

Java Libraries and tools for SED-MIL Combine Workshop 2011 Heidelberg

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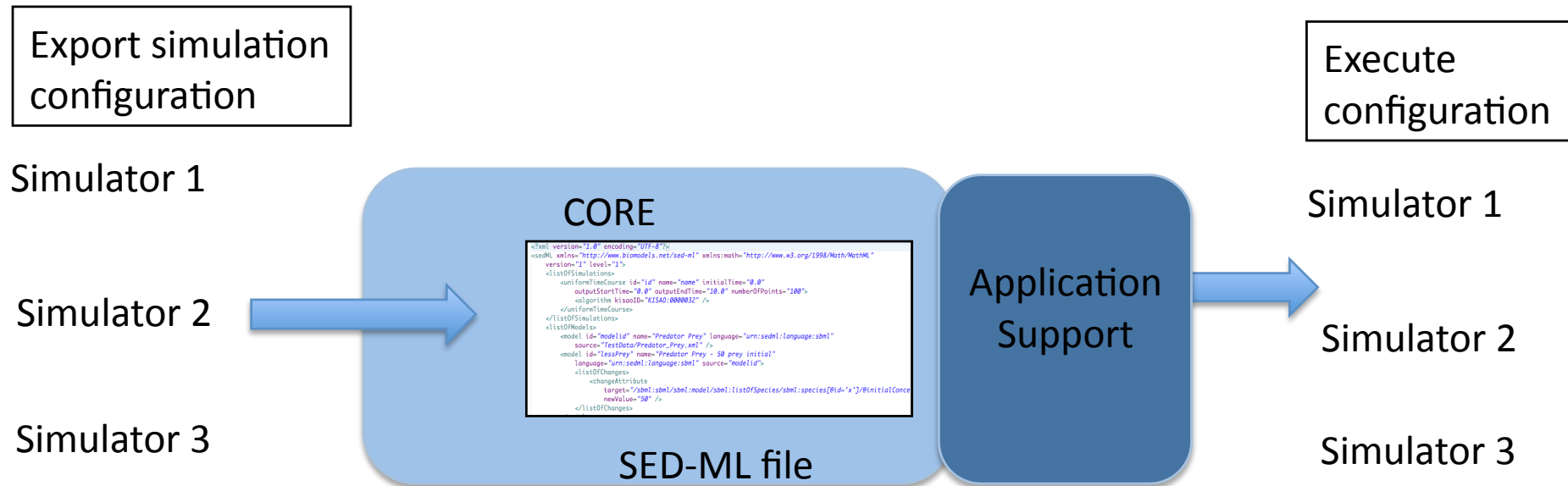
JlibSEDML – a Java library for SED-ML and SED-ED – a graphical editing tool for SED-ML

- 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



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

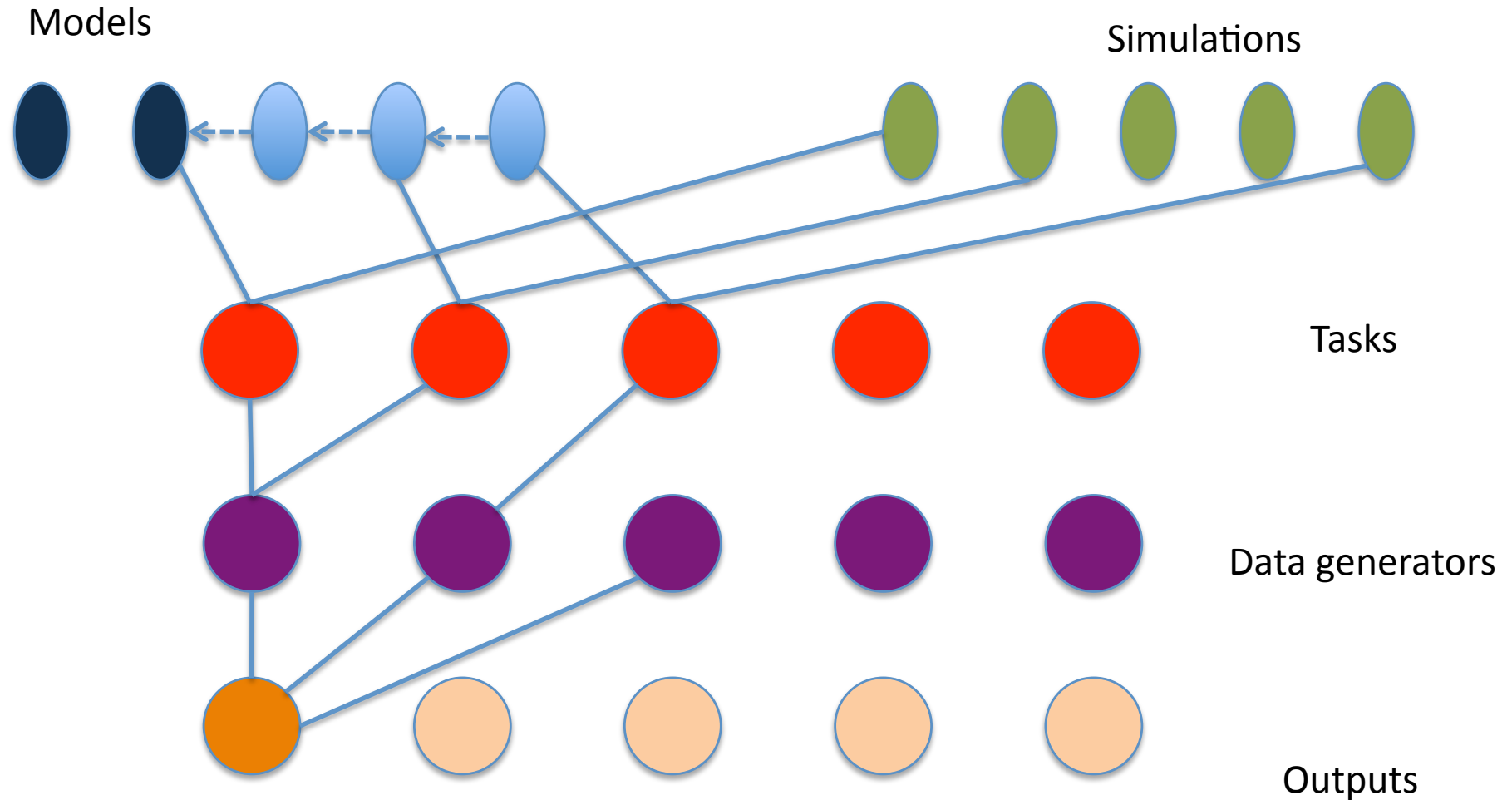
- Separate Java library, **jmathml**
- Supports String, ASTNode and MathML representation of math structures.
- Can add custom symbols
- Supports evaluation of scalar and vector expressions

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

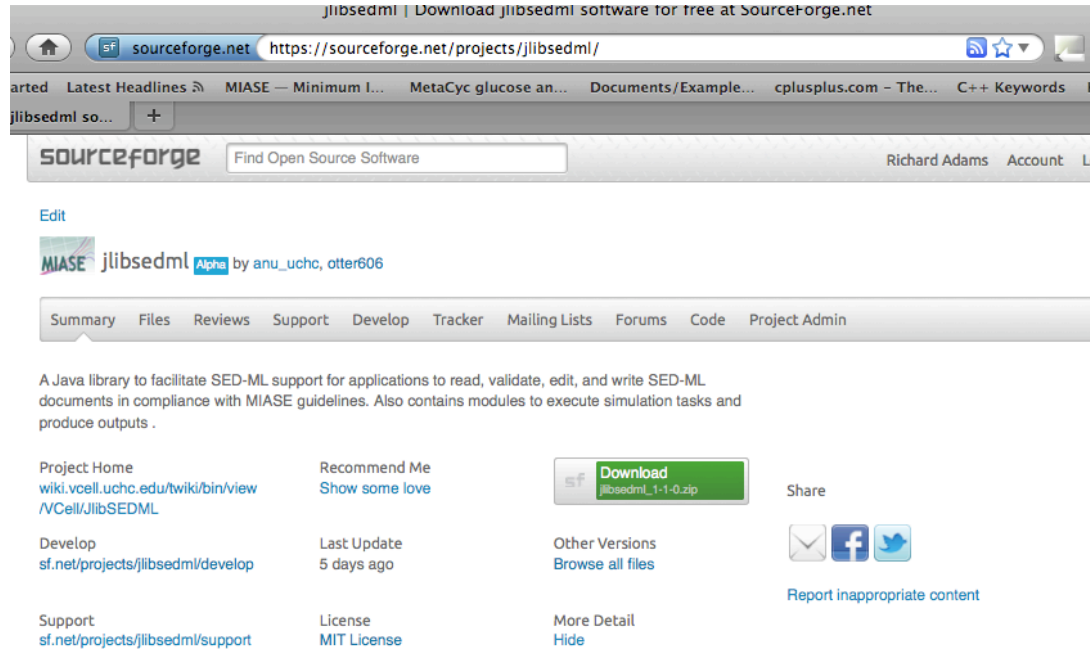
Extensibility

- Validators
- Model retrieval
- Executable SED-ML

Interpreting SED-ML



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



"Pioneering research and infrastructure development to
model the dynamic aspects of biology"



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

Packages
[org.sedml](#)
[org.sedml.execution](#)
[org.sedml.mathsymbols](#)
[org.sedml.modelsupport](#)
[org.sedml.validation](#)
[org.sedml.webtools](#)

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

1. JlibSEDML How-to
 1. Introduction
 1. What can jlibsedml do for me?
 1. Basic support for SED-ML
 2. Support for execution of SED-ML documents
 3. Support for developers
 2. About the authors
 3. Licensing
 2. Installation
 3. Creating a SED-ML document
 1. The basics
 2. Creating a simulation element:
 3. Creating a model element:
 4. Creating a task element:
 5. Creating data generators:
 6. Generating the output
 7. Annotating the document
 8. Writing the document
 1. Basic export
 2. Export as a SED-ML archive.
 9. Conclusions
 4. Reading a SED-ML document.
 1. Reading in a SED-ML file:
 5. Accessing information to run a simulation:
 1. Running the model
 2. Processing the results
 3. A SED-ML execution framework
 1. Executing a simulation
 2. Processing the results:
 3. An example:
 4. Other code snippets
 1. Analysing the KISAO id;
 2. A Simple test analysing the model type:
 6. Manipulating MathML expressions
 1. Vector manipulations
 7. Current issues.
 1. Synchronization and thread safety.
 2. Object identity.
 8. More information
 1. Validation of SED-ML documents
 2. More examples
 3. Javadoc
 4. 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 -

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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" nu
8.</uniformTimeCourse>
9.</listOfSimulations>
10.<listOfModels>
11.<model id="abc1_lj1_2_3e_4_i_1300826091904" name="" language="urn:sedml:language:sbml.level-2.version-2" source="ab
12.<listOfChanges>
13.<changeAttribute newValue="20.00" target="/sbml:sbml/sbml:model/sbml:listOfParameters/sbml:parameter[@id='k_1']/@valu
14.</listOfChanges>
15.</model>
16.</listOfModels>
17.<listOfTasks>
18.<task id="task1" name="default Task" modelReference="abc1_lj1_2_3e_4_i_1300826091904" simulationReference="sim1" />
19.</listOfTasks>
20.<listOfDataGenerators>
21.</listOfDataGenerators>
```

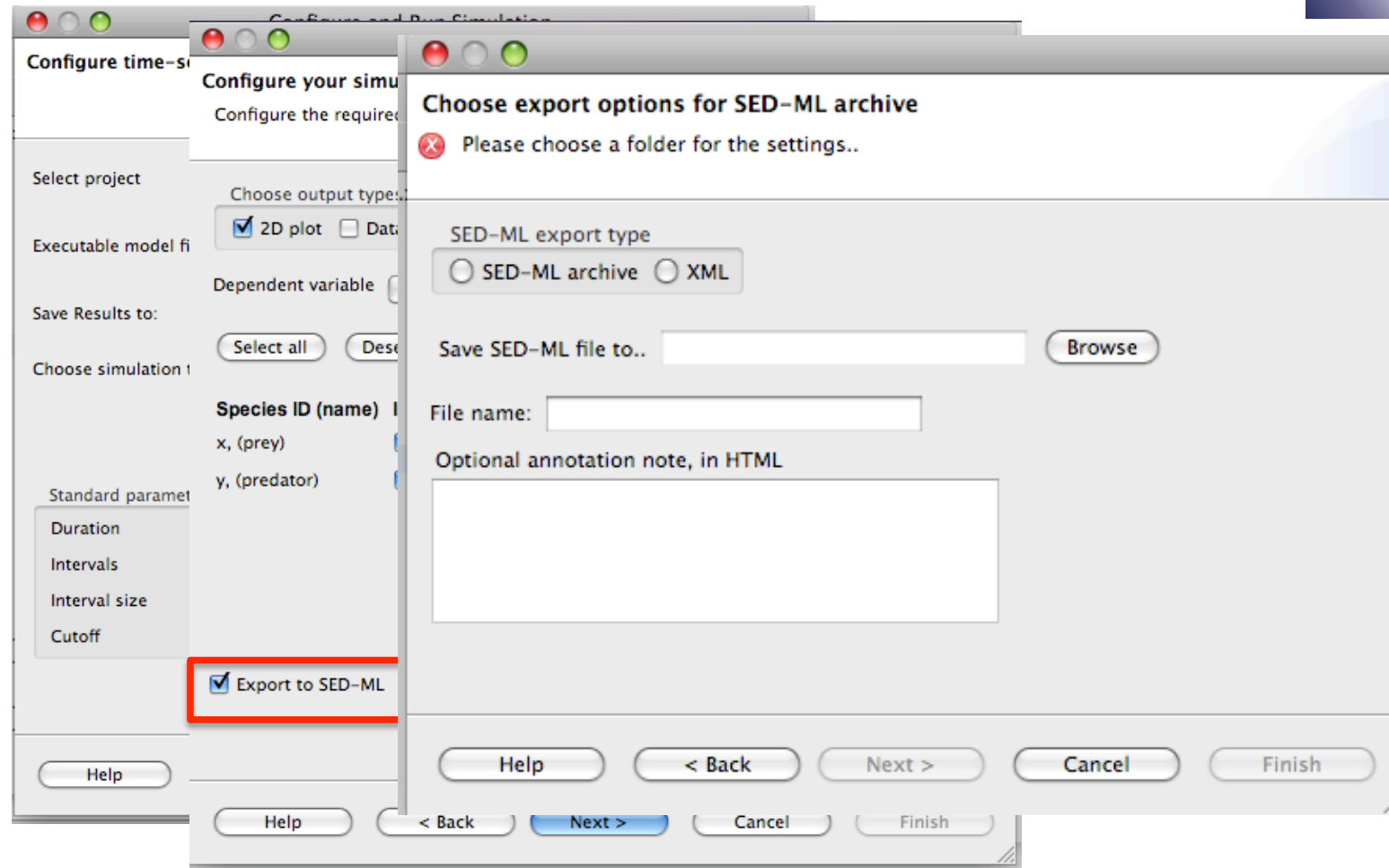
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SBSIN
SBSIV
Project
Downl
Online
Licensi
Contac

SE

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

SED-ML support in SBSI-

www.sbsi.ed.ac.uk



SED-ML support in SBSI – viewing SEDML

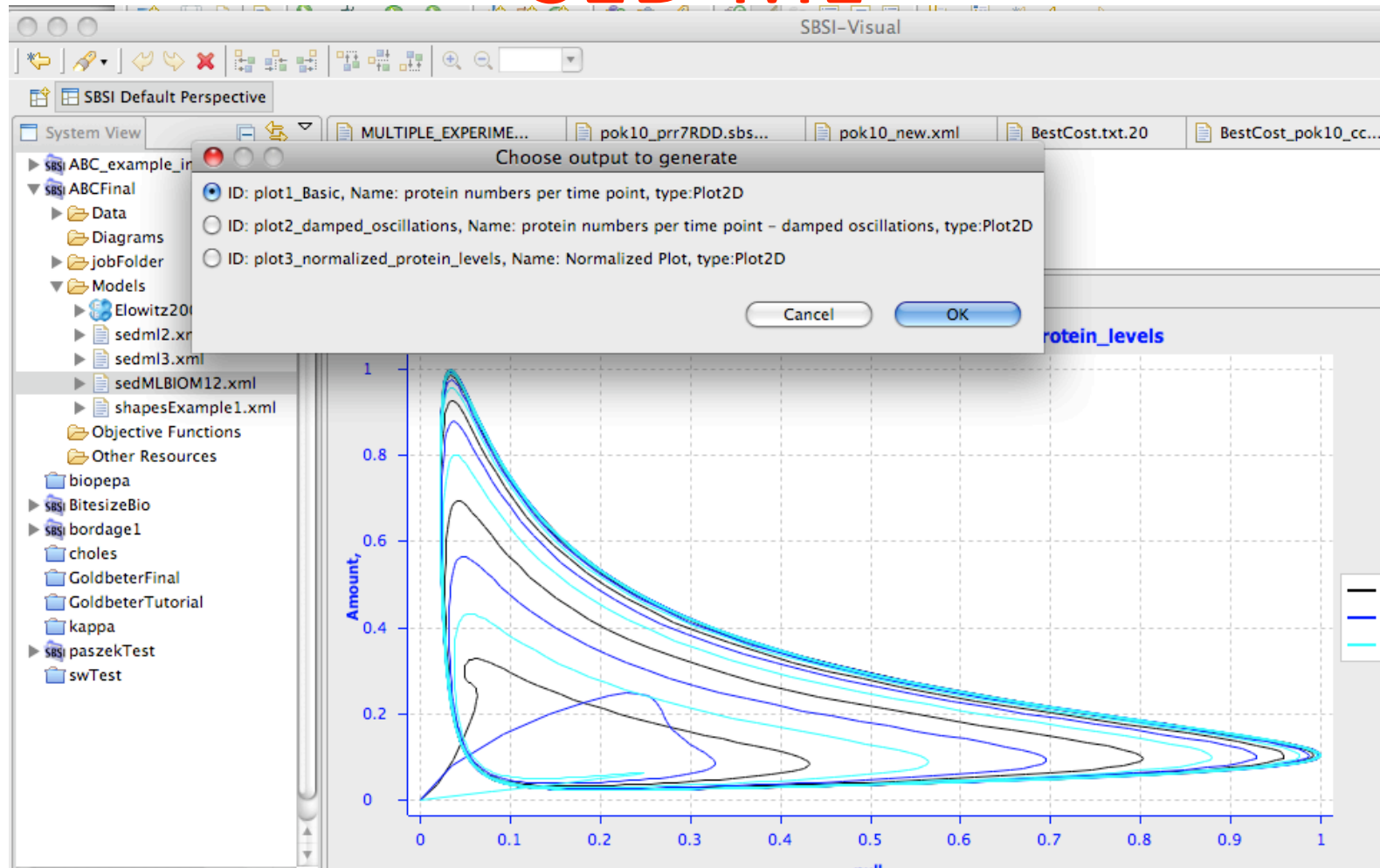
The screenshot shows the SBSI-Visual application interface. On the left, the 'System View' tree shows a project structure with folders like 'Data', 'Diagrams', 'jobFolder', and 'Models'. Under 'Models', the file 'predatorPreySedml.xml' is selected. The main editor window displays the XML content of this file, which includes a simulation definition with parameters like 'id2', 'name', 'initialTime', 'outputStartTime', 'outputEndTime', 'numberOfPoints', and 'algorithm'. The bottom panel shows a 'Problems' view with 2 errors and 8 warnings, specifically listing 'Simulation 'id' not found' errors.

```
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"
```

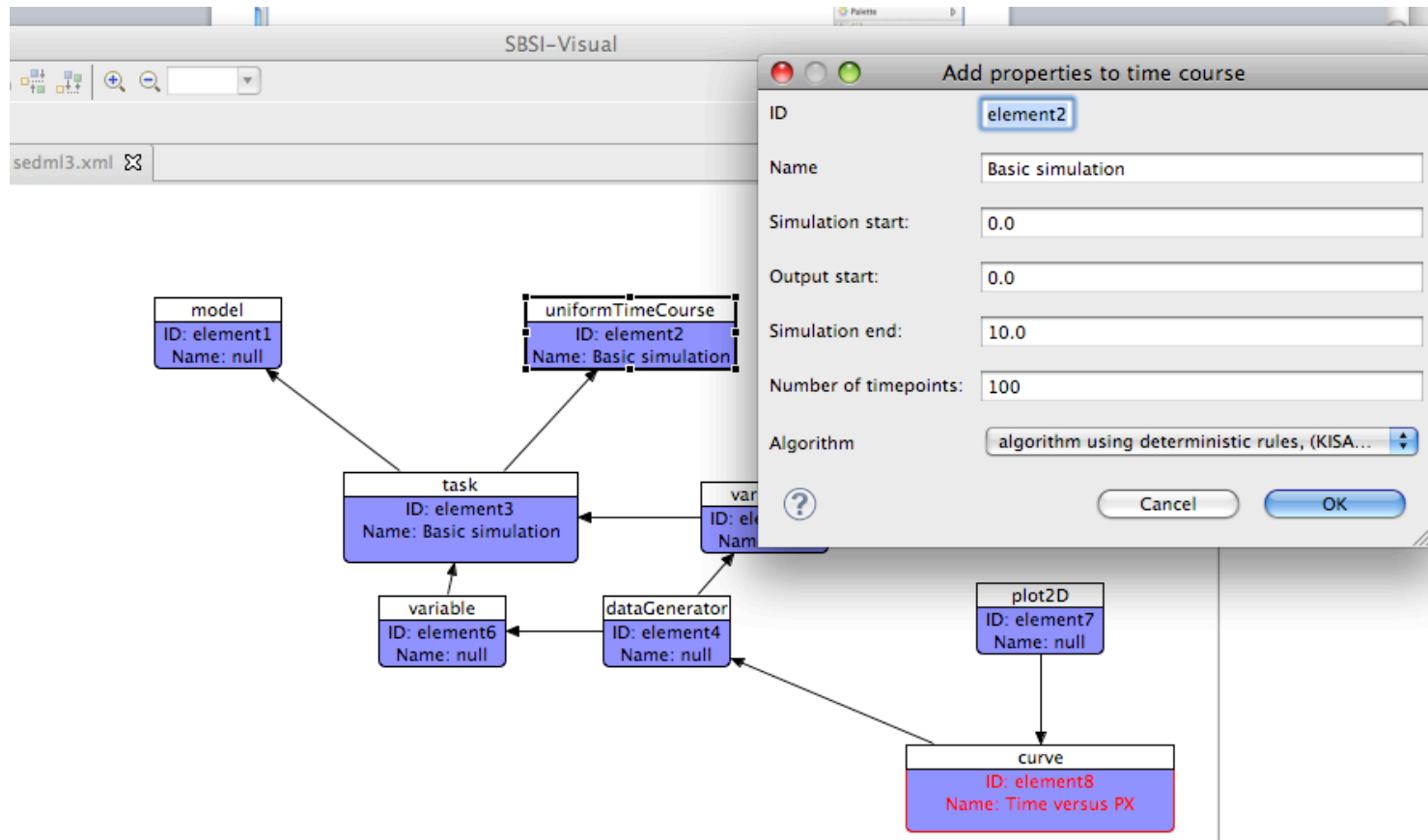
2 errors, 8 warnings, 0 others

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



SED-ED, a SED-ML editor



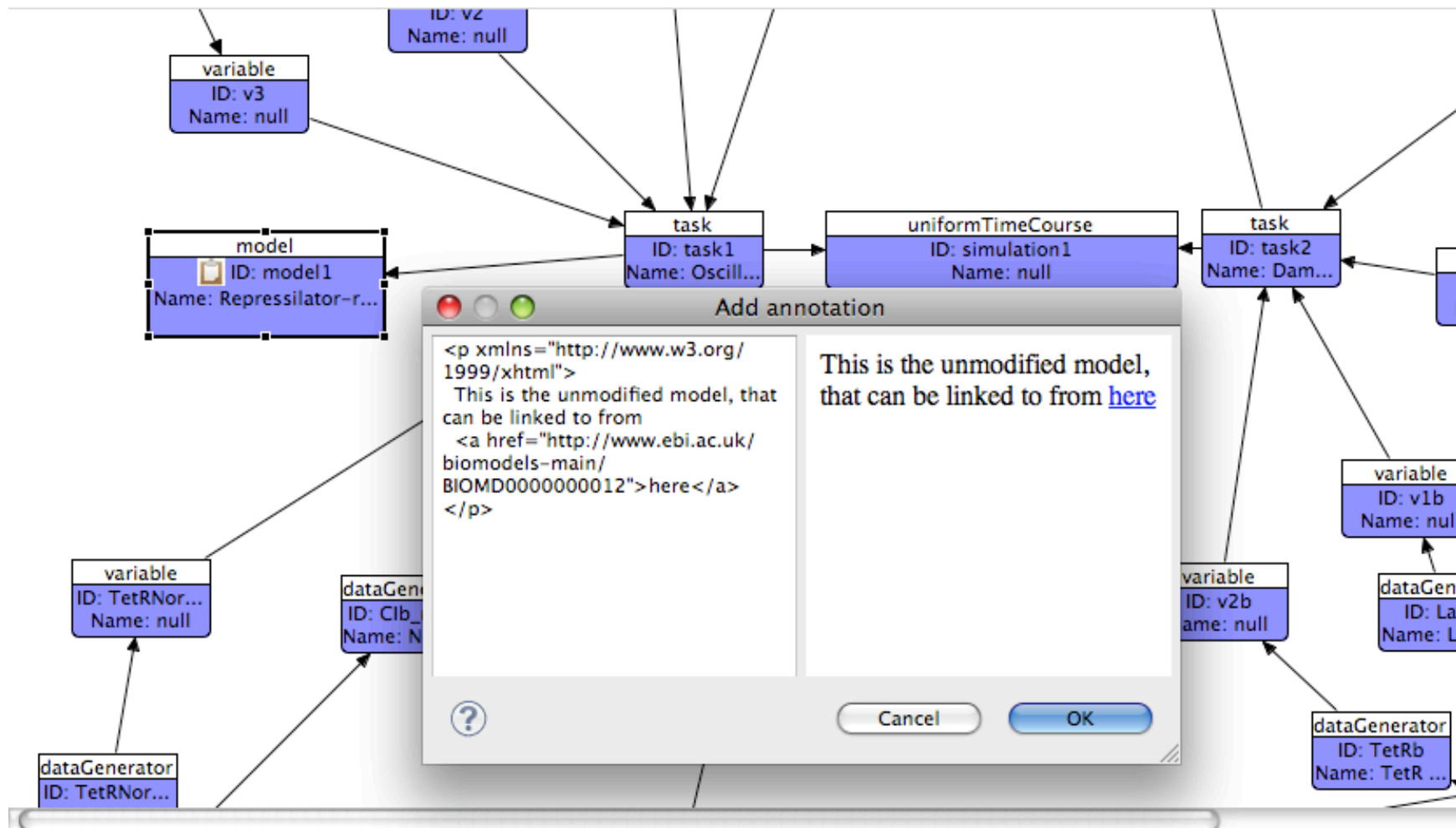
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model the dynamic aspects of biology"**

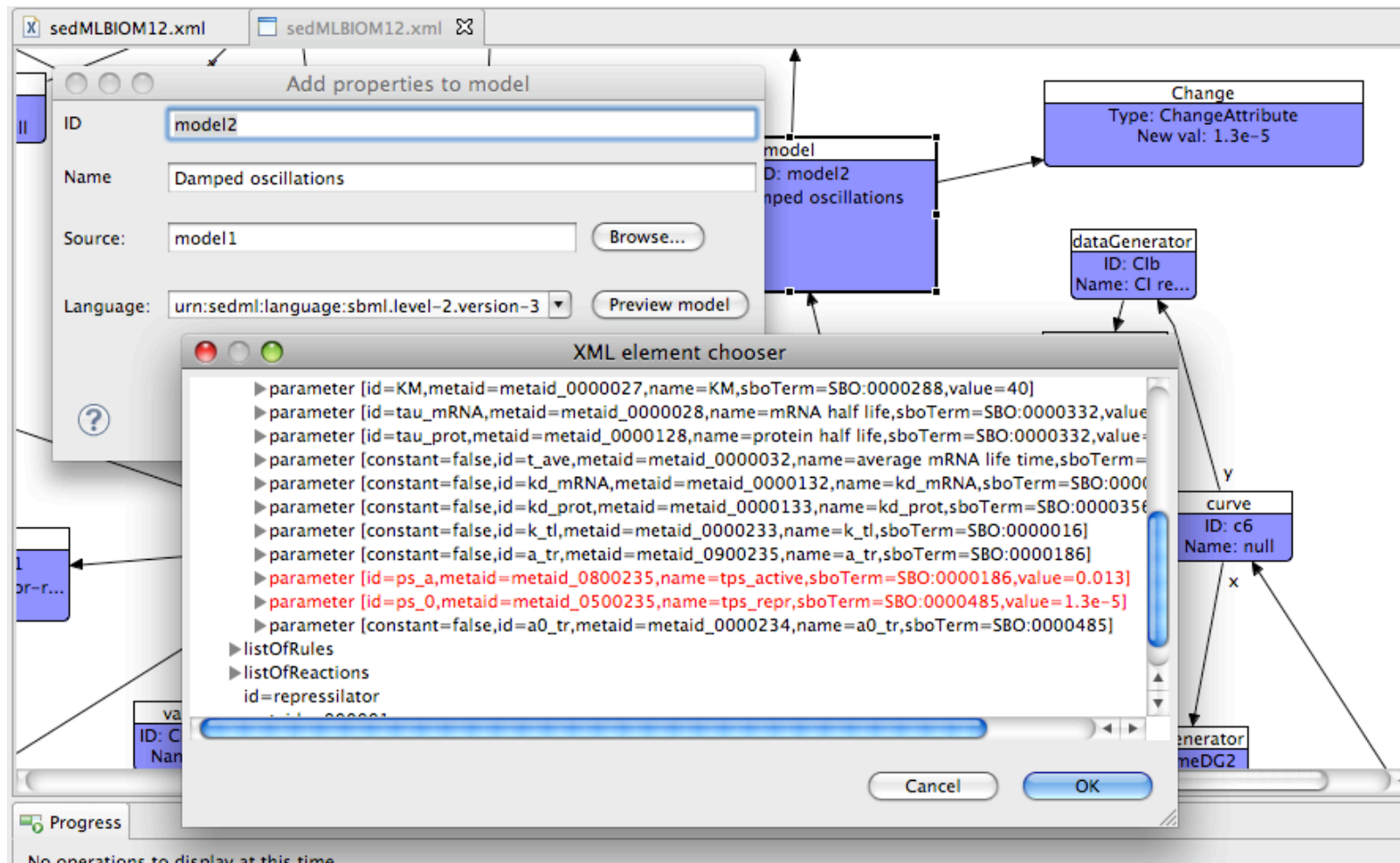
Available as a standalone application : <http://sourceforge.net/projects/jlibsedml/files>
Eclipse or SBSI plugin update site : <http://www.sbsi.ed.ac.uk/update>



Annotating SED-ML



Viewing model changes



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.

Acknowledgements

- VCell
 - Ion Moraru
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- CSBE
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- SED-ML editors
 - Frank Bergmann
 - Dagmar Waltemath
 - Andrew Miller
 - David Nickerson
 - Nicolas Le Novère



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>