



# libSedML Updates and SED-ML Web Tools

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# **LIBSEDML UPDATE**

# LibSedML

## SED-ML Script Editor

```
libSedML 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



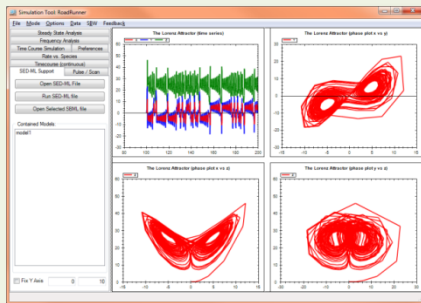
libSedML



libSedMLRunner



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

# What is new - LibSedMLRunner

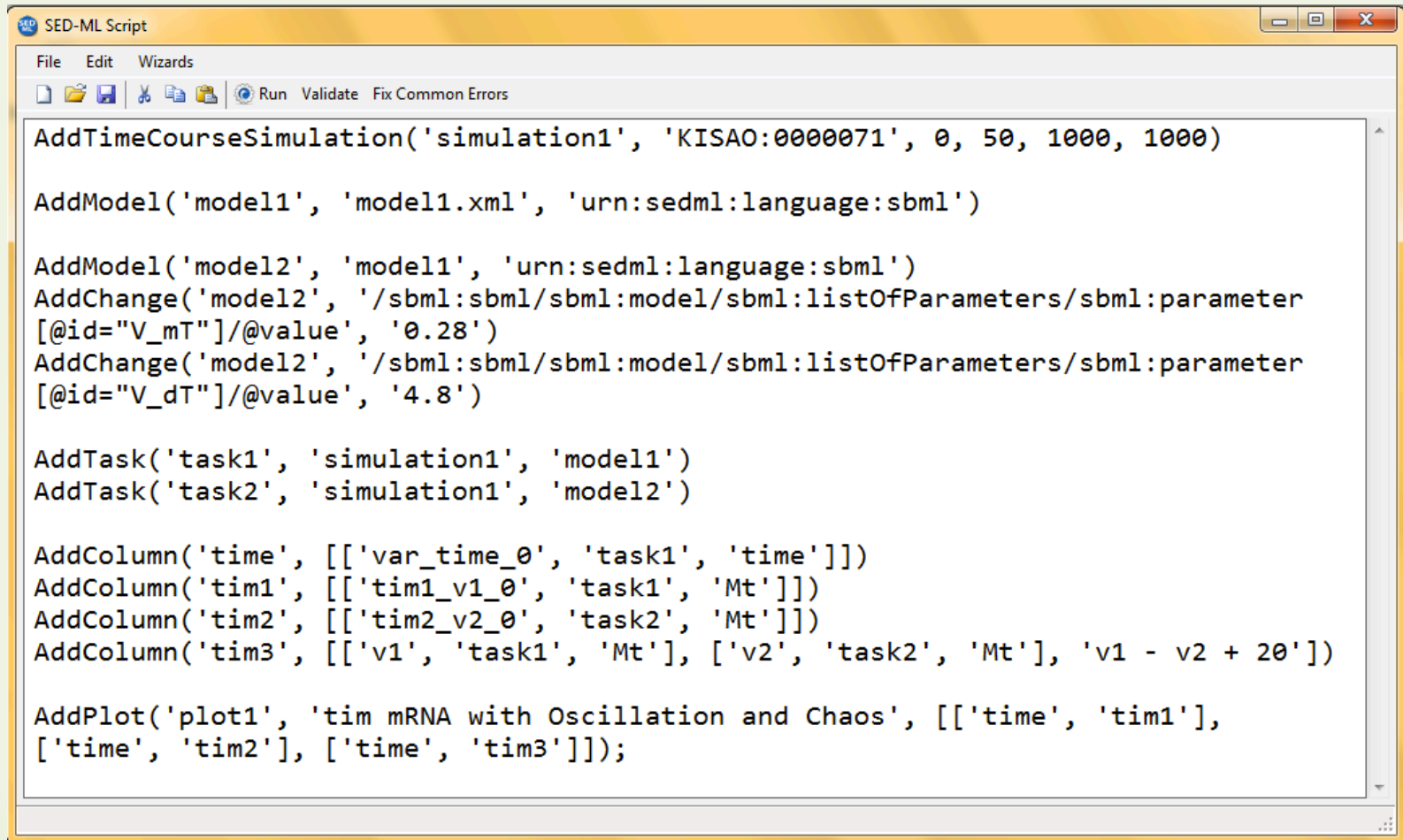
- Similar to LibSedML clear abstraction of supported simulators
- Based on binaries from David Nickerson:
  - Simulation Support for CellML models

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

# **SED-ML SCRIPT EDITOR 1.6**



# SED-ML Script Editor



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

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

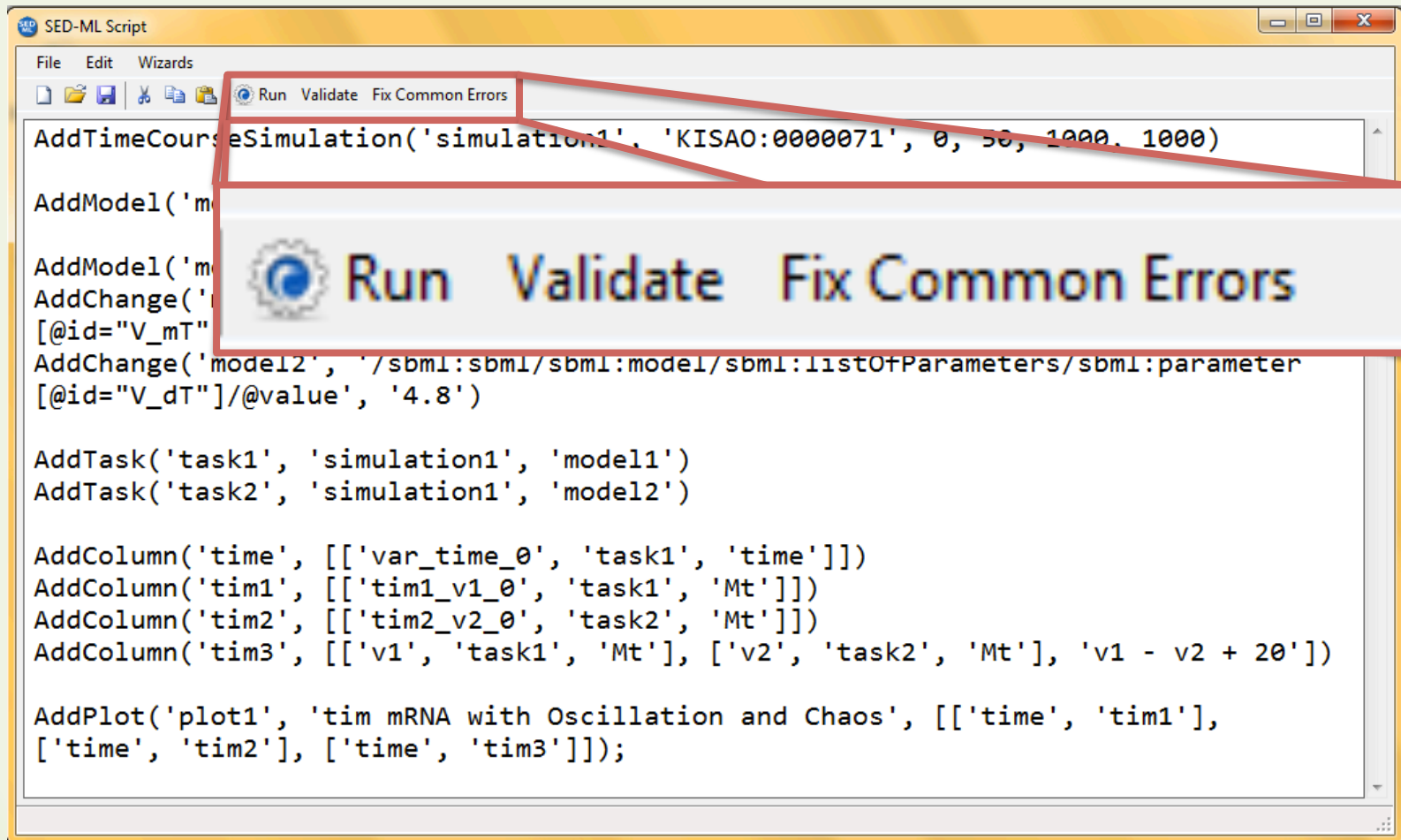
AddModel('model2', 'model1', 'urn:sedml:language:sbml')
AddChange('model2', '/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
[@id="V_mT"]/@value', '0.28')
AddChange('model2', '/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter
[@id="V_dT"]/@value', '4.8')

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

Validation Result

## Validation Results

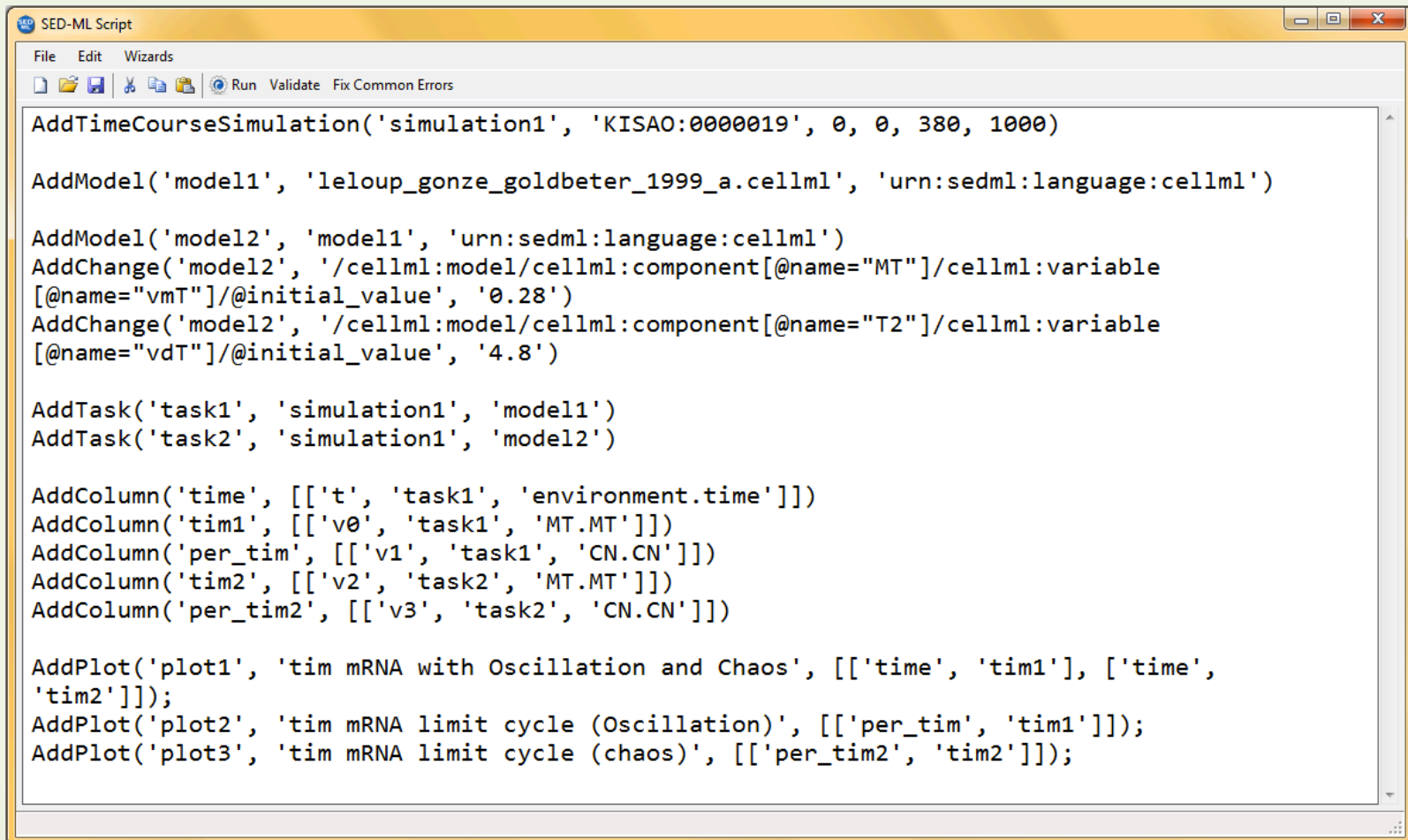
**The document is invalid SED-ML**

0 Fataals(s), 40 Errors(s), 0 Warning(s)

- Error** [Line 2](#) Column 2: The required attribute 'level' is missing.  
<sedML xmlns="http://www.biomodels.net/sed-ml">
- Error** [Line 2](#) Column 2: The required attribute 'version' is missing.  
<sedML xmlns="http://www.biomodels.net/sed-ml">
- Error** [Line 4](#) Column 38: The 'algorithm' attribute is not declared.  
<uniformTimeCourse id="uniform1" algorithm="KISAO:0000019" initialTime="0" outputStartTime="0" outputEndTime="10" numberOfPoints="1000" />
- Error** [Line 4](#) Column 6: The element 'uniformTimeCourse' in namespace 'http://www.biomodels.net/sed-ml' has incomplete content. List of possible elements expected: 'notes, annotation, algorithm' in namespace 'http://www.biomodels.net/sed-ml'.  
<uniformTimeCourse id="uniform1" algorithm="KISAO:0000019" initialTime="0" outputStartTime="0"

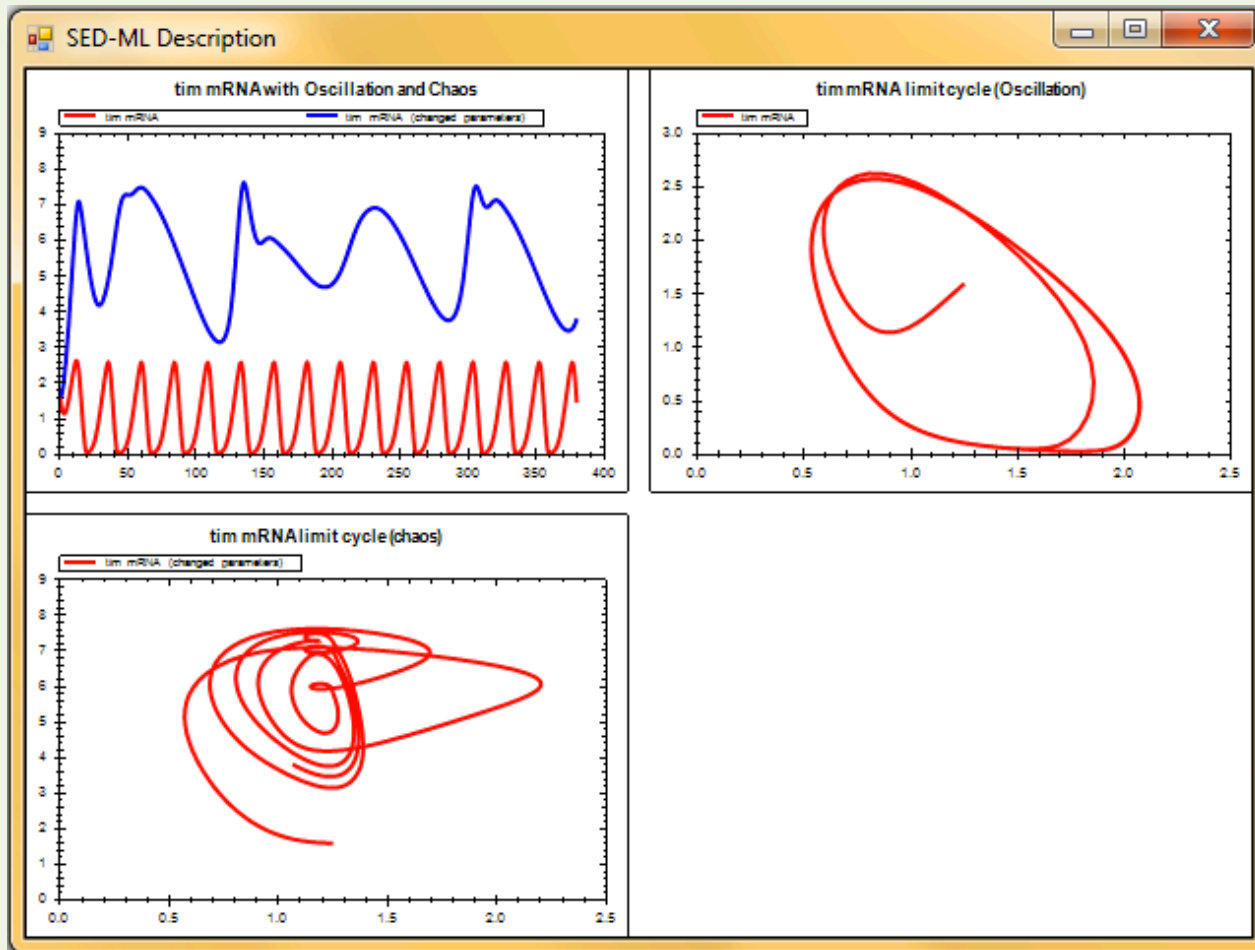
Close

# SED-ML Script Editor - CellML



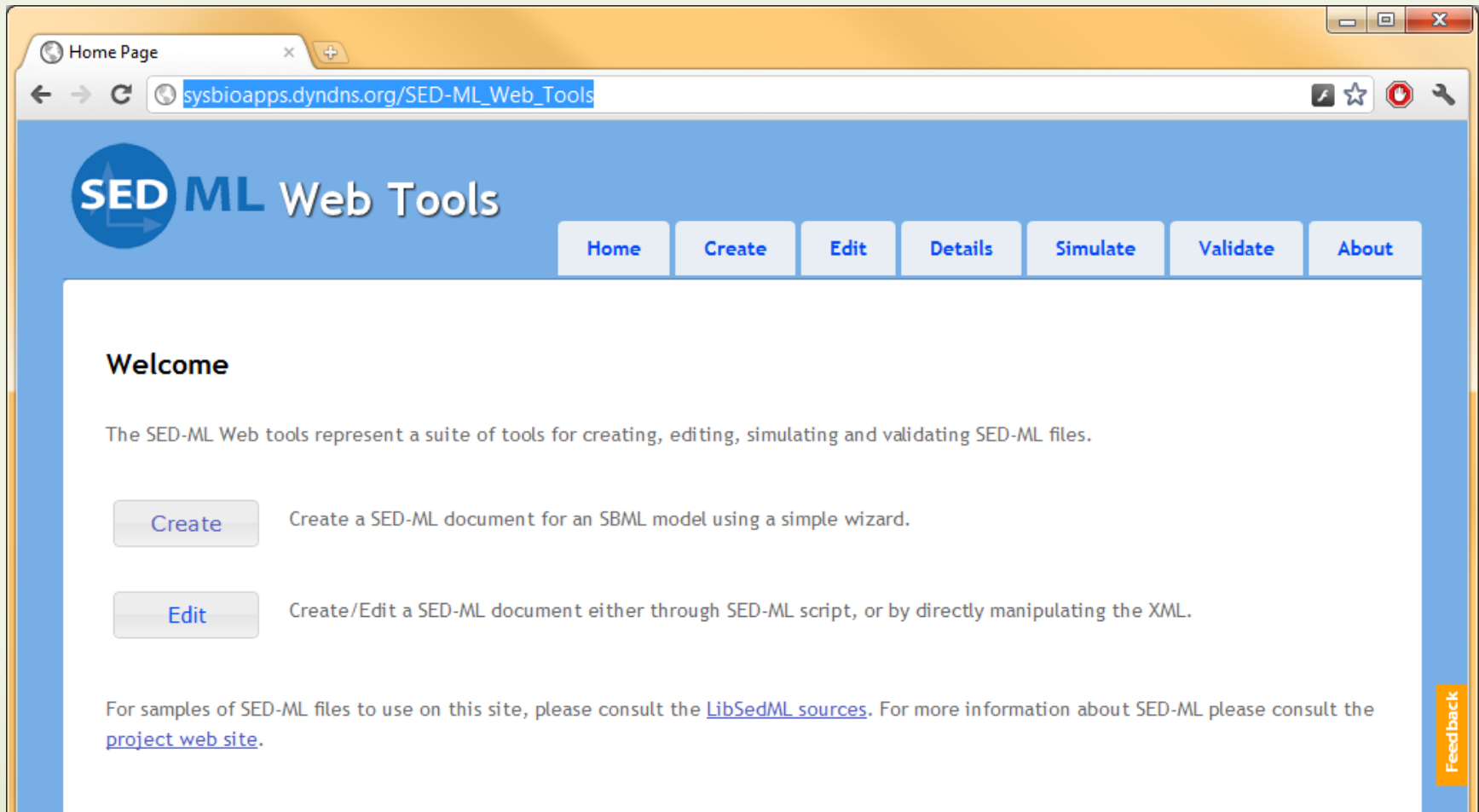
```
SED-ML Script
File Edit Wizards
Run Validate Fix Common Errors
AddTimeCourseSimulation('simulation1', 'KISAO:0000019', 0, 0, 380, 1000)
AddModel('model1', 'leloup_gonze_goldbeter_1999_a.cellml', 'urn:sedml:language:cellml')
AddModel('model2', 'model1', 'urn:sedml:language:cellml')
AddChange('model2', '/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



The screenshot shows a web browser window with the address bar containing [sysbioapps.dyndns.org/SED-ML\\_Web\\_Tools](http://sysbioapps.dyndns.org/SED-ML_Web_Tools). The page features a blue header with the SED-ML logo and the text "Web Tools". Below the header is a navigation menu with buttons for Home, Create, Edit, Details, Simulate, Validate, and About. The main content area has a "Welcome" section followed by a paragraph: "The SED-ML Web tools represent a suite of tools for creating, editing, simulating and validating SED-ML files." Below this are two buttons: "Create" with the description "Create a SED-ML document for an SBML model using a simple wizard." and "Edit" with the description "Create/Edit a SED-ML document either through SED-ML script, or by directly manipulating the XML." At the bottom, there is a paragraph: "For samples of SED-ML files to use on this site, please consult the [LibSedML sources](#). For more information about SED-ML please consult the [project web site](#)." A vertical "Feedback" button is located on the right side of the page.

[http://sysbioapps.dyndns.org/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



# 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')

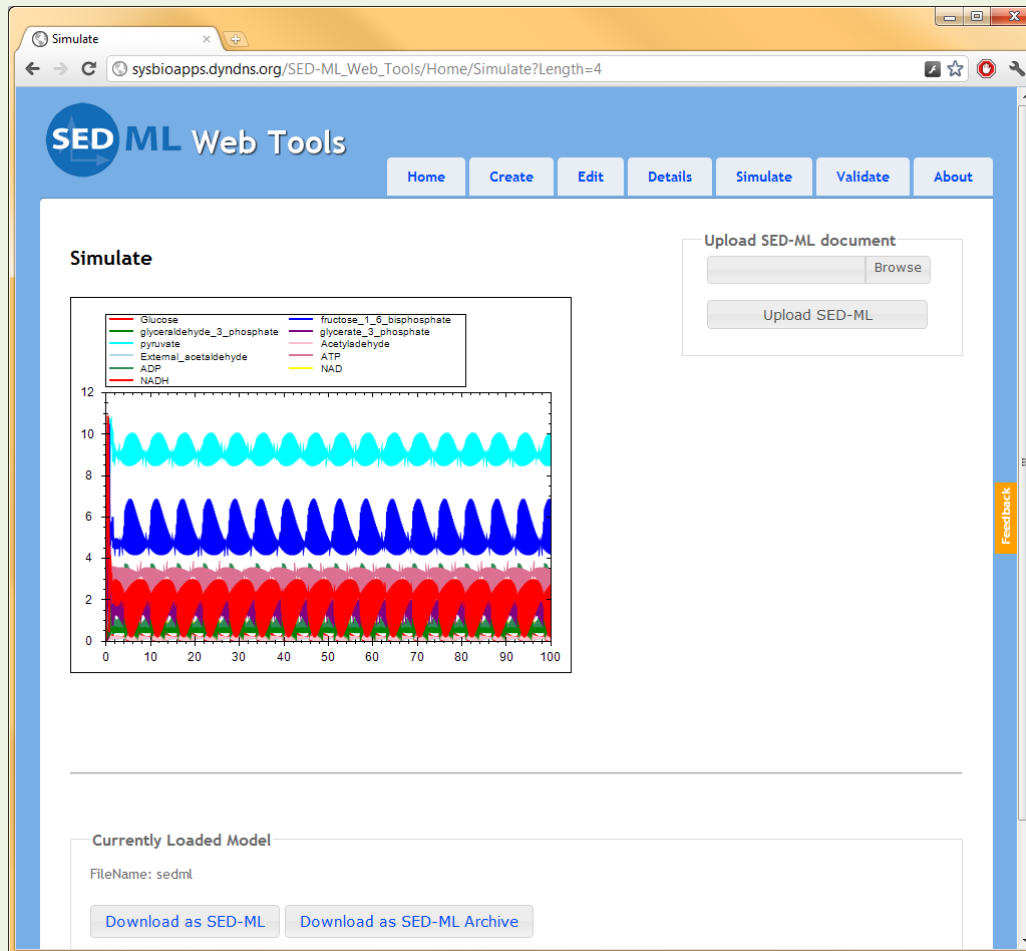
AddTask('task1', 'sim1', 'model1')

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

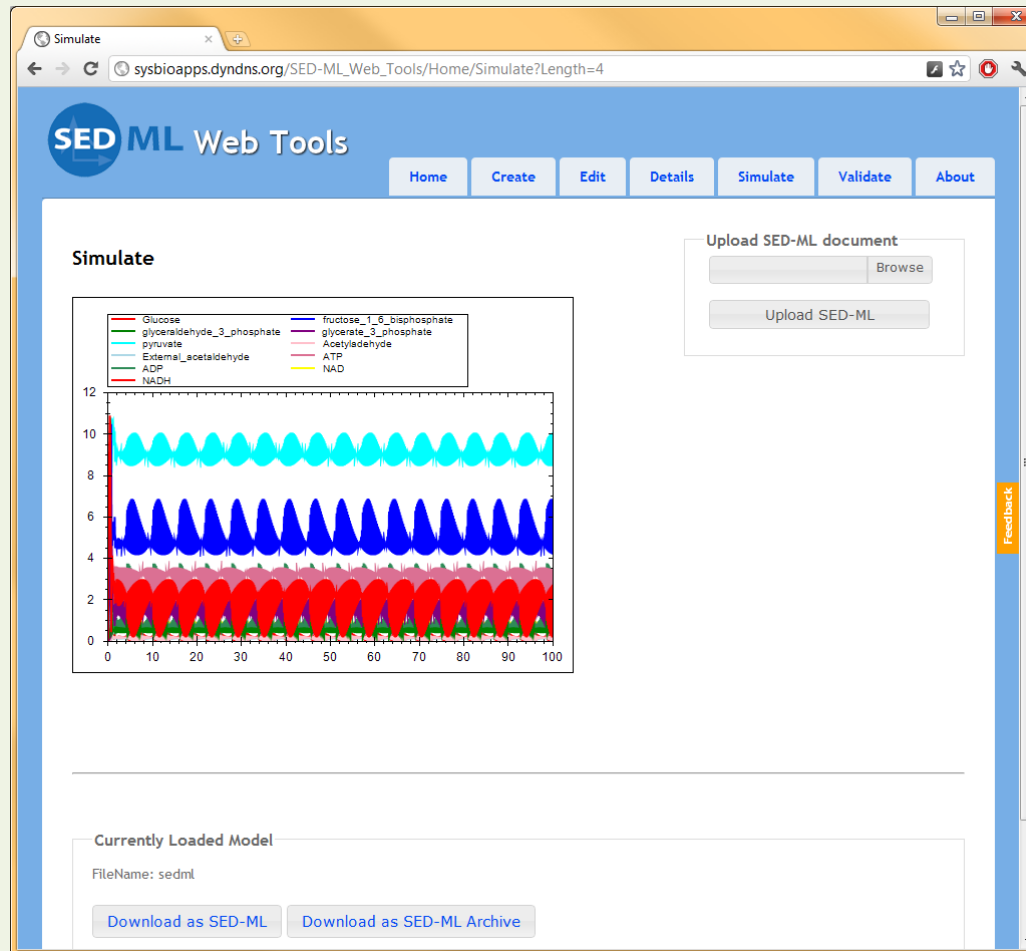
Feedback

# SED-ML Web Tools - Simulate



[http://sysbioapps.dyndns.org/SED-ML\\_Web\\_Tools](http://sysbioapps.dyndns.org/SED-ML_Web_Tools)

# SED-ML Web Tools - Simulate



[http://sysbioapps.dyndns.org/SED-ML\\_Web\\_Tools](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" and the browser tab is "Validate". The page content includes a navigation menu with buttons for Home, Create, Edit, Details, Simulate, Validate, and About. A red banner at the top of the main content area reads "The document is invalid SED-ML". Below this, it states "0 FATALS(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, a snippet of XML code 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 containing a list of 20 lines of XML code. A vertical "Feedback" button is located on the right side of the page.

**SED ML Web Tools**

Home Create Edit Details Simulate Validate About

**The document is invalid SED-ML**

0 FATALS(s), 1 Error(s), 0 Warning(s)

[Fix Common Errors](#)

- **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.

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

**Document Listing**

```
1. <?xml version="1.0" encoding="utf-8"?>
2. <!-- Written by libSedML v1.1.4246.18286 see http://libsedml.sf.net -->
3. <sedML level="1" version="1" xmlns="http://sed-ml.org/">
4. <listOfSimulations>
5.   <uniformTimeCourse id="uniform 1" initialTime="0" outputStartTime="0" outputEndTime="10"
6.     numberOfPoints="1000">
7.     <algorithm kisaoID="KISAO:000019" />
8.   </uniformTimeCourse>
9. </listOfSimulations>
10. <listOfModels>
11.   <model id="model1" language="urn:sedml:language:sbml" source="model1.xml" />
12. </listOfModels>
13. <listOfTasks>
14.   <task id="task1" modelReference="model1" simulationReference="uniform1" />
15. </listOfTasks>
16. <listOfDataGenerators>
17.   <dataGenerator id="time1" name="time">
18.     <listOfVariables>
19.       <variable id="time" taskReference="task1" symbol="urn:sedml:symbol:time" />
20.     </listOfVariables>
21.   </dataGenerator>
22. </listOfDataGenerators>
23. </sedML>
```

Feedback

# SED-ML Web Tools - Download

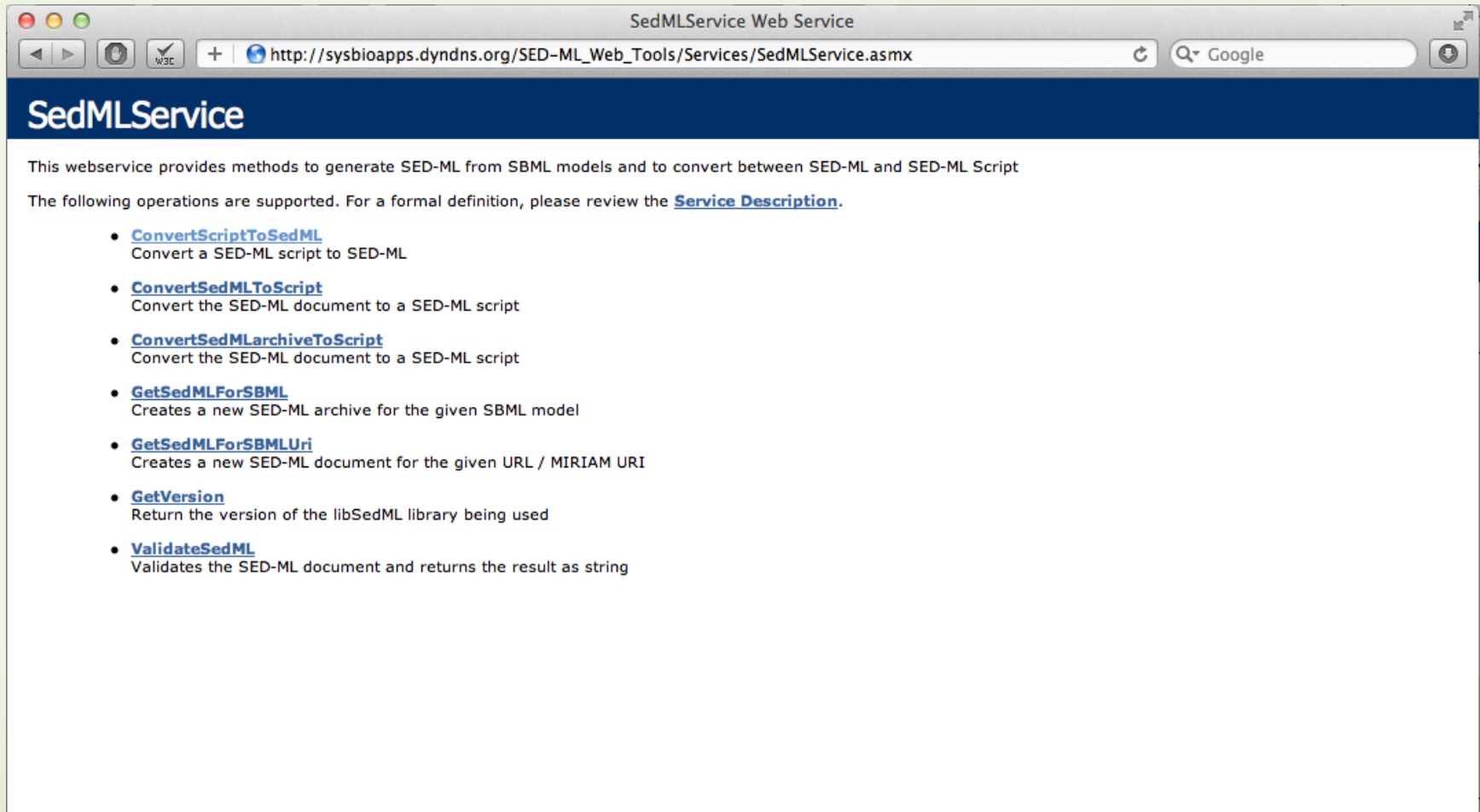
## Currently Loaded Model

FileName: sedml

[Download as SED-ML](#)

[Download as SED-ML Archive](#)

# Web Service (!)



The screenshot shows a web browser window with the title "SedMLService Web Service". The address bar contains the URL "http://sysbioapps.dyndns.org/SED-ML\_Web\_Tools/Services/SedMLService.asmx". The page content includes a blue header with the text "SedMLService". Below the header, there is a paragraph stating: "This webservice provides methods to generate SED-ML from SBML models and to convert between SED-ML and SED-ML Script". This is followed by another paragraph: "The following operations are supported. For a formal definition, please review the [Service Description](#)." Below this, there is a bulleted list of seven operations, each with a blue link and a brief description:

- [ConvertScriptToSedML](#)  
Convert a SED-ML script to SED-ML
- [ConvertSedMLToScript](#)  
Convert the SED-ML document to a SED-ML script
- [ConvertSedMLarchiveToScript](#)  
Convert the SED-ML document to a SED-ML script
- [GetSedMLForSBML](#)  
Creates a new SED-ML archive for the given SBML model
- [GetSedMLForSBMLUri](#)  
Creates a new SED-ML document for the given URL / MIRIAM URI
- [GetVersion](#)  
Return the version of the libSedML library being used
- [ValidateSedML](#)  
Validates the SED-ML document and returns the result as string

# Web Service – Create From SBML

The screenshot shows a web browser window titled "SedMLService Web Service" with the URL [http://sysbioapps.dyndns.org/SED-ML\\_Web\\_Tools/Services/SedMLService.aspx?op=GetSedML](http://sysbioapps.dyndns.org/SED-ML_Web_Tools/Services/SedMLService.aspx?op=GetSedML). The page header is "SedMLService" and includes a link to a complete list of operations. The main section is titled "GetSedMLForSBMLUri" and describes the operation: "Creates a new SED-ML document for the given URL / MIRIAM URI". Below this is a "Test" section with instructions to use the HTTP POST protocol and an "Invoke" button. A form contains input fields for parameters: modeluri, initialTime, startTime, endTime, numPoints, outputFloating, outputBoundary, outputCompartments, outputParameters, generatePlots, and generateReport. At the bottom, there is a "SOAP 1.1" section with a sample request and response in XML format.

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</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

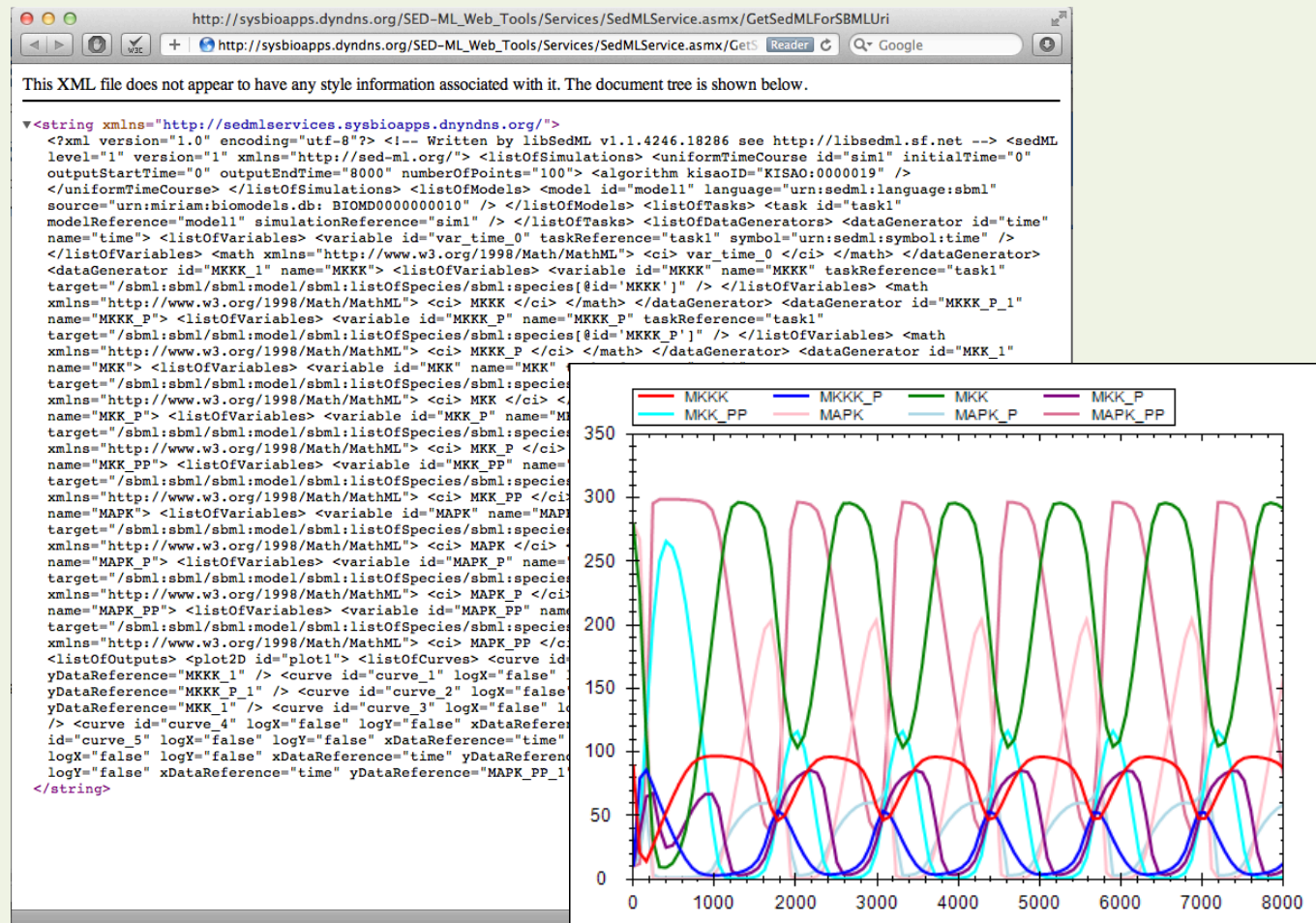
### Test

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>