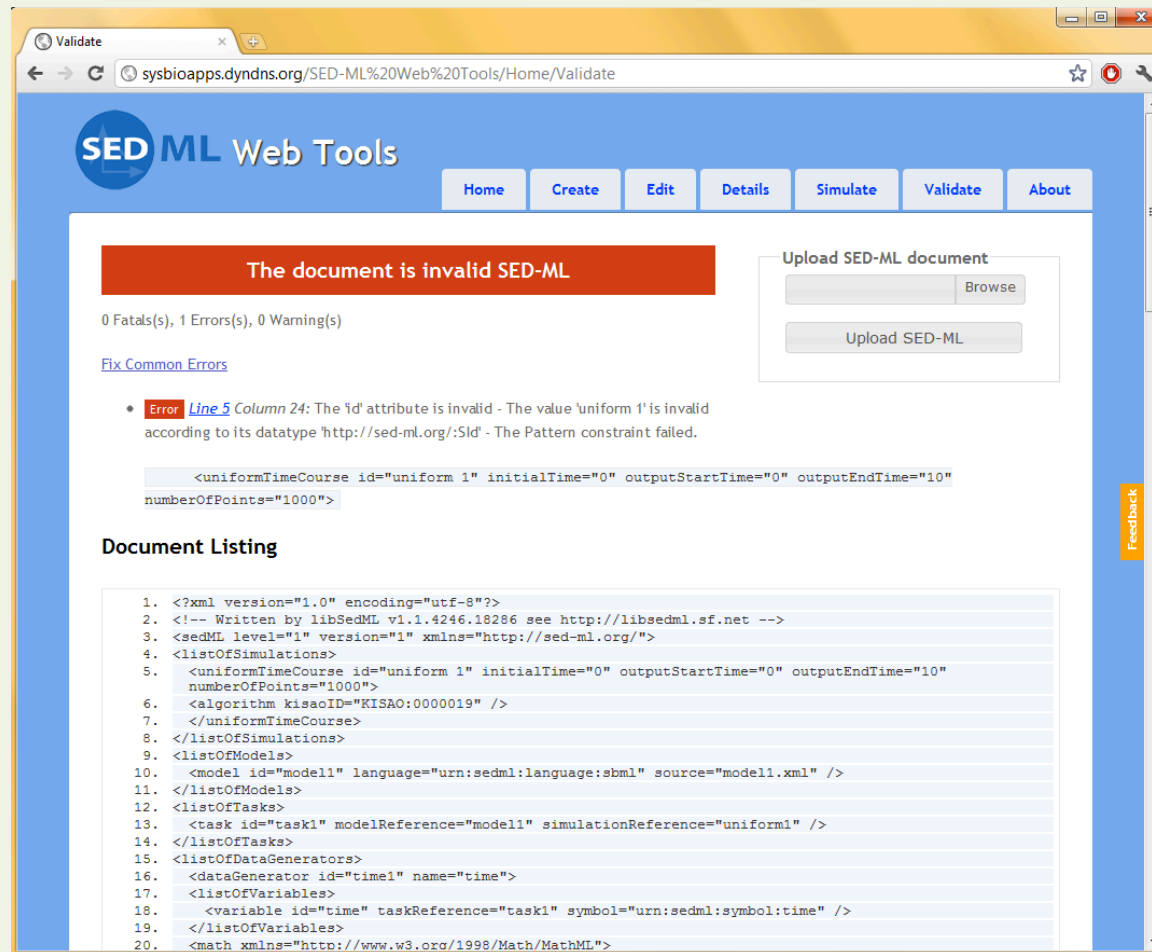
http://sysbioapps.dyndns.org/SED-ML_Web_Tools

SED-ML Web Tools - Simulate



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

SED-ML Web Tools - Validate



The screenshot shows a web browser window with the URL `sysbioapps.dyndns.org/SED-ML%20Web%20Tools/Home/Validate`. The page title is "Validate". The main header is "SED ML Web Tools" with navigation buttons: Home, Create, Edit, Details, Simulate, Validate, and About. A red banner at the top states "The document is invalid SED-ML". Below this, it says "0 Fatal(s), 1 Error(s), 0 Warning(s)" and provides a link to "Fix Common Errors". An error message is displayed: "Error Line 5 Column 24: The 'id' attribute is invalid - The value 'uniform 1' is invalid according to its datatype 'http://sed-ml.org/:SId' - The Pattern constraint failed." Below the error message, the XML snippet is shown:

```
<uniformTimeCourse id="uniform 1" initialTime="0" outputStartTime="0" outputEndTime="10" numberOfPoints="1000">
```

 To the right of the error message is a section titled "Upload SED-ML document" with a "Browse" button and an "Upload SED-ML" button. Below the error message is a "Document Listing" section showing a list of XML elements and their attributes, including `<?xml version="1.0" encoding="utf-8"?>`, `<!-- Written by libSedML v1.1.4246.18286 see http://libsedml.sf.net -->`, `<sedML level="1" version="1" xmlns="http://sed-ml.org/">`, `<listOfSimulations>`, `<uniformTimeCourse id="uniform 1" initialTime="0" outputStartTime="0" outputEndTime="10" numberOfPoints="1000">`, `<algorithm kisaoID="KISAO:000019" />`, `</uniformTimeCourse>`, `</listOfSimulations>`, `<listOfModels>`, `<model id="model1" language="urn:sedml:language:sbml" source="model1.xml" />`, `</listOfModels>`, `<listOfTasks>`, `<task id="task1" modelReference="model1" simulationReference="uniform1" />`, `</listOfTasks>`, `<listOfDataGenerators>`, `<dataGenerator id="time1" name="time">`, `<listOfVariables>`, `<variable id="time" taskReference="task1" symbol="urn:sedml:symbol:time" />`, `</listOfVariables>`, and `<math xmlns="http://www.w3.org/1998/Math/MathML">`.

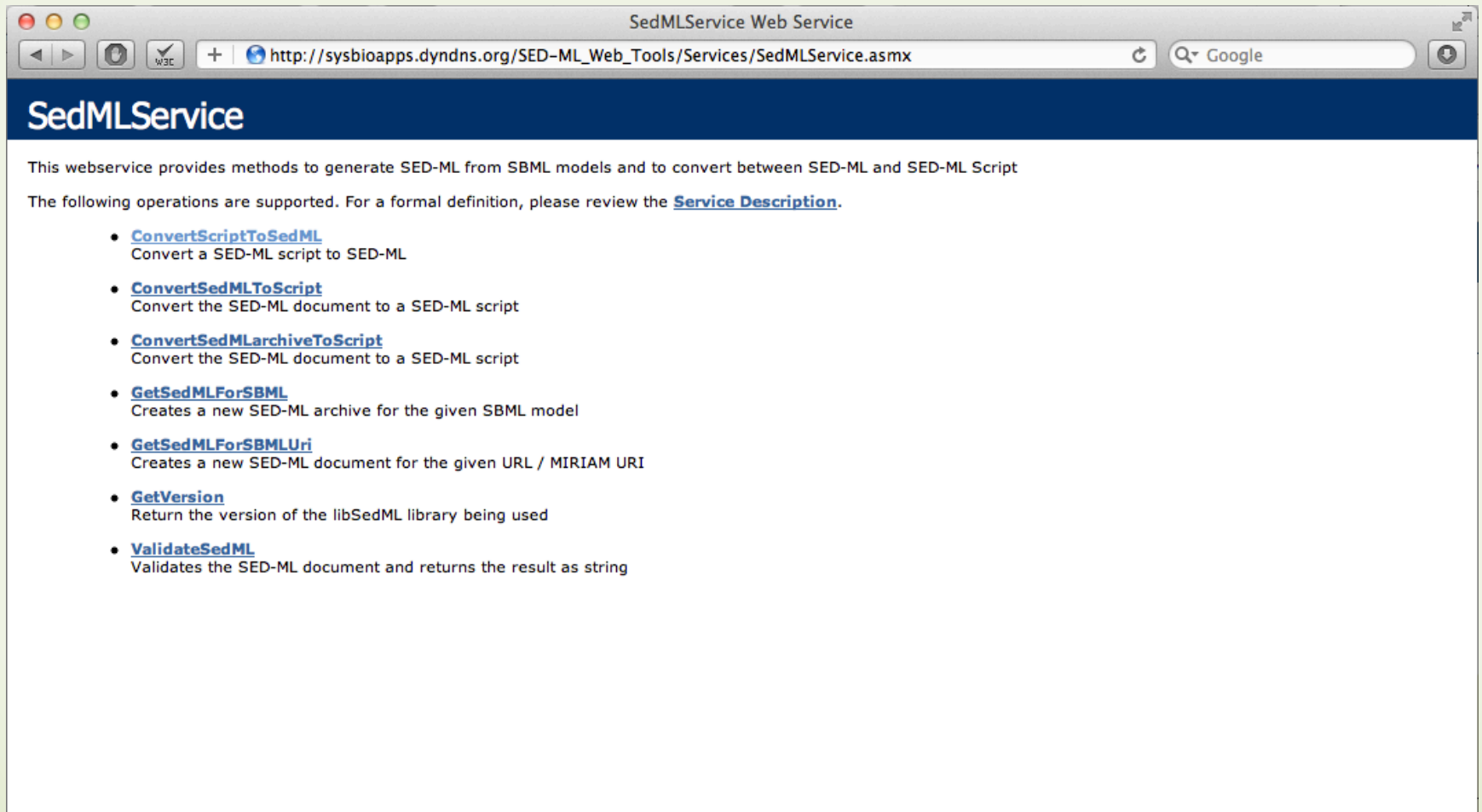
SED-ML Web Tools - Download

Currently Loaded Model

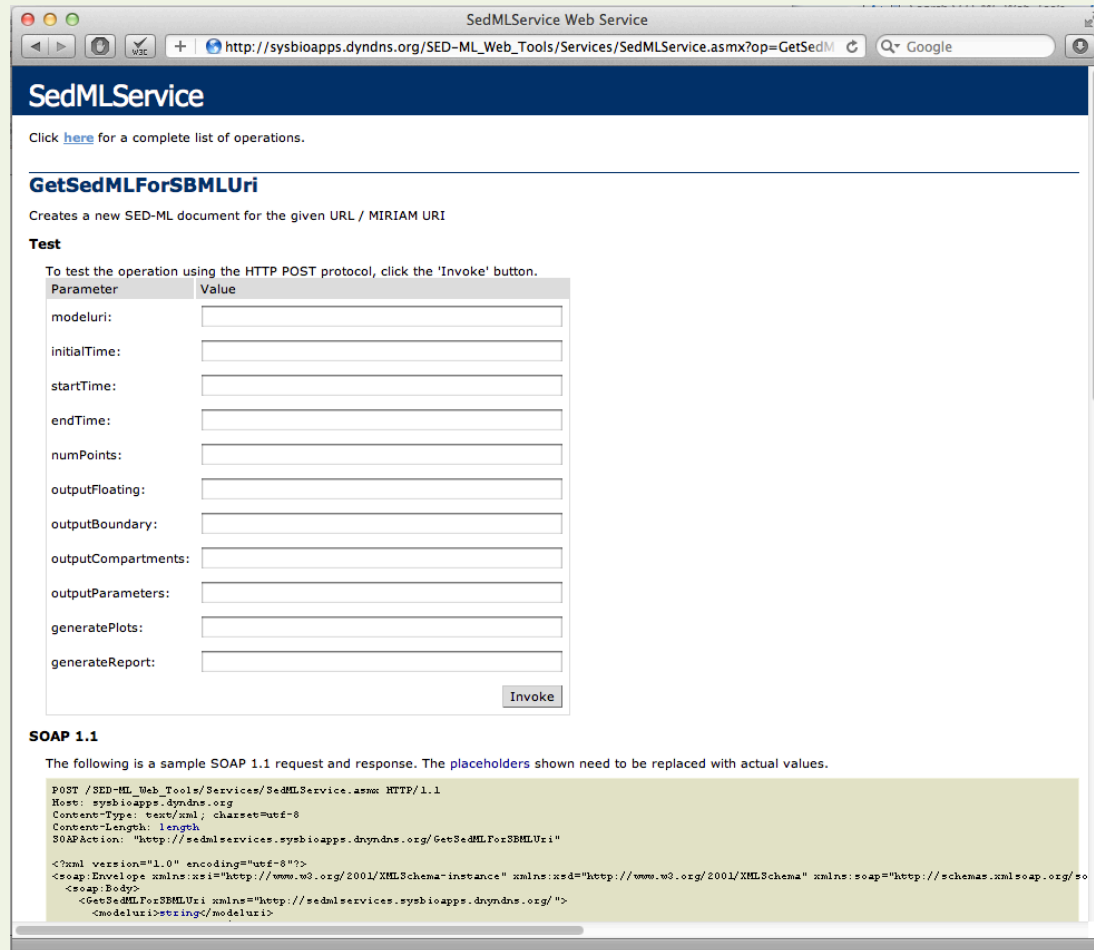
FileName: sedml

[Download as SED-ML](#) [Download as SED-ML Archive](#)

Web Service (!)



Web Service – Create From SBML



SedMLService Web Service

Click [here](#) for a complete list of operations.

GetSedMLForSBMLUri

Creates a new SED-ML document for the given URL / MIRIAM URI

Test

To test the operation using the HTTP POST protocol, click the 'Invoke' button.

| Parameter | Value |
|---------------------|----------------------|
| modelUri: | <input type="text"/> |
| initialTime: | <input type="text"/> |
| startTime: | <input type="text"/> |
| endTime: | <input type="text"/> |
| numPoints: | <input type="text"/> |
| outputFloating: | <input type="text"/> |
| outputBoundary: | <input type="text"/> |
| outputCompartments: | <input type="text"/> |
| outputParameters: | <input type="text"/> |
| generatePlots: | <input type="text"/> |
| generateReport: | <input type="text"/> |

SOAP 1.1

The following is a sample SOAP 1.1 request and response. The placeholders shown need to be replaced with actual values.

```
POST /SED-ML_Web_Tools/Services/SedMLService.aspx HTTP/1.1
Host: sysbioapps.dyndns.org
Content-Type: text/xml; charset=utf-8
Content-Length: length
SOAPAction: "http://sedmlservices.sysbioapps.dyndns.org/GetSedMLForSBMLUri"

<?xml version="1.0" encoding="utf-8"?>
<soap:Envelope xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:xsd="http://www.w3.org/2001/XMLSchema" xmlns:soap="http://schemas.xmlsoap.org/soap/envelope/">
  <soap:Body>
    <GetSedMLForSBMLUri xmlns="http://sedmlservices.sysbioapps.dyndns.org/">
      <modelUri>string</modelUri>
    </GetSedMLForSBMLUri>
  </soap:Body>
</soap:Envelope>
```

Web Service – Create From SBML

Click [here](#) for a complete list of operations.

GetSedMLForSBMLUri

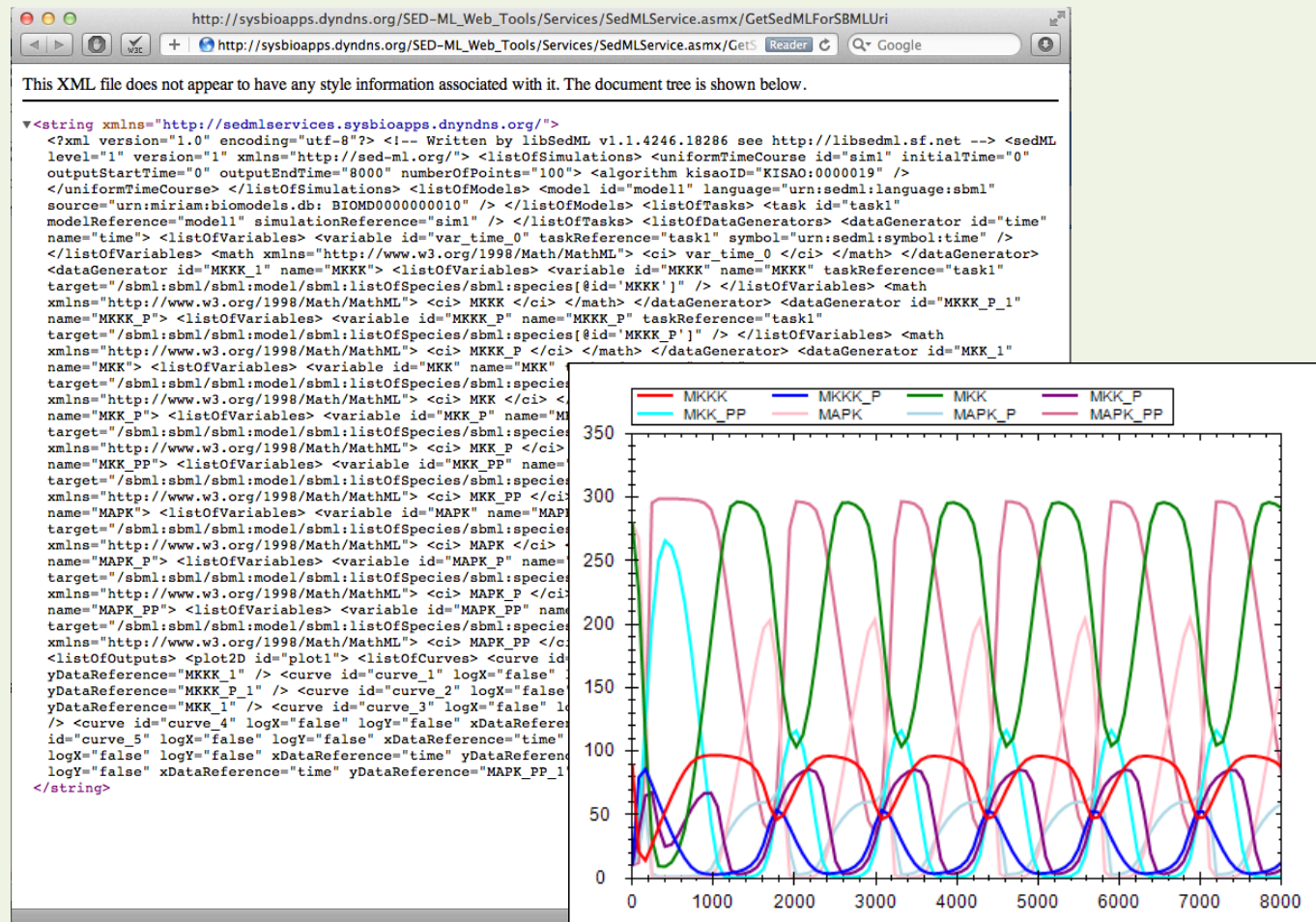
Creates a new SED-ML document for the given URL / MIRIAM URI

Test

To test the operation using the HTTP POST protocol, click the 'Invoke' button.

| Parameter | Value |
|---------------------|---|
| modeluri: | <input type="text" value="urn:miriam:biomodels.db: BIOMD0000000010"/> |
| initialTime: | <input type="text" value="0"/> |
| startTime: | <input type="text" value="0"/> |
| endTime: | <input type="text" value="8000"/> |
| numPoints: | <input type="text" value="100"/> |
| outputFloating: | <input type="text" value="true"/> |
| outputBoundary: | <input type="text" value="false"/> |
| outputCompartments: | <input type="text" value="false"/> |
| outputParameters: | <input type="text" value="false"/> |
| generatePlots: | <input type="text" value="true"/> |
| generateReport: | <input type="text" value="false"/> |

Web Service – Create From SBML



Future Directions

- More simulation types (Nested Simulation Task)
- Referencing data (See the SBRML Interop talk after the break!)
- Support for YOUR model format
 - If you supply the simulator, I'll support it 😊

Acknowledgements

- David Nickerson
- Herbert M. Sauro

Thank You!

- Blog: <http://frank-fbergmann.blogspot.com>
- Web:
 - [http://sysbioapps.dyndns.org/SED-ML Web Tools](http://sysbioapps.dyndns.org/SED-ML_Web_Tools)
 - <http://sysbioapps.dyndns.org>