

SBML L3 Package Development

Sarah Keating



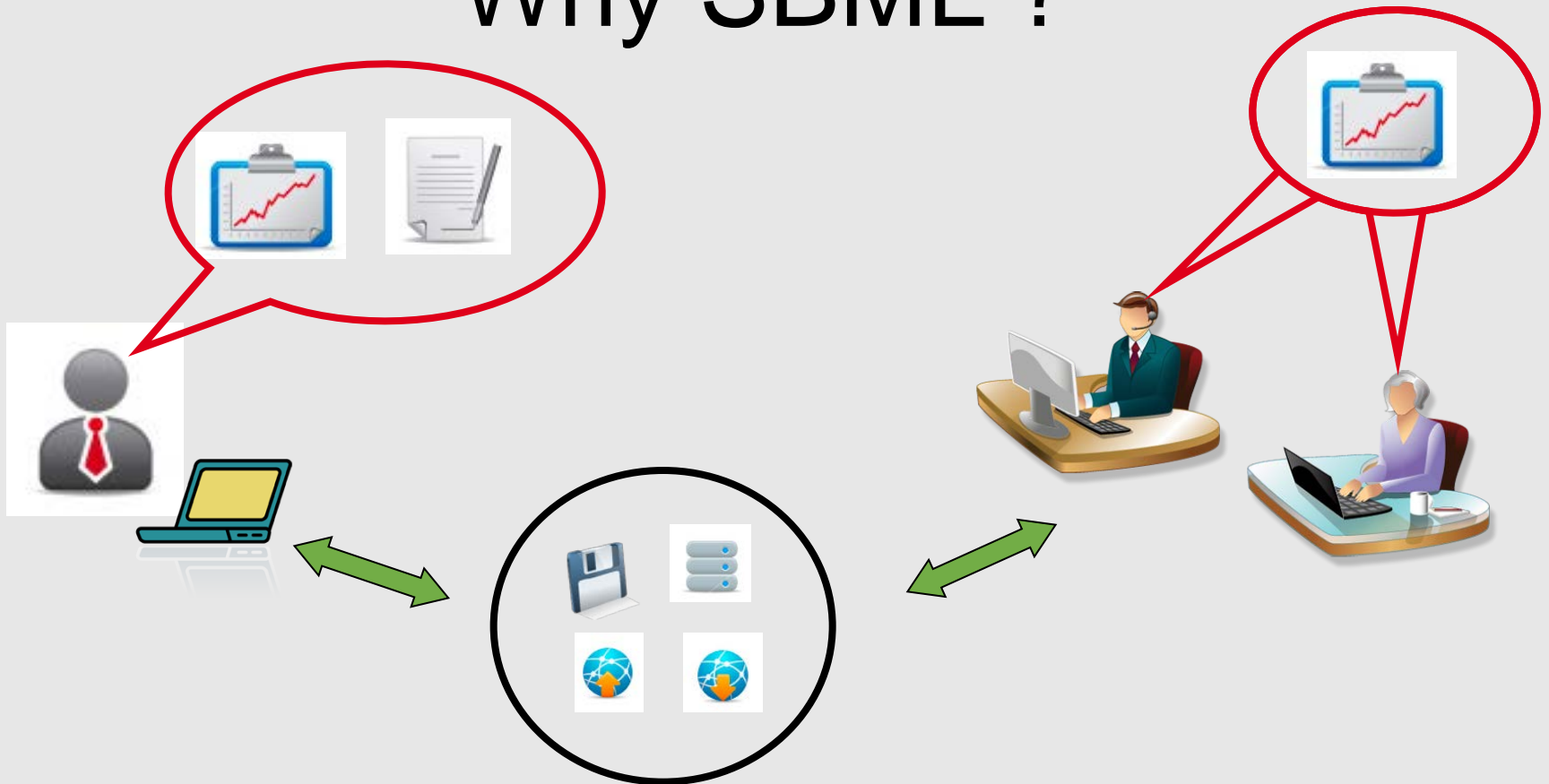
Outline

1. Brief overview of what SBML is and why it was developed
2. Overview of SBML Level 3 modularisation
3. L3 package development
4. libSBML and L3 packages
5. Links and acknowledgements

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Why SBML ?



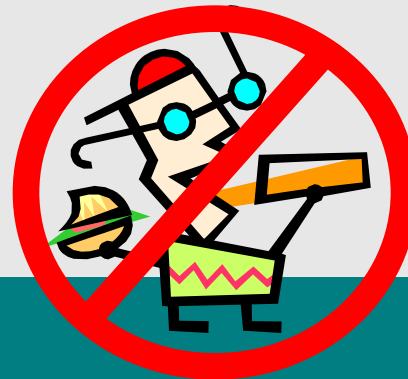
Goal: reproducible and reusable
models and simulations

What is SBML ?

A machine-readable format for representing computational models in systems biology

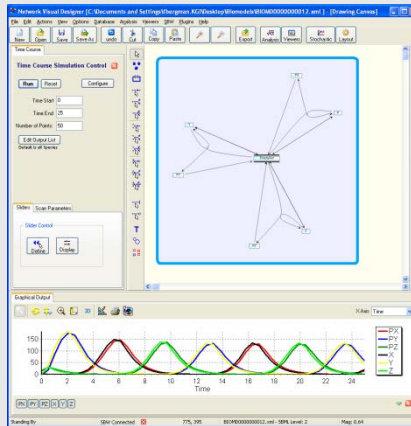
Tool-neutral exchange language for software applications

Expressed in XML



What is SBML ?

- Independent of modelling formalism
- Declares model not procedure



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SBML Level 3

**The Systems Biology Markup Language (SBML):
Language Specification for Level 3 Version 1 Core**

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sbml-editors@sbml.org
core
SBML Level 3 Version 1 Core

Release 1 (Candidate)
31 December 2009

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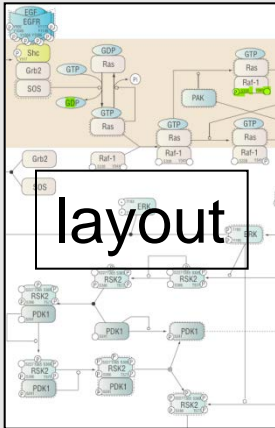
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 **Systems Biology
Markup Language**

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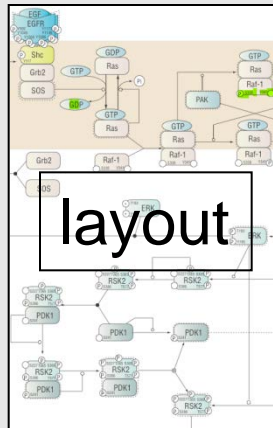
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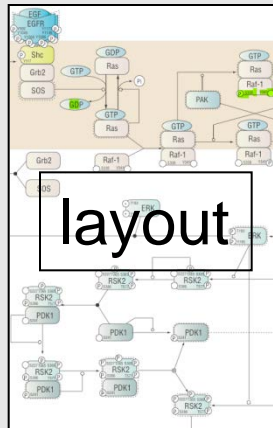
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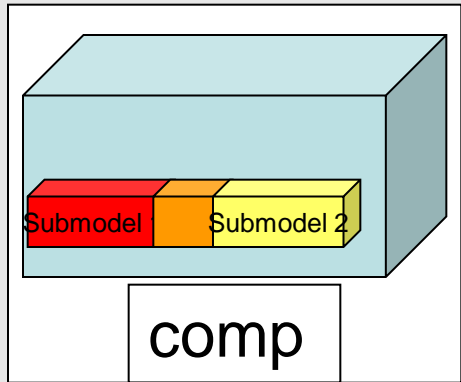
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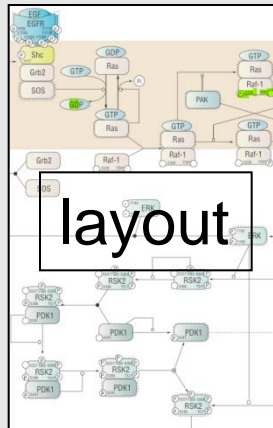
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Markup Language**



SBML Level 3



layout

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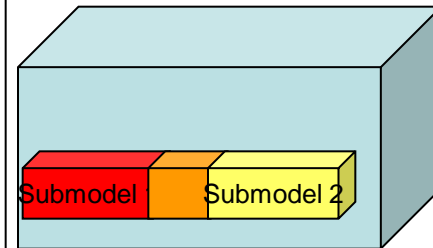
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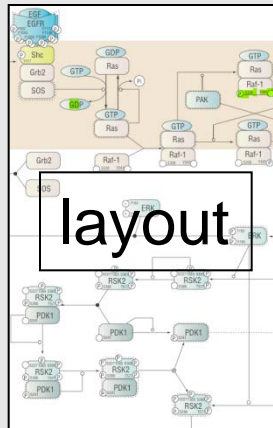
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 **Systems Biology
Markup Language**



comp

SBML Level 3



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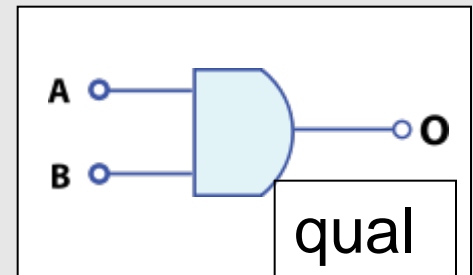
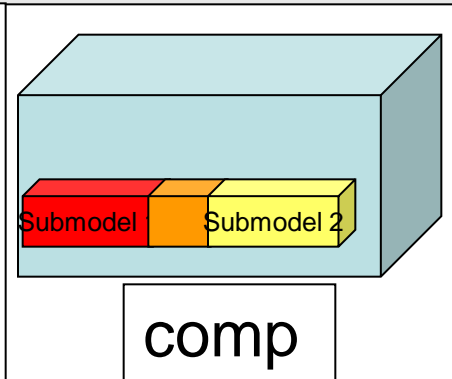
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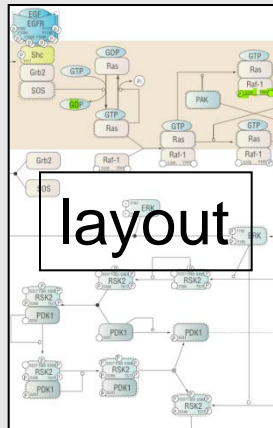
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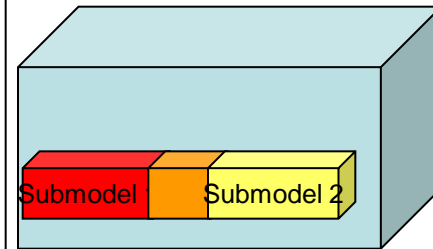
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 **Systems Biology
Markup Language**

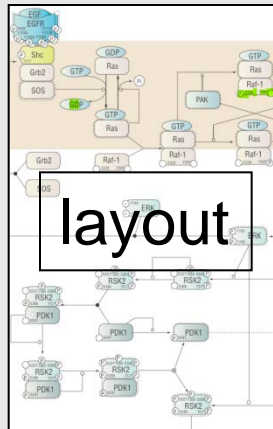
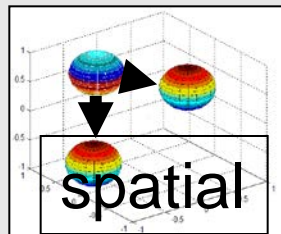


comp



qual

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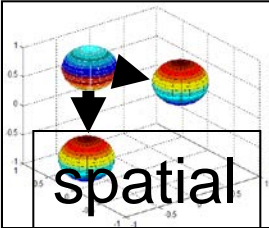

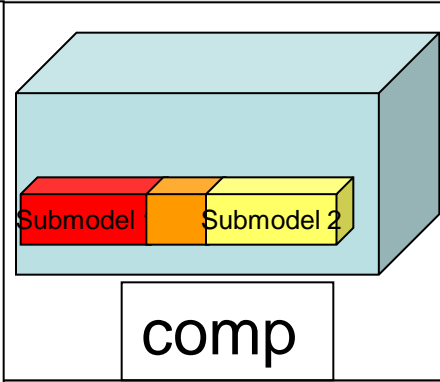
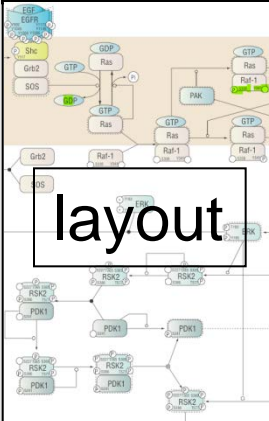
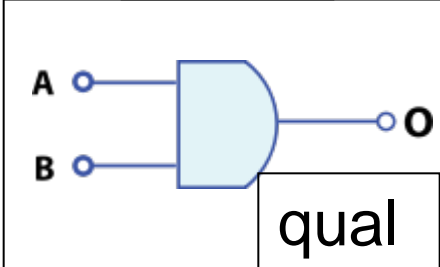
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SBML Systems Biology Markup Language

comp

qual

SBML Level 3

 <p>spatial</p>	<p>The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 1 Core</p> <p>Michael Hucka (Chair) <i>California Institute of Technology, US</i> Frank Bergmann <i>University of Washington, US</i> Stefan Hoops <i>Virginia Bioinformatics Institute, US</i> Sarah M. Keating <i>California Institute of Technology, US</i> Sven Sahle <i>University of Heidelberg, DE</i> Darren J. Wilkinson <i>Newcastle University, GB</i></p> <p>sbml-editors@sbml.org core SBML Level 3 Version 1 Core</p> <p>Release 1 (Candidate) 31 December 2009</p> <p>Please report errors, ambiguities, and other issues in this document using the form at http://sbml.org/specifications/sbml-level-3/version-1/core/issue-report-form</p> <p>Corrections and other changes to this SBML language specification may appear over time. Notifications of new releases are broadcast on the mailing list sbml-announce@sbml.org</p> <p>The latest release of the SBML Level 3 Version 1 Core specification is available at http://sbml.org/specifications/sbml-level-3/version-1/core</p> <p>This release of the specification is available at http://sbml.org/specifications/sbml-level-3/version-1/core/release-1/</p> <p>The list of known issues in all releases of SBML Level 3 Version 1 Core is available at http://sbml.org/specifications/sbml-level-3/version-1/core/errata/</p> <p>Formal schemas for use with XML are available at http://sbml.org/specifications/sbml-level-3/version-1/schemas/</p> <p> Systems Biology Markup Language</p>	 <p>Submodel Submodel 2</p> <p>comp</p>
 <p>layout</p>	 <p>A B O</p> <p>qual</p>	

possibly
necessary

SBML Level 3

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spatial

layout

comp

qual

Submodel 1 Submodel 2

A B

additional
information

mathematically necessary for
correct interpretation

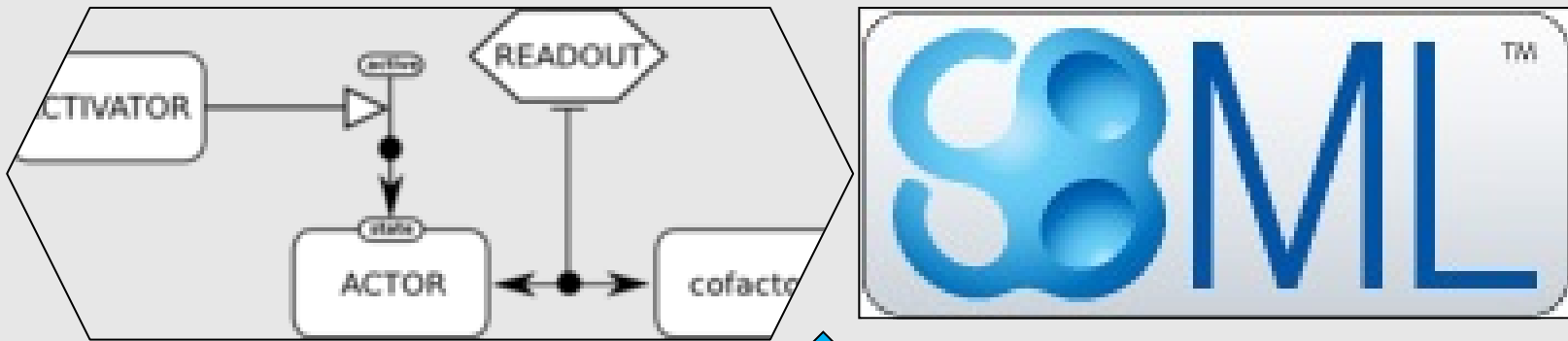
SBML Level 3

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L3 package development



Your model does not fit
with existing SBML

L3 package development

1. Propose a new package



L3 package development

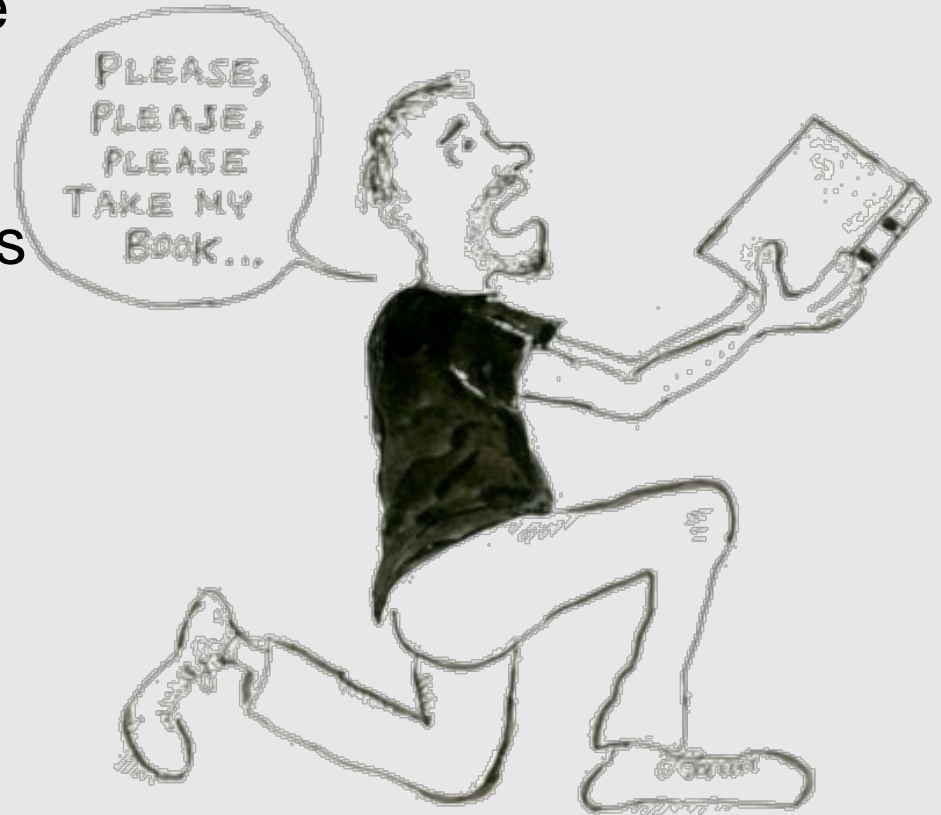
1. Propose a new package



2. Gather interested parties

L3 package development

1. Propose a new package
2. Gather interested parties
3. Write a proposal

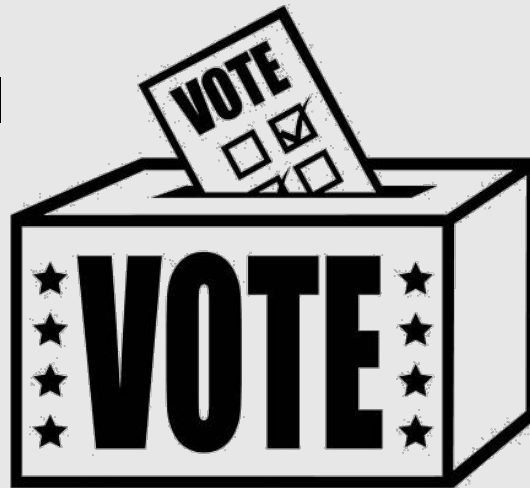


L3 package development

1. Propose a new package

2. Gather interested parties

3. Write a proposal



4. Community vote

L3 package development

1. Propose a new package
2. Gather interested parties
3. Write a proposal
4. Community vote

L3 package development

Voting criteria:

1. Address a problem that SBML users would find useful
2. Biological processes/phenomena
3. Extends SBML naturally from L3 core
4. Not a duplication of something existing

L3 package development



L3 package development

Package Working Group

- Mailing list open to anyone
- One or more of the original proposal authors
- One of the current SBML Editors

L3 package development



Two separate pieces of software that support the specification



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 **Systems Biology
Markup Language**

Formal specification

L3 package development

???

Formal specification

- use official SBML Level 3 package template
- include UML diagrams
- provide full explanation

L3 package development

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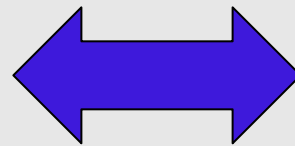
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 **Systems Biology
Markup Language**



**EXPECT
INTERACTION**

Two separate pieces of software that support the specification



Formal specification

L3 package development

Two separate pieces of software that support the specification

???

- manipulate constructs

NOT just store and retrieve

~~libS³ML~~

~~JS³ML~~

L3 package development

Two separate pieces of software that support the specification

???

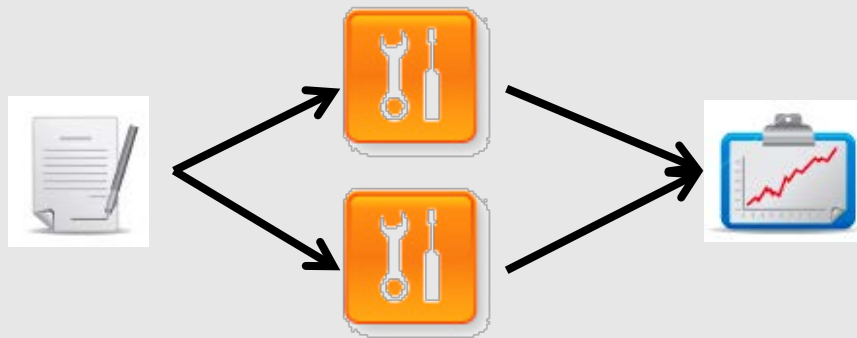
- each tool must **manipulate** a **majority** of the constructs
- between them they must manipulate ALL of the constructs

L3 package development

Two separate pieces of software that support the specification

???

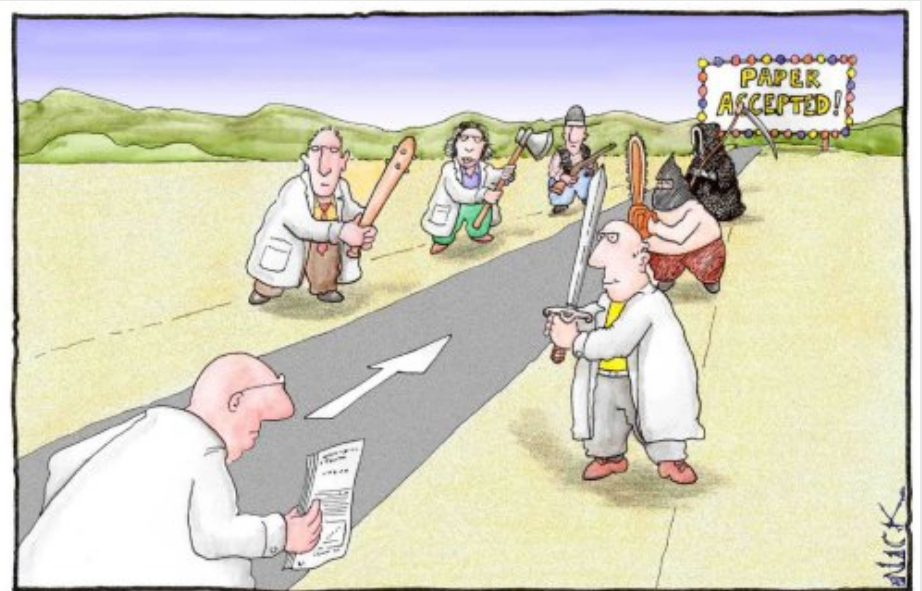
- test models and corresponding test results



(Best case scenario)

L3 package development

SBML Editors
review specification
and
implementations



Most scientists regarded the new streamlined peer-review process as 'quite an improvement.'

L3 package development



L3 package development

Full details of the process:

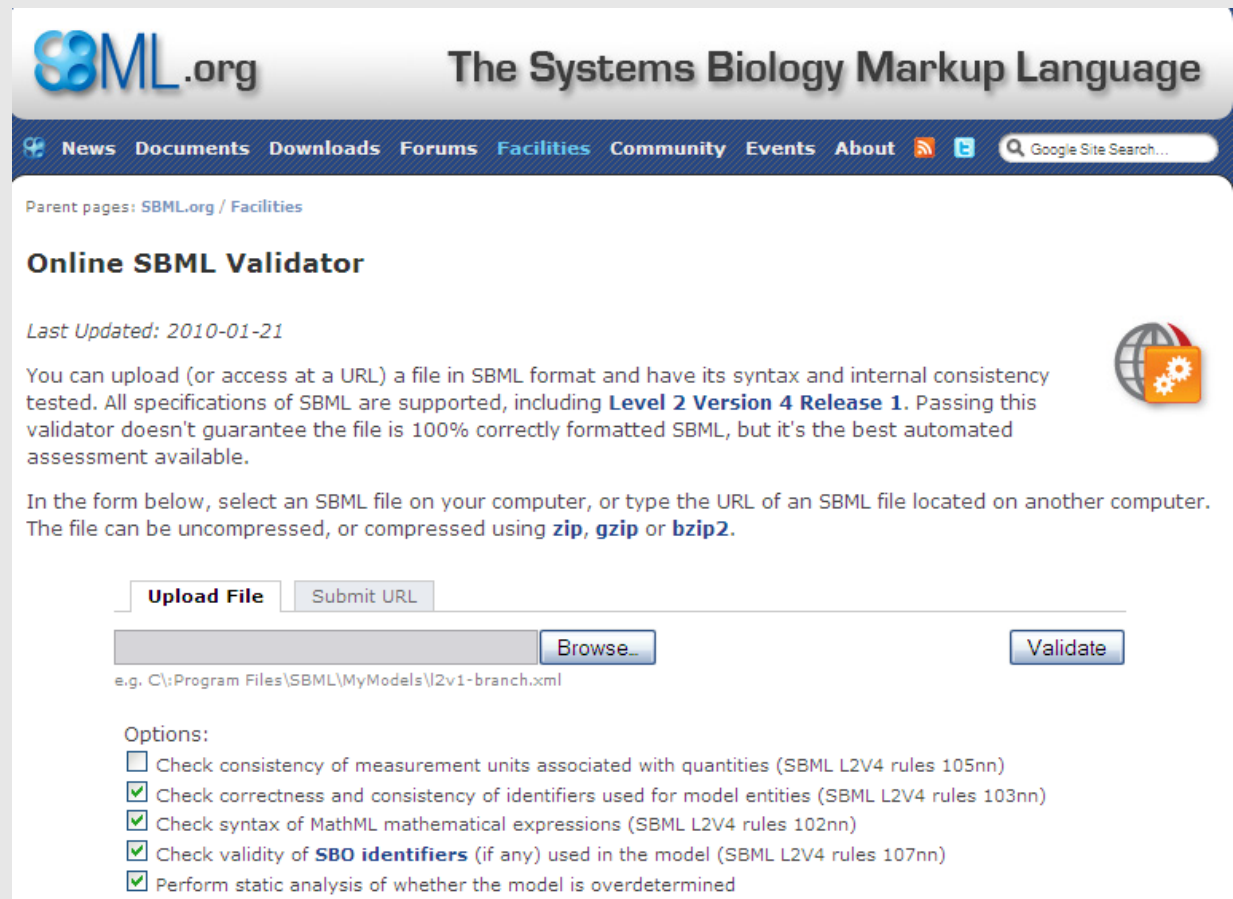
[http://sbml.org/Documents/SBML_Development_Process/
SBML_Development_Process_for_SBML_Level_3](http://sbml.org/Documents/SBML_Development_Process/SBML_Development_Process_for_SBML_Level_3)

Outline

1. Brief overview of what SBML is and why it was developed
2. Overview of SBML Level 3 modularisation
3. L3 package development
- 4. libSBML and L3 packages**
5. Links and acknowledgements

API library for working with SBML

- read
- create
- manipulate
- convert
- write
- validate



The screenshot shows the SBML.org website header with the logo and the text "The Systems Biology Markup Language". Below the header is a navigation menu with links for News, Documents, Downloads, Forums, Facilities, Community, Events, and About. A search bar is also present. The main content area is titled "Online SBML Validator" and includes a "Last Updated: 2010-01-21" date. The text describes the validator's capabilities, mentioning support for Level 2 Version 4 Release 1. A form for uploading a file or submitting a URL is shown, with a "Browse..." button and a "Validate" button. Below the form, there are options for validation, including checkboxes for checking consistency of measurement units, correctness and consistency of identifiers, syntax of MathML mathematical expressions, validity of SBO identifiers, and performing static analysis of whether the model is overdetermined.

SBML.org The Systems Biology Markup Language

News Documents Downloads Forums Facilities Community Events About

Parent pages: SBML.org / Facilities

Online SBML Validator

Last Updated: 2010-01-21

You can upload (or access at a URL) a file in SBML format and have its syntax and internal consistency tested. All specifications of SBML are supported, including **Level 2 Version 4 Release 1**. Passing this validator doesn't guarantee the file is 100% correctly formatted SBML, but it's the best automated assessment available.

In the form below, select an SBML file on your computer, or type the URL of an SBML file located on another computer. The file can be uncompressed, or compressed using **zip**, **gzip** or **bzip2**.

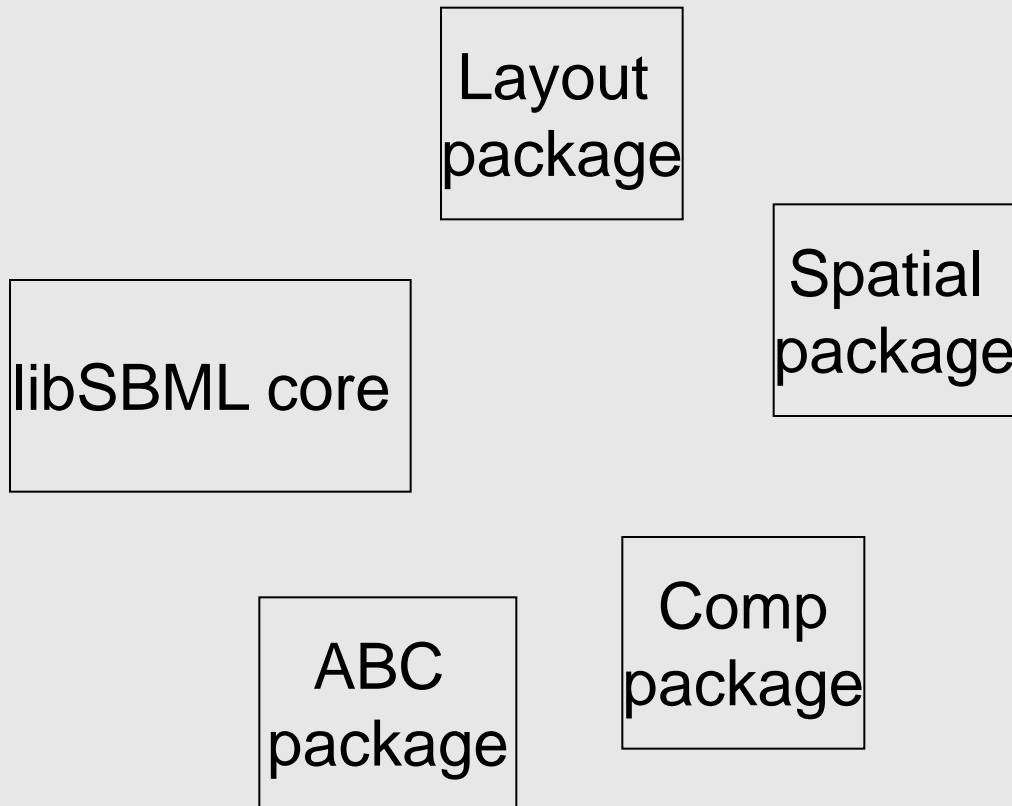
e.g. C:\Program Files\SBML\MyModels\l2v1-branch.xml

Options:

- Check consistency of measurement units associated with quantities (SBML L2V4 rules 105nn)
- Check correctness and consistency of identifiers used for model entities (SBML L2V4 rules 103nn)
- Check syntax of MathML mathematical expressions (SBML L2V4 rules 102nn)
- Check validity of **SBO identifiers** (if any) used in the model (SBML L2V4 rules 107nn)
- Perform static analysis of whether the model is overdetermined

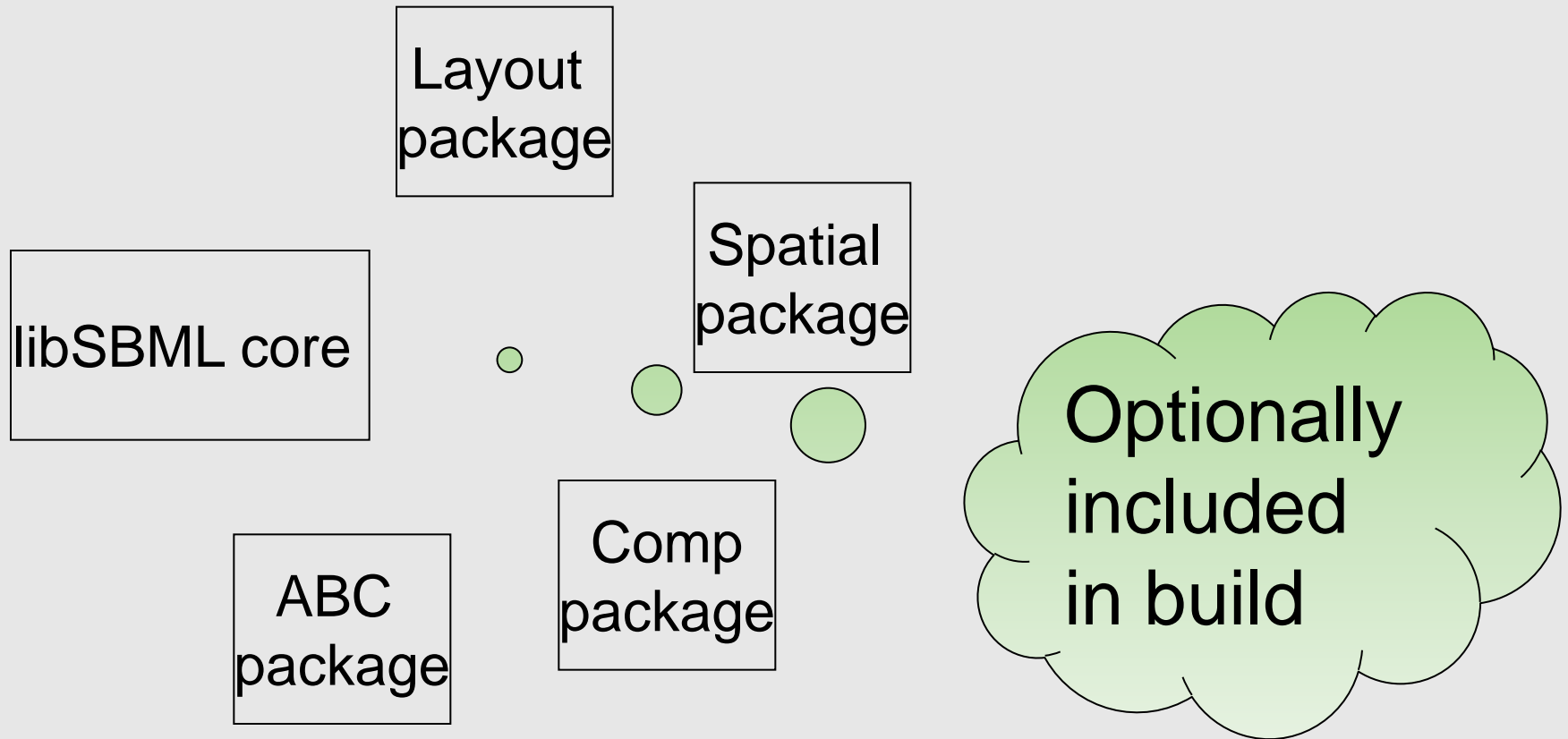
libSBML and L3 packages

libSBML-5

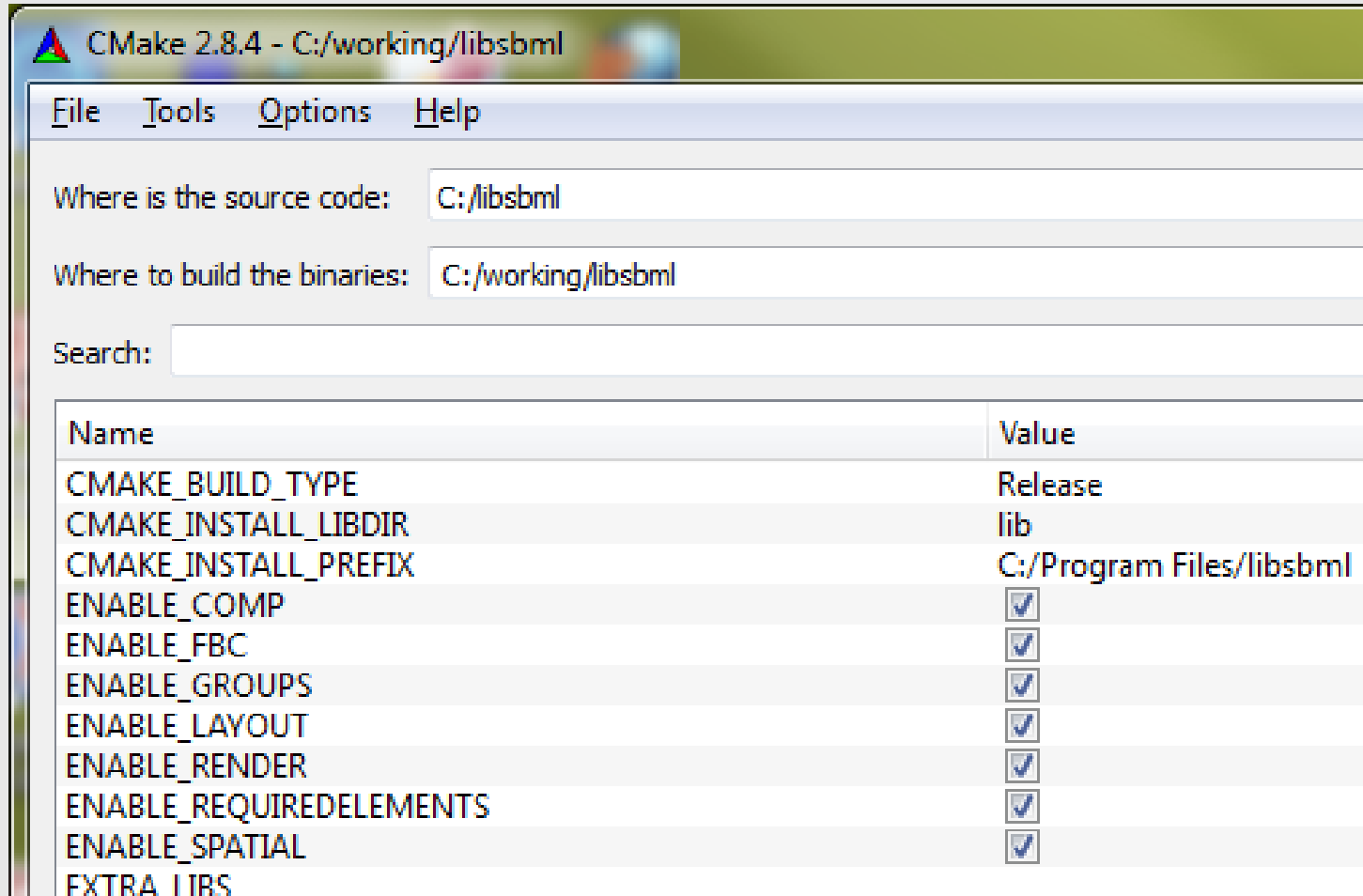


libSBML and L3 packages

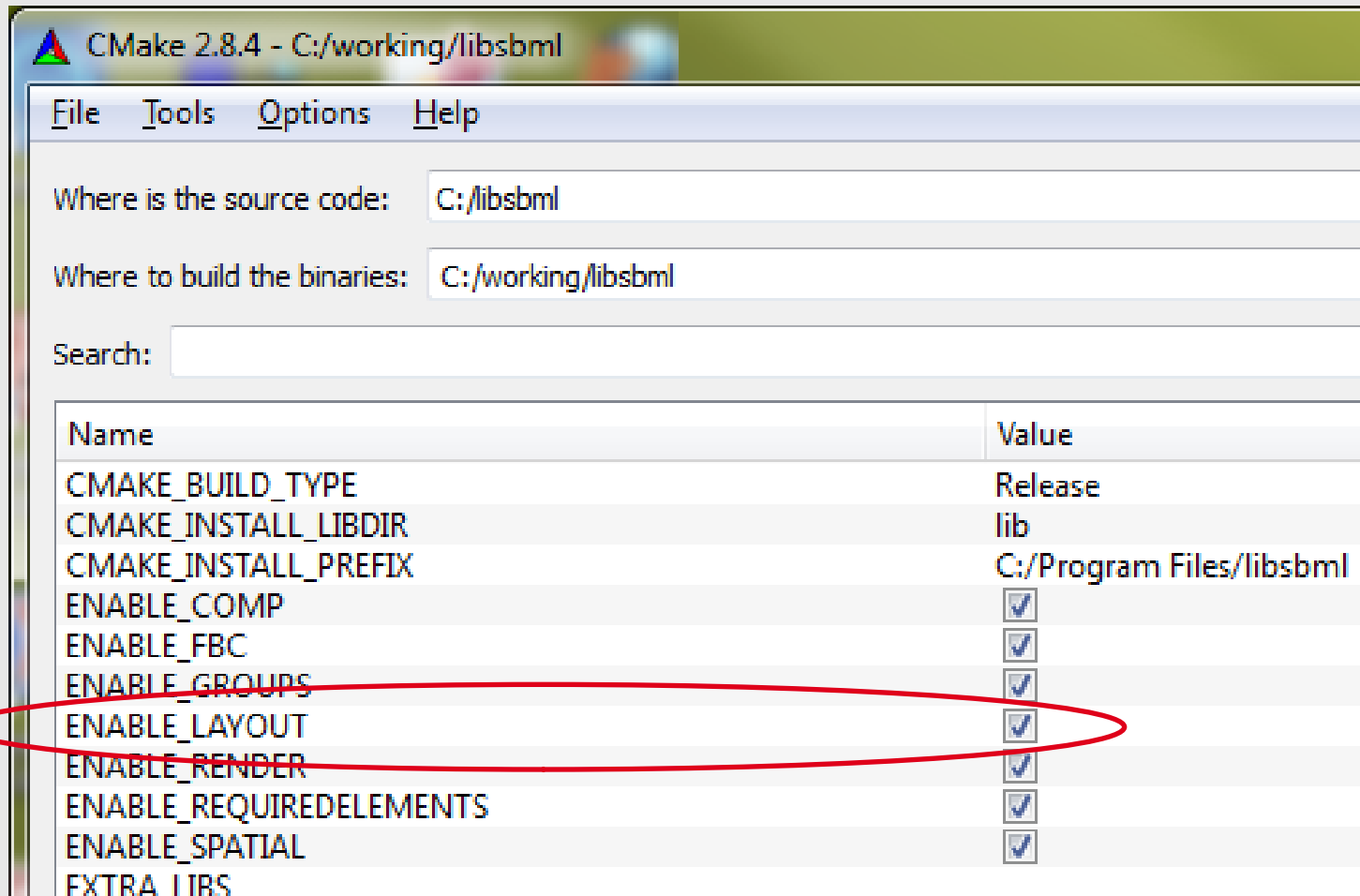
libSBML-5



libSBML and L3 packages



libSBML and L3 packages



libSBML-5

libSBML core
(very minor API changes from libSBML-4)

SBML
Extension

SBasePlugin

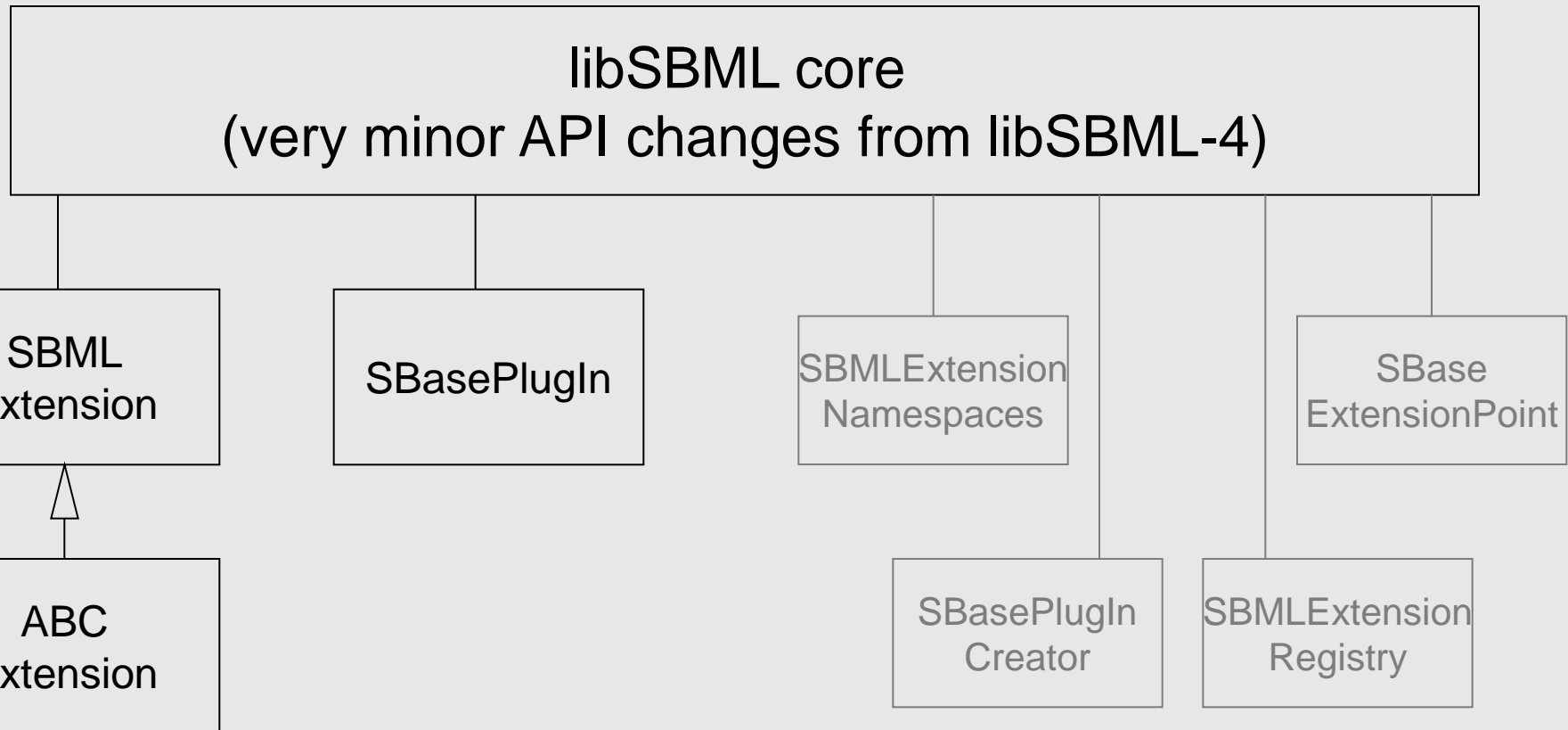
SBMLExtension
Namespaces

SBase
ExtensionPoint

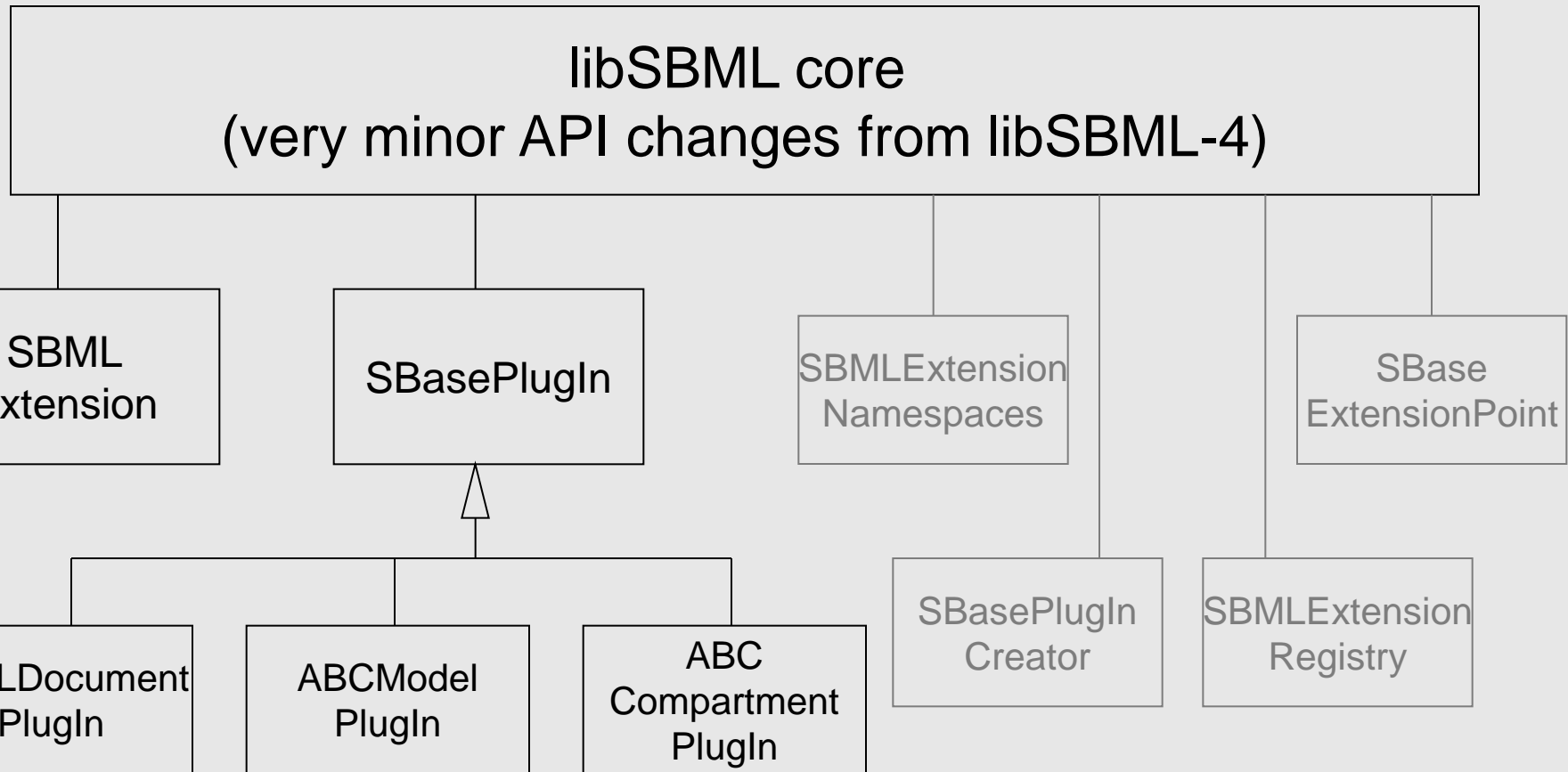
SBasePlugin
Creator

SBMLExtension
Registry

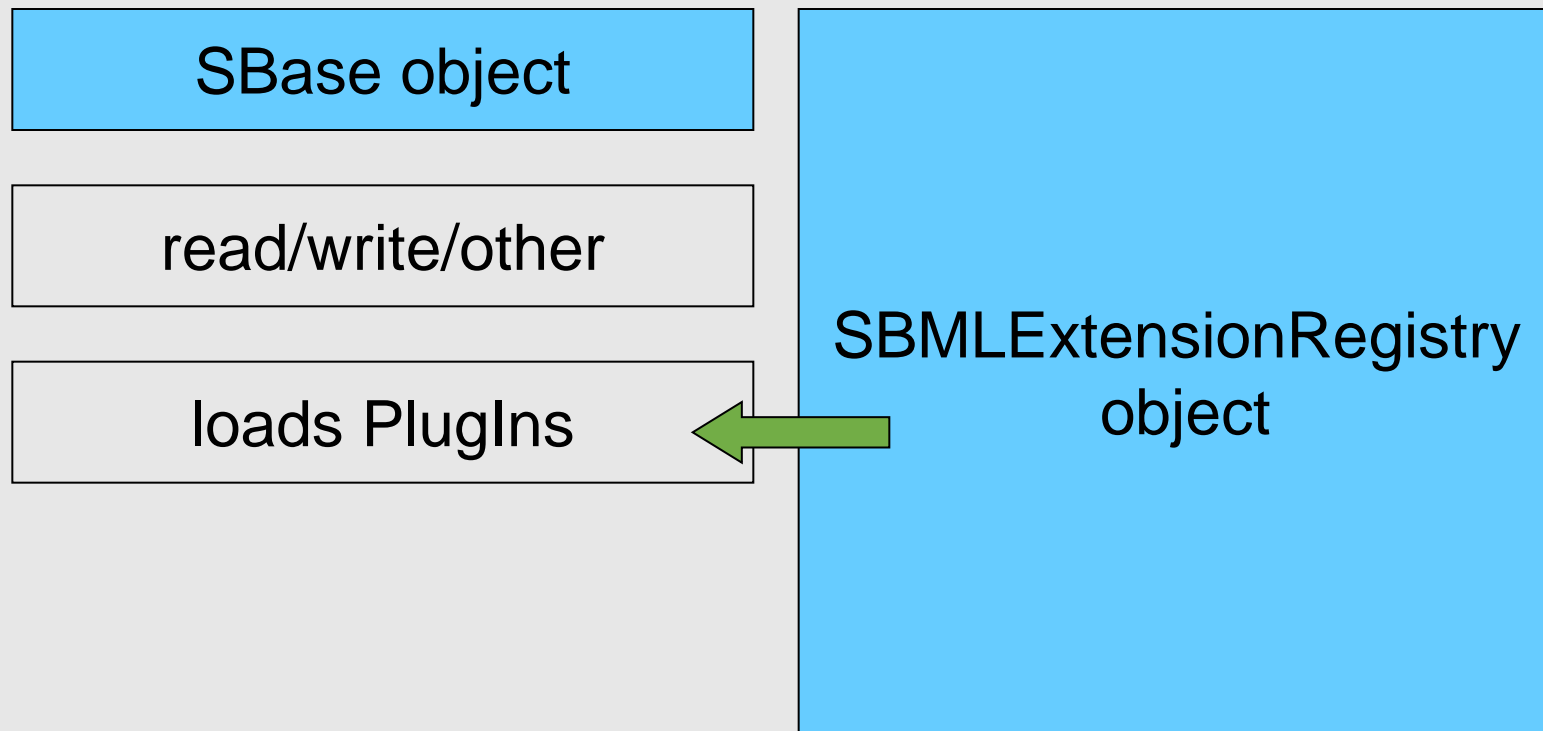
Implementing a package



Implementing a package



How does it work ?



Implementing a package



The Systems Biology Markup Language

News Documents Downloads Forums Facilities Community Events About   

Parent pages: [SBML.org](#) / [Software](#) / [libSBML](#)

Tutorials

The functionality of libSBML is difficult to capture in a single session.

Here we provide access to a number of presentations that deal with particular aspects of using libSBML together with some sample coding exercises (with answers). These are adapted versions of tutorials given in the past.

Presentations

Building and installing

This tutorial shows how to build and install libSBML.

Getting started with programming

Using MIRIAM annotations

Using MATLAB/Octave

L3 Package extensions

This tutorial deals with how to develop the plugin code that allows an SBML Level 3 package to be included with libSBML-5. It deals purely with the libSBML extension classes that register an extension and shows how to include an additional element and also an additional attribute with a core element.

<http://sbml.org/Software/libSBML/Tutorials>



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Links

<http://sbml.org>

Current L3 packages + status:

http://sbml.org/Community/Wiki#SBML_Level_3

Process for developing a package:

[http://sbml.org/Documents/SBML_Development_Process/
SBML_Development_Process_for_SBML_Level_3](http://sbml.org/Documents/SBML_Development_Process/SBML_Development_Process_for_SBML_Level_3)

libSBML tutorial:

<http://sbml.org/Software/libSBML/Tutorials>

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John Doyle; Hiroaki Kitano

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- ◉ JST ERATO-SORST Program (Japan)
- ◉ Japanese Ministry of Agriculture
- ◉ Japanese Ministry of Educ., Culture, Sports, Science and Tech.
- ◉ BBSRC e-Science Initiative (UK)
- ◉ DARPA IPTO Bio-SPICE Bio-Computation Program (USA)
- ◉ Air Force Office of Scientific Research (USA)
- ◉ STRI, University of Hertfordshire (UK)
- ◉ Beckman Institute, Caltech (USA)
- ◉ Molecular Sciences Institute (USA)