SBML L3v2 proposed changes

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L3v2 changes

- Typos, unclear sections, etc.
- Design changes

No more required children

▸ ListOf's may be empty

▸ Reactions may have no reactants or products

▸ All <math> children are optional

▸ The <model> is optional

▸ The event trigger is optional

No more required children

- Justifications:
  - A package may define what is missing (i.e. distrib with function definition math)
  - The modeler may not have that information, but still want to add annotations (i.e. kinetic laws)
- Controversy/Difficulty
  - Valid models may no longer have expected children; will require software to check 'isSetX' more often.

Add 'id' (and 'name') to SBase

- InitialAssignment
- Rule
- Trigger
- Priority
- Delay
- EventAssignment
- Constraint
- All ListOf- elements
- All package elements

Add an 'id' to things that lack it

- Justification:
  - Many packages have different reasons to refer to elements, such as comp (for deletions/replacements) and layout (for display).

- Controversy/Difficulty
  - Existing packages with 'package:id' attributes will have to change to 'id' attributes instead (but SId/PortSId/SpId/etc. scoping may remain unchanged).

Allow some SIdRefs to reference package IDs

- symbol/variable of:
    - AssignmentRule
    - RateRule
    - InitialAssignment
    - EventAssignment
- Any <ci> element
- Referent must have mathematical meaning
- Package not understood = rule not understood

Allow some SIdRefs to reference package IDs

- *NOT:*
  - 'compartment' of Species
  - 'compartment' of Reaction
  - 'species' of SimpleSpeciesReference
  - 'conversionFactor' of Model
  - 'conversionFactor' of Species

Allow some SIdRefs to reference package IDs

▸ Justification:
  ▸ Much easier to change and use package variables if one can reference them directly.
  ▸ Still defines 'fallback' method for when package is not understood ('just ignore it', in most cases).

▸ Controversy/Difficulty
  ▸ Negates old 'validity after reduction' principle.
  ▸ Makes some work of 'spatial' moot (sorry, Jim)

Deprecate 'fast' flag

- If a model has a Reaction with 'fast=true', they get a validation warning
- Future versions of SBML will not have the construct

Deprecate 'fast' flag

- Justification:
  - Only limited existing support
  - Equivalent analysis can be obtained by actual time separation of KineticLaws.

- Controversy/Difficulty
  - Odd to 'deprecate' a required attribute; actually only deprecating the attribute with a value of 'true'.

Create 'rateOf' csymbol

- 'rateOf(x)' means 'dX/dt' **if** X is not solved by an Assignment Rule or an Algebraic Rule, or is a Reaction ID.
- Full differentiation reserved for a package

Create 'rateOf' csymbol

- Justification:
  - Many models use rates of change as independent variables in some equations.
  - A form of 'dX/dt' (often extended function definitions) already in use in tools such as Copasi.
- Controversy/Difficulty:
  - Limitations might be awkward.

New mathML elements

- Old discussions:
  - sbml-discuss: http://sbml.org/Forums/index.php?t=msg&th=2154&rid=0#msg_7991
  - HARMONY 2014: http://www.co.mbine.org/sites/combine/files/harmony2014/2014-04-25-sbml-myers.mov
  - SBML tracker: https://sourceforge.net/p/sbml/sbml-specifications/229/
- Editorial vote: split
  - Only add quotient, rem, max, min, and implies: 3 votes
  - Add everything discussed at HARMONY 2014: 2 votes
  - Either way, add other MathML in MathML-specific packages.

New mathML elements

- Justification:
  - Add all elements that are both easy and potentially useful.
  - Leave for packages all elements that are hard and/or have no clear use-case.
- Controversy/Difficulty
  - Reduces to:
    - Who is SBML's audience? (users/developers; what fields they are from)
    - What is our relationship with other standards?
    - Should SBML be an intersection or a union?

Allow Recursion?

- In FunctionDefinitions:
  - https://sourceforge.net/p/sbml/sbml-specifications/260/
- In AssignmentRules:
  - https://sourceforge.net/p/sbml/sbml-specifications/269/
- Rejected (3:2), but could be revisited

More details at
http://sbml.org/Events/SBML_Editors%27_Meetings/During_HARMONY_2012_05_20/Summary

L3v2 tracker items:
https://sourceforge.net/p/sbml/sbml-specifications/search/?q=labels%3A%22Level+3+Version+1+Core%22