BMC Research Notes

SBMLPkgSpec: A LaTeX Style File for SBML Package Specification Documents

--Manuscript Draft--

Manuscript Number:	RESN-D-17-00585
Full Title:	SBMLPkgSpec: A LaTeX Style File for SBML Package Specification Documents
Article Type:	Research note
Funding Information:	National Institute of General Medical Sciences (GM070923) — Dr. Michael Hucka
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RESEARCH

SBMLPkgSpec: A LaTeX Style File for SBML Package Specification Documents

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Abstract

Objective: SBML (the Systems Biology Markup Language) is a popular open format for storing and exchanging computational models in biology. The definition of SBML is captured in formal specification documents. SBMLPkgSpec is a LaTeX document style intended to fill the need for a standard format for writing such specification documents.

Results: Specification documents for SBML Level 3 extensions (known as *packages* in SBML) are made more uniform with the use of a standard template. SBMLPkgSpec is a LaTeX class that provides a common document format for SBML Level 3 package specifications, to simplify the work of document authors while improving the overall quality of the family of SBML specifications.

Keywords: SBML; XML; data formats; software; simulation; systems biology; computational biology

Introduction

SBML (the Systems Biology Markup Language) is an XML-based (Extensible Markup Language) format that has become a community standard for the storage, communication and interchange of models in systems biology [1, 2]. The format has evolved in a community-driven fashion, with contributions from dozens of people worldwide over more than a decade and a half. The latest generation of SBML is SBML Level 3, which is structured as a self-sufficient core and optional *SBML Level 3 packages* that can be used to extend the core's syntax and semantics [3]. The definition of each SBML Level 3 package is written in a formal specification document that is made freely available to everyone [4, 5]. SBML packages are introduced and ratified according to an explicit SBML Development Process (`http://sbml.org/Documents/SBML_Development_Process`); this process also defines a template for the content that each specification document should contain.

Main Text

SBMLPkgSpec is a LaTeX document class [6] intended to provide a common framework for writing SBML package specifications, as well as provide a uniform look and feel for the family of SBML specifications. SBMLPkgSpec builds on a number of other commonly-available LaTeX document classes, and also defines a number of new commands, so that users of SBMLPkgSpec can focus on the essential aspects of writing clear specification documents for SBML. Among the features provided by SBMLPkgSpec are the following:

- Predefined commands for defining the SBML package version, release date, home web page, and author list, to be printed on the document's front page.
- Commands for defining SBML *validation rules*. A convention developed for the SBML specification documents is to define validation and consistency rules that must or should be satisfied by SBML files that conform to the specification; SBML package specifications likewise define their own validation and consistency rules, and the commands in SBMLPkgSpec provide the means for easily defining and formatting them.
- Commands for formatting the names of common SBML object classes and XML primitive data types, as well as for creating new package-specific definitions. The commands for SBML object names automatically insert hyperlinks to the sections where they are defined from wherever they are referenced within a document.
- Customized commands for cross-referencing sections, tables and figures; these are designed to produce *both* item number and page references that are automatically hyperlinked to the appropriate locations in the finished document. They also obey some common typographical conventions (such as the use of LaTeX ties in the appropriate locations) to save authors the trouble of remembering them.
- Commands for formatting SBML XML examples in a stylized fashion.
- Automatic line numbering of every line in the specification document. This makes it easier to report problems and errors in specification documents, and to issue subsequent lists of errata.
- An option to print the word *DRAFT* on every page in large gray type.
- Commands for different kinds of document notes: notices (with a hand pointer in the left margin), warnings (with a red warning sign in the left margin), and reader notes (formatted as yellow rectangular notes shown in the left margin when the document is formatted in draft mode).
- Other miscellaneous features, such as a number of predefined color names.

To illustrate some of the features of SBMLPkgSpec, Figure 1 shows an image of a page from the user's guide. It illustrates the general look of the document and some of the commands it provides.

Installation and configuration

The use of SBMLPkgSpec should require only a recent and relatively complete installation of LaTeX2e. It was developed and tested with the TeX Live 2011 and 2016 distributions on Mac OS X 10.6–10.11 system, and has been reported to work with TeX Live on Windows and Ubuntu Linux. (For Ubuntu, make sure to install the following packages: "`texlive`", "`texlive-latex-extra`", "`texlive-humantities`", and "`texlive-fonts-extra`".) To use SBMLPkgSpec, you will need to inform your copy of LaTeX where to find the file `sbmlpkgspec.cls` and its accompanying subdirectory "`logos`". This can be done in a variety of ways. Here are two common ones:

- *Per-document installation.* This is probably the simplest approach, although it results in multiple copies of the files. Download the SBMLPkgSpec release from the GitHub repository (https://github.com/sbmlteam/sbmlpkgspec),

copy the contents (specifically, `sbmlpkgspec.cls` and the folder named "`logos`") to the folder where you keep the other files for the SBML Level 3 package specification you are authoring, and you are done. The next time you run LaTeX in that folder, it will find the `.cls` file in the current directory and be on its merry way.

- *"Central" installation.* In this approach, you install `sbmlpkgspec.cls` in a folder where you keep other LaTeX class files, and configure your copy of LaTeX to find things there. Configuring a TeX system in this way on Unix-type systems (Linux, etc.) usually requires setting the environment variable `TEXINPUTS` and possibly others. Please consult the documentation for your TeX installation to determine how to do this.

Once SBMLPkgSpec is installed, users can write specification documents with the standard `documentclass` command in LaTeX to declare the use of the class `sbmlpkgspec`, and write their document using whatever editing environment they prefer, including online shared LaTeX editing environments.

Documentation

SBMLPkgSpec comes with a complete user's guide. Users of SBMLPkgSpec are strongly urged to read the guide; it explains everything needed to know to use the document class, and includes tips for how to make the most of it.

Discussion

LaTeX [6] is a popular document production system in science. In systems biology and the SBML-using community, it is so popular that some software tools have been designed to produce LaTeX output directly [7, 8]. LaTeX provides tremendous power to authors, but it is also relatively difficult to use. Defining new styles is specially difficult, and requires arcane knowledge and significant patience. By simplifying the requirements for producing templated documents and providing a ready-to-use LaTeX style, SBMLPkgSpec can make it easier for SBML specification authors to use LaTeX to produce documents with a uniform format. This in turn permits authors of SBML specifications to concentrate on the technical aspects of the work.

Limitations

SBMLPkgSpec imports many other LaTeX classes when it is used with LaTeX. These additional classes must be installed on the user's computer for SBMLPkgSpec to work. The classes are present in many full-featured TeX distributions such as the TeX Live 2011 and 2016 distributions, but if they are not, the user will need to find and install them separately. The relevant software packages for Ubuntu Linux are noted above.

List of abbreviations

SBML: Systems Biology Markup Language.
XML: Extensible Markup Language.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data and material

SBMLPkgSpec is available in two different forms: as a compressed archive of LaTeX source code and documentation files, and as a public repository that can be cloned using ordinary `git` commands. Both forms are freely available under the terms of the LGPL 2.1 license from the project repository hosted on GitHub at https://github.com/sbmlteam/sbmlpkgspec.

Competing interests

The author declares that he has no competing interests.

Funding

SBMLPkgSpec has been developed thanks to funding from the National Institute of General Medical Sciences under grant R01 GM070923 (Principal Investigator: Michael Hucka).

Authors' contributions

MH developed the software and documentation, and wrote the manuscript.

Acknowledgements

I thank Maciej Swat (from the EMBL European Bioinformatics Institute) for reporting problems with earlier versions of SBMLPkgSpec. I also thank all users for their informal feedback and suggestions.

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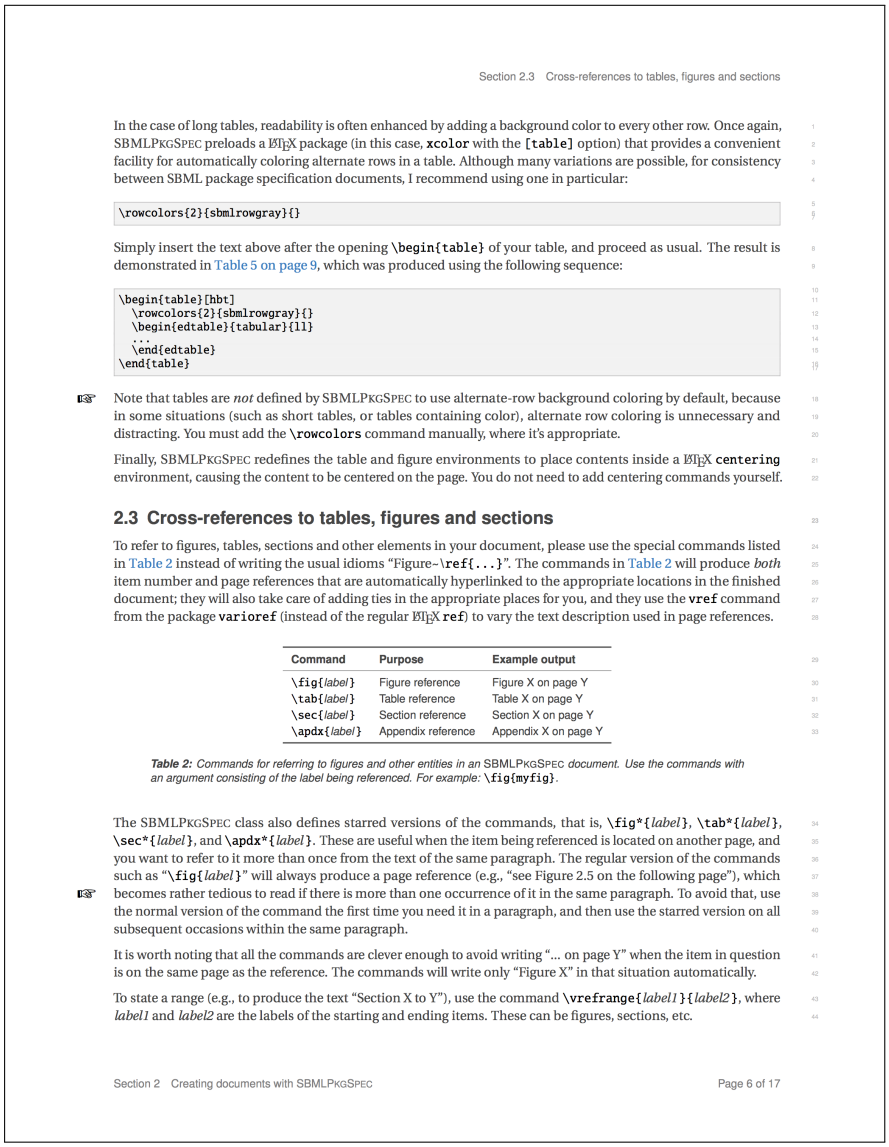
Figure 1 A sample page from the SBMLPkgSpec user's guide, illustrating the look and feel of the document and some of its features.



In the case of long tables, readability is often enhanced by adding a background color to every other row. Once again, SBMLPkgSpec preloads a LaTeX package (in this case, `xcolor` with the `[table]` option) that provides a convenient facility for automatically coloring alternate rows in a table. Although many variations are possible, for consistency between SBML package specification documents, I recommend using one in particular:

```
\rowcolors{2}{sbmlrowgray}{}
```

Simply insert the text above after the opening `\begin{table}` of your table, and proceed as usual. The result is demonstrated in Table 5 on page 9, which was produced using the following sequence:

```
\begin{table}[hbt]
  \rowcolors{2}{sbmlrowgray}{}
  \begin{edtable}{tabular}{ll}
  ...
  \end{edtable}
\end{table}
```

☞ Note that tables are *not* defined by SBMLPkgSpec to use alternate-row background coloring by default, because in some situations (such as short tables, or tables containing color), alternate row coloring is unnecessary and distracting. You must add the `\rowcolors` command manually, where it's appropriate.

Finally, SBMLPkgSpec redefines the table and figure environments to place contents inside a LaTeX `centering` environment, causing the content to be centered on the page. You do not need to add centering commands yourself.

2.3 Cross-references to tables, figures and sections

To refer to figures, tables, sections and other elements in your document, please use the special commands listed in Table 2 instead of writing the usual idioms "Figure~`\ref{...}`". The commands in Table 2 will produce *both* item number and page references that are automatically hyperlinked to the appropriate locations in the finished document; they will also take care of adding ties in the appropriate places for you, and they use the `vref` command from the package `varioref` (instead of the regular LaTeX `ref`) to vary the text description used in page references.

Command	Purpose	Example output
`\fig{`*label*`}`	Figure reference	Figure X on page Y
`\tab{`*label*`}`	Table reference	Table X on page Y
`\sec{`*label*`}`	Section reference	Section X on page Y
`\apdx{`*label*`}`	Appendix reference	Appendix X on page Y

Table 2: *Commands for referring to figures and other entities in an* SBMLPkgSpec *document. Use the commands with an argument consisting of the label being referenced. For example:* `\fig{myfig}`.

The SBMLPkgSpec class also defines starred versions of the commands, that is, `\fig*{`*label*`}`, `\tab*{`*label*`}`, `\sec*{`*label*`}`, and `\apdx*{`*label*`}`. These are useful when the item being referenced is located on another page, and you want to refer to it more than once from the text of the same paragraph. The regular version of the commands such as "`\fig{`*label*`}`" will always produce a page reference (e.g., "see Figure 2.5 on the following page"), which ☞ becomes rather tedious to read if there is more than one occurrence of it in the same paragraph. To avoid that, use the normal version of the command the first time you need it in a paragraph, and then use the starred version on all subsequent occasions within the same paragraph.

It is worth noting that all the commands are clever enough to avoid writing "... on page Y" when the item in question is on the same page as the reference. The commands will write only "Figure X" in that situation automatically.

To state a range (e.g., to produce the text "Section X to Y"), use the command `\vrefrange{`*label1*`}{`*label2*`}`, where *label1* and *label2* are the labels of the starting and ending items. These can be figures, sections, etc.

Figure 1 A sample page from the SBMLPkgSpec user's guide, illustrating the look and feel of the document and some of its features.