JSBML

The SBML Java™ library

Concept of JSBML

- Compromise:
  - High compatibility to libSBML
  - Java-like library

- Main developers
  - Nicolas Rodriguez and Andreas Dräger
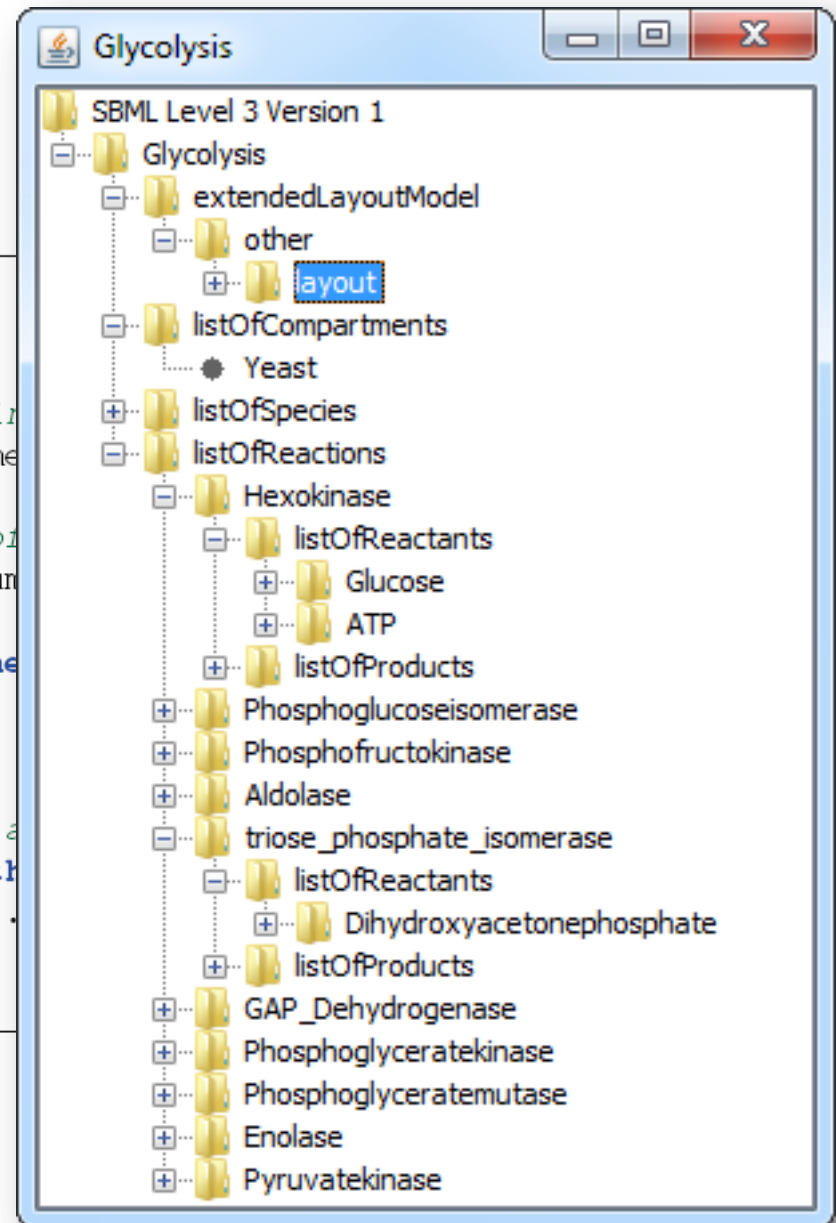 - Both available during the meeting any time to answer JSBML-related questions

JSOML

How to get started?

Obtaining JSBML

- https://sourceforge.net/projects/jsbml/files/jsbml/0.8-b2/

- Download the file `jsbml-0.8-b2-with-dependencies.jar`.

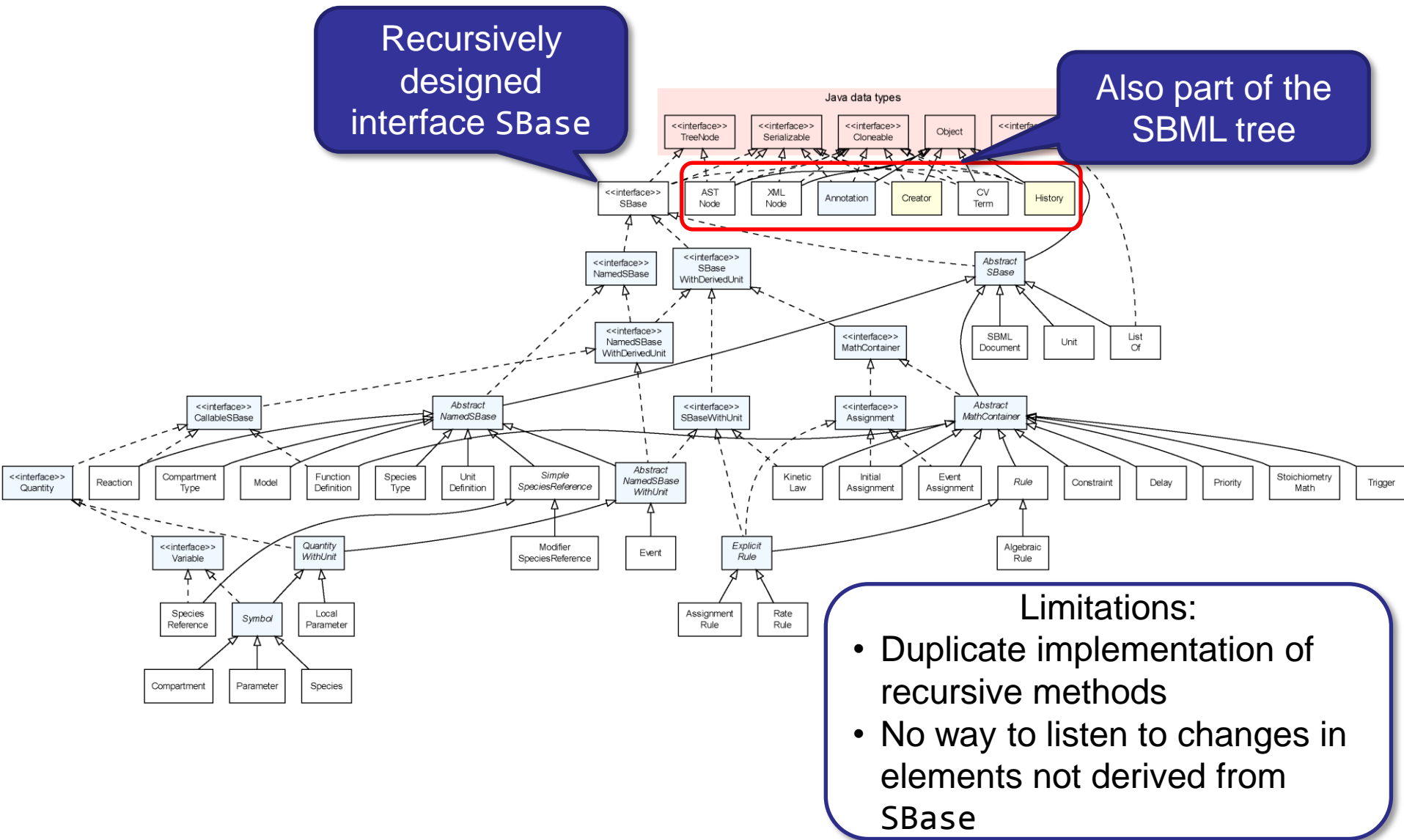- Once you have added it to the Java `CLASSPATH`, you can start working with JSBML.

Visualizing the content of an SBML

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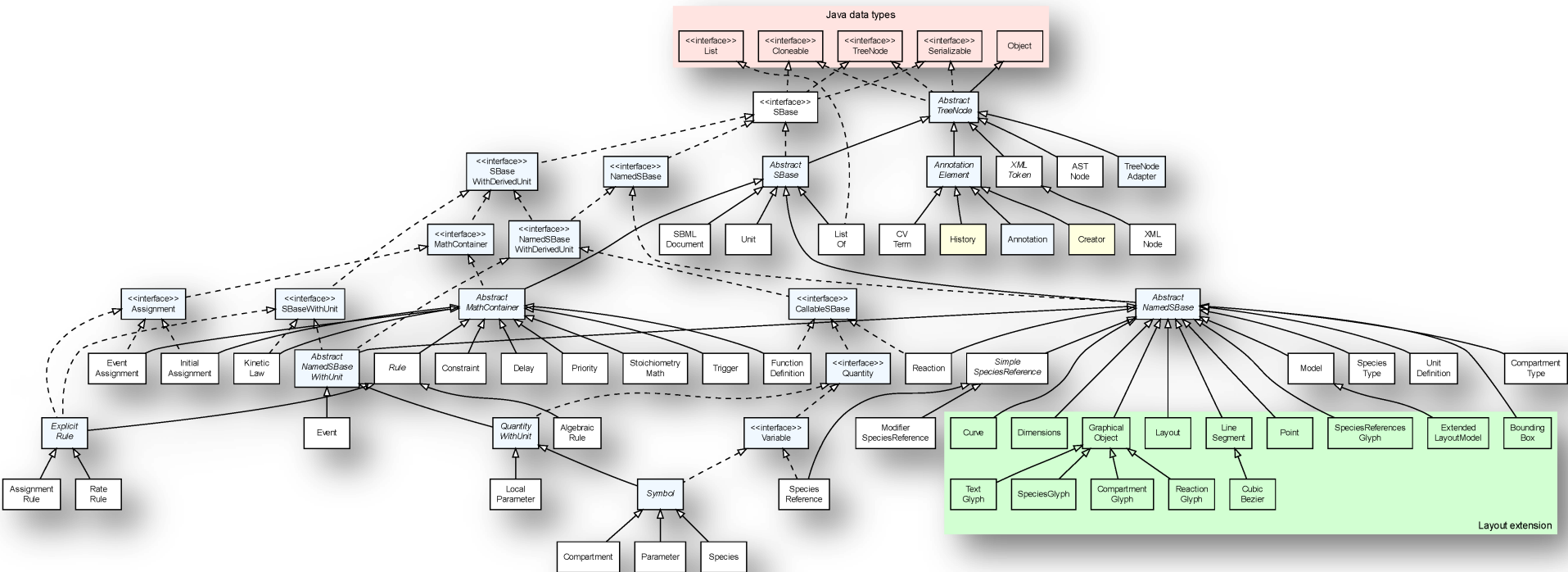
Glycolysis

- SBML Level 3 Version 1
  - Glycolysis
    - extendedLayoutModel
      - other
        - layout
    - listOfCompartments
      - Yeast
    - listOfSpecies
    - listOfReactions
      - Hexokinase
        - listOfReactants
          - Glucose
          - ATP
        - listOfProducts
      - Phosphoglucoseisomerase
      - Phosphofructokinase
      - Aldolase
      - triose_phosphate_isomerase
        - listOfReactants
          - Dihydroxyacetonephosphate
        - listOfProducts
      - GAP_Dehydrogenase
      - Phosphoglyceratekinase
      - Phosphoglyceratemutase
      - Enolase
      - Pyruvatekinase

JS8ML

Data types

Type hierarchy

Recursively designed interface `SBase`

Also part of the SBML tree

Java data types

Limitations:
- Duplicate implementation of recursive methods
- No way to listen to changes in elements not derived from `SBase`

Unified type hierarchy

New top level super class AbstractTreeNode

Java data types

- `<<interface>>` List
- `<<interface>>` Cloneable
- `<<interface>>` TreeNode
- `<<interface>>` Serializable
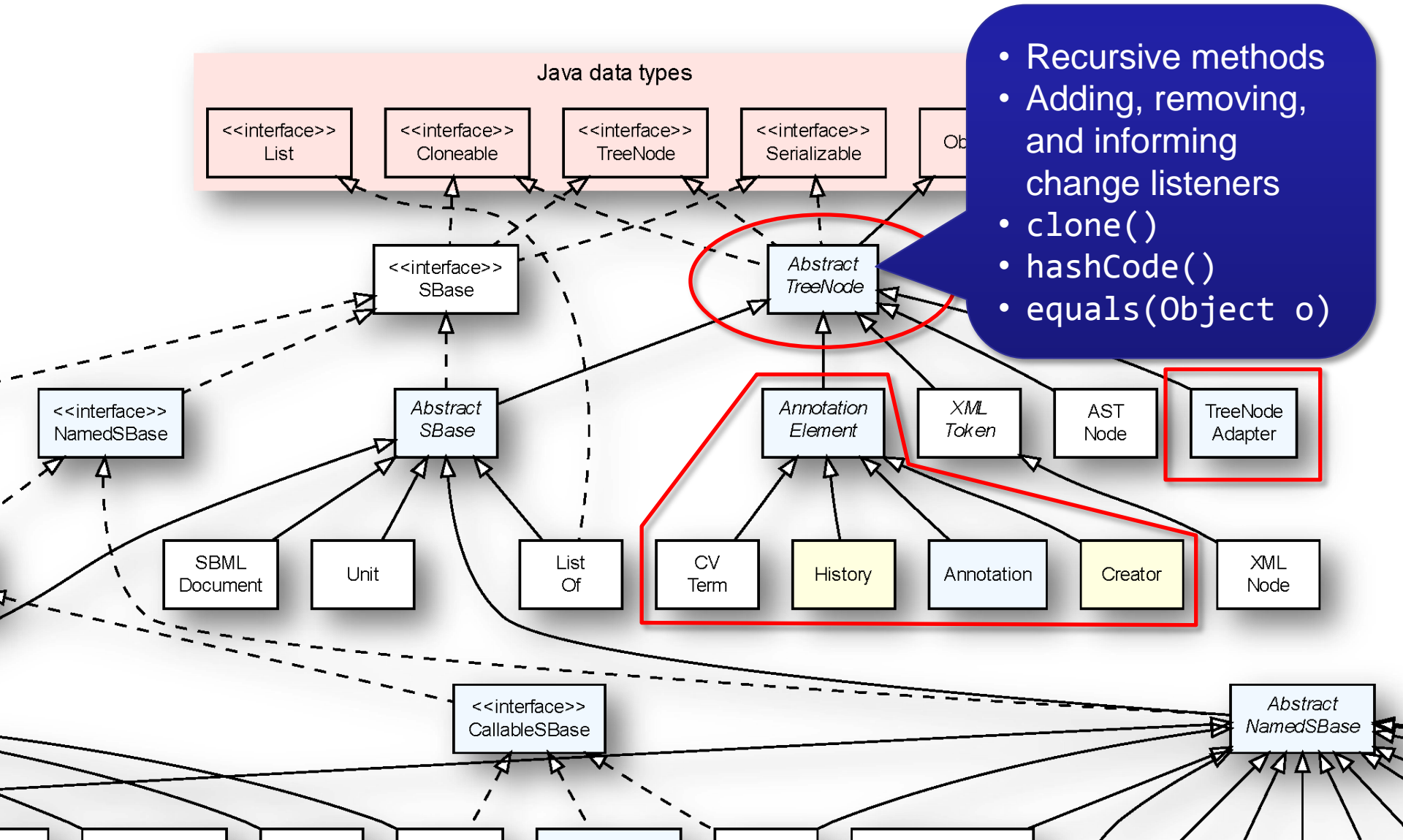
- Recursive methods
- Adding, removing, and informing change listeners
- `clone()`
- `hashCode()`
- `equals(Object o)`

`<<interface>>` SBase

Abstract TreeNode

`<<interface>>` NamedSBase

Abstract SBase

Annotation Element

XML Token

AST Node

TreeNode Adapter

SBML Document

Unit

List Of

CV Term

History

Annotation

Creator

XML Node

`<<interface>>` CallableSBase

Abstract NamedSBase

Listening to changes

SBaseChangedListener in package org.sbml.jsbml

```
public void sbaseAdded(SBase sb) {
   System.out.println("[ADD] " + sb);
}


public void sbaseRemoved(SBase sb) {
   System.out.println("[RMV] " + sb);
}


public void stateChanged(SBaseChangedEvent ev) {
   System.out.println("[CHG] " + ev);
}
```

Improved listener: TreeNodeChangeListener

Package `org.sbml.jsbml.util`, extending `java.beans.PropertyChangeListener`

```java
public void nodeAdded(TreeNode node) {
  System.out.println("[ADD] " + node);
}

public void nodeRemoved(TreeNode node) {
  System.out.println("[RMV] " + node);
}

public void propertyChange(PropertyChangeEvent evt) {
  System.out.println("[CHG] " + evt);
}
```

Specialised event implementation: TreeNodeChangeEvent

JS8ML

New features and bug fixes

New features – an overview

- TreeNodeAdapter as a wrapper for child elements that cannot extend AbstractTreeNode

- SBMLreader: static methods

- Maven script by Igor Rodchenkov

- initDefaults(int level, int version)

- Check for duplicate metaIds

- Automatic, recursive level/version update in case of adding elements with undefined L/V specification to a top element

Most important bug fixes

- General improvements:
  - Closing streams after reading/writing SBML files
  - Support for `NaN` values in formulas and `ASTNodes`
- Improved Level 1 support:
  - Parsing of `Rules` with a type attribute (e.g., `rate`)
  - Denominator attribute in `SpeciesReference` was never read
  - No MathML in `KineticLaw`
  - Exception during conversion between `LocalParameter` and `Parameter` (no `constant` attribute)
- Improved Level 3 support:
  - `getDerivedUnitsInstance()` in `Species`

JS8ML
Modules

Download of modules

- LibSBML input/output:

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

- CellDesigner bridge:

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

- LibSBML compatibility module for switching between libSBML and JSBML still under development

How to contribute

Creating a patch:

- Checkout the sources from sourceforge

  `svn co` **"https://jsbml.svn.sourceforge.net/svnroot/jsbml/trunk jsbml"** `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/tracker/?group_id=279608&atid=1186776

Mailing lists:

- jsbml-development@caltech.edu: public list with discussion about the development of JSBML and support for users.

- jsbml-team@caltech.edu: private list for the JSBML team were anybody can send mails for support or bugs reports.

Systems biology

JSBML: a flexible Java library for working with SBML

Andreas Dräger[1],[*],[†], Nicolas Rodriguez[2],[†], Marine Dumousseau[2], Alexander Dörr[1], Clemens Wrzodek[1], Nicolas Le Novère[2], Andreas Zell[1] and Michael Hucka[3],[*]

[1]Center for Bioinformatics Tuebingen (ZBIT), University of Tuebingen, Tübingen, Germany, [2]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, Cambridge, UK and [3]Computing and Mathematical Sciences, California Institute of Technology, Pasadena, CA, USA

Associate Editor: Jonathan Wren

Thanks for your attention!

http://sbml.org/Software/JSBML