JSBML: a flexible Java library for working with SBML

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ABSTRACT

Summary: 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.

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

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Supplementary information: Supplementary data are available at Bioinformatics online.

1 INTRODUCTION

The XML-based Systems Biology Markup Language (SBML) defines 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.

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specific properties. All ListOf* elements in JSBML implement Java’s List interface, making iteration and the use of generic Java types possible. Figure 1 demonstrates how the hierarchically structured content of an SBML file can be easily visualized in the form of a tree.

JSBML includes parsers that read mathematical formulas in both MathML format and an infix formula syntax. Internally, it converts formulas into an abstract syntax tree representation; it can write out the trees in MathML, infix and \LaTeX{} formula notations. In addition, although JSBML does not implement full-featured consistency checking of SBML models, it does throw Java exceptions in some situations to prevent users from creating invalid content. It implements a check for overdetermined models using the algorithm of Hopcroft and Karp (1973); this is also used to identify variables in algebraic rules. Further, JSBML can automatically derive the units of a mathematical expression. Whenever a property of some SBase is altered, an SBaseChangeEvent is fired that notifies dedicated listeners. As one possible application, graphical user interfaces could automatically react when the model is changed.

Using modules, JSBML capabilities can be further extended; it can therefore be used as a communication layer between an application and libSBML or CellDesigner (Funahashi et al., 2003)—this also facilitates turning an existing application into a plugin for CellDesigner.

3 CONCLUSION

JSBML is an ongoing 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 plugins based on stand-alone programs with very little effort. New versions of SBMLsqueezer (Dräger et al., 2008) and Biomodels Database (Li et al., 2010) have already been released using JSBML. Many other projects are planned.

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REFERENCES


