Combine Workshop 2011 Heidelberg

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CSBE

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

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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

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SED ML

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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

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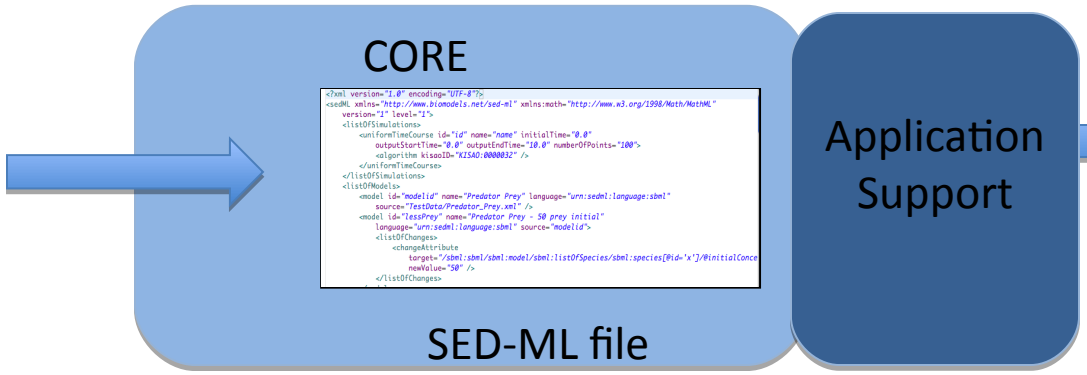
Export simulation configuration

Simulator 1

Simulator 2

Simulator 3



Execute configuration

Simulator 1

Simulator 2

Simulator 3

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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(myOutStream);
```

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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

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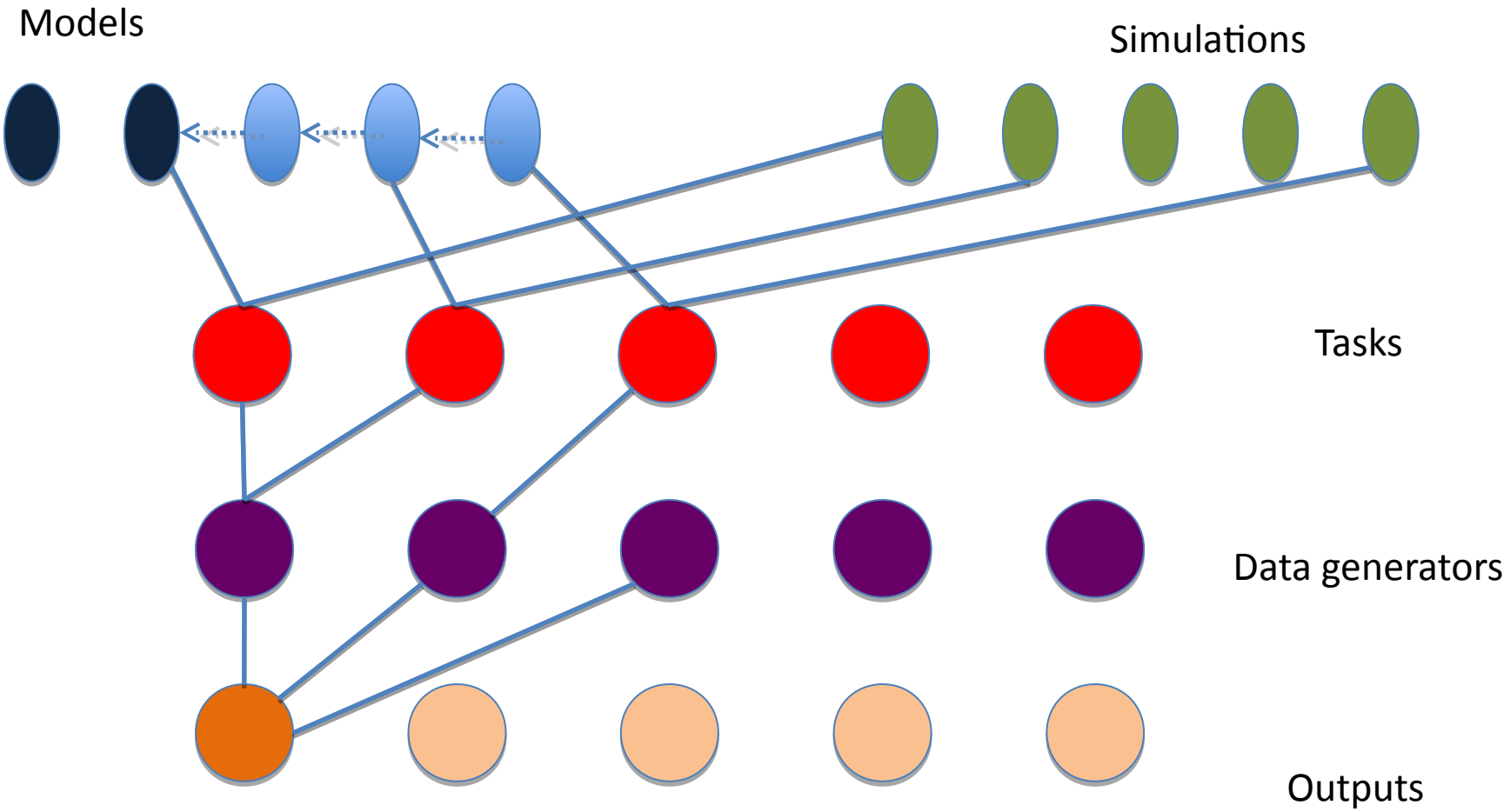
Interpreting SED-ML



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SED ML

JlibSEDML on Sourceforge…

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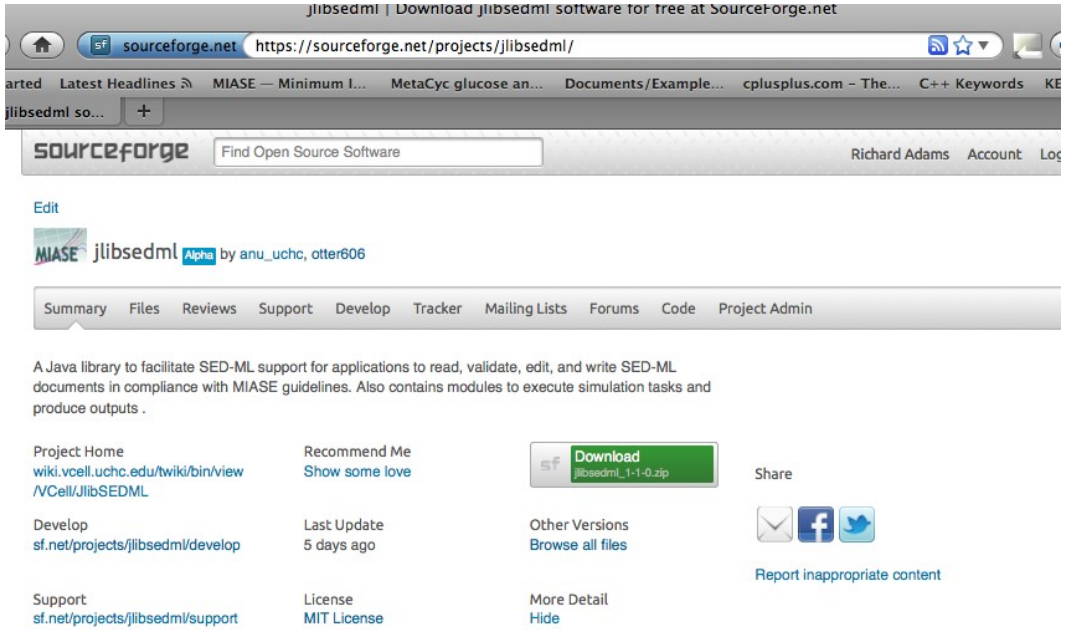

Java library for SED-ML

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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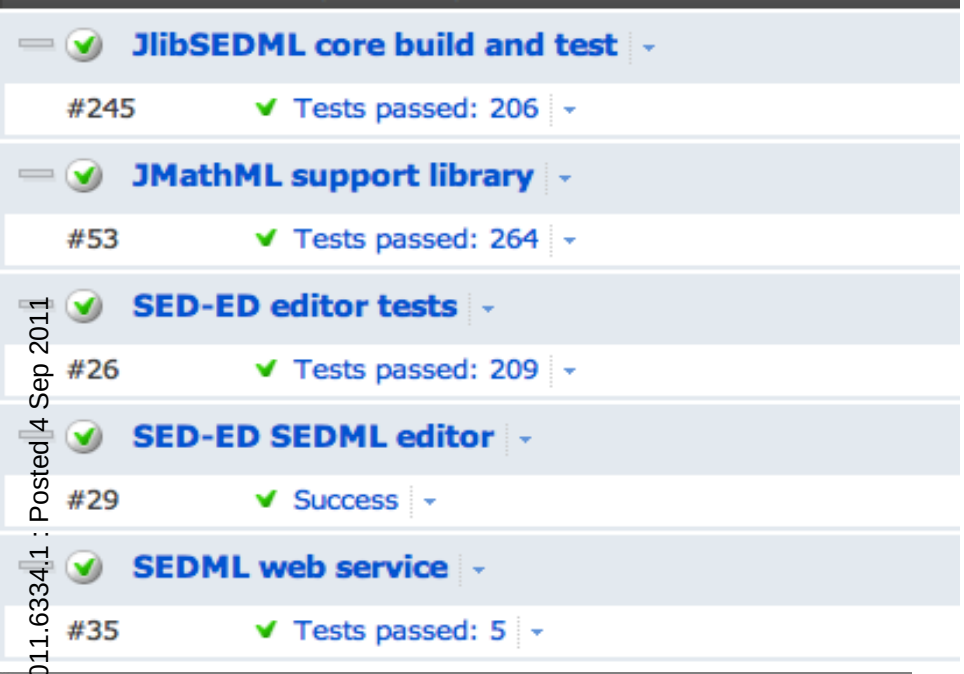

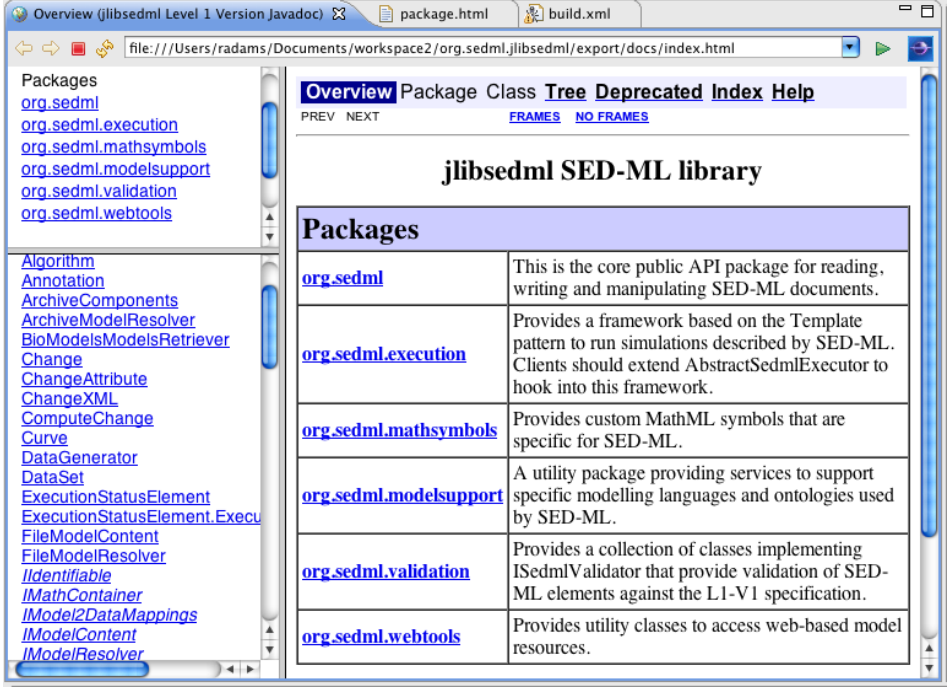

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JlibSEDML How-to

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.

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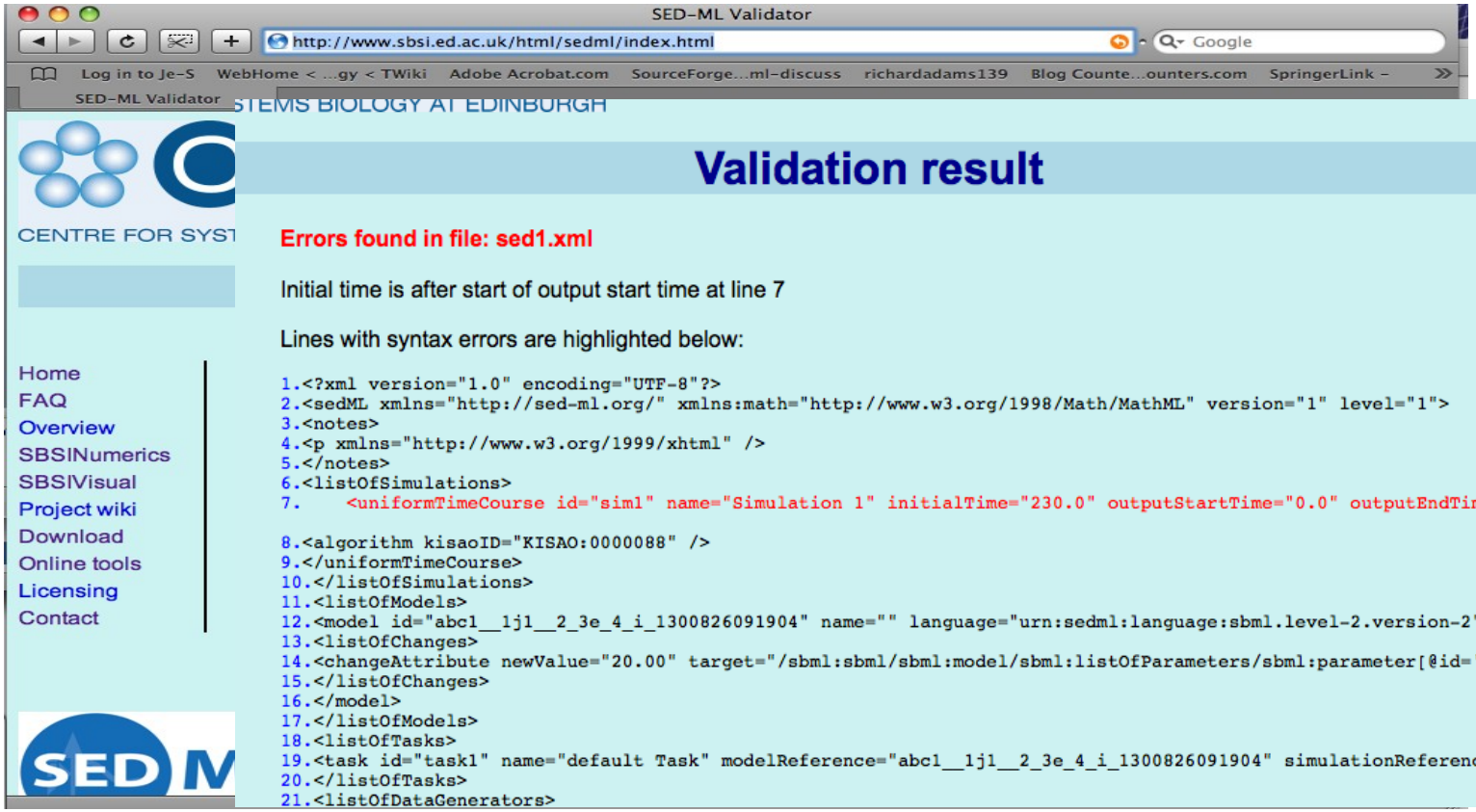
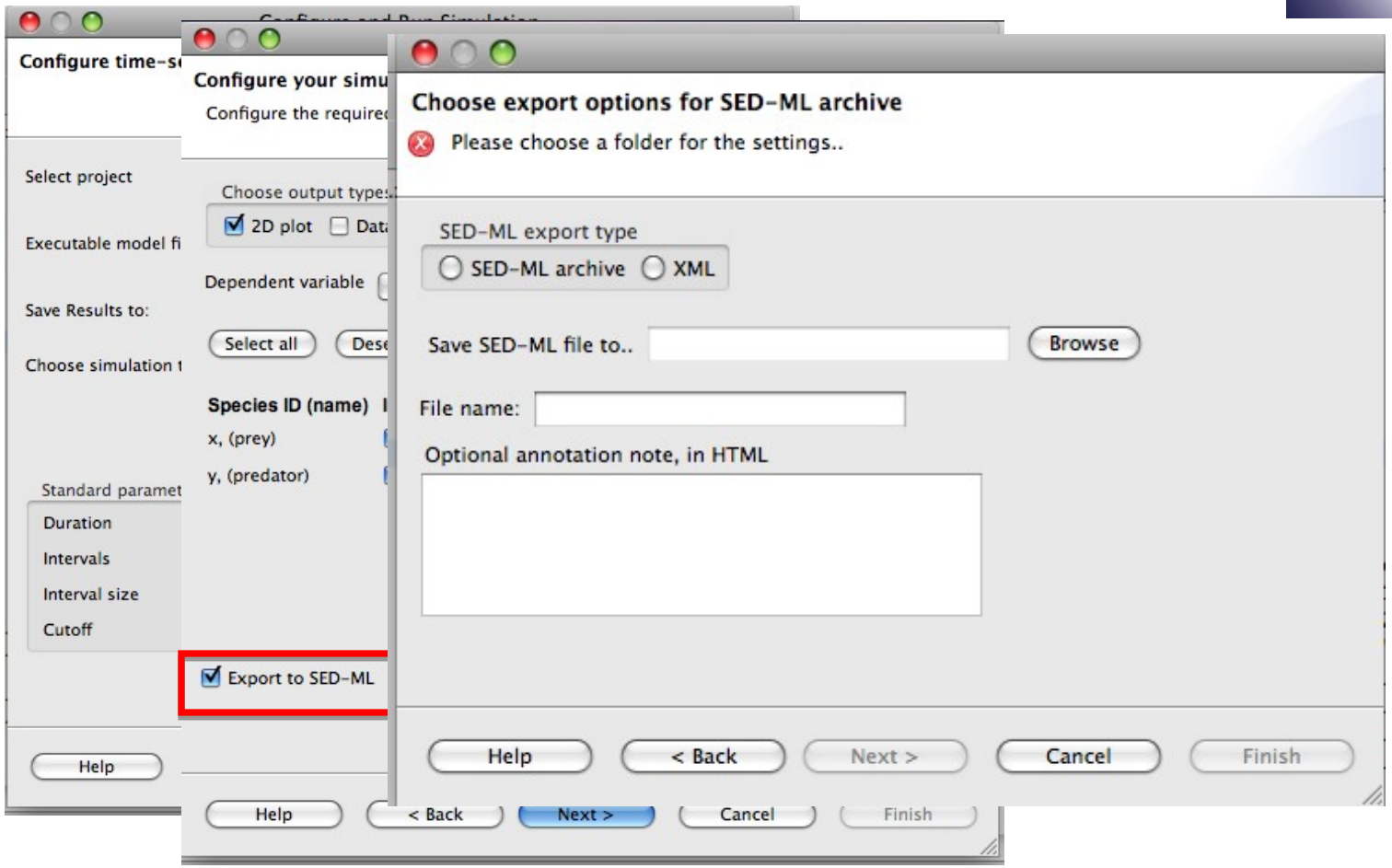
Applications 1 - online SED-ML validator



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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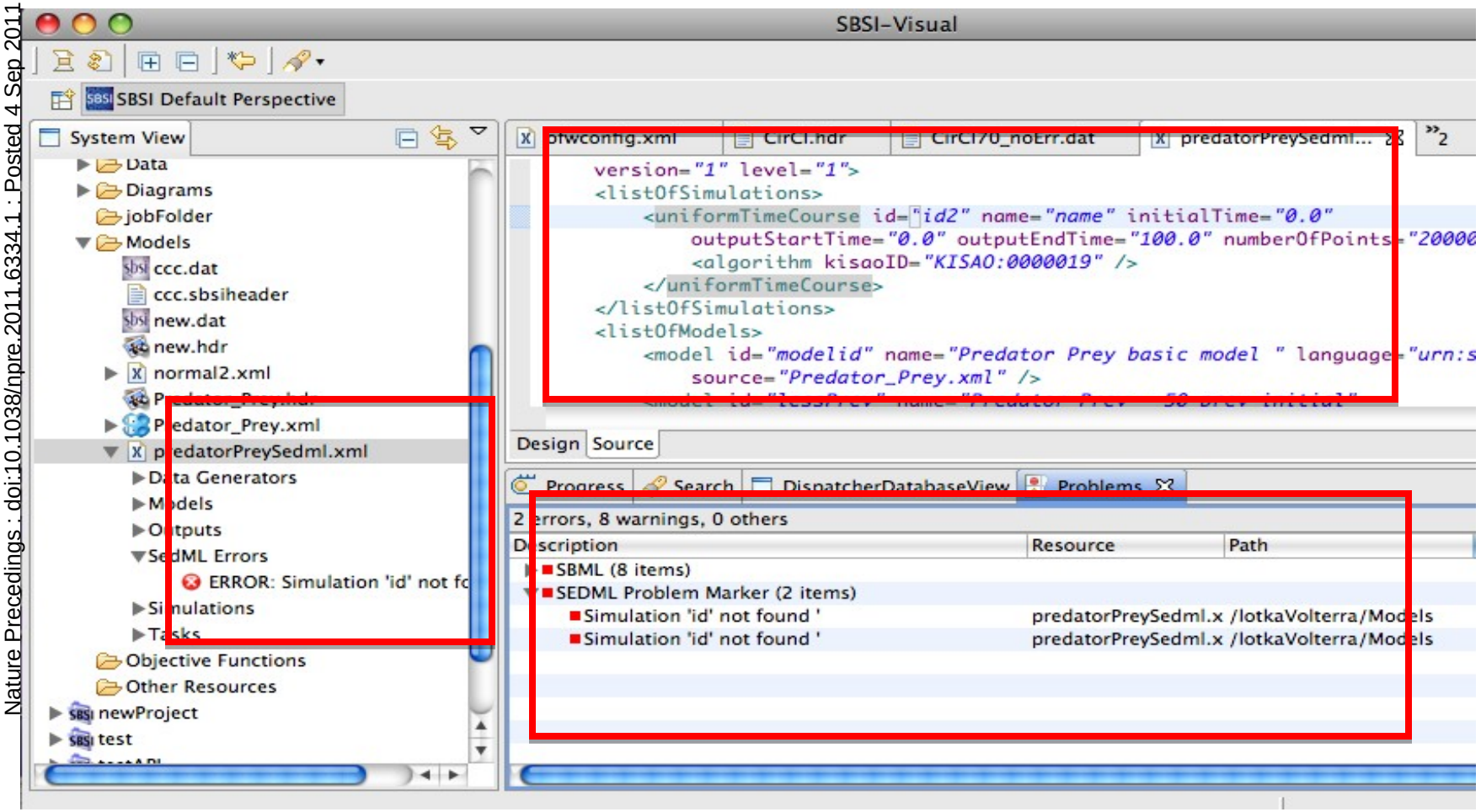

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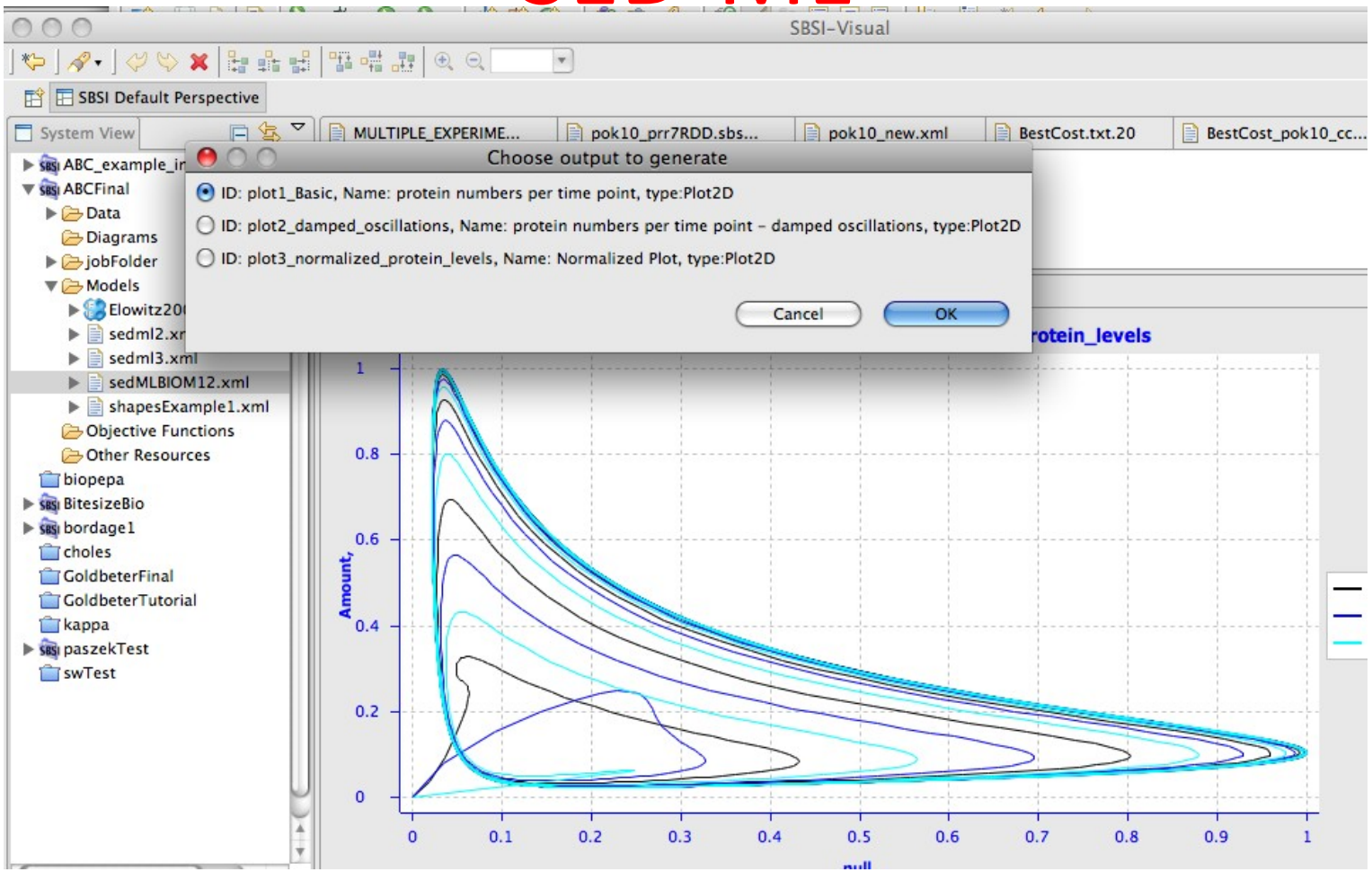
SED ML

SED-ML support in SBSI – executing SED-ML



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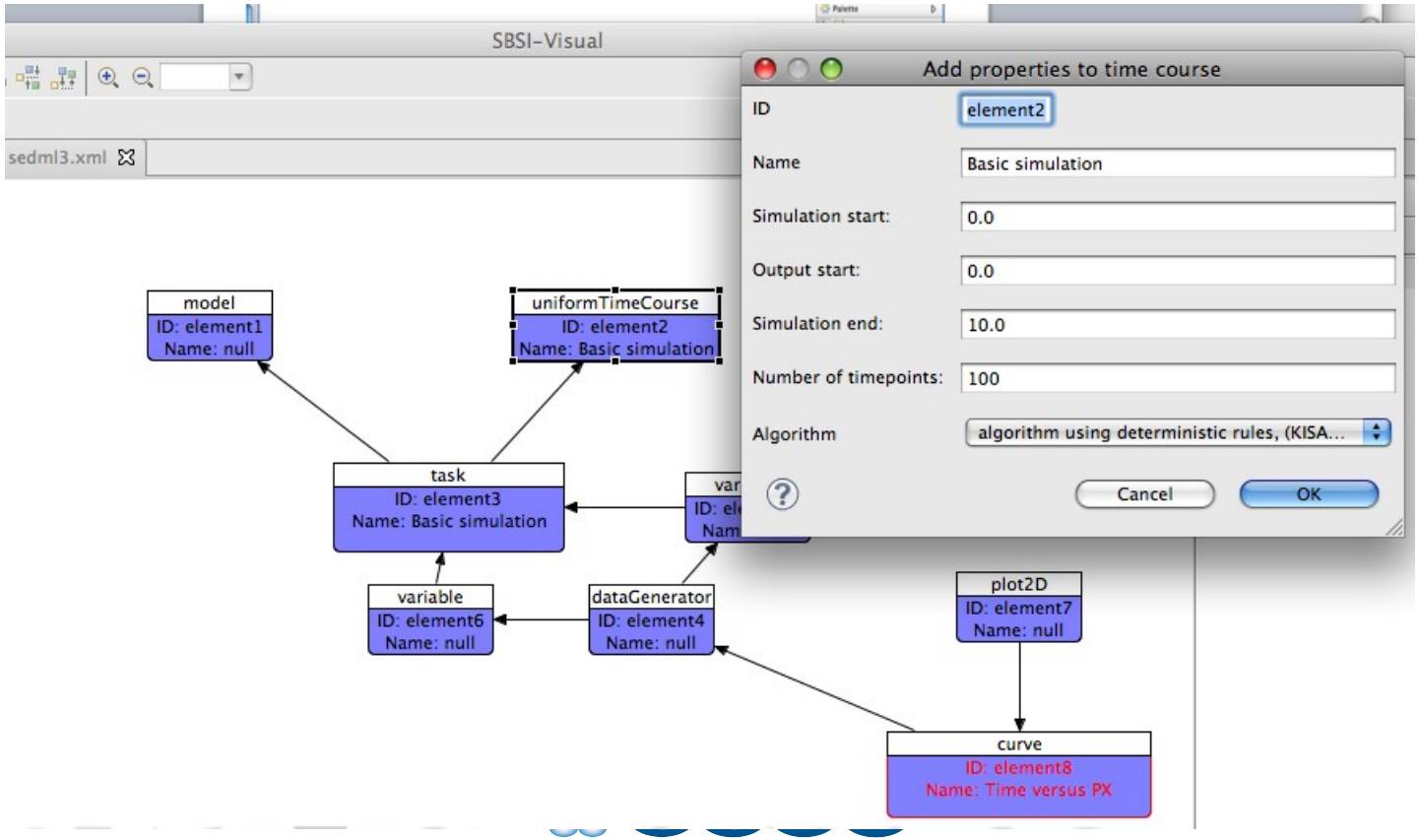
SED ML

SED-ED, a SED-ML editor



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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

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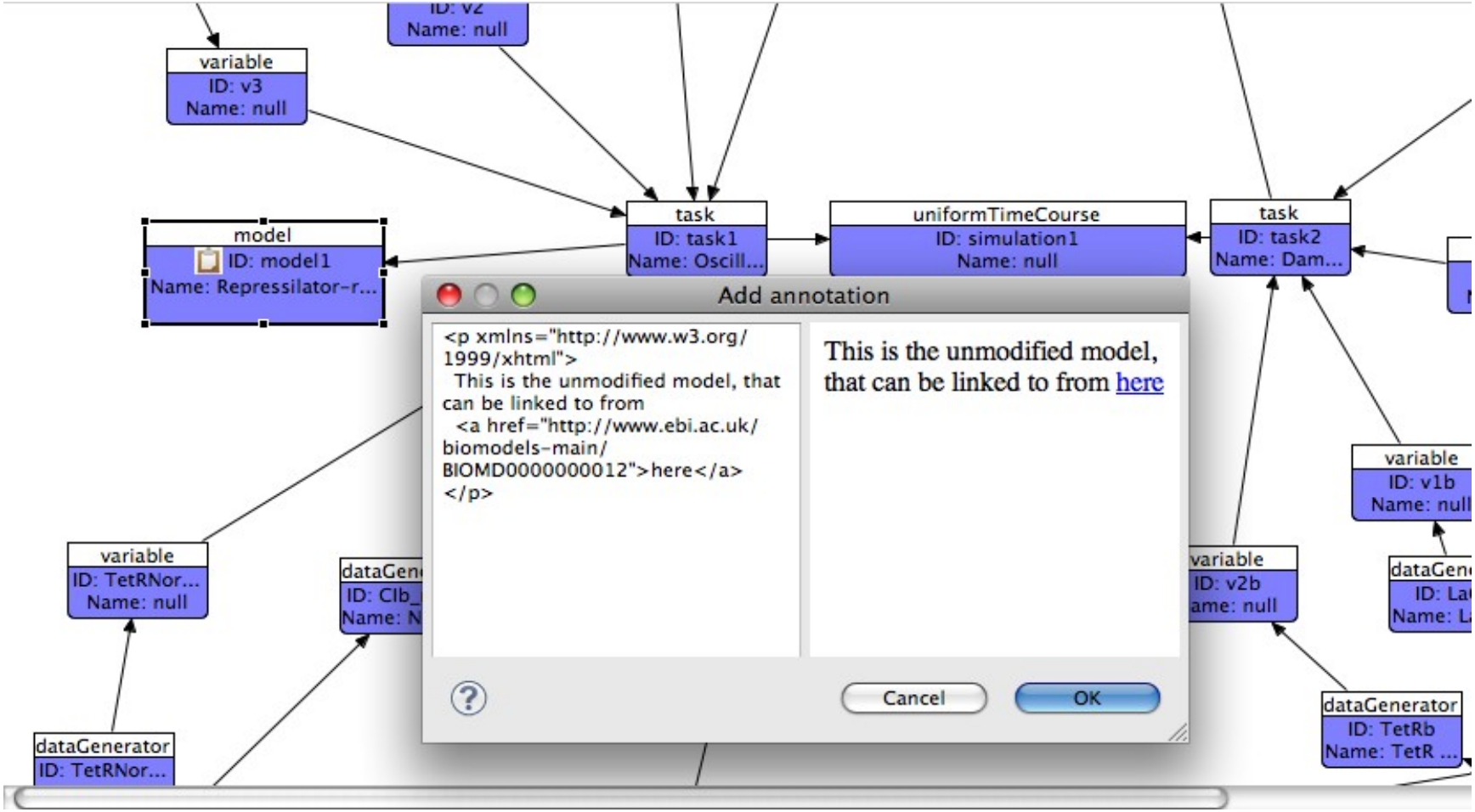
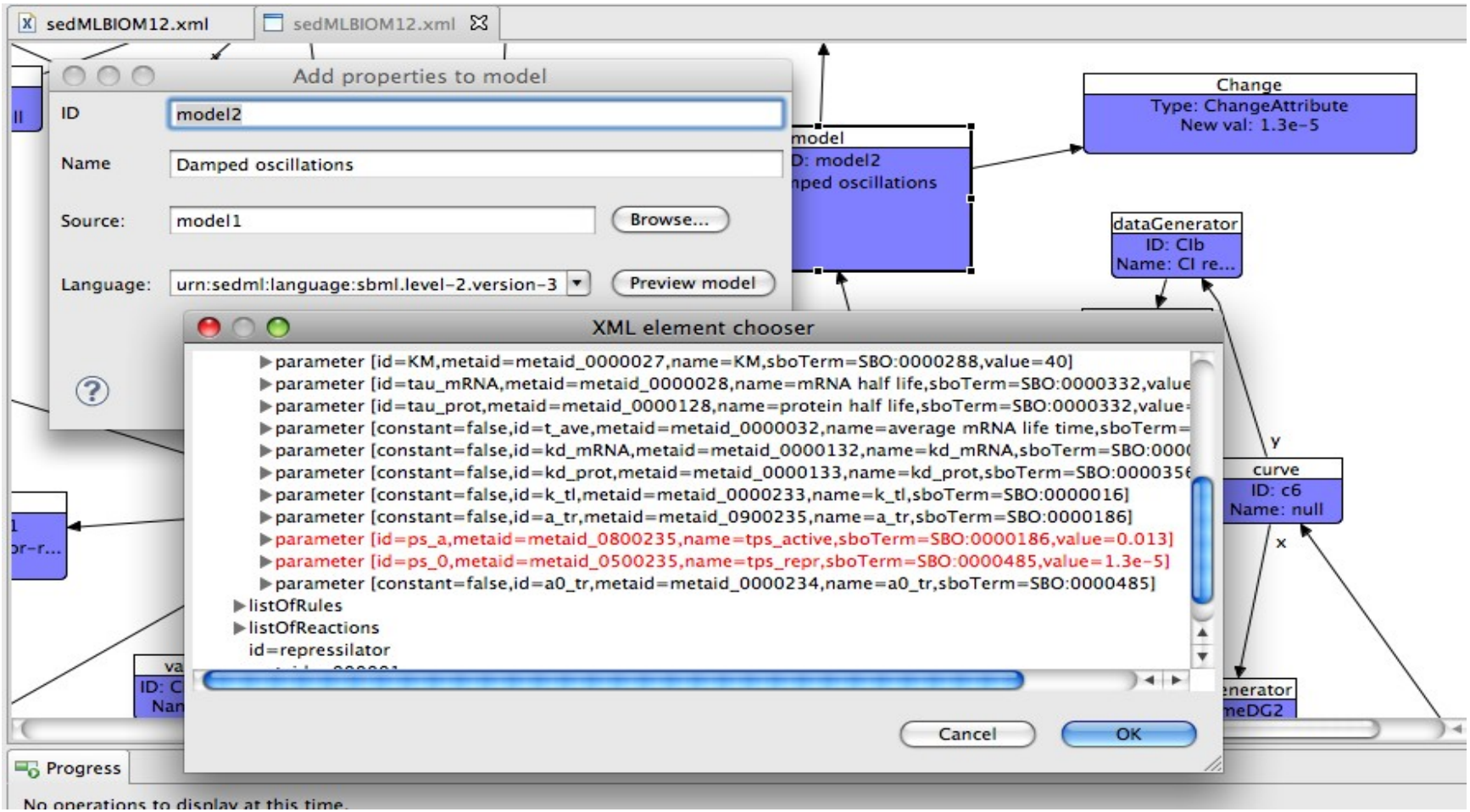
Annotating SED-ML



Viewing model changes



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Other features

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

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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!

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SED ML

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

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