

# SBML Level 3 Math Packages

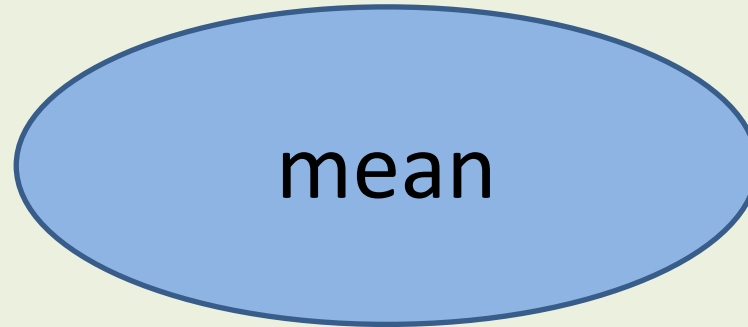
Sarah Keating

# Math in SBML

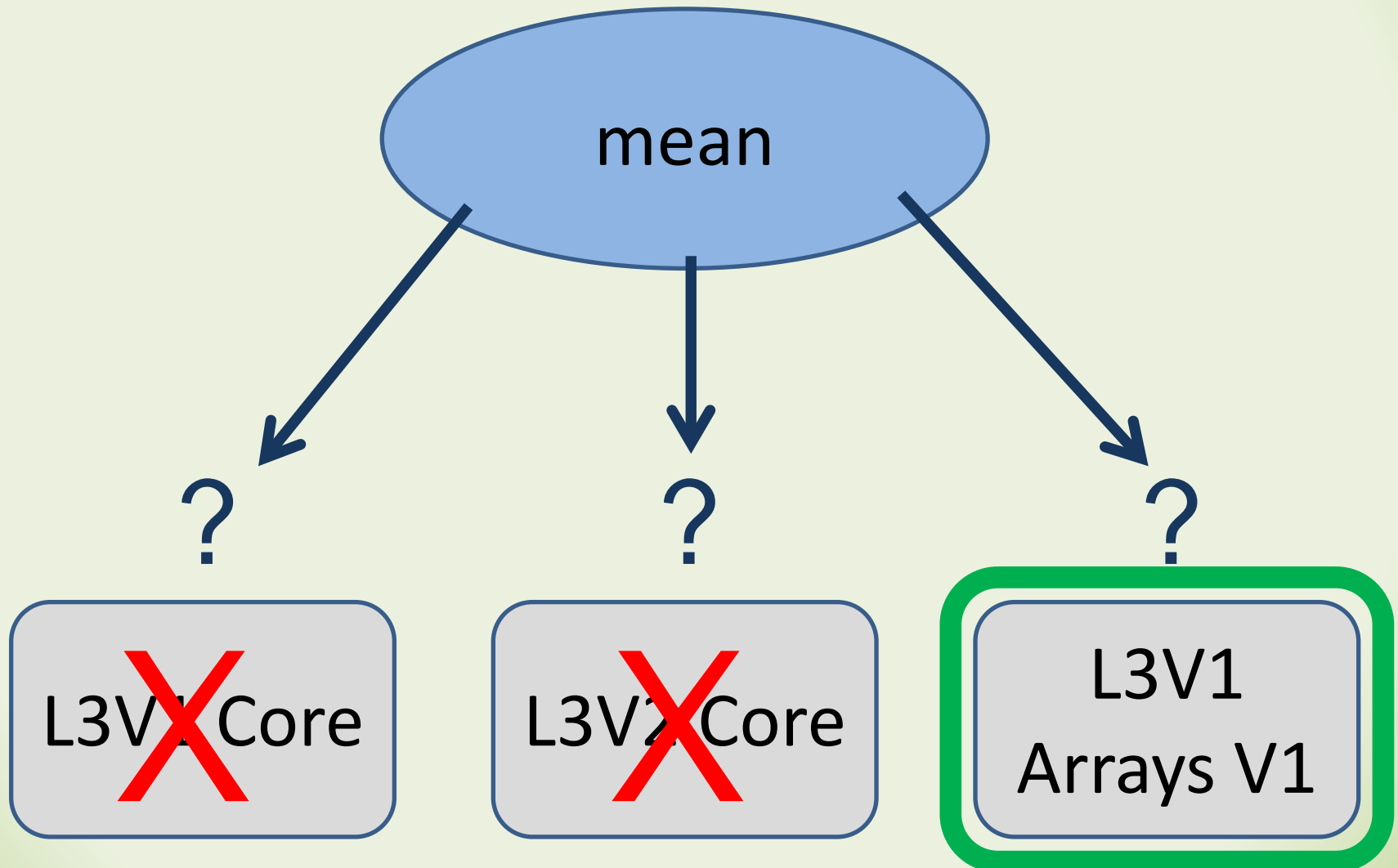
- Limited subset of MathML
- L3V2 core may add further constructs
- Packages can add MathML as needed

***Status Quo***

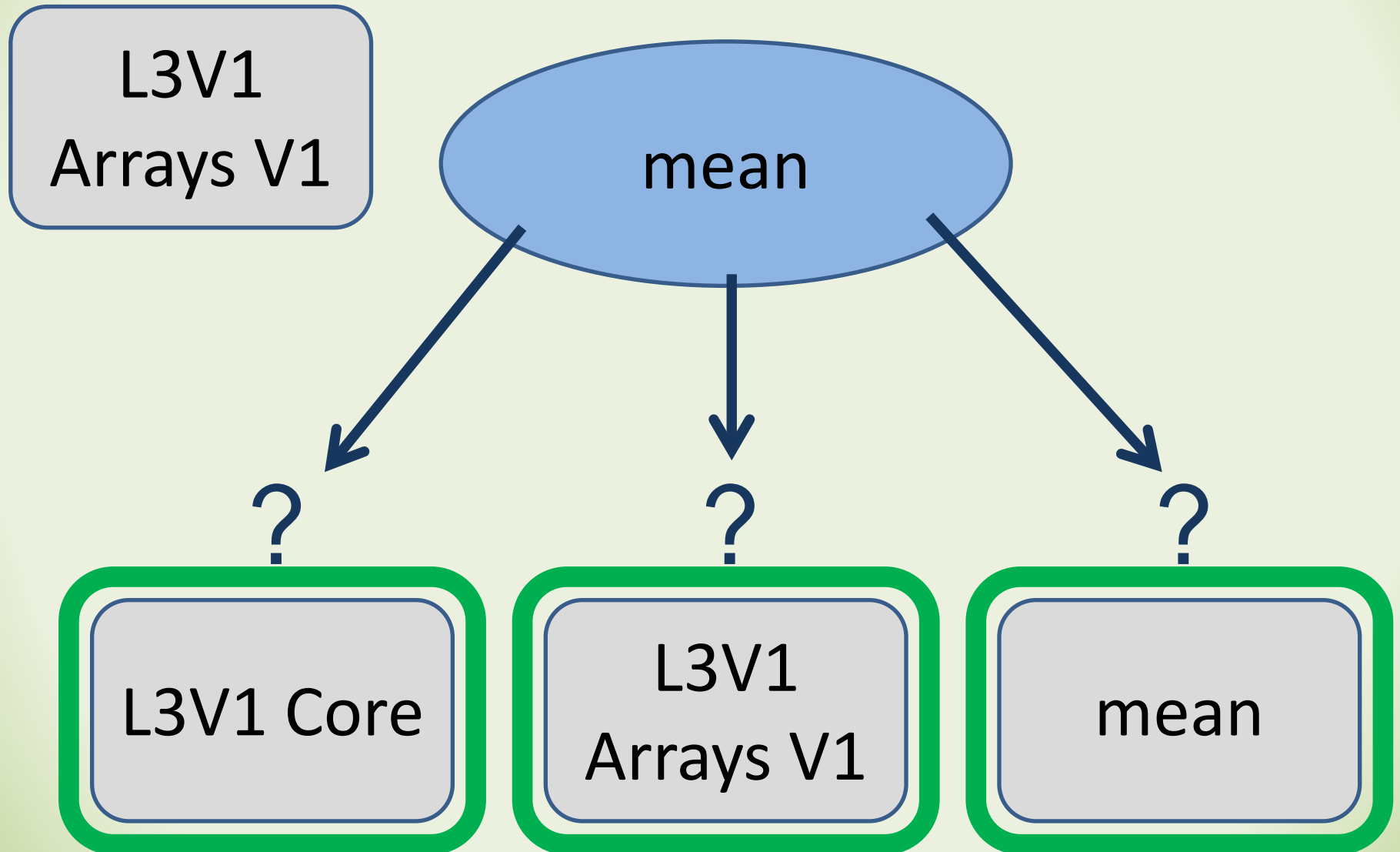
# Need to use a math construct



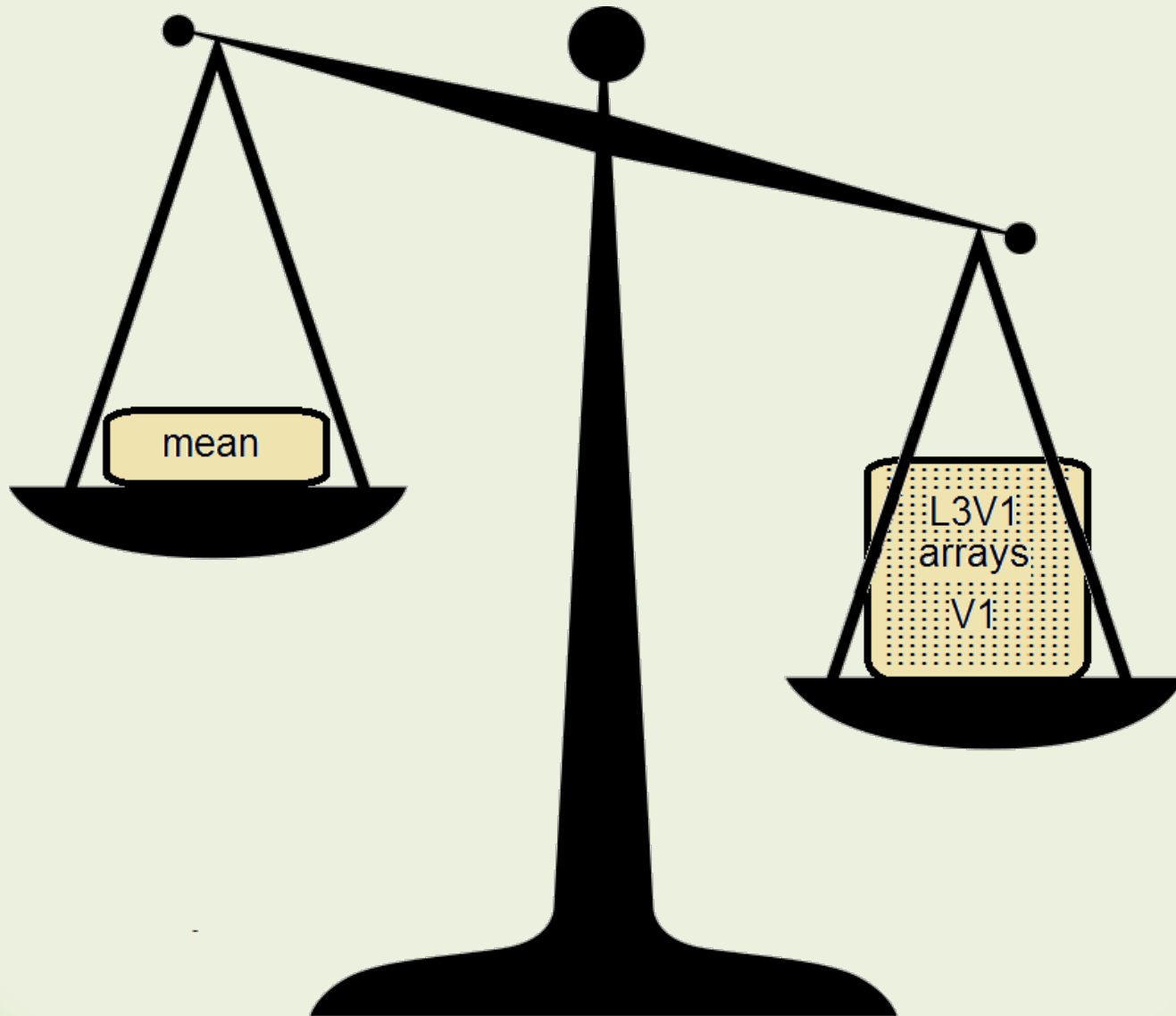
# Where is it specified ?



# Software supporting it ?



# Software wanting to support it ?



# SBML Level 3 Packages

| Package name & link to info page                               | Label   | Description   | Status          |
|--|---------|---|-----------------|
| <b>Annotations</b> <a href="#">↗</a>                           | annot   | Support for richer annotation syntax than the regular annotations in SBML Level 3 Core  | Stalled         |
| <b>Arrays</b> <a href="#">↗</a>                                | arrays  | Support for expressing arrays of things   | Draft available |
| <b>Hierarchical Model Composition</b> <a href="#">↗</a>        | comp    | A means for defining how a model is composed from other models  | Released        |
| <b>Distributions</b> <a href="#">↗</a>                         | distrib | Support for encoding models that sample values from statistical distributions   | Draft available |
| <b>Dynamic Structures</b> <a href="#">↗</a>                    | dyn     | Support for creating and destroying entities during a simulation  | Stalled         |
| <b>Flux Balance Constraints</b> <a href="#">↗</a>              | fbc     | Support for constraint-based (a.k.a. steady-state) models   | Released        |
| <b>Groups</b> <a href="#">↗</a>                                | groups  | A means for grouping elements   | Draft available |
| <b>Layout</b> <a href="#">↗</a>                                | layout  | Support for storing the spatial topology of a network diagram; adjunct to the render package  | Released        |
| <b>Multistate and Multicomponent Species</b> <a href="#">↗</a> | multi   | Object structures for representing entity pools with multiple states and composed of multiple components, and reaction rules involving them | Draft available |
| <b>Qualitative Models</b> <a href="#">↗</a>                    | qual    | Support for models wherein species do not represent quantity of matter & processes are not reactions per se                                 | Released        |
| <b>Rendering</b> <a href="#">↗</a>                             | render  | Support for defining the graphical symbols and glyphs used in a diagram of the model; adjunct to the layout package                         | Draft available |
| <b>Required Elements</b> <a href="#">↗</a>                     | req     | Support for fine-grained indication of SBML elements that have been changed by the presence of another package                              | Draft available |
| <b>Spatial Processes</b> <a href="#">↗</a>                     | spatial | Support for describing processes that involve a spatial component, and describing the geometries involved                                   | Draft available |

# Limited subset of MathML





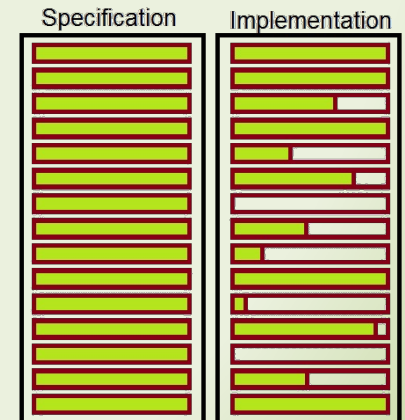
# Way forward ...

- Allow any MathML



# Huge burden on software development

# Mismatch between specification and implementation



# Way forward ...

- Allow any MathML
- Put useful functions into L3V2 core

Discussed at  
HARMONY



# Radical thought ...

Create  
several small  
math only  
packages



# Radical thought ...

- Group similar MathML constructs into small math package
  - e.g. vectors/stats
- Core/Packages do not extend MathML
  - depend on necessary math package
  - e.g. arrays would depend on ‘vectors’

# Advantages

- Any math construct is only defined once but can be used by any package that requires it
- Additional math in packages would be usable with L3V1
- Developers will have smaller targets to support

# Possible packages

## Additional content elements

interval

## Extra arithmetic

quotient (L3V2?)

max

min

rem (L3V2?)

implies (L3V2?)

gcd

lcm (MathML 2.0)

## Extra logic

condition

forall

exists

## Theory of sets

emptyset (MathML2.0) set

list union

intersect in

notin subset

prsubset notsubset

notprsubset setdiff

card (MathML 2.0)

cartesianproduct (MathML 2.0)

## Sum and product

lowlimit

uplimit

sum

product

# Possible packages

## Statistics

|                          |        |
|--------------------------|--------|
| mean                     | sdev   |
| variance                 | median |
| mode                     | moment |
| momentabout (MathML 2.0) |        |

## Array math

|          |
|----------|
| vector   |
| selector |

## Linear algebra

|                            |             |
|----------------------------|-------------|
| matrix                     | matrixrow   |
| inverse                    | determinant |
| transpose                  |             |
| vectorproduct (MathML 2.0) |             |
| scalarproduct (MathML 2.0) |             |
| outerproduct (MathML 2.0)  |             |