







## JSBML: a flexible and entirely Java-based library for working with SBML

Andreas Dräger<sup>1\*</sup>, Nicolas Rodriguez<sup>2\*</sup>, Marine Dumousseau<sup>2</sup>, Alexander Dörr<sup>1</sup>, Clemens Wrzodek<sup>1</sup>, Roland Keller<sup>1</sup>, Sebastian Fröhlich<sup>4</sup>, Nicolas Le Novère<sup>2</sup>, Andreas Zell<sup>1</sup>, and Michael Hucka<sup>3</sup>

The specifications of the Systems Biology Markup Language (SBML) define standards for storing and exchanging computer models of biological processes in text files. In order to perform model simulations, graphical visualizations and other software manipulations, an in-memory representation of SBML is required. We developed JSBML for this purpose. In contrast to prior implementations of SBML APIs, JSBML has been designed from the ground up for the Java™ programming language, and can therefore be used on all platforms supported by a Java Runtime Environment. This offers important benefits for Java users, including the ability to distribute software as Java Web Start applications. JSBML supports all SBML Levels and Versions through Level 3 Version 1, and we have strived to maintain the highest possible degree of compatibility with the popular library libSBML. JSBML also supports modules that can facilitate the development of plugins for end user applications, as well as ease migration from a libSBML-based backend.

Source code, binaries and documentation for JSBML can be freely obtained under the terms of the LGPL 2.1 from the website http://sbml.org/Software/JSBML.

## Scope

JSBML provides an SBML parser and programming library that maps all SBML elements to a flexible and extended type hierarchy (Fig. 1). JSBML strives to attain compatibility with libSBML's Java API, to ease a switch from one library to the other. JSBML supports all constructs for SBML up to the latest Level 3 Version 1, including an API to add SBML extensions. More complex functions of libSBML, e.g., model consistency checking, SBML validation, and the conversion between different SBML Levels and Versions are expected to be included as separate community efforts via web services.

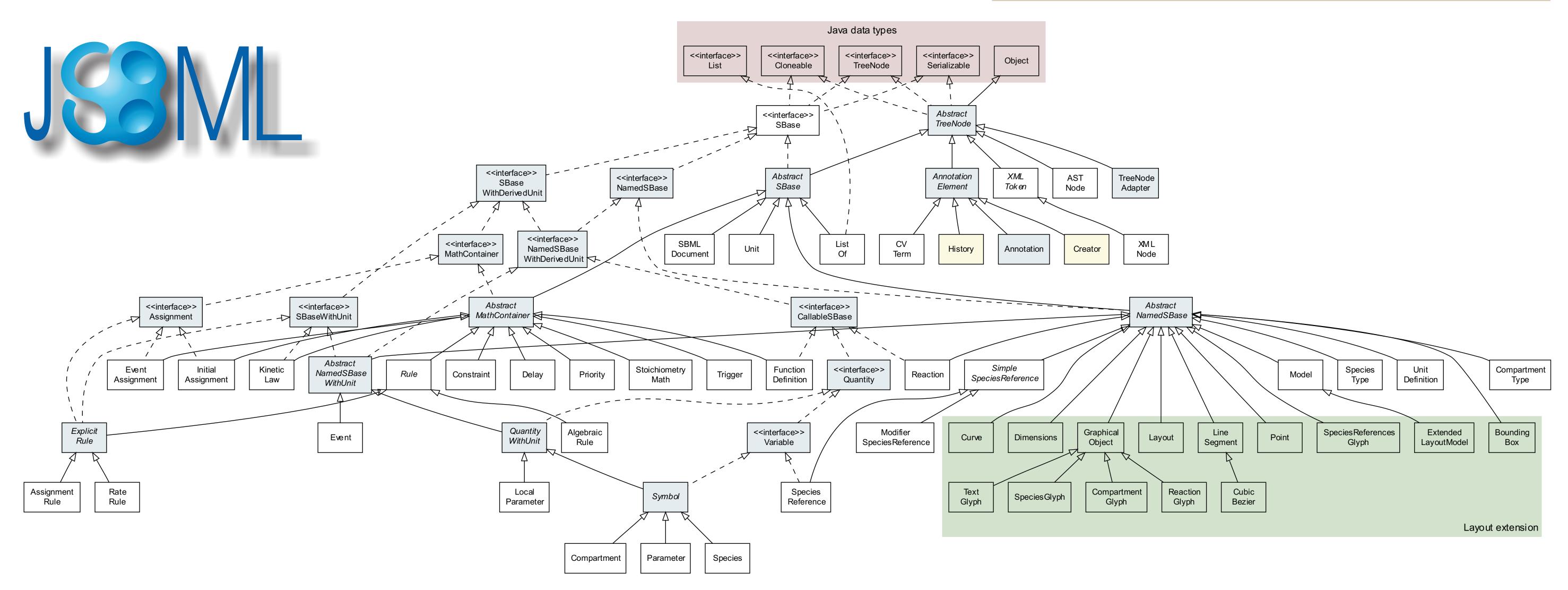


Fig. 1: The type hierarchy of the main SBML constructs in JSBML. With letting SBase implement the Java interfaces Cloneable, Serializable, and TreeNode, all derived elements also implement these types. The basic implementation of the interface SBase is AbstractSBase, which inherits from AbstractTreeNode. In this way, many recursive methods have been shifted into this very general super class, including reaction to dedicated ChangeListener implementations. Also SBML elements that do not inherit from SBase extend AbstractTreeNode. In this way, the type hierarchy provides a unified way of accessing data types. Elements colored in blue have been introduced as additional, in most cases abstract, data types in JSBML but do not have a corresponding element in libSBML. The yellow types Creator and History correspond to ModelCreator and ModelHistory in libSBML.

## Summary

JSBML is written entirely in Java version 1.5 and does not require additional non-Java software. It is distributed in source-code form as well as pre-compiled JAR files in different versions (including/excluding third-party libraries). JSBML is a young, ongoing software project that provides comprehensive and entirely Java-based data structures to read, write, and manipulate SBML files. Its layered architecture allows for the creation of Java web start applications and CellDesigner plug-ins based on stand-alone programs with very little effort. One program, SBMLsqueezer [4] 1.3, has already been re-implemented and released using JSBML, a simulator that is benchmarked on the SBML test suit will be available soon, and many other projects are planned.

A minimal example for a visual representation of the content of an SBML file using JSBML with source code and output for an SBML test model of the glycolysis that includes a layout extension:

```
Glycolysis

                                                       SBML Level 3 Version 1
import javax.swing.*;
                                                        Glycolysis
import org.sbml.jsbml.SBMLDocument;
                                                        import org.sbml.jsbml.xml.stax.SBMLReader;
                                                         listOfCompartments
public class JSBMLvisualizer extends JFrame {
                                                            Yeast
                                                           listOfSpecies
  public JSBMLvisualizer(SBMLDocument document)
                                                        super(document.getModel().getId);
                                                            getContentPane().add(new JTree(document));

⊕ Glucose

                                                              · ATP
    pack();
                                                            setVisible(true);
                                                              Phosphoglucoseisomerase
                                                              Phosphofructokinase
  // Expects file name as command line argument
                                                          in ______ triose_phosphate_isomerase
  public static void main(String args[])
                                                            throws Exception {
                                                              Dihydroxyacetonephosphate
                                                            new JSBMLvisualizer(
                                                             GAP_Dehydrogenase
      SBMLReader.readSBML(args[0]));
                                                              Phosphoglyceratekinase
                                                              Phosphoglyceratemutase
                                                              Enolase
                                                          ⊕... Pyruvatekinase
```

## References

- [1] Hucka M, Finney A, Sauro HM et al. The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models. Bioinformatics 19 (4): 524–31, 2003.
- [2] Bornstein BJ, Keating SM, Jouraku A, Hucka M. LibSBML: An API Library for SBML. Bioinformatics, 24(6):880–881, 2008.
- [3] Dräger A, Rodriguez N, Dumousseau M, Dörr A, Wrzodek C, Le Novère N, Zell A, Hucka M. JSBML: a flexible Java library for working with SBML. Bioinformatics, 27(15):2167-2168, 2011.
- [4] Dräger A, Hassis N, Supper J, Schröder A, Zell A. SBMLsqueezer: a CellDesigner plug-in to generate kinetic rate equations for biochemical networks, BMC Systems Biology 2008, 2:39, 2008.





