

Jlibsedml – a Java library for manipulating Sedml files

Richard Adams

CSBE, University of Edinburgh,
Edinburgh, Scotland



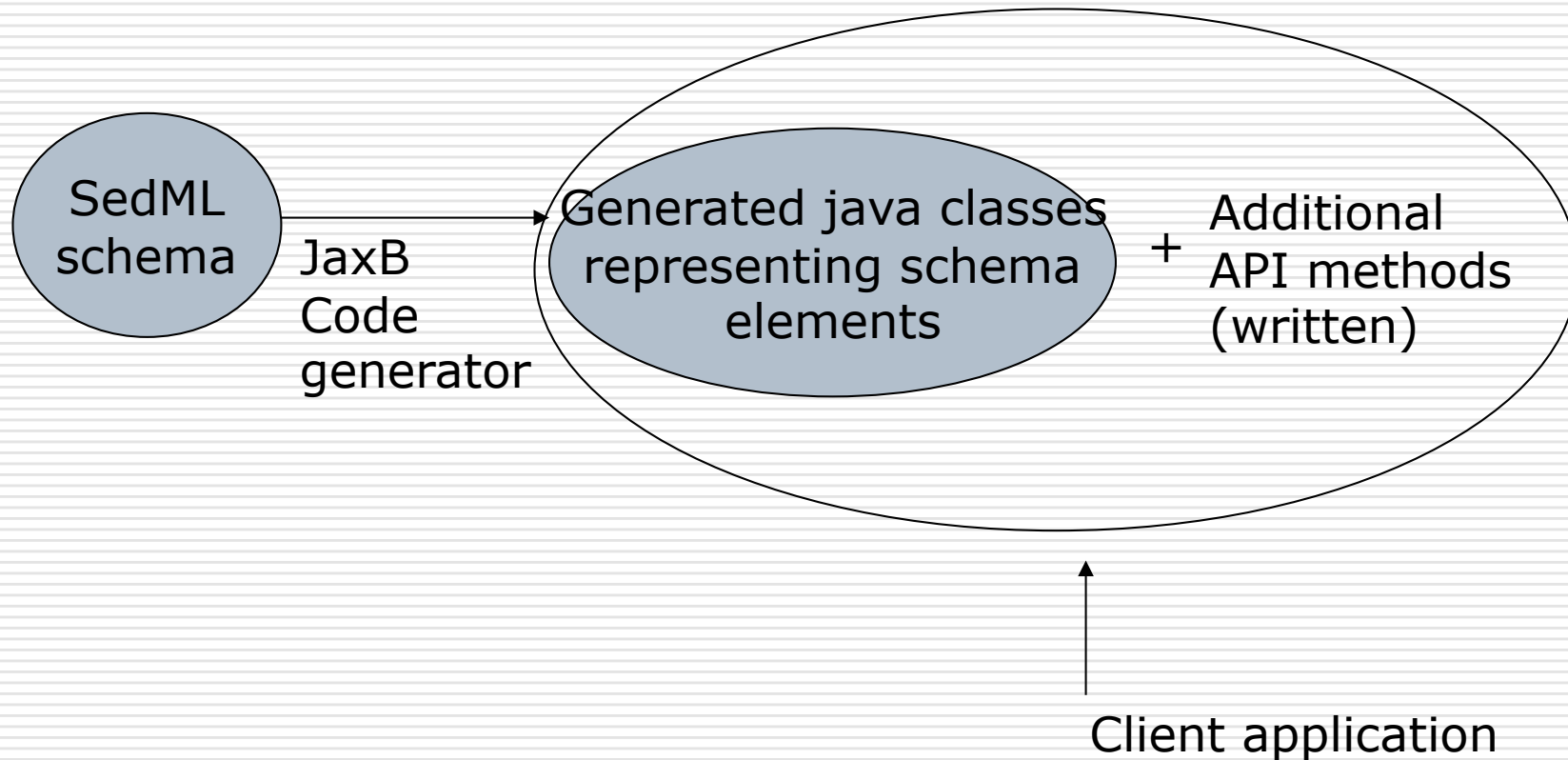
Justification

A good library can help with adoption of standards. E.g., libSBML

Why Java?

- ease of use in Java applications (building a cross-platform app with libSBML can be tricky)
 - Need to develop an exchange format internally in our SBSI project.
- Since we're starting from scratch we may as well develop to a standard.
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Current components



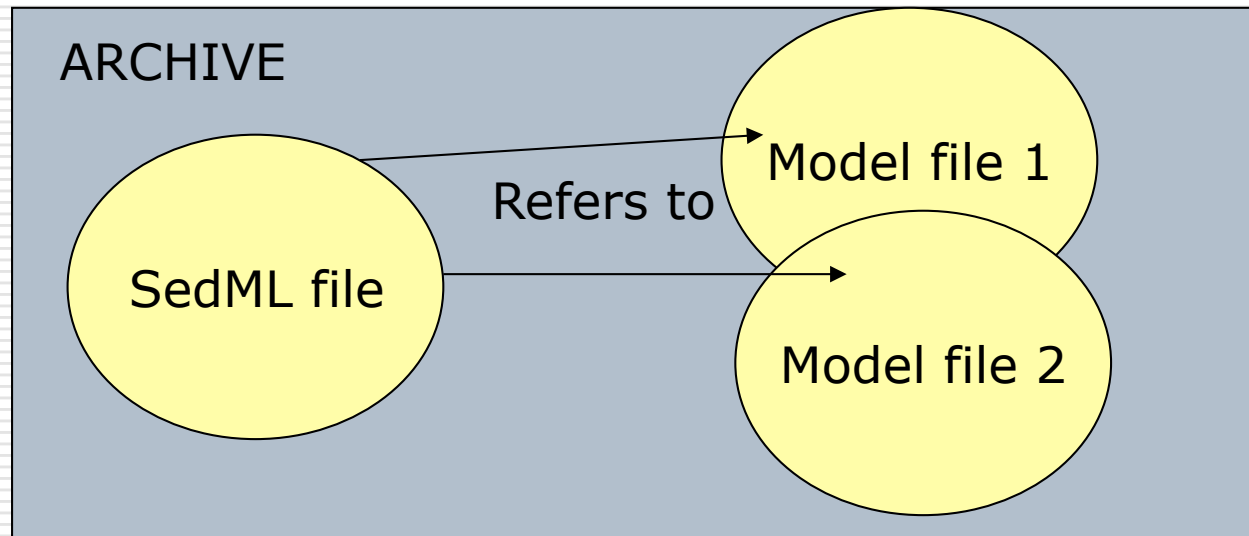
miase.svn.sourceforge.net/svnroot/miase

Coordinating simulation description with model

- ❑ Sedml describes operations on a model.
 - ❑ How to reference the model? It could be in a public repository, in which case it can be accessed via http, or else it needs to be accessible to software reproducing a simulation.
 - ❑ Therefore an archive format proposed
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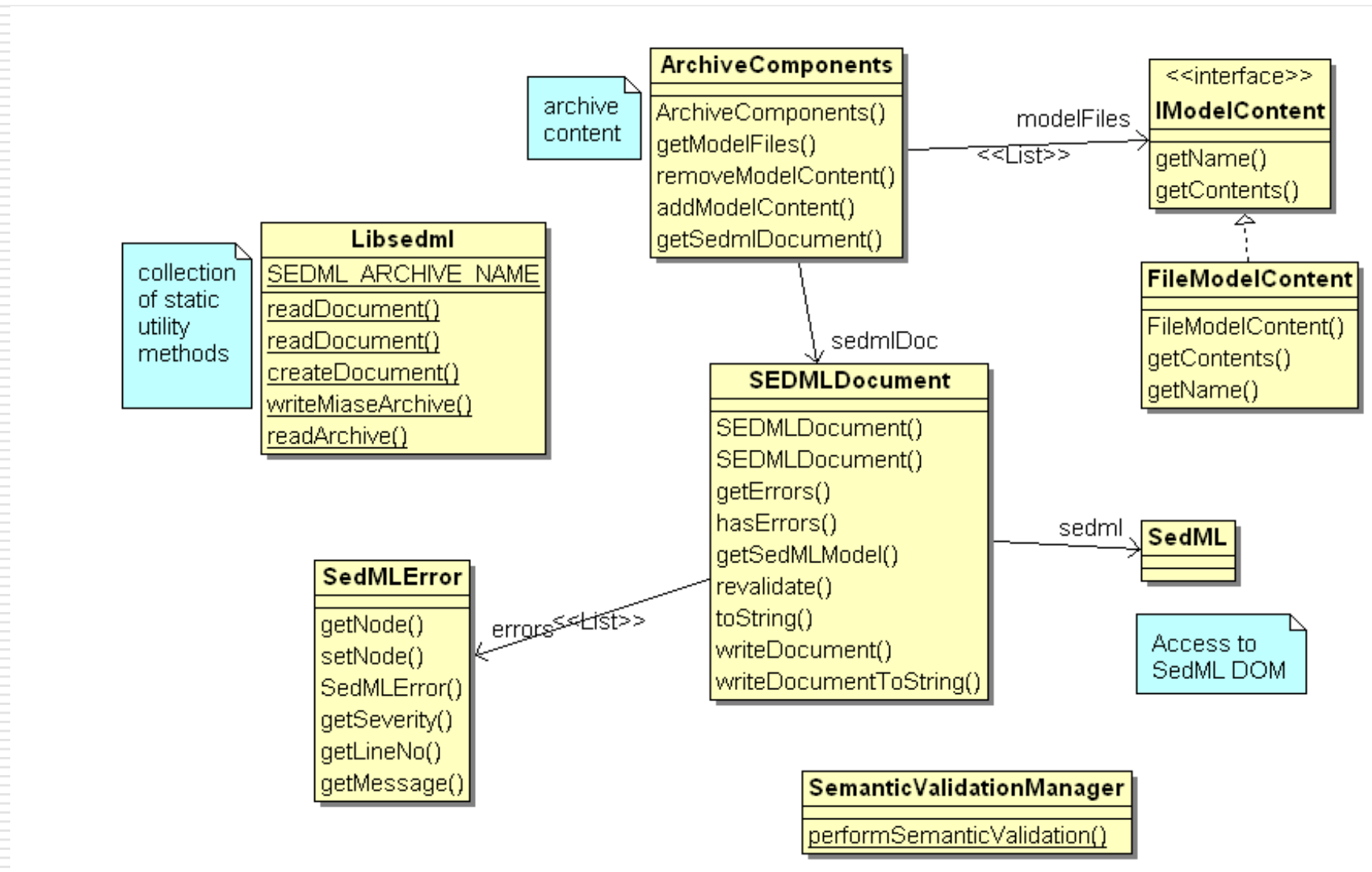
Proposed archive format (Frank Bergmann)

The archive contains models and info needed to run simulation



Essentially is a zipped archive. Downside is we need a specialized software tool to inspect its contents.

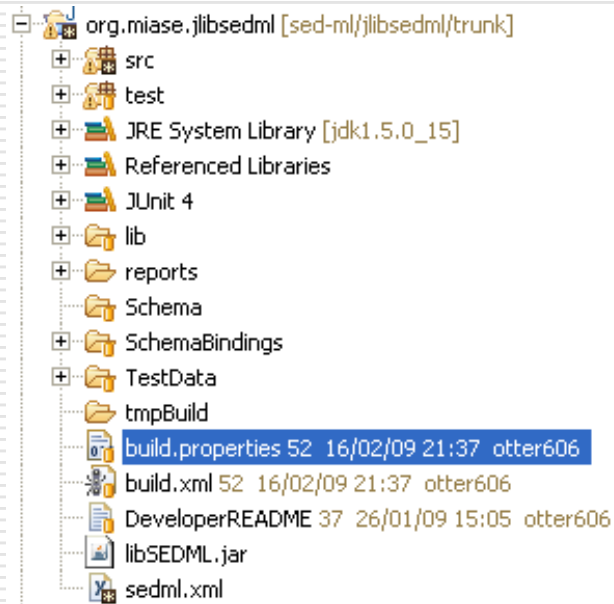
Similar API organisation to libsbml



Project resources:

Eclipse Java project on MIASE sourceforge site.

<http://miase.svn.sourceforge.net/viewvc/miase/sed-ml/jlibsedml/>



Ant script to generate classes, build and deploy library jar, run tests and generate reports.

JUnit test suite checks example models in sedml sourceforge project.

Available under Apache Licence, v2

Example code

```
SEDMLDocument doc = Libsedml.readDocument(myFile);  
// get errors  
List<SedMLError> errors = doc.getErrors();
```

```
// de novo document creation  
doc = LibsedML.createDocument();  
//get model  
Sedml model = doc.getSedMLModel();
```

```
// apply changes to your model using the SedML dom
```

```
// write document back to file  
doc.writeDocument(myFile);
```

Example code (II)

To write a .miase archive file with the model file included:

// add files to archive

```
List<IModelFile> models = new ArrayList<IModelFile>();  
models.add(new FileModelContent(myModelFile));
```

```
// get zipped archive
```

```
ArchiveComponents comps = new ArchiveComponents(models,  
    sedmldoc);  
byte [] zippedBytes = LibSedml.writeMiaseArchive(comps);
```

Outstanding issues I

Jaxb generated classes produce a rather awkward API. Perhaps when schema is more stable we replace with handcoded classes and Jaxb annotations

E.g., No add/ remove operations for ListOf objects, we have to access underlying `java.util.List` object

```
sedml.getListOfModels().addModel(Model m);
```

would be better than the current:

```
sedml.getListOfModels().getModels().addModel(Model m);
```

Outstanding issues II

- MathML handling

LibSBML has nice handling and interconversion of Mathml and String formats

This is not available in libSedml yet; operations using autogenerated classes are extremely inconvenient.

Outstanding issues III

- ❑ Current spec rather limited to time course simulations.
 - ❑ We need to be able to archive optimisation procedures as well, with references to experimental data etc.,
 - ❑ How to refer to data?
 - SBRML? A bit too verbose
 - XML metadata and tabular exptal data could be good compromise
 - Header file / Data file – has reusable header files but overhead of maintaining integrity of data.
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Acknowledgements

- ☐ Dagmar Koehn
 - ☐ Frank Bergmann
 - ☐ Nicholas Le Novere
and Miase mailing list!
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