

User guide for JSBML

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The specifications of the Systems Biology Markup Language (SBML) define a standard for storing and exchanging biochemical models in XML-formatted text files. To perform higher-level operations on these models, e.g., numerical simulation or visual representation, an appropriate mapping to in-memory objects is required. To this end, the JSBML library has been developed. JSBML supports all SBML levels and versions that are available today. In addition, JSBML provides modules that facilitate the development of CellDesigner plugins or ease the migration from a libSBML backend.

This document should help you getting started with JSBML. It is not only intended for users, developing their applications from scratch, but also for users, switching from libSBML to JSBML.

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1 Getting started with JSBML

The following are quick-start instructions for getting started with JSBML. This document is based on JSBML version 0.8. Before doing any of the steps below, you will need to obtain a copy of JSBML either via the SourceForge download page¹ or using Subversion (SVN) as described below.

1.1 Introduction

JSBML is a library that will help you to manipulate SBML files. If you are not familiar with SBML, a good starting point would be to read the latest SBML specification² (Hucka *et al.*, 2010). If you have some other questions about SBML, you may find the answer in the SBML FAQ³. JSBML is written in JavaTM. To use it, you will need a Java Runtime Environment (JRE) 1.5 or higher. See, for example, the Java SE download page⁴. JSBML also provides several modules. Two of them should ease developers to interact with CellDesigner or libSBML and one module eases switching from libSBML to JSBML or the other way around.

1.2 Obtaining and setting up JSBML

1.2.1 Using the JSBML JAR file distribution

Before starting to use JSBML, you will need to configure your class path. JSBML provides two versions of the JAR file:

1. including all dependencies - it is sufficient to include just this file in your class path.
2. without any dependencies - you need to take care of all the dependencies of JSBML by yourself.

The JSBML JAR file with dependencies is a merged JAR file that includes all of its dependencies. In this case, it is sufficient to include it into your build or class path to use JSBML.

¹<https://sourceforge.net/projects/jsbml/files/jsbml/>

²<http://sbml.org/Documents/Specifications/>

³<http://sbml.org/Documents/FAQ>

⁴<http://www.oracle.com/technetwork/java/javase/downloads/index.html>

Dependencies

When using the JSBML JAR file without dependencies, you need the JSBML dependencies in addition to the JSBML library. The following list gives you an overview of all these libraries:

biojava-1.7-ontology.jar This is a stripped down version of the biojava-1.7⁵ containing mostly ontology-related classes (Holland *et al.*, 2008).

junit-4.8.jar This library is only needed, if you want to run the JUnit⁶ tests of JSBML (located in the `test` folder).

stax2-api-3.0.3.jar Used to read and write the XML files⁷.

stax-api-1.0.1.jar Used to read and write the XML files⁸.

woodstox-core-lgpl-4.0.9.jar Used to read and write the XML files. This the stax parser implementation we use⁹.

staxmate-2.0.0.jar Used to read and write the XML files. This library allow to use stax in a more friendly manner¹⁰.

xstream-1.3.1.jar Used to read and write the XML files. This parser is used to parse the result from the SBML validator, we might use it more in the future or drop it to use only stax/-woodstox¹¹.

jigsaw-dateParser.jar This is a stripped down version of the jigsaw-library, containing one class to manipulate dates. It has been created with the most recent version from 2010-12-16¹².

log4j-1.2.8.jar JSBML uses the Apache log4j logger¹³. If you want to use logging, you should include this logger.

JSBML was developed and tested with these versions of the libraries described above. Some more recent versions might work, too. When you have all of these dependencies in your build or class path alongside the JSBML JAR file, you are ready to work with JSBML.

⁵<http://biojava.org>

⁶<http://www.junit.org>

⁷<http://docs.codehaus.org/display/WSTX/StAX2>

⁸<http://stax.codehaus.org>

⁹<http://woodstox.codehaus.org>

¹⁰<http://staxmate.codehaus.org>

¹¹<http://xstream.codehaus.org>

¹²<http://jigsaw.w3.org>

¹³<http://logging.apache.org/log4j/>

1.2.2 Download and usage of the source distribution

As an alternative to using the JAR files, you can check out the source tree from SVN and compile JSBML yourself. To do that, you will need to have a Java JDK⁴ installed, the Apache Ant¹⁴ build system, and Subversion¹⁵, a version control system.

Use the following command to download the latest JSBML classes (requires Subversion¹⁵):

```
svn co "https://jsbml.svn.sourceforge.net/svnroot/jsbml/trunk" jsbml
cd jsbml
```

To compile the JSBML library to a single JAR file, type the following command (requires Apache Ant¹⁴):

```
ant jar
```

If you want to run the JUnit tests on your compiled JAR file, please use the following command:

```
ant test
```

If you performed all the steps above, you should have a JSBML library, based on the latest version of all classes. You can now include the created JAR file into your build or class path and start using JSBML.

1.2.3 Download and usage of the JSBML modules

JSBML provides today, two additional modules. Please type the following Subversion¹⁵ commands on your command line to obtain the corresponding modules.

The CellDesigner bridge module should help CellDesigner plugin developers to use JSBML as internal datastructure.

```
svn co "https://jsbml.svn.sourceforge.net/svnroot/jsbml/modules/cellDesigner"
cellDesigner
```

Developers, who still want to make use of libSBML, might want to have a look at the libSBML communication layer.

```
svn co "https://jsbml.svn.sourceforge.net/svnroot/jsbml/modules/libSBMLio/"
libSBMLio
```

¹⁴<http://ant.apache.org/>

¹⁵<http://subversion.apache.org/>


```
1 import javax.swing.*;
2 import org.sbml.jsbml.*;
3
4 /** Displays the content of an SBML file in a {@link JTree} */
5 public class JSBMLvisualizer extends JFrame {
6
7     /** @param document The sbml root node of an SBML file */
8     public JSBMLvisualizer(SBMLDocument document) {
9         super(document.getModel().getId());
10        getContentPane().add(new JScrollPane(new JTree(document)));
11        pack();
12        setVisible(true);
13    }
14    /** @param args Expects a valid path to an SBML file. */
15    public static void main(String[] args) throws Exception {
16        new JSBMLvisualizer((new SBMLReader()).readSBML(args[0]));
17    }
18 }
```

Listing 1.1: Parsing and visualizing the content of an SBML file

1.3 Hello World: writing your first JSBML applications

This section presents two examples for using JSBML. One example reads an existing `SBMLDocument` from a file and visualizes it on a `JFrame`. The second example creates a new `SBMLDocument` from scratch and writes its content into a file. This should help you getting started and writing your own JSBML applications.

1.3.1 Reading and visualizing an `SBMLDocument`

Listing 1.1 demonstrates in a simple code example how to parse an SBML file (submitted as first argument) and to immediately display its content on a `JFrame`. Fig. 1.1 on page 11 shows an example output when applying the program to an SBML test model. Line 19 in Listing 1.1 shows how to read an `SBMLDocument` from a file, using the `SBMLReader`. Afterwards, the `JSBMLvisualizer` constructor is called, which first creates a new `JFrame` with the model's id as title (line 10). Since JSBML's `SBase` object, and all derived elements, implement the `TreeNode` interface, it is possible to create a `JTree` from the information in the `SBMLDocument` only. This is done in line 11.

1.3.2 Creating and writing an `SBMLDocument`

Listing 1.2 on the next page shows a more complex example. A new `SBMLDocument` is created from scratch. It mainly consists of one `Compartment`, one `Model`, two `Species`, and a `Reaction` in which both `Species` are involved. This `SBMLDocument` is written into a file, using

```

1  import org.sbml.jsbml.*;
2
3  /** Creates an {@link SBMLDocument} and writes it's content to disk. */
4  public class JSBMLexample implements SBaseChangedListener {
5      public JSBMLexample() throws Exception {
6
7          // Create a new SBMLDocument, using SBML level 2 version 4.
8          SBMLDocument doc = new SBMLDocument(2, 4);
9          doc.addChangeListener(this);
10
11         // Create a new SBML-Model and compartment in the document
12         Model model = doc.createModel("test_model");
13         model.setMetaId("meta_"+model.getId());
14         Compartment compartment = model.createCompartment("default");
15         compartment.setSize(1d);
16
17         // Create model history
18         History hist = new History();
19         Creator creator = new Creator("Given_Name", "Family_Name",
20             "My_Organisation", "My@EMail.com");
21         hist.addCreator(creator);
22         model.setHistory(hist);
23
24         // Create some example content in the document
25         Species specOne = model.createSpecies("test_spec1", compartment);
26         Species specTwo = model.createSpecies("test_spec2", compartment);
27         Reaction sbReaction = model.createReaction("reaction_id");
28
29         // Add a substrate (SBO: 15) and product (SBO: 11).
30         SpeciesReference subs = sbReaction.createReactant(specOne);
31         subs.setSBOTerm(15);
32         SpeciesReference prod = sbReaction.createProduct(specTwo);
33         prod.setSBOTerm(11);
34
35         // Write the SBML document to disk
36         new SBMLWriter().write(doc, "test.sbml.xml", "ProgName", "Version");
37     }
38
39     /** Just an example main */
40     public static void main(String[] args) throws Exception {
41         new JSBMLexample();
42     }
43
44     /** Those three methods respond to events from SBaseChangedListener */
45     public void sbaseAdded(SBase sb) {System.out.println("[ADD]_" + sb);}
46     public void sbaseRemoved(SBase sb) {System.out.println("[RMV]_" + sb);}
47     public void stateChanged(SBaseChangedEvent ev) {System.out.println("[CHG]_"
48         + ev);}

```

Listing 1.2: Creating a new SBMLDocument and writing its content into a file

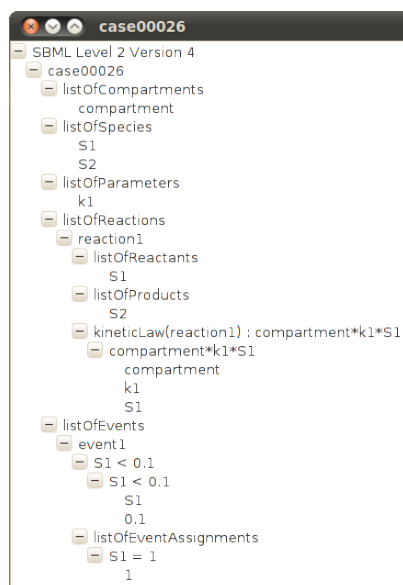


Figure 1.1: A tree representation of the content of SBML test model case00026. In JSBML, the hierarchically structured SBML-Document can be traversed recursively because all instances of SBase implement the interface `TreeNode`.

SBMLWriter.

1.3.3 Further examples

Listing 2.4 on page 30 shows how to convert libSBML data structures into JSBML data objects. Listing 2.5 on page 31 demonstrates the implementation of CellDesigner's abstract class `PluginAction` and Listing 2.6 on page 32 gives a complete example for writing CellDesigner plugins with JSBML.

2 Main differences between JSBML and libSBML

Until today, libSBML has been the main library for developing Java applications that use SBML. Thus, many Java developers are used to the methods and commands, libSBML provides. The JSBML team made some effort to allow those developers a fast and easy switch to this new library. For example, a libSBML compatibility module has been developed, that implements existing libSBML methods and simply redirects the parameters to the corresponding JSBML methods. But it is important that developers, coming from libSBML, know the main differences between the two libraries. The following sections give a brief description of those main differences.

2.1 Introduction

The intention of implementing a pure Java™ Application Programming Interface (API) for working with SBML files was not to re-implement the existing Java API of libSBML (Bornstein *et al.*, 2008). From the very beginning, JSBML has been designed based on the SBML specifications (Hucka *et al.*, 2003, 2008, 2010) but with respect to naming conventions of methods and variables from libSBML. Similarly to the SBML specifications, the libSBML library has grown historically. The implementation of JSBML permitted to entirely re-design the type hierarchy of the SBML elements and the way to implement what is specified in the SBML specifications. However, it is important to keep in mind that SBML is a language that defines how to store of biological processes and how to exchange these models between different software tools. It does not specify how to represent its elements in memory. Furthermore, during the evolution of SBML some elements or properties of elements have become obsolete. It is therefore up to an implementing library to decide how to deal with those constructs. To facilitate switching from libSBML to JSBML and the other way around, JSBML has been designed to behave similarly to libSBML but, due to the different background of both libraries and the fact that libSBML is based on C and C++ code, some differences are unavoidable. In cases of doubt JSBML tries to mirror the SBML specifications rather than libSBML. Finally, JSBML has also been developed as a library that does not “only” provide reading, manipulating, and writing abilities for SBML files. It is intended to be directly used as a flexible internal data structure for numerical computation, visualization and much more. With the help of its modules JSBML can also be used as a communication layer between applications, such as CellDesigner (Funahashi *et al.*, 2003). The following sections will not only give a detailed overview about the most important differences between JSBML and libSBML, but also provide some programming examples and hints about how to use and work with JSBML.

2.2 An extended type hierarchy

Whenever multiple elements defined in at least one of the SBML specifications share some attributes, JSBML provides a common superclass or at least a common interface that gathers methods for the manipulation of the shared properties. In this way, the type hierarchy of JSBML has become quite complex (see Figs. 2.1 to 2.5 on pages 14–18). Just as in libSBML, all elements extend the abstract type `SBase`, but in JSBML, `SBase` has become an interface. This allows more complex relations between derived data types. In contrast to libSBML, `SBase` in JSBML extends three other interfaces: `Cloneable`, `Serializable`, and `TreeNode`. As all elements defined in JSBML override the `clone()` method from the class `java.lang.Object`, all JSBML elements can be deeply copied and are therefore *cloneable*. By extending the interface `Serializable`, it is possible to store JSBML elements in binary form without explicitly writing them to an SBML file. In this way, programs can easily load and save their in-memory objects or send complex data structures through a network connection without the need of additional file encoding and subsequent parsing. The third interface, `TreeNode` is actually defined in Java's `swing` package. `TreeNode` is a type that is independent of any graphical information. It basically defines recursive methods on hierarchically structured data types, such as iteration over all of its successors. In this way, all instances of JSBML's `SBase` interface can be directly passed to the `swing` class `JTree` and can hence be easily visualized. Listing 1.1 on page 9 demonstrates in a simple code example how to parse an SBML file and to immediately display its content on a `JFrame`. The `ASTNode` class in JSBML also implements all these three interfaces and can hence be cloned, serialized, and visualized in the same way.

2.2.1 Characteristic features of SBases

The SBML specifications define the data type `SBase` as the supertype for all other SBML elements. In JSBML, `SBase` has become an interface and most elements therefore extend its abstract implementation `AbstractSBase`.

In contrast to libSBML, the Level and Version of such an `AbstractSBase` is stored in a special object, a `ValuePair`. The class `ValuePair` takes two values of any type that both implement the interface `Comparable`. Storing the Level/Version combination in such a `ValuePair`, which itself implements the `Comparable` interface, allows users to perform checks for an expected Level/Version combination of an element more easily, as the example in Listing 2.1 on page 19 demonstrates. The method `getLevelAndVersion()` in `AbstractSBase` delivers an instance of `ValuePair` with the Level and Version combination for the respective element.

Some types derived from `SBase` contain a unique identifier, an `id`. JSBML gathers all these elements under the common interface `NamedSBase`. The class `AbstractNamedSBase`, which extends `AbstractSBase`, implements this interface.

Many SBML elements represent some quantitative value, which is associated with a unit. However, the value does not necessarily have to be defined explicitly. In many cases, it needs to be computed from a formula contained in the instance of `SBase` in form of an abstract syntax tree, i.e.,



Figure 2.1: 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. 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.

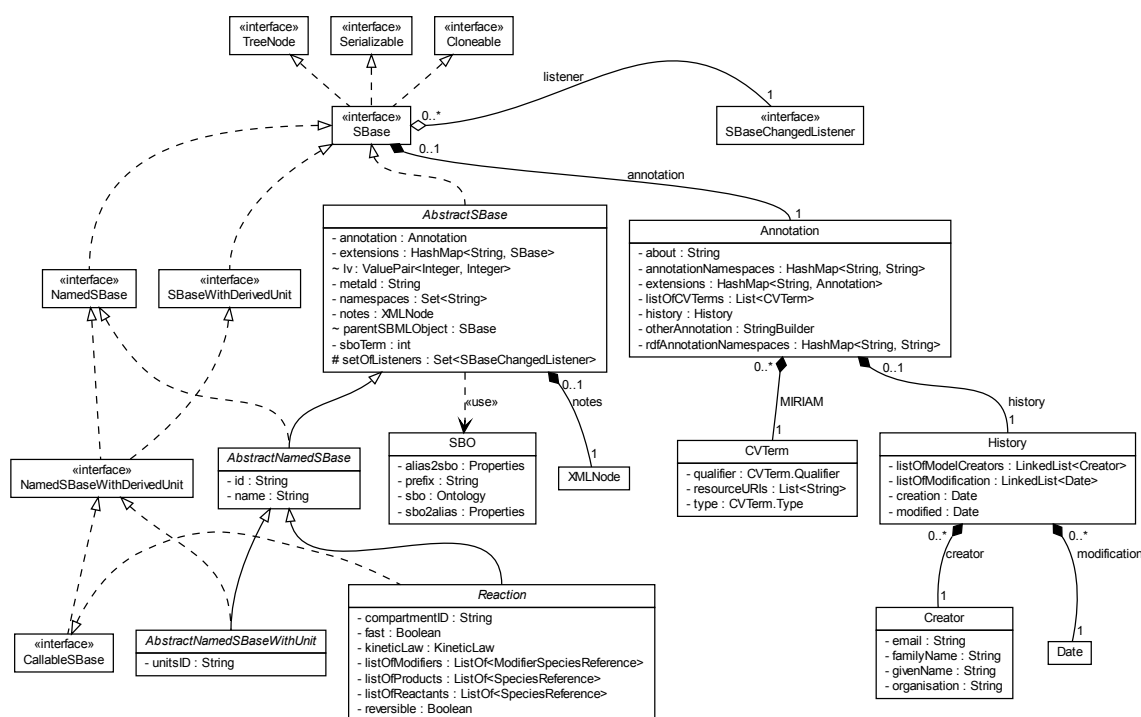


Figure 2.2: The interface `SBase`, adapted from Dräger (2011). This figure displays the most important top-level data structures of JSBML with main focus on the differences to libSBML. All other data types that represent SBML constructs in JSBML extend either one of the two abstract classes `AbstractSBase` or `AbstractNamedSBase`. The class `SBO` parses the ontology file provided on the SBO web site (<http://www.ebi.ac.uk/sbo/main/>) in OBO format (Open Biomedical Ontologies) using a parser provided by the BioJava project (Holland *et al.*, 2008). For the sake of a clear arrangement, this figure omits all methods in the UML diagram.

`ASTNode`. Therefore, also the associated unit may not be set explicitly but can be derived when evaluating the formula. In JSBML, the interface `SBaseWithDerivedUnit` unifies all those elements that either explicitly or implicitly contain some unit. If these elements can also be addressed using an identifier, they also implement the interface `NamedSBaseWithDerivedUnit`. Within formulas, i.e., `ASTNodes`, references can only be made to instances of `CallableSBase`, which is a special case of `NamedSBaseWithDerivedUnit`. Fig. 2.3 on the next page shows this part of JSBML's type hierarchy in more detail.

As a special case, these elements may explicitly declare a unit. The interface `SBaseWithUnit` serves as the supertype for all those elements that may be explicitly equipped with a unit. The convenient class `AbstractNamedSBaseWithUnit` extends `AbstractNamedSBase` and implements both interfaces `SBaseWithUnit` and `NamedSBaseWithDerivedUnit`. All elements derived from this abstract class may therefore declare a unit and can be addressed using a

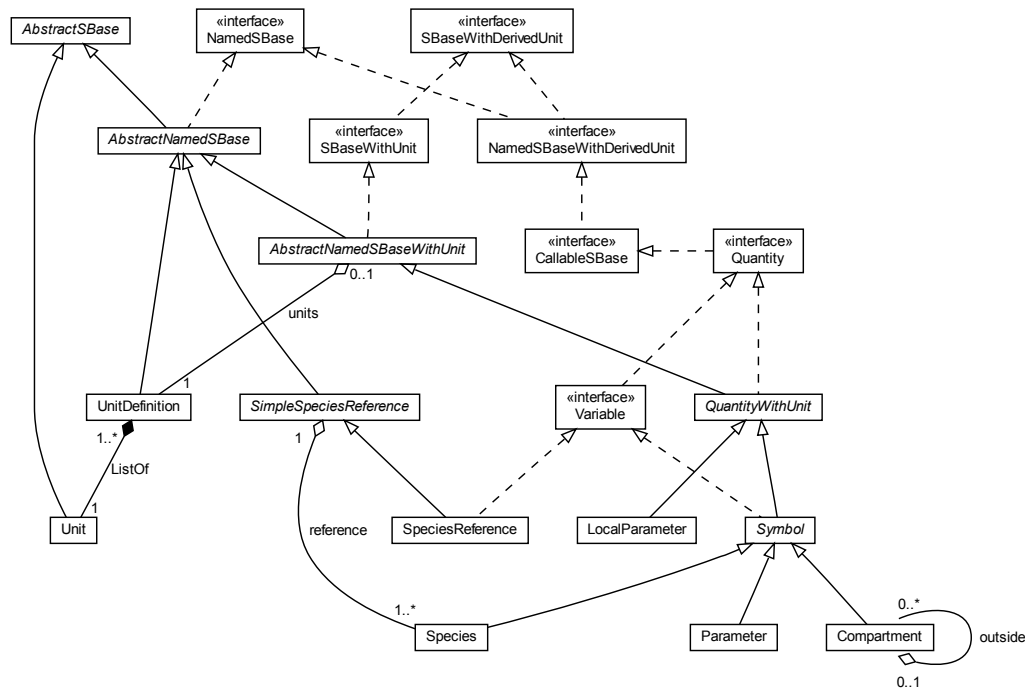


Figure 2.3: The interface `Variable`, adapted from Dräger (2011). JSBML refers to those components of a model that may change their value during a simulation as `Variables`. The class `Symbol` serves as the abstract superclass for variables that can also be equipped with a unit. Instances of `Parameter` do not contain any additional field. In `Species`, a Boolean switch decides whether its value is to be interpreted as an initial amount or as an initial concentration. In contrast to `Variables`, `LocalParameters` represent constant unit-value pairs that can only be accessed within their declaring `KineticLaw`.

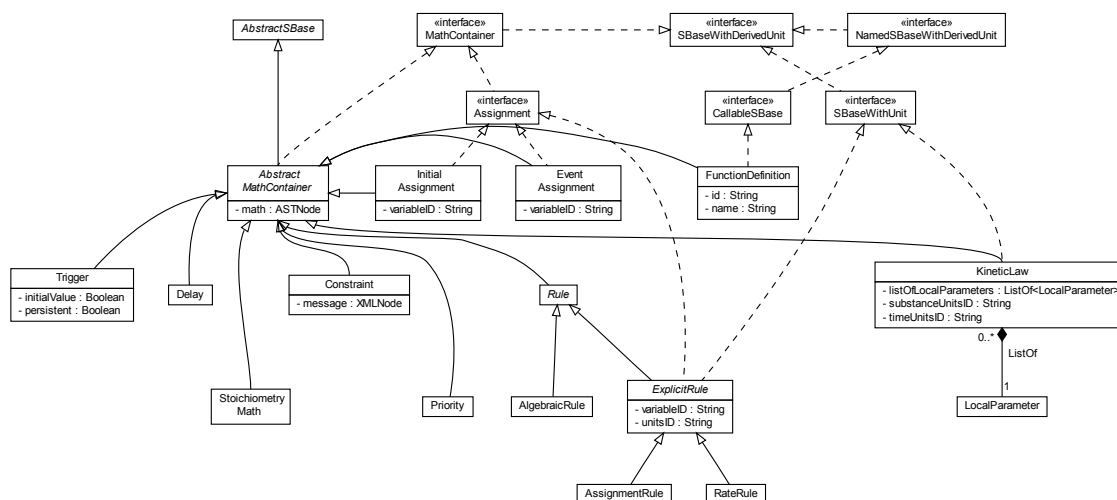


Figure 2.5: MathContainer, adapted from Dräger (2011). Instances of the interface MathContainer, particularly its directly derived class AbstractMathContainer, constitute the superclass for all elements that store and manipulate mathematical formulas in JSBML, which is done in form of ASTNode objects. These can be evaluated using an implementation of ASTNode-Compiler. Note that some classes that extend AbstractMathContainer do not contain any own fields or methods: Delay, Priority, StoichiometryMath, or AlgebraicRule.

The specification of SBML Level 3 introduces another type of Variable, which does not explicitly declare its unit: SpeciesReference. On the other hand, a LocalParameter is a QuantityWithUnit, but not a Variable, because it is always constant.

2.2.2 The MathContainer interface

This interface gathers all those elements that may contain mathematical expressions encoded in abstract syntax trees (instances of ASTNode). The abstract class AbstractMathContainer serves as actual superclass for most of the derived types. Figs. 2.4 to 2.5 on pages 17–18 give a better overview of how this data structure is intended to function.

2.2.3 The Assignment interface

JSBML unifies all those elements that may change the value of some *variable* in SBML under the interface Assignment. This interface uses the term *variable* for the element whose value is to be changed depending on some mathematical expression that is also present in the Assignment (because Assignment extends the interface MathContainer). Therefore, an Assignment contains methods such as `set-/getVariable(Variable v)` and also `isSetVariable()` as well as `unsetVariable()`. In addition to that, JSBML also provides the methods

```

1  if (mySBase.getLevelAndVersion().compareTo(Integer.valueOf(2),
2      Integer.valueOf(2)) < 0) {
3      throw new IllegalArgumentException(String.format(
4          "Cannot_create_a_%s_with_Level_%s_and_Version_%s.",
5          mySBase.getElementName(), getLevel(), getVersion()));
6  }

```

Listing 2.1: Check for a minimal expected Level/Version combination

set-/getSymbol(String symbol) in the InitialAssignment class to make sure that switching from libSBML to JSBML is quite smoothly. However, the preferred way in JSBML is to apply the methods setVariable either with String or Variable instances as arguments. Fig. 2.5 on the facing page displays the type hierarchy of the Assignment interface in more detail.

2.3 Differences in the abstract programming interface

JSBML strives to attain an almost complete compatibility to libSBML. However, the differences in the programming languages C++ and JavaTM lead to the necessity of introducing some differences. In some cases, a direct “translation” from C++ and C code to Java would not be very elegant. JSBML wants to provide a Java API, whose classes and methods are structured, named, and behave like classes and methods in other Java libraries. In this section, we will discuss the most important differences in the APIs of JSBML and libSBML.

2.3.1 Abstract syntax trees

Both libraries define a class ASTNode for in-memory manipulation and evaluation of abstract syntax trees that represent mathematical formulas and equations. These can either be parsed from a representation in C language-like Strings, or from a MathML representation. The JSBML ASTNode provides various methods to transform these trees to other formats, for instance, L^AT_EX Strings. In JSBML, several static methods allow easy creation of new syntax trees, for instance, the following code

```
ASTNode myNode = ASTNode.plus(myLeftAstNode, myRightASTNode);
```

creates a new instance of ASTNode which represents the sum of the two other ASTNodes. In this way, even complex trees can be easily manipulated.

In SBML, abstract syntax trees may refer to the following elements: Parameters, LocalParameters, FunctionDefinitions, Reactions, Compartments, Species, and, since Level 3, also SpeciesReferences. JSBML gathers all these elements under the common interface CallableSBase, which extends the interface NamedSBaseWithDerivedUnit. In

2 Main differences between JSBML and libSBML

this way, JSBML ensures that only identifiers of those elements can be set in instances of `ASTNode`. JSBML provides a set of convenient constructors and methods to work with instances of `CallableSBase`, of which we here give a short overview. The `set` method allows users to change

Getter and setter:

```
public void setVariable(CallableSBase variable) { ... }

public CallableSBase getVariable() { ... }
```

the type of an `ASTNode` to `ASTNode.Type.NAME` and to directly set the name to the identifier of the given `CallableSBase`. The `get` method directly looks for the corresponding element in the `Model` and returns this element. If no such element can be found or the type of the `ASTNode` is something different from `ASTNode.Type.NAME`, an exception will be thrown.

Some examples for convenient manipulation methods, of which some are static:

```
public static ASTNode frac(MathContainer container,
    CallableSBase numerator, CallableSBase denominator) {...}

public static ASTNode pow(MathContainer container,
    CallableSBase basis, CallableSBase exponent) { ... }

public ASTNode plus(CallableSBase nsb) { ... }
```

Methods like these above facilitate creating or manipulating complex abstract syntax trees. Several static methods are available that directly create small trees from given elements in memory, whereas some methods such as the `plus` method changes the structure of existing syntax trees.

Some examples for convenient constructors:

```
public ASTNode(CallableSBase nsb) { ... }

public ASTNode(CallableSBase nsb, MathContainer parent) { ... }
```

With these constructors, dedicated single nodes can be created whose type (from the enumeration `ASTNode.Type`) will be `NAME` and whose name will be set to the identifier of the given `CallableSBase`.

2.3.2 The `ASTNodeCompiler` class

This interface allows users to create customized interpreters for the content of mathematical equations encoded in abstract syntax trees. It is directly and recursively called from the `ASTNode`

class and returns an `ASTNodeValue` object, which wraps the possible evaluation results of the interpretation. JSBML already provides several implementations of this interface, for instance, `ASTNode` objects can be directly translated to C language-like `Strings`, `LaTeX`, or `MathML` for further processing. Furthermore, the class `UnitsCompiler`, which JSBML uses to derive the unit of an abstract syntax tree, also implements this interface.

2.3.3 Cloning when adding child nodes to instances of `SBase`

When adding elements such as a `Species` to a `Model`, `libSBML` will clone the object and add the clone to the `Model`. In contrast, JSBML does not automatically perform cloning. The advantage is that modifications on the object belonging to the original pointer will also propagate to the element added to the `Model`. Furthermore, this is more efficient with respect to the run time and also more intuitive for Java programmers. If cloning is necessary, users should call the `clone()` method manually. Since all instances of `SBase` and also `Annotation`, `ASTNode`, `CVTerm`, and `History` implement the interface `Cloneable` (see Fig. 2.1 on page 14), all these elements can be naturally cloned. However, when cloning an object in JSBML, such as an `AbstractNamedSBase`, all children of this element will recursively be cloned before adding them to the new element. This is necessary, because the data structures specified in SBML define a tree, in which each element has exactly one parental node.

2.3.4 Compartments

In SBML Level 3 (Hucka *et al.*, 2010), the domain of the `spatialDimensions` attribute in `Compartments` was changed from $\{0, 1, 2, 3\}$, which can be represented with a `short` value in Java, to a value in \mathbb{R} , i.e., a `double` value. For this reason, the method `getSpatialDimensions()` in JSBML always returns a `double` value. For consistency with `libSBML`, the `Compartment` class in JSBML also provides the redundant method `getSpatialDimensionsAsDouble()` that returns the identical value, but that is marked as a deprecated method.

2.3.5 Deprecation

The intention of JSBML is to provide a Java library that supports the latest specifications of SBML. But we also want to support earlier specifications. So JSBML provides methods and classes to cover elements and properties from earlier SBML specifications as well, but these are often marked as being deprecated to avoid creating models that refer to these elements.

2.3.6 Exceptions

In case of an error, JSBML throws often an exception while `libSBML` methods return some error codes instead. This behavior helps programmers and users to avoid creating invalid SBML data structures already when dealing with these in memory. Furthermore, exception handling is very

well implemented in Java and it is therefore a better programming style in this language. Methods can already declare that these may potentially throw exceptions. In this way, programmers can be aware of potential sources of problems already at the time of writing the source code. Examples are the `ParseException` that may be thrown if a given formula cannot be parsed properly into an `ASTNode` data structure, or `InvalidArgumentExceptions` if inappropriate values are passed to methods. For instance,

- An object representing a constant such as a `Parameter` whose `constant` attribute has been set to `true` cannot be used as the `Variable` element in an `Assignment`.
- An instance of `Priority` can only be assigned to an `Events` if its `level` attribute has at least been set to three.
- Another example is the `InvalidArgumentException` that is thrown when trying to set an invalid identifier `String` for an instance of `AbstractNamedSBase`.

Hence, you have to be aware of potential exceptions and errors when using JSBML, on the other hand this will prevent you from doing obvious mistakes. The class `SBMLReader` in JSBML catches those errors and exceptions. With the help of the logging utility, JSBML notifies users about syntactical problems in SBML files. JSBML follows the rule that illegal or invalid properties are not set.

2.3.7 Model history

In earlier versions of SBML, only the model itself could be associated with a history, i.e., a description about the person(s) who build this model, including names, e-mail addresses, modification and creation dates. Nowadays, it has become possible to annotate each individual construct of an SBML model with such a history. This is reflected by naming the corresponding object `History` in JSBML, whereas it is still called `ModelHistory` in libSBML. Hence, all instances of `SBase` in JSBML contain methods to access and manipulate its `History`. Furthermore, you will not find the classes `ModelCreator` and `ModelCreatorList` because JSBML gathers its `Creator` objects in a generic `List<Creator>` in the `History`.

2.3.8 Replacement of the interface `libSBMLConstants` by Java enums

You won't find a corresponding implementation of the interface `libSBMLConstants` in JSBML. The reason is that the JSBML team decided to encode constants using the Java construct `enum`. For instance, all the fields starting with the prefix `AST_TYPE_*` have a corresponding field in the `ASTNode` class itself. There you can find the `enum Type`. Instead of typing `libSBMLConstants.AST_TYPE_PLUS`, you would therefore type `ASTNode.Type.PLUS`.

The same holds true for `Unit.Kind.*` corresponding to the `libSBMLConstants.UNIT_KIND_*` fields.

2.3.9 The classes `libSBML` and `JSBML`

There is no class `libSBML` because this library is called `JSBML`. You can therefore only find a class `JSBML`. This class provides some similar methods as the `libSBML` class in `libSBML`, such as `getJSBMLDottedVersion()` to obtain the current version of the `JSBML` library, which is 0.8.* at the time of writing this document. However, many other methods that you might expect to find there, if you are used to `libSBML`, are located in the actual classes that are related with the function. For instance, the method to convert between a `String` and a corresponding `Unit.Kind` can be done by using the method

```
Unit.Kind myKind = Unit.Kind.valueOf(myString);
```

In a similar way, the `ASTNode` class provides a method to parse C-like formula `Strings` according to the specification of SBML Level 1 (Hucka *et al.*, 2003) into an abstract syntax tree. Therefore, in contrast to the `libSBML` class, the class `JSBML` contains only a few methods.

2.3.10 Various types of `ListOf*` classes

In `JSBML`, there is not a specific `ListOf*` class for each type of `SBase` elements. We used a generic implementation `ListOf<? extends SBase>` that allows us to use the same class for each of the different `ListOf*` classes defined in `libSBML` while keeping a type safe class. We defined several methods that use the `Filter` interface to search or filter a `ListOf` object. For example, to query an instance of `ListOf` in `JSBML` for names or identifiers or both, you can apply the following filter:

```
NamedSBase nsb = myList.firstHit(new NameFilter(identifier));
```

This will give you the first element in the list with the given identifier. Various filters are already implemented, but you can easily add your customized filter. To this end, you only have to implement the `Filter` interface in `org.sbml.jsbml.util.filters`. There you can also find an `OrFilter` and an `AndFilter`, which take as arguments multiple other filters. With the `SBOFilter` you can query for certain SBO annotations (Le Novère, 2006; Le Novère *et al.*, 2006) in your list, whereas the `CVTermFilter` helps you to identify `SBase` instances with a desired MIRIAM (Minimal Information Required In the Annotation of Models) annotation (Le Novère *et al.*, 2005). For instances of `ListOf<Species>` you can apply the `BoundaryConditionFilter` to look for those species that operate on the boundary of the reaction system.

2.3.11 Units and unit definitions

The exponent attribute of units

Since SBML Level 3 (Hucka *et al.*, 2010) the data type of the exponent attribute in the `Unit` class has been changed from `int` to `double` values. `JSBML` reflects this in the method `getExponent()` by returning `double` values only. For a better compatibility with `libSBML`, whose

corresponding method still returns `int` values, JSBML also provides the method `getExponentAsDouble()`. This method returns the value from the `getExponent()` method and is therefore absolutely redundant.

Predefined unit definitions

A model in JSBML always also contains all predefined units in the model if there are any, i.e., for models encoded with SBML versions before Level 3. These can be accessed from an instance of model by calling the method `getPredefinedUnit(String unit)`.

MIRIAM annotations (Le Novère *et al.*, 2005) have become an integral part of SBML models since Level 2 Version 2. Recently, the Unit Ontology¹ (UO) has been included in the set of supported ontology and online resources of MIRIAM. Since all the predefined units in SBML have corresponding entries in the UO, JSBML automatically equips those predefined units with the correct MIRIAM URI in form of a controlled vocabulary term (CVTerm) if the Level/Version combination of the model supports MIRIAM annotations.

Note that the enum `Unit.Kind` also provides methods to directly obtain the entry from the UO that corresponds to a certain unit kind and also to generate MIRIAM URIs accordingly. In this way, JSBML facilitates the annotation of user-defined units and unit definitions with MIRIAM-compliant information.

Access to the units of an element

In JSBML, all SBML elements, that can be associated with some unit, implement the interface `SBaseWithUnit`. This interface provides methods to directly access an object representing their unit. Currently, the following elements implement this interface:

- `AbstractNamedSBaseWithUnit`
- `ExplicitRule`
- `KineticLaw`

Fig. 2.1 on page 14 provides a better overview about the relationships between all the classes explained here. Note that `AbstractNamedSBaseWithUnit` serves as the abstract superclass for `Event` and `QuantityWithUnit`. In the class `Event`, all methods to deal with units are deprecated because the `timeUnits` attribute was removed in SBML Level 2 Version 2. The same holds true for instances of `ExplicitRule` and `KineticLaw`, which both can only be explicitly populated with units in SBML Level 1 for `ExplicitRule` and before SBML in Level 2, Version 3 for `KineticLaw`. In contrast, `QuantityWithUnit` serves as the abstract superclass for `LocalParameter` and `Symbol`, which is then again the super type of `Compartment`, `Species`, and (global) `Parameter`.

¹<http://www.obofoundry.org/cgi-bin/detail.cgi?id=unit>

With `SBaseWithUnit` being a subtype of `SBaseWithDerivedUnit` users can access the units of such an element in two different ways:

`getUnit ()` This method returns the `String` of the unit kind or the unit definition in the model that has been directly set by the user during the life time of the element. If nothing has been declared, an empty `String` will be delivered.

`getDerivedUnit ()` This method gives either the same result as `getUnit ()` if some unit has been declared explicitly, or it returns the predefined unit of the element for the given SBML Level/Version combination. Only if neither a user-defined nor a predefined unit is available, this method returns an empty `String`.

Both methods have corresponding methods to directly obtain an instance of `UnitDefinition` for convenience.

However, care must be taken when obtaining an instance of `UnitDefinition` from one of the classes implementing `SBaseWithUnit` because it might happen that the model containing this `SBaseWithUnit` does actually not contain the required instance of `UnitDefinition` and the method returns a `UnitDefinition` that has just been created for convenience from the information provided by the class. It might therefore be useful to either check if the `Model` contains this `UnitDefinition` or to add it to the `Model`.

In case of `KineticLaw` it is even more difficult, because SBML Level 1 allows to separately set the substance unit and the time unit of the element. To unify the API, we decided to also provide methods that allow the user to simply pass one `UnitDefinition` or its identifier to `KineticLaw`. These methods then try to guess if a substance unit or time unit is given. Furthermore, it is possible to pass a `UnitDefinition` representing a variant of substance per time directly. In this case, the `KineticLaw` will memorize a direct link to this `UnitDefinition` in the model and also try to save separate links to the time unit and the substance unit. However, this may cause a problem if the containing `Model` does not contain separate `UnitDefinitions` for both entries.

Generally, this approach provides a more general way to access and to manipulate units of SBML elements.

2.4 Additional features of JSBML

The JSBML library also provides some features that cannot be found in `libSBML`. This section briefly introduces its most important additional capabilities.

2.4.1 Change listeners

JSBML introduces the possibility to listen to change events in the life of an SBML document. To benefit from this advantage, simply let your class implement the interface `SBaseChangedListener` and add it to the list of listeners in your instance of `SBMLDocument`. You only have to implement three methods

sbaseAdded(SBase sbase) This method notifies the listener that the given SBase has just been added to the SBMLDocument

sbaseRemoved(SBase sbase) The SBase instance passed to this method is no longer part of the SBMLDocument as it has just been removed.

stateChanged(SBaseChangedEvent event) This method provides detailed information about some value change within the SBMLDocument. The object passed to this method is an SBaseChangedEvent, which provides information about the SBase that has been changed, its property whose value has been changed (this is a String representation of the name of the property), along with the previous value and the new value.

With the help of these methods, you can keep track of what your SBMLDocument does at any time. Furthermore, one could consider to make use of this functionality in a graphical user interface, where the user should be asked if he or she really wants to delete some element or to approve changes before making these persistent. Another idea of using this, would be to write log files of the model building process automatically. To this end, JSBML already provides the implementation SimpleSBaseChangedListener, which notifies a logger about each change.

Note that the class SBaseChangedEvent extends the class java.util.EventObject and that the interface SBaseChangedListener extends the interface EventListener in the java.util package. In this way, the event and listener data structures fit into the common Java™ API (Application Programming Interface) and allow users also to make use of, e.g., EventHandlers to deal with changes in a model. It should also be noted that SBaseChangedListeners only keep track of changes in instances of SBase directly. This means that changes inside of, e.g., CVTerm or History may not be traced with the current implementation.

2.4.2 Determination of the variable in AlgebraicRules

The class OverdeterminationValidator in JSBML provides methods to determine if a model is over determined. This is done using the algorithm of Hopcroft and Karp (1973). While doing that, it also determines the variable element for each AlgebraicRule if possible. In JSBML, AlgebraicRule even provides a method getDerivedVariable() to directly obtain a pointer to its free variable.

2.4.3 find* methods

JSBML provides users with several find* methods on a Model to quickly query for elements, based on their identifier or name. Developers can search for various instances of SBase (for instance, CallableSBase, NamedSBase, NamedSBaseWithDerivedUnit) or use the methods findLocalParameters, findQuantity, findQuantityWithUnit, findQuantityWithUnit, findSymbol, and findVariable to search for the corresponding element in the model. This enables a quick and easy way to work with SBML models, without having to iterate through the elements of a Model again and again.

2.4.4 Utility classes provided by JSBML

JSBML also provides some convenient additional utility classes. We here discuss some of these classes in more detail, which are all gathered in the package `org.sbml.jsbml.util`. There you can also find a growing number of additional helpful classes.

Preimplemented mathematic functions and constants

The class `org.sbml.jsbml.util.Maths` contains several static methods for mathematic operations not provided by the standard Java class `java.lang.Math`. Most of these methods are basic operations, for instance, `cot(double x)` or `ln(double x)`. However, the class `Maths` also provides some less commonly used methods, such as `csc(double x)` or `sech(double x)` as well as double constants representing Avogadro's number ($6.02214199 \cdot 10^{23} \text{ mol}^{-1}$) and the universal gas constant $R = 8.314472 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. In this way, the functions and constants implemented in class `Maths` complement standard Java with methods and numbers required by the SBML specifications (Hucka *et al.*, 2003, 2008, 2010).

Some tools for String manipulation

The class `StringTools` provides several methods for convenient `String` manipulation. These methods are particularly useful when parsing or displaying double numbers in a `Locale`-dependent way. To this end, this class predefines a selection of usefull number formats. It can also wrap `String` elements into HTML code, mask non-ASCII characters using corresponding HTML codes, efficiently concatenate `Strings`, or deliver the operating system-dependent new line character.

2.4.5 Logging functionality

JSBML makes use of the logger provided by the `log4j` project. `Log4j` allow to use six levels of logging (TRACE, DEBUG, INFO, WARN, ERROR and FATAL) but inside JSBML we are mainly using ERROR, WARN and DEBUG. The default configuration of `log4j` used in JSBML can be found in the package `org.sbml.jsbml.resources.cfg` with the name `log4j.properties`. In this file, you will found some documentation of which JSBML classes do some logging and at which levels.

If you do not change anything, all the log messages, starting at the info level (meaning info, warn, error and fatal), will be printing on the console. Some of these messages might be usefull to the end-users to warn them that they are doing something wrong.

If you want to modify the default `log4j` behavior, you will need to create a customized `log4j` configuration file. The best way of doing this, according to the `log4j` manual ², is to define and use the '`log4j.configuration`' environment variable to point to the `log4j` configuration file to use. One

²<http://logging.apache.org/log4j/1.2/manual.html>

way of doing this is to add '-Dlog4j.configuration=/home/user/myLog4j.properties' to your java command.

Some examples configurations

Listing 2.2 gives a short overview about how to customize the configuration file to log all the changes that happen to the SBML elements by putting the threshold of all the loggers in the `org.sbml.jsbml.util` package to `DEBUG`. The class `SimpleSBBaseChangeListener` will then output the old value and the new value whenever a setter methods is used on the SBML elements.

```
# All logging output sent to the console
log4j.rootCategory=INFO, console

#
# Console Display
#
log4j.appender.console=org.apache.log4j.ConsoleAppender
log4j.appender.console.layout=org.apache.log4j.PatternLayout

# Pattern to output the caller's file name and line number.
log4j.appender.console.layout.ConversionPattern=%d{yyyy-MM-dd HH:mm:ss} - %5p
    (%F:%L) - %m%n

# Log the messages from the SimpleSBBaseChangeListener at the DEBUG Level
# Allow to see all the changes that hapenned to the SBML elements
log4j.logger.org.sbml.jsbml.util=DEBUG
```

Listing 2.2: A simple log4j example.

When you enable the debug level on some loggers, the output can became quite large and the help of some log viewers software³ can become handy to filter the log output.

If you are deploying your application in an application server like Tomcat, you could define an appender that would send some messages by email, listing 2.3 give an example of that, were any messages from the error level are send by mail. All the messages are also written to a rolling log file.

```
# Logging is sent to a file and by email from the info level.
log4j.rootLogger=info, file, mail

#
# email appender definition
# it will send by email all messages from the error level.
```

³http://en.wikipedia.org/wiki/Log4j#Log_Viewers

```
#
log4j.appender.mail=org.apache.log4j.net.SMTPAppender
#defines how othen emails are send
log4j.appender.mail.BufferSize=1
log4j.appender.mail.SMTPHost="smtp.myservername.xx"
log4j.appender.mail.From=fromemail@myservername.xx
log4j.appender.mail.To=toemail@myservername.xx
log4j.appender.mail.Subject=Log ...
log4j.appender.mail.threshold=error
log4j.appender.mail.layout=org.apache.log4j.PatternLayout
log4j.appender.mail.layout.ConversionPattern=%d{ABSOLUTE} %5p %c{1}:%L - %m%n

### file appender
log4j.appender.file=org.apache.log4j.RollingFileAppender
log4j.appender.file.maxFileSize=100KB
log4j.appender.file.maxBackupIndex=5
log4j.appender.file.File=test.log
log4j.appender.file.threshold=info
log4j.appender.file.layout=org.apache.log4j.PatternLayout
log4j.appender.file.layout.ConversionPattern=%d{ISO8601} %5p %c{1}:%L - %m%n
```

Listing 2.3: SMTPAppender log4j example.

Using XML instead of a properties file to define the log4j configuration, you can even send some log levels to one appender and others to an other appender, using the LevelRange filter. This way, you could output the DEBUG messages only to a separate file.

2.4.6 JSBML modules

JSBML modules extend the functionality of JSBML and are provided as separate libraries (JAR files). With the help of the current JSBML modules, JSBML can be used as a communication layer between your application and libSBML (Bornstein *et al.*, 2008) or between your program and the program known as CellDesigner (Funahashi *et al.*, 2003). Furthermore, a compatibility module will try to provide the same package structure and API as in the libSBML Java bindings. In this section, we will give small code examples of how to make use of these modules.

How to use libSBML for parsing SBML into JSBML data structures?

The capabilities of the SBML validator constitute the major strength of libSBML (Bornstein *et al.*, 2008) in comparison to JSBML, whose SBML validation is not yet fully implemented. Furthermore, if the platform-dependency of libSBML does not hamper your application, or you want to slowly switch from libSBML to JSBML, you may want to be able to still read and write SBML models using libSBML. To this end, the JSBML module `libSBMLio` provies the classes `LibSBMLReader` and `LibSBMLWriter`. Listing 2.4 on the next page gives a small example of how to use the `LibSBMLReader`. For this example to run, please make sure to have libSBML installed

```
1  /** @param args the path to a valid SBML file. */
2  public static void main(String[] args) {
3      try {
4          // Load libSBML:
5          System.loadLibrary("sbmlj");
6          // Extra check to be sure we have access to libSBML:
7          Class.forName("org.sbml.libsbml.libsbml");
8
9          // Read SBML file using libSBML and convert it to JSBML:
10         LibSBMLReader reader = new LibSBMLReader();
11         SBMLDocument doc = reader.convertSBMLDocument(args[0]);
12
13         // Run some application:
14         new JSBMLvisualizer(doc);
15
16     } catch (Throwable e) {
17         e.printStackTrace();
18     }
19 }
```

Listing 2.4: A simple example for converting libSBML data structures into JSBML data objects

correctly on your system. The current version of the libSBML/JSBML interface at the time of writing this document requires libSBML version 4.2.0. To this end, you may have to set environment variables, e.g., the `LD_LIBRARY_PATH` under Linux operating system, appropriately. For details, see the documentation of libSBML⁴. Writing SBML works similarly. This example will display the content of an SBML file in a `JTree`, similar as shown in Fig. 1.1 on page 11.

How to turn a JSBML-based application into a CellDesigner plugin?

Once an application has been implemented based on JSBML, it can easily be accessed from CellDesigner's plugin menu (Funahashi *et al.*, 2003). To this end, it is necessary to extend two classes that are defined in CellDesigner's plugin API (Application Programming Interface). The Listings 2.5 to 2.6 on pages 31–32 show a very simple example of how to pass CellDesigner plugin model data structures to the translator in JSBML, which creates then a JSBML `Model` data structure. The examples described by Listings 2.5 to 2.6 on pages 31–32 create a plugin for CellDesigner, which displays the SBML data structure in a tree, like the example in Fig. 1.1 on page 11. This example only shows how to translate a plugin data structure from CellDesigner into a corresponding JSBML data structure. With the help of the class `PluginSBMLWriter` it is possible to notify CellDesigner about changes in the model data structure. Note that Listing 2.6 on page 32 is only completed by implementing the methods from the superclass. In this example it is sufficient to leave the implementation empty.

⁴<http://sbml.org/Software/libSBML>

```
1 package org.sbml.jsbml.cdplugin;
2
3 import java.awt.event.ActionEvent;
4 import javax.swing.JMenuItem;
5 import jp.sbi.celldesigner.plugin.PluginAction;
6
7 /** A simple implementation of an action for a CellDesigner plug-in */
8 public class SimpleCellDesignerPluginAction extends PluginAction {
9
10     private SimpleCellDesignerPlugin plugin;
11
12     /** Constructor memorizes the plug-in data structure. */
13     public SimpleCellDesignerPluginAction(SimpleCellDesignerPlugin plugin) {
14         this.plugin = plugin;
15     }
16
17     /** Executes an action if the given command occurs. */
18     public void myActionPerformed(ActionEvent ae) {
19         if (ae.getSource() instanceof JMenuItem) {
20             String itemText = ((JMenuItem) ae.getSource()).getText();
21             if (itemText.equals(SimpleCellDesignerPlugin.ACTION)) {
22                 plugin.startPlugin();
23             }
24         } else {
25             System.err.printf("Unsupported_source_of_action_%s\n", ae
26                 .getSource().getClass().getName());
27         }
28     }
29 }
30 }
```

Listing 2.5: A simple implementation of CellDesigner's abstract class PluginAction

```

1 package org.sbml.jsbml.cdplugin;
2
3 import javax.swing.*;
4 import jp.sbi.celldesigner.plugin.*;
5 import org.sbml.jsbml.*;
6 import org.sbml.jsbml.gui.*;
7
8 /** A very simple implementation of a plugin for CellDesigner. */
9 public class SimpleCellDesignerPlugin extends CellDesignerPlugin {
10
11     public static final String ACTION = "Display_full_model_tree";
12     public static final String APPLICATION_NAME = "Simple_Plugin";
13
14     /** Creates a new CellDesigner plugin with an entry in the menu bar. */
15     public SimpleCellDesignerPlugin() {
16         super();
17         try {
18             System.out.printf("\n\nLoading_%s\n\n", APPLICATION_NAME);
19             SimpleCellDesignerPluginAction action = new
20                 SimpleCellDesignerPluginAction(this);
21             PluginMenu menu = new PluginMenu(APPLICATION_NAME);
22             PluginMenuItem menuItem = new PluginMenuItem(ACTION, action);
23             menu.add(menuItem);
24             addCellDesignerPluginMenu(menu);
25         } catch (Exception exc) {
26             exc.printStackTrace();
27         }
28
29         /** This method is to be called by our CellDesignerPluginAction. */
30         public void startPlugin() {
31             PluginSBMLReader reader = new PluginSBMLReader(getSelectedModel(), SBO
32                 .getDefaultPossibleEnzymes());
33             Model model = reader.getModel();
34             SBMLDocument doc = new SBMLDocument(model.getLevel(), model
35                 .getVersion());
36             doc.setModel(model);
37             new JSBMLvisualizer(doc);
38         }
39
40         // Include also methods from superclass, not needed in this example.
41         public void addPluginMenu() { }
42         public void modelClosed(PluginSBase psb) { }
43         public void modelOpened(PluginSBase psb) { }
44         public void modelSelectChanged(PluginSBase psb) { }
45         public void SBaseAdded(PluginSBase psb) { }
46         public void SBaseChanged(PluginSBase psb) { }
47         public void SBaseDeleted(PluginSBase psb) { }
48     }

```

Listing 2.6: A simple example for a CellDesigner plugin using JSBML as a communication layer

libSBMLcompat, the JSBML compatibility module for libSBML

The compatibility module of JSBML will use the same package structure as the libSBML java bindings and provides identically named classes and API. Using the module, it will be possible to switch an existing application from libSBML to JSBML or the other way around without changing any code.

This module is in development and will be available with the version 1.0 of JSBML.

3 Open tasks in JSBML

- JSBML does not yet provide a complete validator for SBML.
- The support for SBML Level 3 should be completed, particularly extension packages.
- The `toSBML()` methods in `SBase` are still missing.
- Constructors and methods with namespaces are not yet provided.
- The `libSBML` compatibility module needs to be fully implemented.

Appendix A

Frequently Asked Questions (FAQ)

For questions regarding SBML, please see the SBML FAQ at <http://sbml.org/Documents/FAQ>.

Why does the class `LocalParameter` not inherit from `Parameter`? The reason is the Boolean attribute `constant`, which is present in `Parameter` and can be set to `false`. A parameter in the meaning of SBML is not a constant, it might be some system variable and can therefore be the subject of `Rules`, `Events`, `InitialAssignments` and so on, i.e., all instances of `Assignment`, whereas a `LocalParameter` is defined as a constant quantity that never changes its value during the evaluation of a model. It would therefore only be possible to let `Parameter` inherit from `LocalParameter` but this could lead to a semantic misinterpretation.

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