SBML status update

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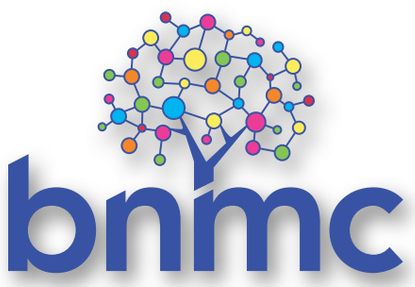


Outline

1. Status of the SBML specifications
2. Status of the SBML Level 3 packages
3. Status of the SBML Development Process
4. Status of the SBML Test Suite
5. Status of the SBML libraries

SBML = Systems Biology Markup Language

Format for representing quantitative models

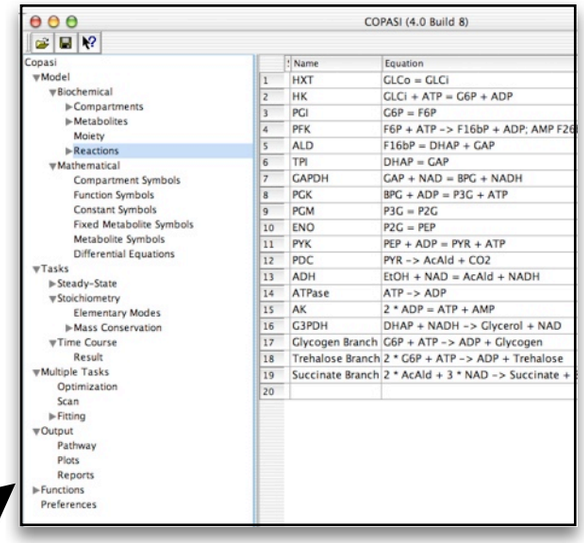
- Defines object model + rules for its use
  - Serialized to XML

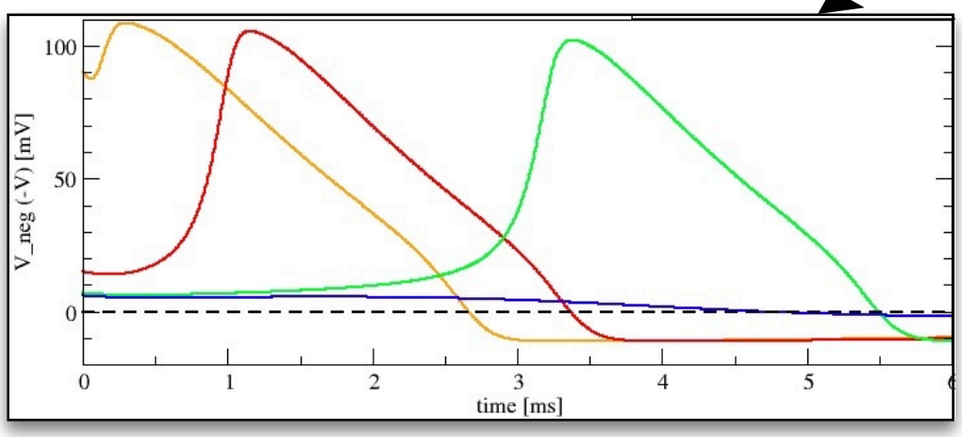
Neutral with respect to modeling framework

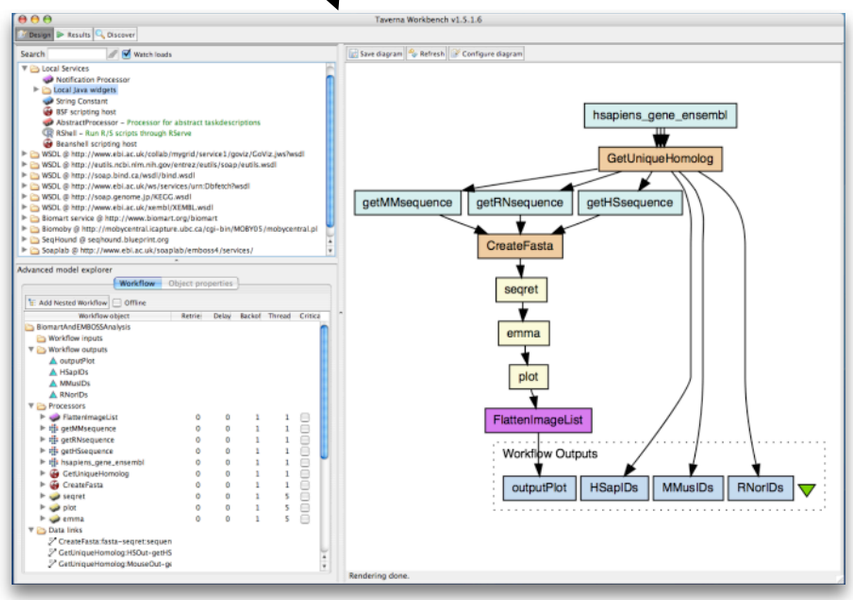
- ODE vs. stochastic vs. ...

A lingua franca for software

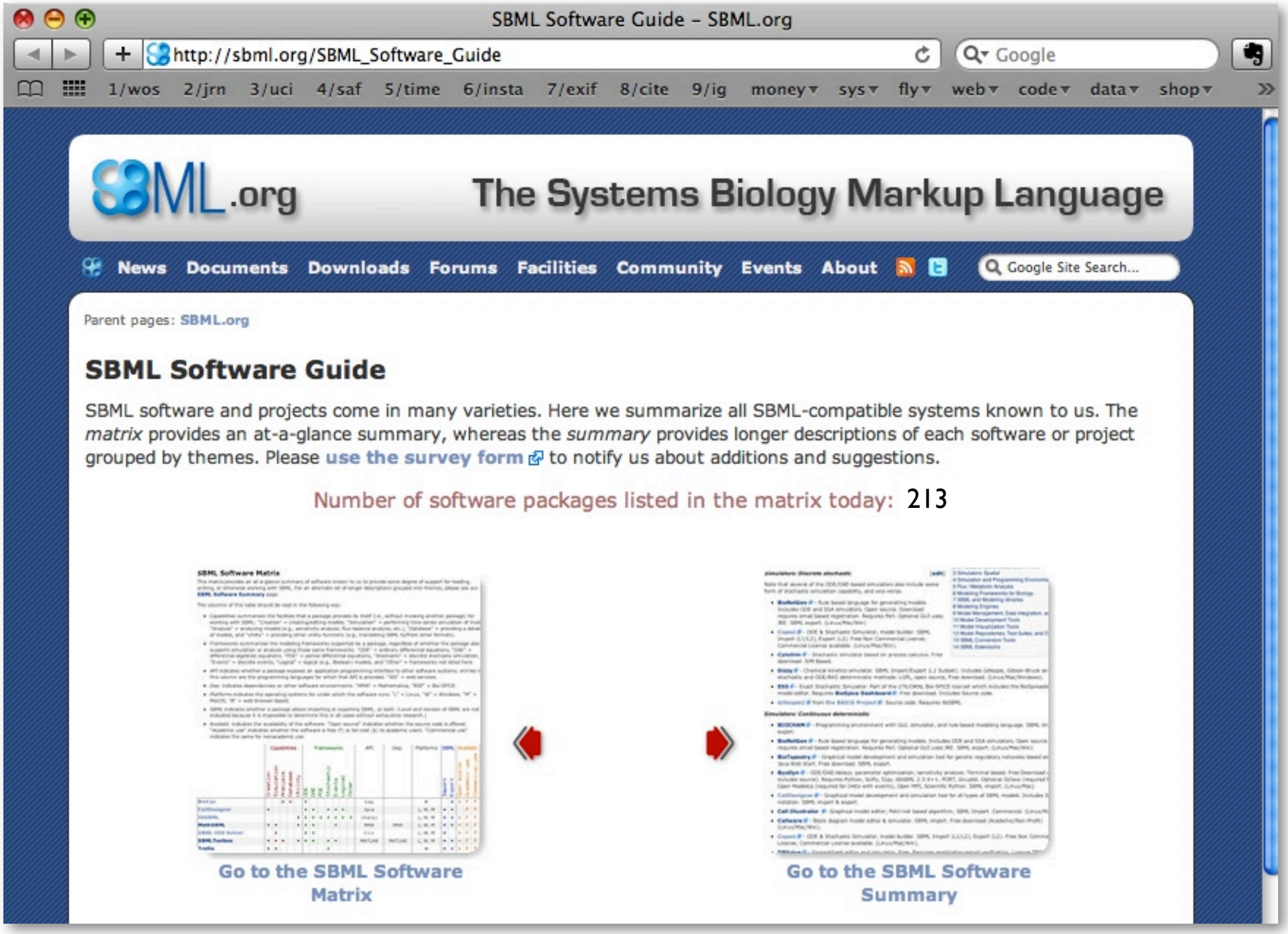
- Not procedural







For a list of tools, see the SBML Software Guide



Basic parts of SBML

The **reaction** is central: a process occurring at a given rate

- Participants are pools of entities (**species**)

$$n_a A + n_b B \xrightarrow{f([A],[B],[P],\ldots)} n_p P$$

$$n_c C \xrightarrow{f(\ldots)} n_d D + n_e E + n_f F$$

$$\vdots$$

Models can further include:

- Other constants & variables
- Compartments
- Explicit math
- Discontinuous events
- Unit definitions
- Annotations

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Can be anything conceptually compatible

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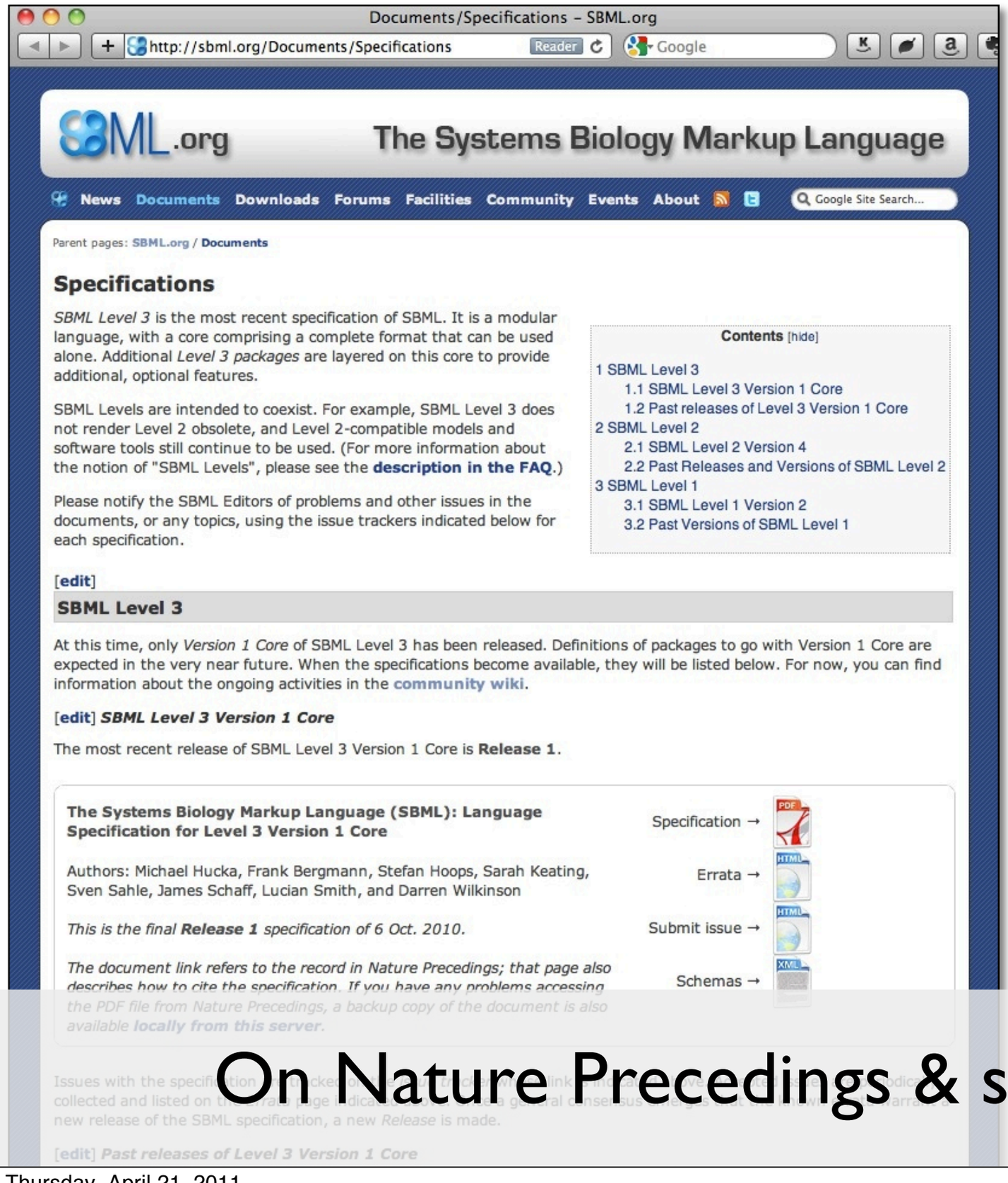
Current SBML specifications



Current specifications:

- **Level 3 Version 1 Core**
  - 6 Oct. 2010
- **Level 2 Version 4**
  - 22 Dec. 2008
- **Level 1 Version 2**
  - 28 Aug. 2003

On Nature Precedings & sbml.org/Documents

Evolution of features took time & practical experience

Level 1	Level 2	Level 3
predefined math functions	user-defined functions	user-defined functions
text-string math notation	MathML subset	MathML subset
reserved namespaces for annotations	no reserved namespaces for annotations	no reserved namespaces for annotations
no controlled annotation scheme	RDF-based controlled annotation scheme	RDF-based controlled annotation scheme
no discrete events	discrete events	discrete events
default values defined	default values defined	no default values
monolithic	monolithic	modular

Cannot keep growing the feature set indefinitely

SBML Level 3 is modular:

- "Core" defines common aspects
- "Packages" add optional features
  - Models declare which packages they use
  - Tools can tell their users which packages they support
- Analogy to XML — XML is core, then there's XPath, MathML, etc.

Rationale: even if a tool isn't equipped to handle a given package, probably can still interpret *some* aspects of the model

Additional expected benefit: decouple development of individual L3 pkgs

Level 3 package	Active?	libSBML 5 implementation?
Graph layout	✓	★
Groups	✓	★
Spatial	✓	★
Flux balance constraints	✓	★
Hierarchical composition	✓	★ (in progress)
Multicomponent species	✓	
Annotations	✓	
Graph rendering	✓	
Distribution & ranges	✓	
Qualitative models	✓	
Dynamic structures		
Arrays & sets		

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Storing model diagrams inside SBML files

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Grouping model entities together, for conceptual and annotation purposes

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2-D and 3-D spatial geometries and spatial processes

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Models composed of submodels

Level 3 package	Active?	libSBML 5 implementation?
Graph layout	✓	★
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A.k.a. steady-state models, flux balance analysis models

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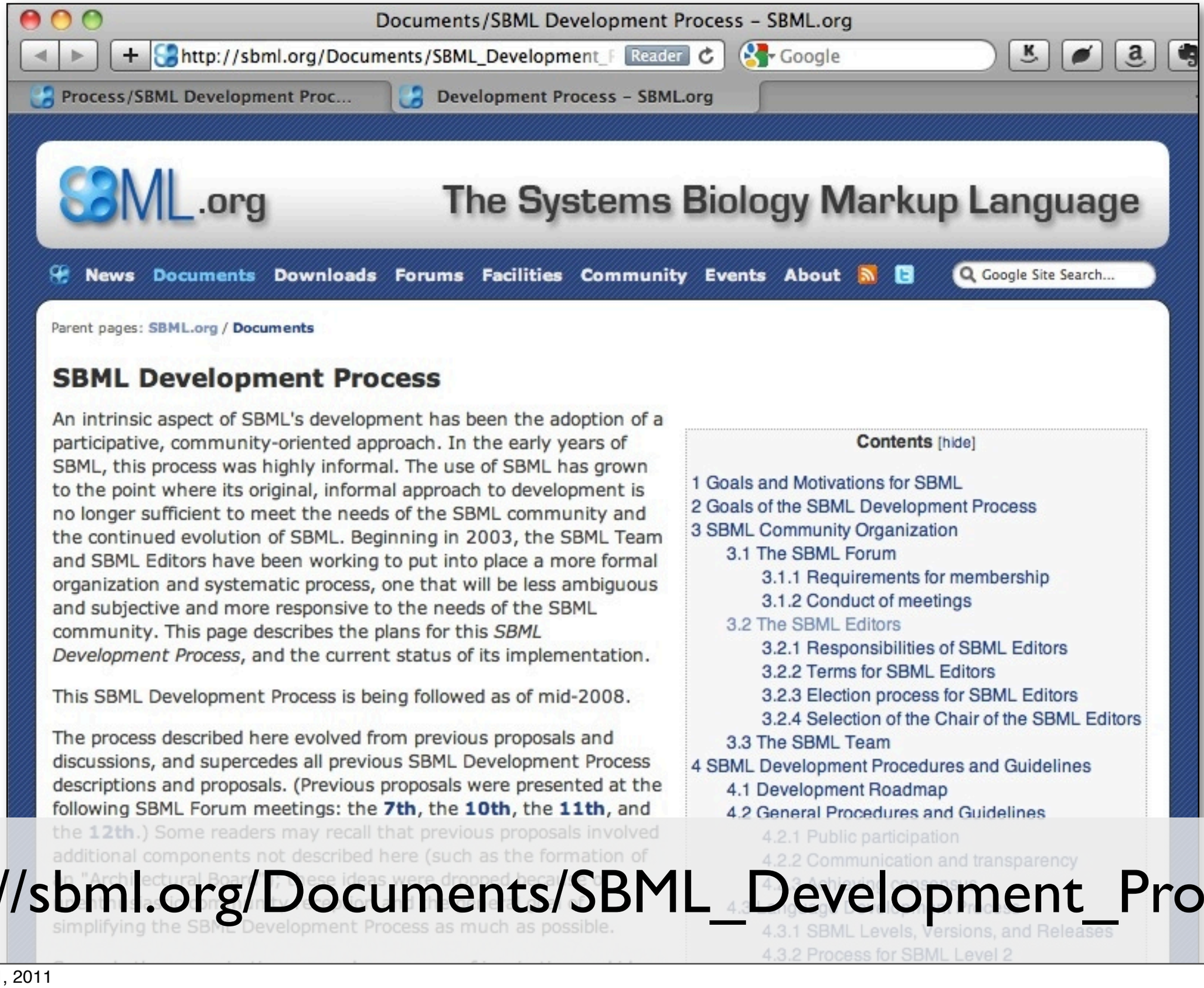
The excitement is palpable

Overheard at this meeting:

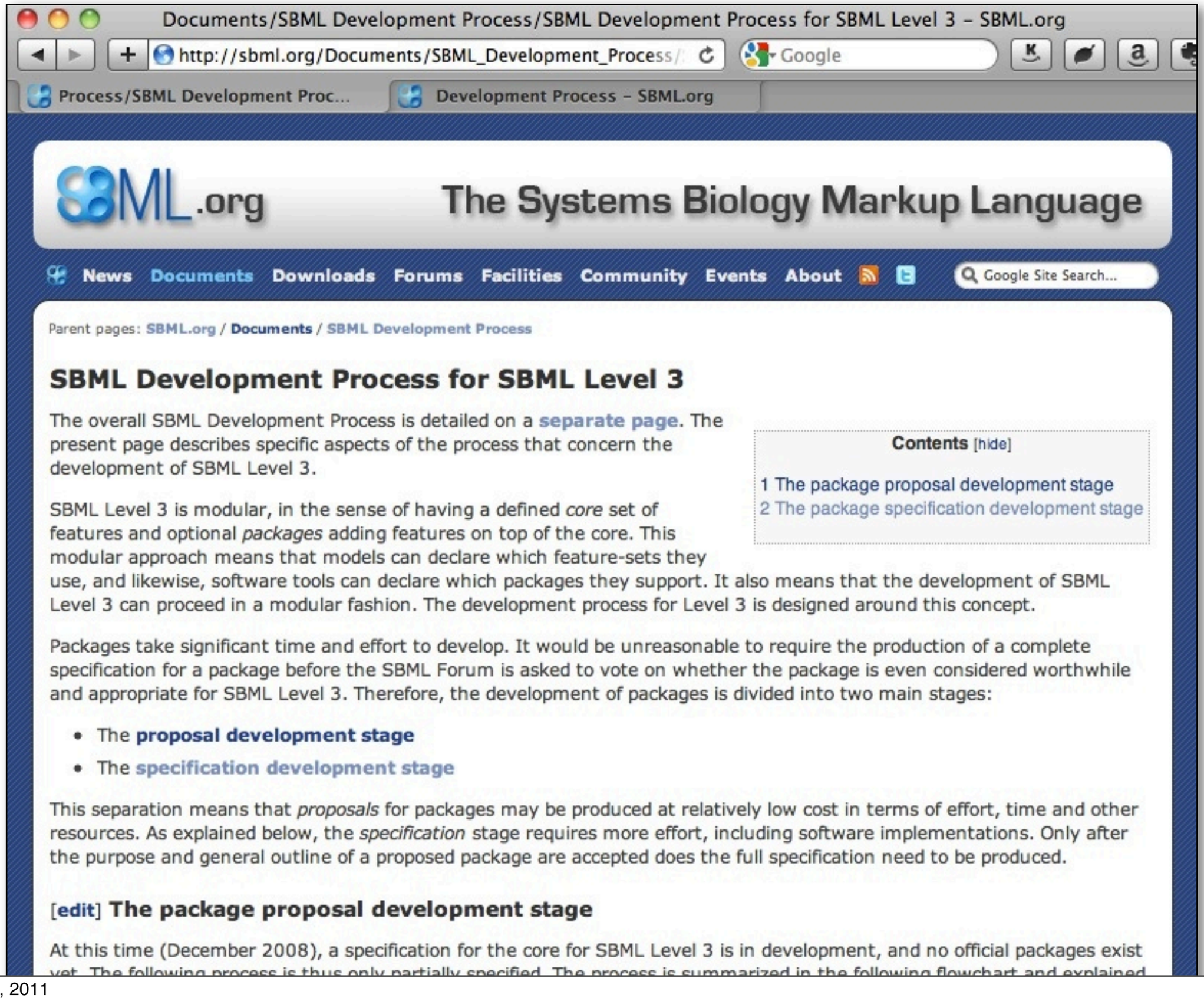
- "There's been a massive appearance of packages overnight!"
- "This package stuff is really easy. It's almost as if you planned it."

SBML Development Process Progress



http://sbml.org/Documents/SBML_Development_Process

Elaboration of process for Level 3 packages



Documents/SBML Development Process/SBML Development Process for SBML Level 3 – SBML.org

http://sbml.org/Documents/SBML_Development_Process/

3. The proposal voting/selection stage:
   a. After the period of discussion described in (2.d), either the proposer(s), or the SBML Editors, can call for a formal vote on whether the proposal should be pursued further. The timing and other conditions for issuing a vote are left to the judgment of the SBML Editors. The request can be made by posting a public request on **sbml-discuss** or by contacting the SBML Editors directly.
   b. The SBML Editors will construct a survey for the purpose of holding a public vote on the proposal. The survey will allow members of the SBML community to indicate one of 3 choices: (i) *accept*: the proposal addresses a need that SBML should cover, and proposes a reasonable method of doing so; (ii) *revise*: the proposal addresses a need that SBML should cover, but the proposed approach is not considered desirable, and a different attempt should be made; (iii) *reject*: the proposal does not address a need that SBML should cover.
      - The voting form may also contain the option for voters to sign up for the relevant *Package Working Group* (PWG) described in (3.e) below.
   c. The Chair of the SBML Editors will issue the call for votes. A *minimum* period of 2 weeks will be given before the vote is closed to give the SBML community sufficient time to evaluate the technical aspects of the proposal. At the Chair's discretion, a longer period may be chosen if it is deemed to be warranted.
   d. At the end of the voting period, the SBML Editors will report the outcome publicly.
      - For the decision to be (i) *accept*, 50% or more of the voters must choose the *accept* option.
      - For the decision to be (iii) *reject*, more than 50% of the voters must choose the *reject option*.
      - Any other outcome is deemed equivalent to (ii) *revise*.
   e. If the outcome of the previous step is not *reject*, the SBML Editors will proceed to form a Package Working Group (PWG) consisting of at least one of the package proposers, at least one SBML Editor, and any other members of the **sbml-discuss** mailing list who request to be part of the PWG. The Editors will further create a mailing list that will serve as both a basic notification/communication mechanism as well as a membership list for the PWG. The Editors will announce the formation of the PWG on the **sbml-discuss** mailing, and optionally via other means.
      - The mailing list shall have the name `sbml-label`, where `label` is the short-form label for the package. (Example: `sbml-multi`.)
      - In recognition of the fact that many package proposals were in existence for some years before these SBML process rules were created, and have achieved a type of de facto acceptance in the SBML community as being desirable packages, the formation of the PWG for these existing packages may be initiated at the same time as the call for votes described in (3.c). The justification is that the probability of these package proposals being ultimately rejected is considered low enough that the effort of creating the PWG is warranted: in other words, it appears clear that the packages are desired by the SBML community and what remains is to work out the details of their formulations. The packages recognized under these terms are the following (listed here using their short labels): `layout`, `render`, `multi`, `comp`, `qual`, `distrib`, `spatial`, `geom`, `arrays`, `dyn` [illegible] proposal, it merely hastens the formation of the PWG. This is viewed as desirable to help the process of working out the details with a larger group of interested participants.

Steps 3 & 4 of *package proposal development stage* fleshed out

Notable parts elaborated

Voting/acceptance of package **proposals** (note: not the specifications)

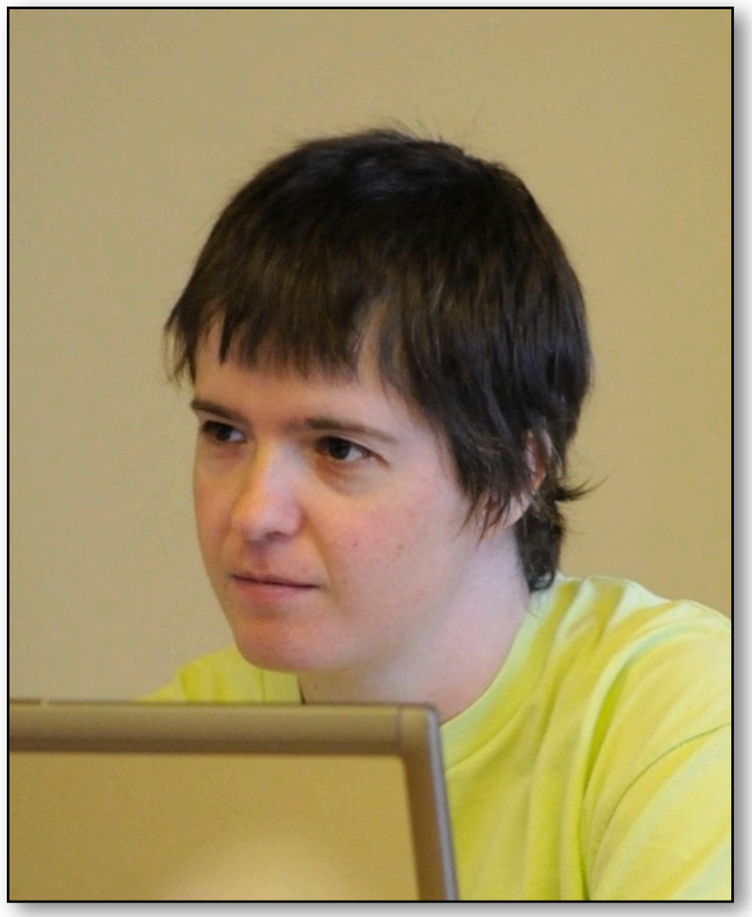
- Call for votes for existing package proposals will be issued within a matter of days

Introduction of *Package Working Groups* (PWGs)

- Group members will be
  - At least one author of the package proposal
  - At least one SBML Editor
  - Optionally, other interested persons
- Call for joining PWG will be issued for existing proposals with upcoming call for votes

New SBML Editors for 2011

Sarah Keating



Chris Myers

Status of the SBML Test Suite

Since COMBINE 2010:

- 65 new test cases
  - Includes tests for new Event features such as "persistence"
- Where possible, case results determined using analytical solutions

So far this year: informal alpha release of cases provided to some groups

- 2 groups reported tests were critical to correcting defects in their sw

Next steps:

- New test case archive + updated online system: within days of today
  - Will include SED-ML files
- Standalone test system to be rewritten after this meeting
  - Previous system to be replaced by Frank's more feature-rich system

Status of SBML libraries

libSBML version 5 (full featured, many language interfaces, validation, etc.)

JSBML version 0.8 (lean, mean, pure Java machine)

— Watch the next two presentations —