



The SBML Java™ library

# Concept of JSBML

## Compromise

- High compatibility to libSBML
- Java-like library

## Main developers



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How to get started?

# Obtaining JSBML

- Every stable and experimental release is available for download at <http://sourceforge.net/projects/jsbml/files/jsbml/>
- Download the file `jsbml-X.Y-with-dependencies.jar`
- Once you have added it to the Java CLASSPATH, you can start working with JSBML.

# How to compile JSBML-qual

## Creating a JAR file with the latest code from the repository:

- Checkout the sources from sourceforge  
`svn co svn://svn.code.sf.net/p/jsbml/code/trunk JSBML`  
`cd JSBML/core`  
`ant jar`  
`cd ../extensions/qual`  
`ant jar`  
now, include the jar file from core/build, core/lib, extension/qual/build

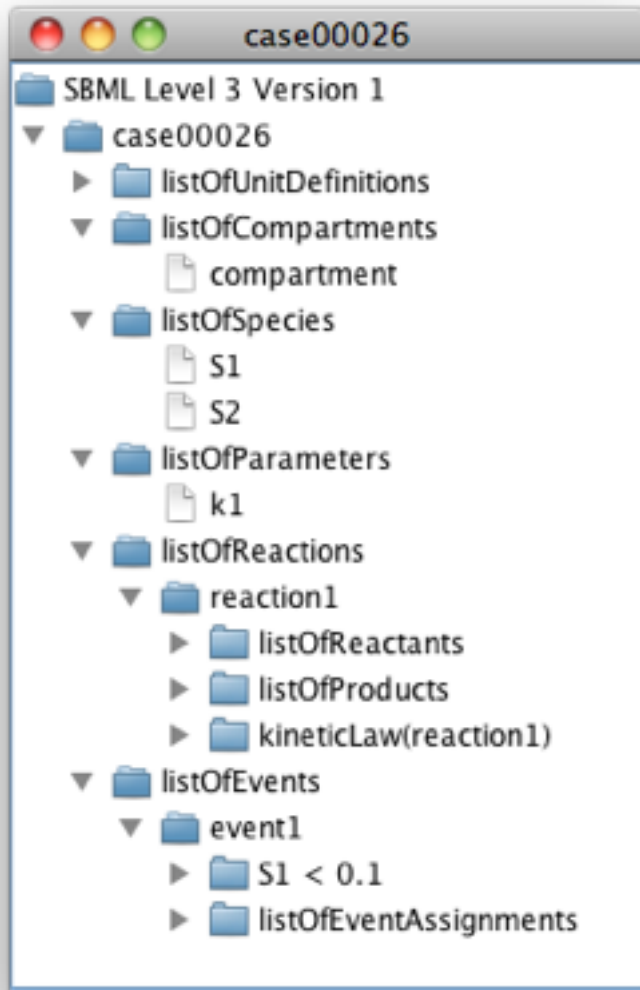
## Generating a big jar, including JSBML-qual:

```
cd ../../  
cp -v extensions/qual/build/*.jar core/lib/  
cd core  
ant bigjar
```

now, you have a jsbml-X.Y-with-dependencies.jar that contains JSBML-qual as well

- Since JSBML 1.0β1 a precompiled version of JSBML-qual is already available for download at <http://sourceforge.net/projects/jsbml/files/jsbml/>

# Visualizing the content of an SBML file



```
import java.io.File;
import javax.swing.*;
import org.sbml.jsbml.*;

/**
 * Displays the content of an SBML file in a {@link JTree}
 */
public class JSBMLvisualizer extends JFrame {

    /**
     * @param document The SBML root node of an SBML file
     */
    public JSBMLvisualizer(SBMLDocument document) {
        super(document.getModel().getId());
        getContentPane().add(new JScrollPane(new JTree(document)));
        pack();
        setVisible(true);
    }

    /**
     * Main routine. Note: this does not perform any error checking,
     * but should. It is an illustration only.
     * @param args Expects a valid path to an SBML file.
     */
    public static void main(String[] args) throws Exception {
        UIManager.setLookAndFeel(UIManager.getSystemLookAndFeelClassName());
        new JSBMLvisualizer(SBMLReader.read(new File(args[0])));
    }
}
```

Example output when reading an SBML file with the code on the left from the SBML Test Suite with JSBML (on Mac OS X)

# How does XML parsing work?

- Mapping between SBML elements and Java classes: `/jsbml-trunk/resources/org/sbml/jsbml/resources/cfg/SBMLCoreElements.xml`
- Then each SBase has a `readAttributes` and `writeAttributes` methods that take care of reading and writing the attributes of the element.
- The parsing is done in:
  - `org.sbml.jsbml.xml.stax`: main entry point of the parsing, using Stax.
  - `org.sbml.jsbml.xml.parsers`: parser independent of the underlying XML parsing library used.
- For extension packages a similar parsing/writing mechanism is used

# Creating a new SBML model from scratch

```
public JSBMLexample() throws Exception {
    // Create a new SBMLDocument object, using SBML Level 3 Version 1.
    SBMLDocument doc = new SBMLDocument(3, 1);
    doc.addTreeNodeChangeListener(this);

    // Create a new SBML model, and add a compartment to it.
    Model model = doc.createModel("test_model");
    Compartment compartment = model.createCompartment("default");
    compartment.setSize(1d);

    // Create a model history object and add author information to it.
    History hist = model.getHistory(); // Will create the History, if it does not exist
    Creator creator = new Creator("Given Name", "Family Name", "Organization", "My@EMail.com");
    hist.addCreator(creator);

    // Create some sample content in the SBML model.
    Species specOne = model.createSpecies("test_spec1", compartment);
    Species specTwo = model.createSpecies("test_spec2", compartment);
    Reaction sbReaction = model.createReaction("reaction_id");

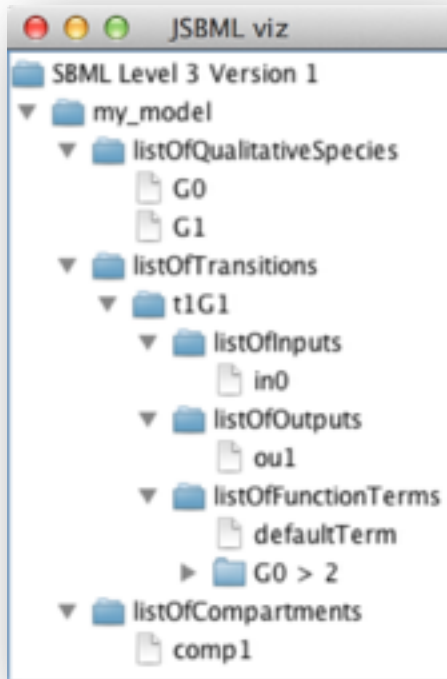
    // Add a substrate (SB0:0000015) and product (SB0:0000011) to the reaction.
    SpeciesReference subs = sbReaction.createReactant(specOne);
    subs.setSBOTerm(15);
    SpeciesReference prod = sbReaction.createProduct(specTwo);
    prod.setSBOTerm(11);

    // For brevity, WE DO NOT PERFORM ERROR CHECKING, but you should,
    // using the method doc.checkConsistency() and then checking the error log.

    // Write the SBML document to a file.
    SBMLWriter.write(doc, "test.xml", "JSBMLexample", "1.0");
}
```



# How to create a simple qual model in JSBML?



```
int level = 3, version = 1;
SBMLDocument doc = new SBMLDocument(level, version);
Model model = doc.createModel("my_model");

// Creating the qualitative model extension and adding it to the document
QualModelPlugin qualPlugin = new QualModelPlugin(model);
model.addExtension(QualConstants.getNamespaceURI(level, version), qualPlugin);

// ListOfCompartments
Compartment comp1 = model.createCompartment("comp1");
comp1.setConstant(true);

// ListOfQualitativeSpecies
QualitativeSpecies g0 = qualPlugin.createQualitativeSpecies("G0", comp1, false);
QualitativeSpecies g1 = qualPlugin.createQualitativeSpecies("G1", comp1, false);

// ListOfTransitions
Transition t1G1 = qualPlugin.createTransition("t1G1");

// ListOfInputs
t1G1.createInput("in0", g0, InputTransitionEffect.consumption);
// ListOfOutputs
t1G1.createOutput("ou1", g1, OutputTransitionEffect.assignmentLevel);

// ListOfFunctionTerms
FunctionTerm defTerm = new FunctionTerm(level, version);
defTerm.setDefaultTerm(true);
defTerm.setResultLevel(0);

FunctionTerm ft1 = new FunctionTerm(level, version);
ft1.setResultLevel(1);

try {
    ft1.setMath(ASTNode.parseFormula("G0 > 2"));
} catch (ParseException exc) {
    exc.printStackTrace();
}

// G0 and G1
ASTNode andNode = new ASTNode(ASTNode.Type.LOGICAL_AND);
andNode.addChild(new ASTNode(g0.getId()));
andNode.addChild(new ASTNode(g1.getId()));

t1G1.addFunctionTerm(defTerm);
t1G1.addFunctionTerm(ft1);
```

# The resulting Qual model

```
<?xml version='1.0' encoding='UTF-8' standalone='no'?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" qual:required="true" level="3"
xmlns:qual="http://www.sbml.org/sbml/level3/version1/qual/version1" version="1">
  <model id="my_model">
    <qual:listOfQualitativeSpecies xmlns:qual="http://www.sbml.org/sbml/level3/version1/qual/version1">
      <qual:qualitativeSpecies qual:constant="false" qual:compartment="comp1" qual:id="G0"/>
      <qual:qualitativeSpecies qual:constant="false" qual:compartment="comp1" qual:id="G1"/>
    </qual:listOfQualitativeSpecies>
    <qual:listOfTransitions xmlns:qual="http://www.sbml.org/sbml/level3/version1/qual/version1">
      <qual:transition qual:id="t1G1">
        <qual:listOfInputs>
          <qual:input qual:transitionEffect="consumption" qual:qualitativeSpecies="G0" qual:id="in0"/>
        </qual:listOfInputs>
        <qual:listOfOutputs>
          <qual:output qual:transitionEffect="assignmentLevel" qual:qualitativeSpecies="G1" qual:id="ou1"/>
        </qual:listOfOutputs>
        <qual:listOfFunctionTerms>
          <qual:defaultTerm qual:resultLevel="0">
            </qual:defaultTerm>
          <qual:functionTerm qual:resultLevel="1">
            <math xmlns="http://www.w3.org/1998/Math/MathML">
              <apply>
                <gt;/>
                <ci> G0 </ci>
                <cn type="integer"> 2 </cn>
              </apply>
            </math>
          </qual:functionTerm>
        </qual:listOfFunctionTerms>
      </qual:transition>
    </qual:listOfTransitions>
    <listOfCompartments>
      <compartment id="comp1" constant="true"/>
    </listOfCompartments>
  </model>
</sbml>
```

# Recent Changes in JSBML with relevance for qual

- File `/core/resources/org/sbml/jsbml/resources/cfg/PackageParserNamespaces.xml` has been deleted
- SBMLReader and SBMLWriter now based on Java annotations → when using Eclipse and directly operating on the trunk, configuration needs to be updated as described here: <https://code.google.com/p/spi/wiki/EclipseSettings>
- libSBML now also supports qual and the SBML online validator validates qual models
- Naming conventions of qual objects: `QualitativeModel` is now deprecated (at the moment in the trunk, but at latest with the next release of 1.0 also in the stable version)
- Please use `QualModelPlugin` instead. Reason: Compatibility to libSBML's naming conventions
- Improved support for MAVEN: All `pom.xml` files have been updated



# Download of modules

- LibSBML input/output:  
`svn co svn://svn.code.sf.net/p/jsbml/code/trunk/modules/libSBMLio libSBMLio`
- CellDesigner bridge:  
`svn co svn://svn.code.sf.net/p/jsbml/code/trunk/modules/celldesigner celldesigner`
- **Further modules:** Android, compare, libSBMLcompat
- LibSBML compatibility module for switching between libSBML and JSBML still under development

# LibSBML module

```
public static void main(String[] args) {
    try {
        // Load LibSBML:
        System.loadLibrary("sbmlj");
        // Extra check to be sure we have access to libSBML:
        Class.forName("org.sbml.libsbml.libsbml");

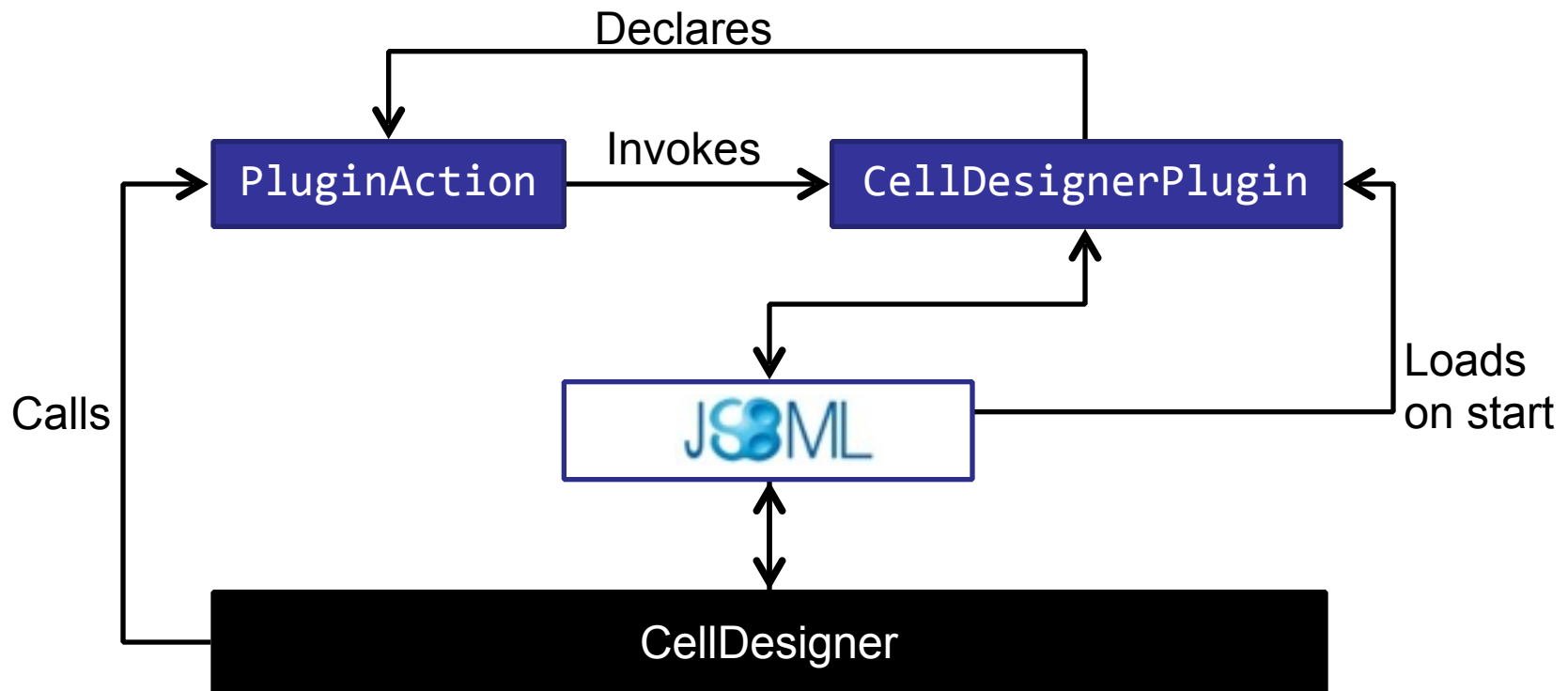
        // Read SBML file using LibSBML and convert it to JSBML:
        SBMLInputConverter<org.sbml.libsbml.Model> reader = new LibSBMLReader();
        SBMLDocument doc = reader.convertSBMLDocument(args[0]);
        //SBMLDocument doc = new SBMLDocument(2,4);

        org.sbml.libsbml.SBMLDocument libDoc = reader.getOriginalModel().getSBMLDocument();
        //org.sbml.libsbml.SBMLDocument libDoc = new org.sbml.libsbml.SBMLDocument(2,4);
        doc.addTreeNodeChangeListener(new LibSBMLChangeListener(libDoc));

        // Run some application:
        new JSBMLVisualizer(doc);
    } catch (Throwable exc) {
        exc.printStackTrace();
    }
}
```

# CellDesigner module

- Turning an existing application into a plugin for CellDesigner
- Only implementation of two abstract classes required



# CellDesigner module: Example for a PluginAction

```
public class SimpleCellDesignerPluginAction extends PluginAction {
    /** The plugin that is triggered when this object receives appropriate actions. */
    private SimpleCellDesignerPlugin plugin;

    /** @param plugin */
    public SimpleCellDesignerPluginAction(SimpleCellDesignerPlugin plugin) {
        this.plugin = plugin;
    }

    @Override
    public void myActionPerformed(ActionEvent evt) {
        if (evt.getSource() instanceof JMenuItem) {
            JMenuItem item = (JMenuItem) evt.getSource();
            if (item.getText().equals(SimpleCellDesignerPlugin.ACTION)) {
                try {
                    plugin.startPlugin();
                } catch (XMLStreamException exc) {
                    JOptionPane.showMessageDialog(item, exc.getMessage(),
                        exc.getClass().toString(), JOptionPane.ERROR_MESSAGE);
                    exc.printStackTrace();
                }
            }
        } else {
            JOptionPane.showMessageDialog(null, "Unsupported source of action "
                + evt.getSource().getClass().getName(), "Invalid Action",
                JOptionPane.WARNING_MESSAGE);
        }
    }
}
```



# CellDesigner module: Example for a CellDesignerPlugin

```
public class SimpleCellDesignerPlugin extends AbstractCellDesignerPlugin {

    public static final String ACTION = "Display full model tree";
    public static final String APPLICATION_NAME = "Simple Plugin";

    private PluginSBMLReader reader;

    /** Creates a new CellDesigner plugin with an entry in the menu bar. */
    public SimpleCellDesignerPlugin() {
        try {
            reader = new PluginSBMLReader(SB0.getPossibleEnzymes());
            addPluginMenu();
        } catch (Throwable exc) {
            exc.printStackTrace();
        }
    }

    @Override
    public void addPluginMenu() {
        PluginMenu menu = new PluginMenu(APPLICATION_NAME);
        PluginMenuItem menuItem = new PluginMenuItem(ACTION, new SimpleCellDesignerPluginAction(this));
        menu.add(menuItem);
    }

    /** Performs the action for which this plugin is designed.
     * @throws XMLStreamException If the given SBML model contains errors.
     */
    public void startPlugin() throws XMLStreamException {
        Model model = reader.convertModel(getSelectedModel());
        model.getSBMLDocument().addTreeNodeChangeListener(new PluginChangeListener(this));
        new JSBMLvisualizer(model.getSBMLDocument());
    }
}
```



Some more details

# Using annotation

```
Species species = model.createSpecies("species", comp1);
species.addCVTerm(new CVTerm(CVTerm.Qualifier.BQB_IS,
    "http://identifiers.org/go/G0:0006915",
    "http://identifiers.org/kegg.genes/hsa:321"));
species.addCVTerm(new CVTerm(CVTerm.Qualifier.BQB_IS_DESCRIBED_BY,
    "http://identifiers.org/pubmed/16333295"));
species.addCVTerm(new CVTerm(CVTerm.Qualifier.BQB_IS_ENCODED_BY,
    "http://identifiers.org/ensembl/ENSG00000085662"));
species.addCVTerm(new CVTerm(CVTerm.Qualifier.BQB_OCCURS_IN,
    "http://identifiers.org/kegg.reaction/R01787"));

/* This method call will return a List of Species that are annotated with the Qualifier
 * 'occursIn' and a resource attached to this qualifier that contains the String 'kegg'.
 */
model.getListOfSpecies().filter(new CVTermFilter(CVTerm.Qualifier.BQB_OCCURS_IN, ".*kegg.*"));
```

# How to contribute

## Creating a patch:

- Checkout the sources from sourceforge  
`svn co svn://svn.code.sf.net/p/jsbml/code/trunk JSBML`
- Do your modifications, then create a patch file:  
`svn diff > jsbml-patch.txt`
- Attach it to a tracker item or send it through the development list.

**Bug tracker:** <http://sourceforge.net/p/jsbml/bugs/>

**Pivotal :** <https://www.pivotaltracker.com/projects/499447>

## Mailing lists:

- [jsbml-development@caltech.edu](mailto:jsbml-development@caltech.edu): public list with discussion about the development of JSBML and support for users.
- [jsbml-team@caltech.edu](mailto:jsbml-team@caltech.edu): private list for the JSBML team where anybody can send mails for support or bugs reports.

**JSBML: a flexible Java library for working with SBML**

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# Thanks

<http://sbml.org/Software/JSBML>