Systems Biology Markup Language: Proposed Level 2 Modifications Generalizing Compartments

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1 Introduction

In this document, we propose modifications to the Systems Biology Markup Language (SBML) Level 2 feature set that generalize the compartment element to allow inclusion of `compartments` of varying dimensionality. The biological motivation for this effort is the inclusion of membranes; while membranes can be included to some extent in the SBML Level 1 and proposed Level 2 specifications, such a representation is inadequate, in that it is unclear how to distinguish "membrane" compartments from "volume" compartments; thus, it is not clear when to apply the concentration unit conversions (that is, the conversion between volumetric concentrations in units of substance per volume, and membrane concentrations in units of substance per area) necessary for maintaining proper mass conservation relationships.

2 Proposed Level 2 Modifications

We propose to generalize the `compartment` element by the addition of the `dimensions` attribute, and by changing the name of the `volume` attribute to `size`, as illustrated in Table 1. Our proposal to change the name of the `volume`

Compartment
name: SName
dimension: double {use="optional" default="3"}
size: double {use="optional" default="1"}
units: SName {use="optional"}
outside: SName {use="optional"}

Table 1: Proposed SBML Level 2 `compartment` element.

attribute is based solely on our desire to emphasize that compartments are not inherently three-dimensional, and the type of the `dimension` attribute, double, allows inclusion of fractal dimensions (although we currently see no way of interpreting this in terms of compartments, and expect most developers will be forced to reject models with fractal dimensions).

We also propose the addition of two built-in quantities, specifically, `area` and `length`, with default units of square meters, and meters, respectively. These built-in quantities are useful in the `compartment` element's `units` attribute, similar to the current use of `volume` for specifying default units. Along these lines, we ask that the Level 2 proposal be modified to clarify the description of the `units` attribute in the `compartment` element. In particular, it should be made clear that the `units` attribute is not restricted to volumetric units, and that the intent is for the units specified in the `units` attribute should be consistent with respect to the value of the `dimension` attribute.

3 Other Impacts

There has been discussion of modifying the units of the `initialAmount` attribute of the `species` element, as well as the units associated with the `kineticLaw` attribute of the `reaction` element. Currently, the units are specified as

substance and substance/time, respectively, although tools do not seem to handle either correctly. Thus, one proposal is to change the units of `initialAmount` to concentration; this is well-defined, given that species are associated with compartments. It has similarly been proposed to change the units associated with `kineticLaw` to concentration/time; however, this is not well-defined, since reactions cannot be associated with only one compartment. Moreover, given that reactions involving species associated with compartments of different dimension must be computed in terms of fluxes, with units substance/time, we see no way around maintaining the current units definitions for both `initialAmount` and `kineticLaw`. This would, of course, mean that tools developers would need to conform to the specification.