

Combine Workshop 2011 Heidelberg

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JlibSEDML – a Java library for SED-ML and SED-ED – a graphical editing tool for SED-ML

- JlibSEDML update
- SED-ML application support in SBSI and SED-ED

Aims and current status of JlibSEDML

- API to read/write and interpret SED-ML files.
- Native Java, light-weight, few dependencies.
- Two independent implementations from VCell and SBSI teams merged in Spring 2010.
- Current release **1.1.2** fully supports **SED-ML level 1 version 1**

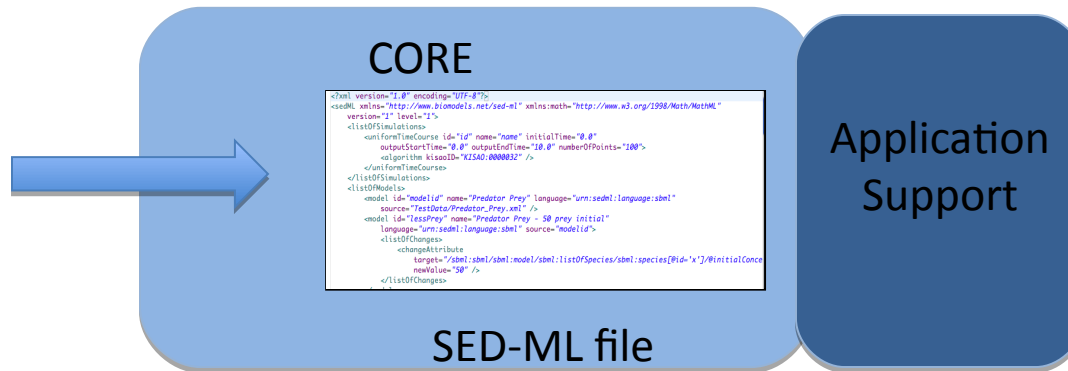
Scope of jlibSEDML

Export simulation configuration

Simulator 1

Simulator 2

Simulator 3



Execute configuration

Simulator 1

Simulator 2

Simulator 3

Core API

- Based on familiar libSBML conventions.
- E.g.,

```
SEDMLDocument doc = Libsedml.readSEDML(myInputStream);  
List<SedMLError> errs = doc.validate();  
SedML sedml = doc.getSEDML();  
  
//manipulate your SED-ML object model  
  
doc.writeDocument(myOutputStream);
```

MathML support

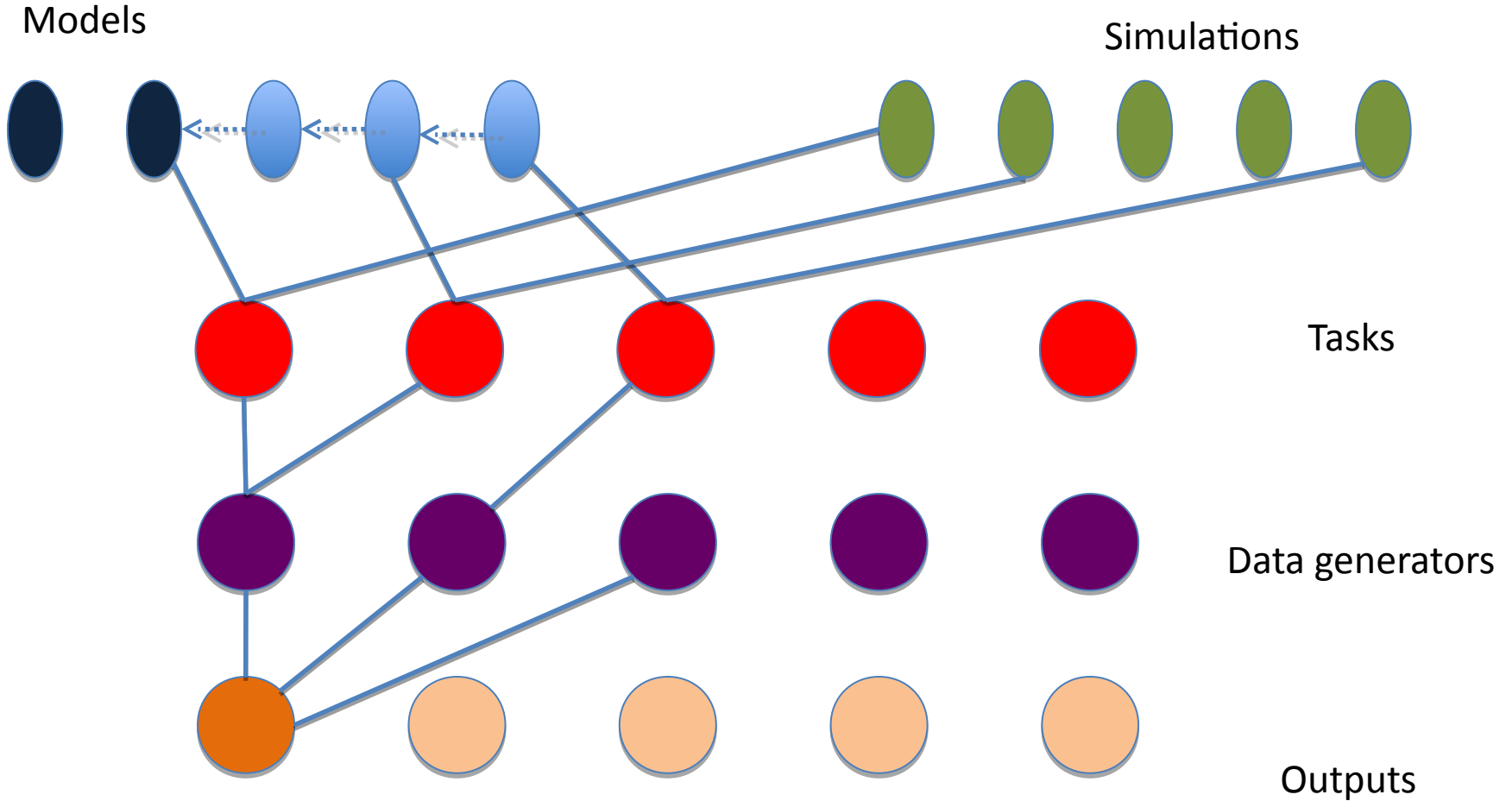
- Separate Java library, **jmathml**
- Supports String, ASTNode and MathML representation of math structures.
- Can add custom symbols
- Supports evaluation of scalar and vector expressions

```
ASTNode root = parser.parse("a + b");  
EvaluationContext ec = new EvaluationContext();  
ec.setValueFor("a", 1);  
ec.setValueFor("b", 2);  
Double result = root.evaluate(ec).getValue();
```

Extensibility

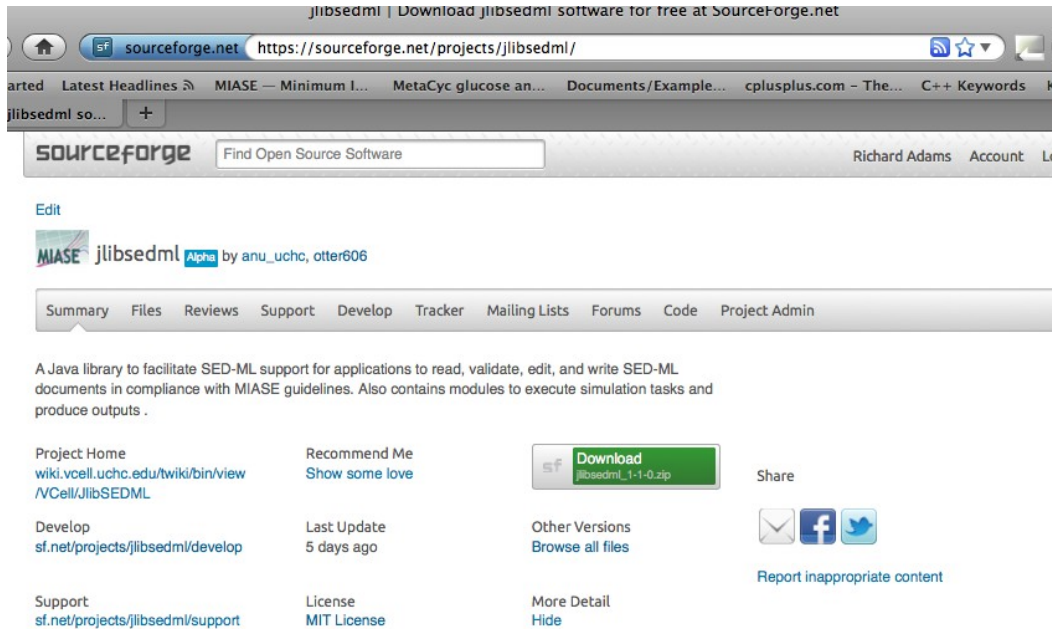
- Validators
- Model retrieval
- Executable SED-ML

Interpreting SED-ML



Nature Precedings : doi:10.1038/npre.2011.6334.1 : Posted 4 Sep 2011

JlibSEDML on Sourceforge...



Java library for SED-ML

Open-source MIT license

**Version 1.1.2 implements
SED-ML level 1 version 1**

<http://sourceforge.net/projects/jlibsedml/>

Binaries, source (Ant build and tests), OSGi bundle



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JlibSEDML core build and test ✓ #245 Tests passed: 206

JMathML support library ✓ #53 Tests passed: 264

SED-ED editor tests ✓ #26 Tests passed: 209

SED-ED SEDML editor ✓ #29 Success

SEDML web service ✓ #35 Tests passed: 5

Overview (jlibsedml Level 1 Version Javadoc) package.html build.xml

file:///Users/radams/Documents/workspace2/org.sedml.jlibsedml/export/docs/index.html

Overview Package Class Tree Deprecated Index Help
PREV NEXT FRAMES NO FRAMES

jlibsedml SED-ML library

Packages	
org.sedml	This is the core public API package for reading, writing and manipulating SED-ML documents.
org.sedml.execution	Provides a framework based on the Template pattern to run simulations described by SED-ML. Clients should extend AbstractSedmlExecutor to hook into this framework.
org.sedml.mathsymbols	Provides custom MathML symbols that are specific for SED-ML.
org.sedml.modelsupport	A utility package providing services to support specific modelling languages and ontologies used by SED-ML.
org.sedml.validation	Provides a collection of classes implementing ISedmlValidator that provide validation of SED-ML elements against the L1-V1 specification.
org.sedml.webtools	Provides utility classes to access web-based model resources.

[Algorithm](#)
[Annotation](#)
[ArchiveComponents](#)
[ArchiveModelResolver](#)
[BioModelsModelsRetriever](#)
[Change](#)
[ChangeAttribute](#)
[ChangeXML](#)
[ComputeChange](#)
[Curve](#)
[DataGenerator](#)
[DataSet](#)
[ExecutionStatusElement](#)
[ExecutionStatusElement_Execu](#)
[FileModelContent](#)
[FileModelResolver](#)
[Identifiable](#)
[IMathContainer](#)
[IModel2DataMappings](#)
[IModelContent](#)
[IModelResolver](#)

JlibSEDML How-to

- JlibSEDML How-to
 - Introduction
 - What can jlibsedml do for me?
 - Basic support for SED-ML
 - Support for execution of SED-ML documents
 - Support for developers
 - About the authors
 - Licensing
 - Installation
 - Creating a SED-ML document
 - The basics
 - Creating a simulation element:
 - Creating a model element:
 - Creating a task element:
 - Creating data generators:
 - Generating the output
 - Annotating the document
 - Writing the document
 - Basic export
 - Export as a SED-ML archive.
 - Conclusions
 - Reading a SED-ML document.
 - Reading in a SED-ML file:
 - Accessing information to run a simulation:
 - Running the model
 - Processing the results
 - A SED-ML execution framework
 - Executing a simulation
 - Processing the results:
 - An example:
 - Other code snippets
 - Analysing the KISAO id:
 - A Simple test analysing the model type:
 - Manipulating MathML expressions
 - Vector manipulations
 - Current issues.
 - Synchronization and thread safety.
 - Object identity.
 - More information
 - Validation of SED-ML documents
 - More examples
 - Javadoc
 - Getting involved

Jlibsedml

- Documentation: Javadoc & user manual
- Xpath support
- Extensible model retrieval framework.
- Extensible execution framework.

Applications 1 - online SED-ML validator

SED-ML Validator

http://www.sbsi.ed.ac.uk/html/sedml/index.html

Log in to Je-S WebHome < ...gy < TWiki Adobe Acrobat.com SourceForge...ml-discuss richardadams139 Blog Counte...ounters.com SpringerLink -

SED-ML Validator SYSTEMS BIOLOGY AT EDINBURGH

Validation result

Errors found in file: sed1.xml

Initial time is after start of output start time at line 7

Lines with syntax errors are highlighted below:

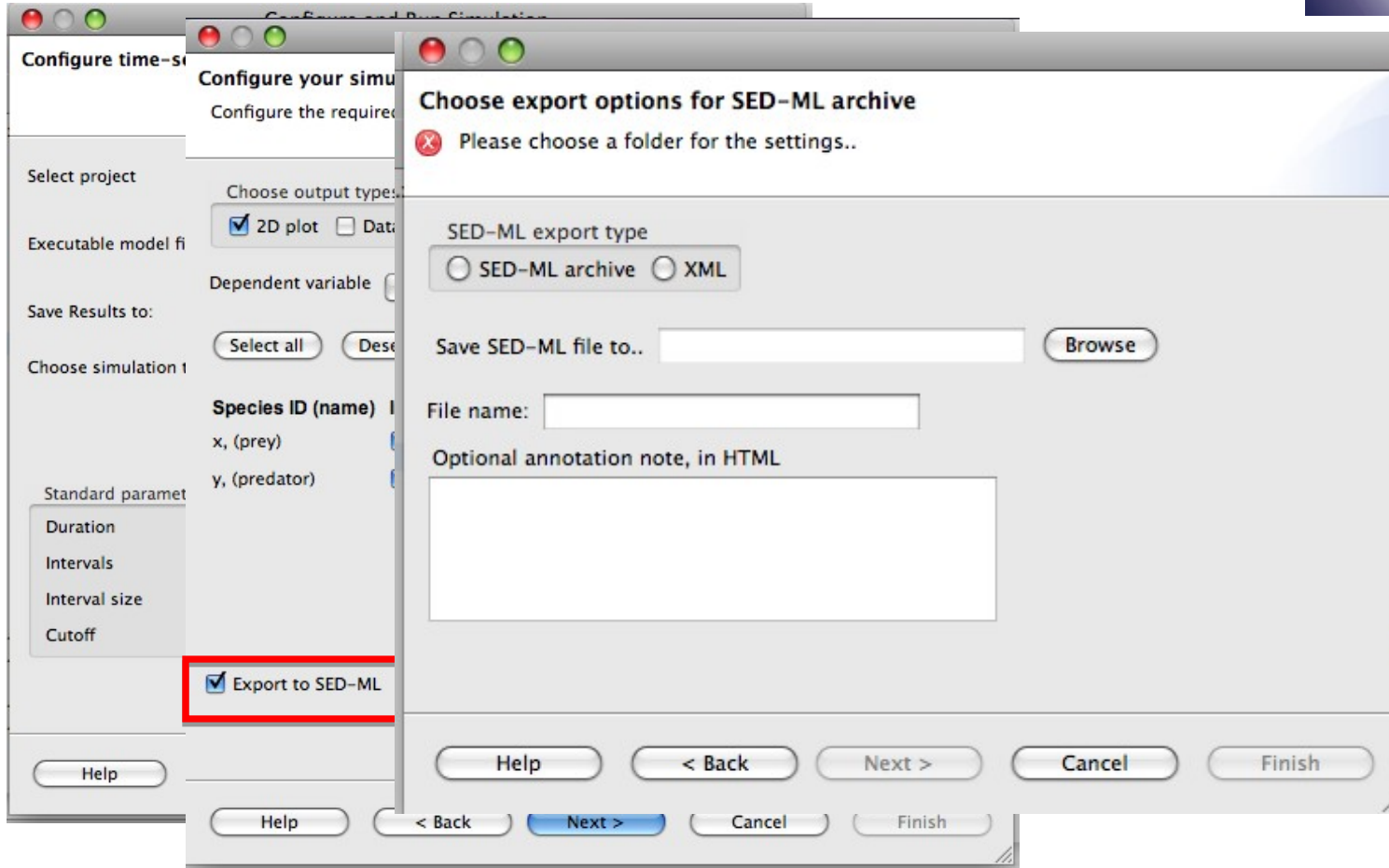
```
1.<?xml version="1.0" encoding="UTF-8"?>
2.<sedML xmlns="http://sed-ml.org/" xmlns:math="http://www.w3.org/1998/Math/MathML" version="1" level="1">
3.<notes>
4.<p xmlns="http://www.w3.org/1999/xhtml" />
5.</notes>
6.<listOfSimulations>
7.  <uniformTimeCourse id="sim1" name="Simulation 1" initialTime="230.0" outputStartTime="0.0" outputEndTime="10.0" num
8.<algorithm kisaoID="KISAO:0000088" />
9.</uniformTimeCourse>
10.</listOfSimulations>
11.<listOfModels>
12.<model id="abc1_1j1_2_3e_4_i_1300826091904" name="" language="urn:sedml:language:sbml.level-2.version-2" source="ab
13.<listOfChanges>
14.<changeAttribute newValue="20.00" target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k_1']/@valu
15.</listOfChanges>
16.</model>
17.</listOfModels>
18.<listOfTasks>
19.<task id="task1" name="default Task" modelReference="abc1_1j1_2_3e_4_i_1300826091904" simulationReference="sim1" />
20.</listOfTasks>
21.<listOfDataGenerators>
```

Home
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SBSINumerics
SBSIVisual
Project wiki
Download
Online tools
Licensing
Contact

SED ML

<http://www.sbsi.ed.ac.uk/html/sedml/>

SED-ML support in SBSI- www.sbsi.ed.ac.uk



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SED-ML support in SBSI – viewing SEDML

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The screenshot displays the SBSI-Visual software interface. On the left, the 'System View' tree shows a project structure with folders for Data, Diagrams, jobFolder, and Models. The 'Models' folder is expanded, showing files like ccc.dat, ccc.sbsiheader, new.dat, new.hdr, normal2.xml, Predator_Prey.hdr, Predator_Prey.xml, and predatorPreySedml.xml. The 'predatorPreySedml.xml' file is selected. The main window shows the XML code for this file, with a red box highlighting the simulation and model definitions. Below the code, the 'Problems' window shows a list of errors and warnings, with a red box highlighting the error messages.

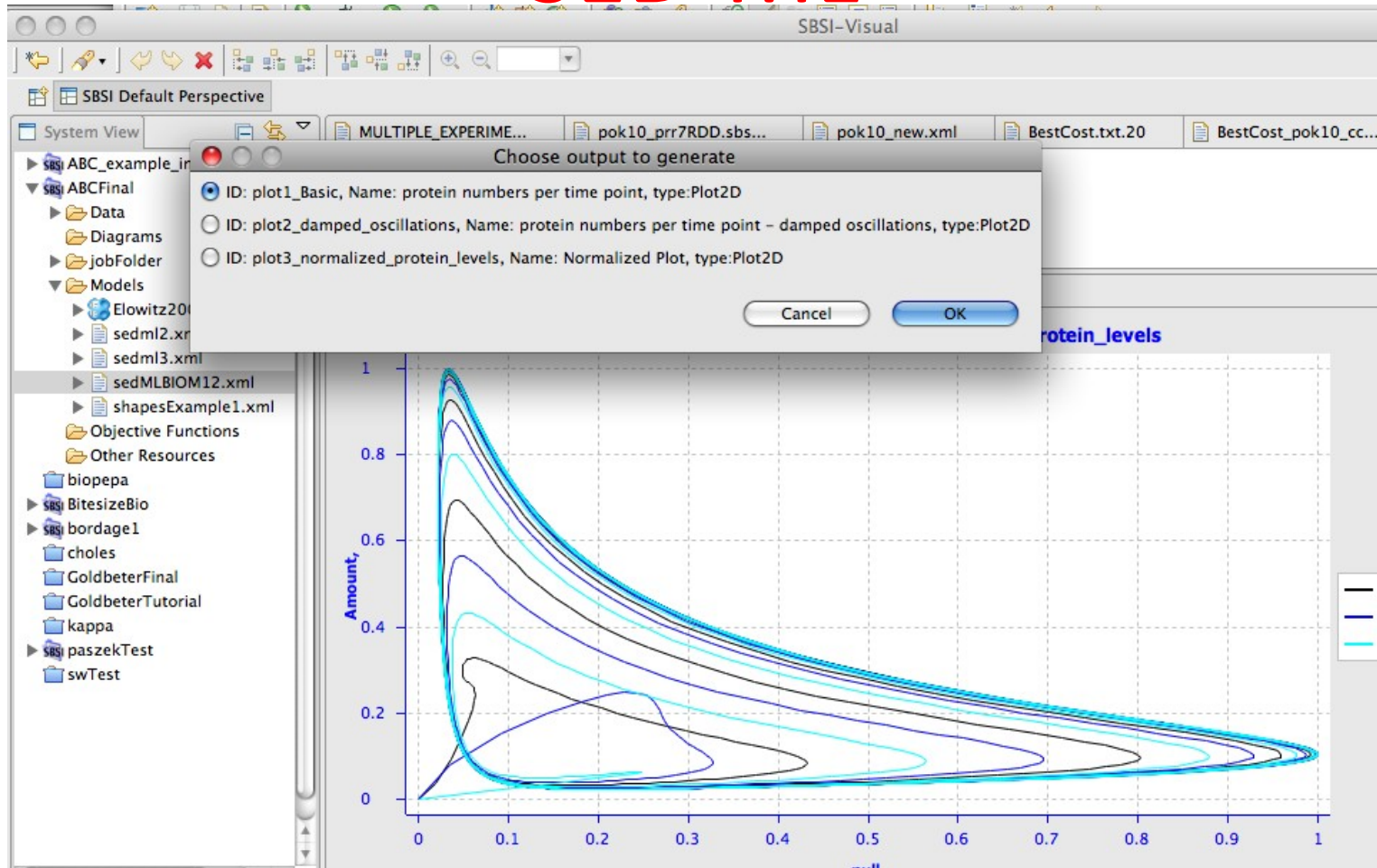
```
version="1" level="1">
<listOfSimulations>
  <uniformTimeCourse id="id2" name="name" initialTime="0.0"
    outputStartTime="0.0" outputEndTime="100.0" numberOfPoints="20000"
    <algorithm kisaoID="KISAO:0000019" />
  </uniformTimeCourse>
</listOfSimulations>
<listOfModels>
  <model id="modelid" name="Predator Prey basic model " language="urn:s
    source="Predator_Prey.xml" />
  <model id="lessPrey" name="Predator_Prey_50 prey initial"
```

2 errors, 8 warnings, 0 others

Description	Resource	Path
SBML (8 items)		
SEDML Problem Marker (2 items)		
Simulation 'id' not found'	predatorPreySedml.x	/lotkaVolterra/Models
Simulation 'id' not found'	predatorPreySedml.x	/lotkaVolterra/Models

SED-ML support in SBSI – executing SED-ML

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SED-ED, a SED-ML editor

The screenshot shows the SBSI-Visual application interface. On the left, a hierarchical diagram represents the simulation structure. The root node is 'task' (ID: element3, Name: Basic simulation). It has two children: 'model' (ID: element1, Name: null) and 'uniformTimeCourse' (ID: element2, Name: Basic simulation). The 'uniformTimeCourse' node has a child 'var' (ID: element5, Name: null). The 'task' node also has a child 'variable' (ID: element6, Name: null). The 'variable' node has a child 'dataGenerator' (ID: element4, Name: null). The 'dataGenerator' node has a child 'plot2D' (ID: element7, Name: null). The 'plot2D' node has a child 'curve' (ID: element8, Name: Time versus PX). A dialog box titled 'Add properties to time course' is open over the 'uniformTimeCourse' node. The dialog contains the following fields: ID (element2), Name (Basic simulation), Simulation start (0.0), Output start (0.0), Simulation end (10.0), Number of timepoints (100), and Algorithm (algorithm using deterministic rules, (KISA...)). The dialog has 'Cancel' and 'OK' buttons.



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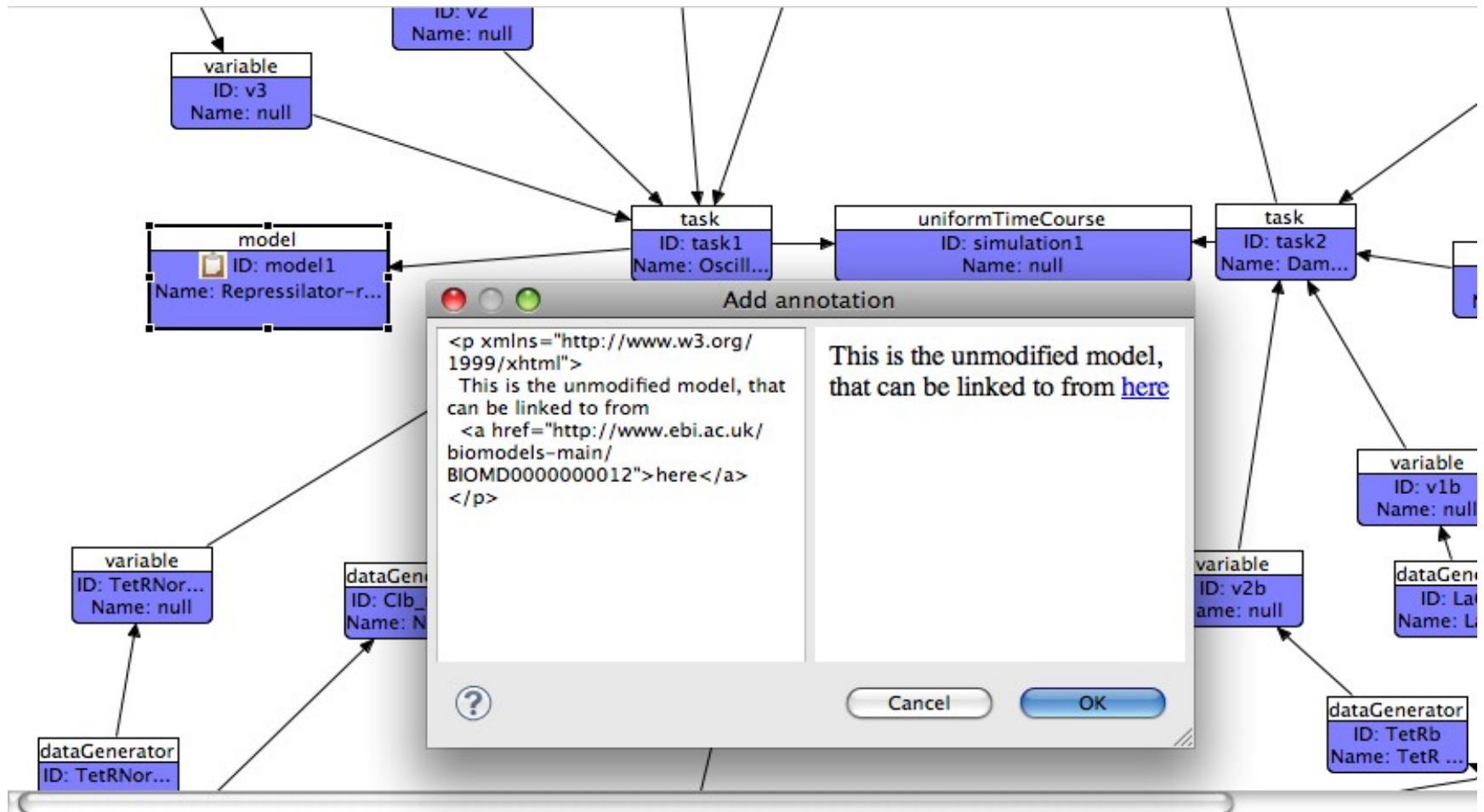
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Available as a standalone application : <http://sourceforge.net/projects/jlibsedml/files>
Eclipse or SBSI plugin update site : <http://www.sbsi.ed.ac.uk/update>



Annotating SED-ML



Viewing model changes

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The screenshot displays a software interface for editing SBML models. It features several overlapping windows:

- Add properties to model:** A dialog box with fields for ID (model2), Name (Damped oscillations), Source (model1), and Language (urn:sedml:language:sbml.level-2.version-3). It includes buttons for 'Browse...', 'Preview model', and a help icon.
- XML element chooser:** A window listing XML elements with their attributes. The following parameters are highlighted in red:
 - parameter [id=ps_a,metaid=metaid_0800235,name=tps_active,sboTerm=SBO:0000186,value=0.013]
 - parameter [id=ps_0,metaid=metaid_0500235,name=tps_repr,sboTerm=SBO:0000485,value=1.3e-5]
- Change:** A box indicating a change to the 'model2' element, specifically a 'ChangeAttribute' where the 'New val:' is '1.3e-5'.
- dataGenerator:** A box showing details for a data generator with ID 'Clb' and Name 'Cl re...'.
- curve:** A box showing details for a curve with ID 'c6' and Name 'null'.

At the bottom, a progress bar shows 'No operations to display at this time.' and buttons for 'Cancel' and 'OK' are visible.

Other features

- Inspect and edit SEDX archives directly.
- Inflate / generate SEDX archives.
- Optional auto-layout of SED-ML workflows.
- Auto-generation of XPath expressions.

Future implementation work

- SED-ED
 - work towards a stable release.
 - Integrated Kisao 2 support
- Jlibsedml
 - Bugfix /maintenance releases for level 1 v1 support.
 - Rapid support of future SED-ML features.

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 - Andrew Miller
 - David Nickerson
 - Nicolas Le Novere



Thanks for listening!

Applications 2 - SED-ML web service

Embryonic SOAP web service

// Applies changes to a model and returns the new model

String applyChanges(String modelID, String originalModel, String sedML)

//Validates the SEDML document and returns errors
SedmlError validate (String sedMLDoc)

// Implementing
ProcessedResult simulate (String sedML)

<http://mook.inf.ed.ac.uk:8848/SedMLWebService/sedmlws?wsdl>