

SBMLEditor toward SBML level 3 and modularisation

Nicolas Rodriguez^{1,*}, Anika Oellrich¹, Nicolas Le Novère¹

1. EMBL - European Bioinformatics Institute, Cambridge, UK

*E-mail: rodrigue@ebi.ac.uk

In Systems Biology, complementary computational tools are often used to model and analyse different characteristics of a particular system. Unfortunately most tools have their own format for entering and storing models. The Systems Biology Markup Language (SBML) [1] is a free, open format designed to promote interoperability between those different modeling tools so that model descriptions produced by one tool can be read and processed by other programs. It also offers a standard representation for model storage, transmission, and re-use. Although SBML is specified as a set of classes, it is instantiated as an XML language. But, even if SBML is text-based, and can be edited in a simple text editor, it is intended to be written and read by machines, rather than humans. As such it requires specific user-interface to translate a modeler's intention into its computer representation.

In order to prepare for SBML Level 3, being currently designed, and its modularity, we had to change the architecture of SBMLEditor [2] (see Table 1 for a list of SBML features). Instead of DOM, we use the Apache Digester to read the XML. It reads the SBML file in a SAX manner and creates Java objects while reading the file. These Java objects are derived from the SBML specifications, which contain UML definitions for each SBML element.

The new libsbml-3.0.0 release contains a lot more validation rules and will fully support SBML Level 2 Version 3 specifications. However we expect some users to keep using the previous stable release as they will need time to switch and all tools will not immediately support libsbml-3.0.0. To be able to support both libsbml-2.3.4 and libsbml-3.0.0 releases, we had to build a separate jar to call libsbml functions. It allows SBMLEditor to support both libsbml releases, even if they have differences in their APIs.

Furthermore, we had to formalize possible extensions of SBMLEditor, such as the one that supports RDF annotations. For the next release of SBMLEditor (2.0), we defined a set of interfaces allowing the application to work, with the help of a plugin, on new SBML elements that it doesn't know, or on elements which internal structure has been changed. The `SBaseFilter` class must be implemented by each extensions to define which type of elements they will be responsible for. The extension will then have to provide all the functionalities to manipulate these types of SBML elements. Several other interfaces, like `SBMLTreeNode` to create the `JTree` nodes and `SBaseFactory` to edit the element, help the writer of the extension to achieve this. We already worked on one of these extensions to support a modified multistate components proposal [3]. We worked on a set of annotations to be able to use SBML as input for StochSim. A library was written to generate most of the StochSim configuration files from a properly annotated SBML file. The needed XML necessary is complex and prone to human errors. Therefore, a graphical interface, through the SBMLEditor, was warmly welcome by model writers.

Feature	Details	Completion
RDF annotation	We implemented it first as a proposal, before its inclusion in the SBML specifications, since Level 2 Version 2	1.0
math editor	Possibility to edit equations in infix notation instead of the Mathematical Markup Language (MathML)	1.0
Integration in SBW	Application that support the System Biology Workbench (SBW) can open their model for edition with SBMLEditor	1.0
libsbml-3.0.x support	Because of changes in APIs between libsbml versions 2.3.4 and 3.0.0, a separate library was created to regroup all the libsbml method's call	1.3
SBO support	Ability to search and browse the System Biology Ontology (SBO)	2.0
Extension/Plugin APIs	Definitions of a set of interfaces to allow easier extension of SBMLEditor	2.0
StochSim Multistate	A first extension example, based on a multistate proposal, adapted to produce StochSim INI files	2.0
Simulation launching	Ability to launch different simulation software. We can already do that through SBW but it would be nice to be able to launch SOSlib, StochSim, Ecell...	planned extension
Integration in Taverna	This would allow easier interactions with other software, tools, workflow...	planned extension

Table 1: List of SBMLEditor Features

References

- [1] Hucka M, Finney A, Sauro HM and all the SBML forum (2003) **The Systems Biology Markup Language (SBML): A Medium for Representation and Exchange of Biochemical Network Models**. *Bioinformatics*, **19**: 524-531.
- [2] Rodriguez N, Donizelli M, Le Novère N (2007) **SBMLeditor: effective creation of models in the Systems Biology Markup Language (SBML)**. *BMC Bioinformatics*, **8**:79
- [3] Le Novère N, Oellrich A (2007) **Systems Biology Markup Language (SBML) Level 3 Proposal: multistate components** Technical report. available via the World Wide Web <http://www.ebi.ac.uk/compneur-srv/sbml/proposals/multistatesNEW.pdf>