SBML Level 3 Package Specification

Required Elements

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The latest release, past releases, and other materials related to this specification are available at
http://sbml.org/Documents/Specifications/SBML_Level_3/Packages/req

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TBD

Contents

1 Introduction

The SBML Level 3 Required Elements package is a small package that allows models to declare exactly which components of a model have the meaning of their mathematical semantics changed by another package or by custom annotations. It does this simply by defining an optional child of **SBase** which can be attached to any component of a model with associated mathematics. The rest of this specification explains the package constructs and how they can be used.

1.1 Proposal corresponding to this package specification

This specification for Required Elements in SBML Level 3 Version 1 is based on the draft located at this URL:

http://sbml.svn.sf.net/svnroot/sbml/trunk/specifications/sbml-level-3/version-1/req/specification/

The tracking number in the SBML issue tracking system (SBML Team, 2010) for Required Elements package activities is 3594695. The version of the proposal used as the starting point for this specification is the version of August, 2011 (Smith, 2011).

1.2 Package dependencies

The Required Elements package has no dependencies on other SBML Level 3 packages.

1.3 Document conventions

UML 1.0 (Unified Modeling Language; Eriksson and Penker 1998; Oestereich 1999) notation is used in this document to define the constructs provided by this package. Colors in the diagrams carry the following additional information for the benefit of those viewing the document on media that can display color:

- *Black*: Items colored black in the UML diagrams are components taken unchanged from their definition in the SBML Level 3 Core specification document.

- *Green*: Items colored green are components that exist in SBML Level 3 Core, but are extended by this package. Class boxes are also drawn with dashed lines to further distinguish them.

- *Blue*: Items colored blue are new components introduced in this package specification. They have no equivalent in the SBML Level 3 Core specification.

The following typographical conventions distinguish the names of objects and data types from other entities; these conventions are identical to the conventions used in the SBML Level 3 Core specification document:

Class: Names of ordinary (concrete) classes begin with a capital letter and are printed in an upright, bold, sans-serif typeface. In electronic document formats, the class names are also hyperlinked to their definitions in this specification document. (However, class names are not hyperlinked if they are for classes that are unchanged from their definitions in their original specification.)

`SomeThing`, `otherThing`: Attributes of classes, data type names, literal XML, and tokens *other* than SBML class names, are printed in an upright typewriter typeface.

For other matters involving the use of UML and XML, this document follows the conventions used in the SBML Level 3 Core specification document.

2 Background and context

At the heart of many SBML models is mathematics. When present, the mathematics is considered to be of principle importance to understanding the model. Many SBML Level 3 packages replace the mathematical interpretation of elements present in SBML Level 3 Version 1 Core. Models with these package namespaces defined must add a `required`="`true`" flag on the definition of that namespace. However, for software tools that wish to manipulate and augment SBML models with extended mathematics which they do not understand, a blanket `required`="`true`" flag on the namespace is not granular enough. The tools need to know which *specific* model elements have had their mathematics changed (if any), so that they can understand which parts of the model are safe to manipulate freely and which must be treated with care. In addition, some software tools add custom annotations to SBML models that are intended to change the mathematical meaning of the element. Any model consumer that receives such a model but doesn't understand that annotation won't even have a `required` flag to let them know that the math is supposed to be different.

The Required Elements package is an exceedingly small package that allows model writers to declare specifically which components of the model have had their mathematics changed, by which package or annotation, and whether interpretation of those components in the absence of any package information results in a workable model. It accomplishes this by defining a class that can be added as an optional child of any SBML element with mathematical meaning.

3 Package syntax and semantics

This section contains a definition of the syntax and semantics of the Required Element package for SBML Level 3 Version 1 Core.

3.1 Namespace URI and other declarations necessary for using this package

Every SBML Level 3 package is identified uniquely by an XML namespace URI. For an SBML document to be able to use a given Level 3 package, it must declare the use of that package by referencing its URI. The following is the namespace URI for this version of the Required Elements package for SBML Level 3 Version 1 Core:

"`http://www.sbml.org/sbml/level3/version1/req/version1`"

In addition, SBML documents using a given package must indicate whether the package can be used to change the mathematical interpretation of a model. This is done using the attribute `required` on the `<sbml>` element in the SBML document. For the Required Elements package, the value of this attribute must be "`false`", because while the Required Elements package is designed to clarify how other packages change the mathematical meaning of the model, it cannot itself do so.

The following fragment illustrates the beginning of a typical SBML model using SBML Level 3 Version 1 Core and this version of the Required Elements package:

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1"
      xmlns:req="http://www.sbml.org/sbml/level3/version1/req/version1" req:required="false">
```

3.2 Primitive data types

The Required Elements package uses three of the data types described in Section 3.1 of the SBML Level 3 Version 1 Core specification, specifically `SId`, `string` and `boolean`. The package does not define any new types.
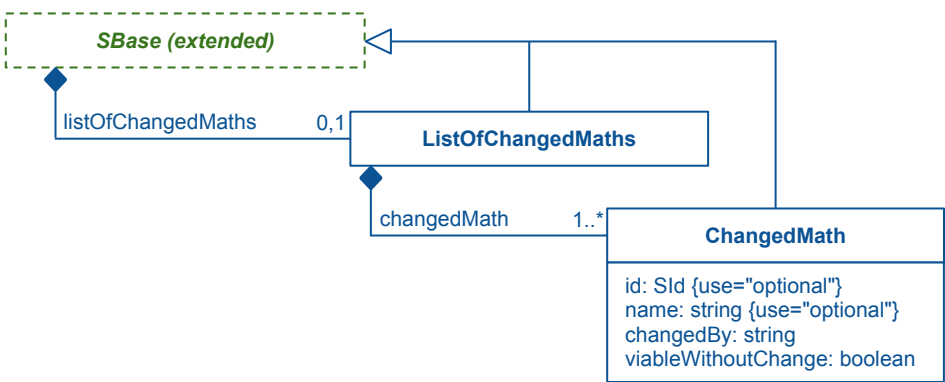
Figure 1: *The definition of the extended **SBase** class, and the new **ListOfChangedMaths** and **ChangedMath** classes.*

3.3 The extended SBase class

As mentioned above, this package's reason for being is to define an optional child of the SBML Level 3 **SBase** class. Figure 1 provides the definition of this **SBase** extension, and its optional **ChangedMath** children. These children are added to **SBase** instead of to those elements that have math in them (such as **InitialAssignment**, **KineticLaw**,

etc.) or that have mathematical meaning (such as **Parameter** or **Species**) because this approach allows other SBML
Level 3 packages to define new elements with mathematics which may, in turn, be overridden by other packages.

3.4   The ListOfChangedMaths class

As is standard in SBML specifications, any time more than one child of the same class is to be added to an
element, a 'ListOf' that element is provided to store them, and to collect annotations about the list itself. The child
'listOfChangedMaths' on SBase is optional, but if present, must contain one or more 'changedMath' children.

3.5   The ChangedMath class

The **ChangedMath** class defines an element, one or more of which may be added to any SBML element that either has
mathematical meaning, or that contains a **Math** child. In SBML Level 3 Core, the former group includes the classes
Compartment, **Parameter**, **Reaction**, **Species**, and **SpeciesReference**, and the latter group includes the classes
Constraint, **Delay**, **EventAssignment**, **FunctionDefinition**, **InitialAssignment**, **KineticLaw**, **Priority**, **Rule**, and **Trigger**.
Event elements do not have any direct **Math** children, but do indirectly, and may thus be given a **ChangedMath**
child. Packages that introduce elements that have mathematical meaning and/or that contain **Math** children may
also be extended through the addition of a **ChangedMath** child, when some other package changes that element's
mathematical interpretation.

Elements with mathematical meaning may have a **ChangedMath** child when a package alters the value or meaning
of that symbol. As an example, a **Submodel** from the Hierarchical Model Composition package may contain an
Event or **Rule** that assigns new values to a parameter. Because an interpreter that did not understand submodels
would not catch this change, the Hierarchical Model Composition package can be seen to change the math of that
element, and it would be appropriate to denote this by adding a **ChangedMath** child to the affected parameter.

Similarly, models that use the proposed Spatial Processes package can change the meaning of a **Compartment** by
turning it into a bounded object with an size implied by those boundaries (and how they change over time), instead
of using the element's `size` attribute. Spatial Processes elements may also change a **Species** to be spatially defined,
and therefore represent different values depending on what coordinates in space are under consideration. Affected
compartments and species could be given **ChangedMath** children to denote this fact.

Elements with **Math** children may also be changed by the addition of package elements. Some packages may
instruct the modeler to disregard the **Math** and to use some other construct instead. For example, the proposed
Distrubtions package adds a new child to **FunctionDefinition**, which replaces the old mathematics with a new set
of mathematics returning a draw from a random distribution (something impossible with **Math**).

Each package may define for itself when it would be appropriate or necessary, given the package's structure, to add
a **ChangedMath** element to something. If no such definition exists, a user may add **ChangedMath** elements where
they understand the math to be changing.

For packages with no such rules, the addition of **ChangedMath** children cannot be guaranteed to be normative, that
is, software that understands the Required Elements package, but which does not understand some other package
flagged `required`="`true`" will not be able to assert that every element with altered mathematics has been given
a **ChangedMath** child. However, a package may define its own validation rules in conjunction with this Required
Elements package, and a user may then be able to guarantee that any affected element has been denoted as such.

In addition, some software tools introduce custom annotations that are intended to change the mathematics of
a model. In the simplest cases, this has been done to accomplish what eventually might be covered by packages,
before the package itself has been finalized. For example, many software tools have introduced custom annotations
of function definitions to allow them to sample from random distributions, before the Distributions package allows
them to do so in an 'official' manner. Other tools work with models that go beyond the scope of core SBML in other
ways, but still use SBML to store and exchange the basic parts. To promote more nuanced exchangeability, the
ChangedMath element may point to any arbitrary annotation namespace when that annotation is used to change
the mathematical interpretation of an SBML element.

Note that a **ChangedMath** element should be added to the model component that is directly affected only, and not on a component that is indirectly affected by the changed mathematics. For example, if a model contains a **FunctionDefinition** object whose mathematics are extended by the SBML Level 3 package for Distributions, and elsewhere in the model there is an **InitialAssignment** object that uses that function, a **ChangedMath** child should be added only to the **FunctionDefinition** object and not the **InitialAssignment** nor on the element that assigns to, because the latter are only indirectly affected, through processes understood without reference to package definitions.

Multiple packages may affect the mathematics of the same object in different ways. For example, a construct from the Spatial Process package could change a **Species** to be spatially defined, and that same model may have a **Submodel** from the Hierarchical Model Composition package which contains a **Reaction** that affects that **Species**. In that case, the **Species** would have two **ChangedMath** children, one for each package that affects it.

Since **ChangedMath** itself has no mathematical meaning and no child **Math** object, it may not itself have a **ChangedMath** child.

3.5.1   The `id` and `name` attributes

The optional `id` attribute on the **ChangedMath** object class serves to provide a way to identify the element. The attribute takes a value of type `SId`. Note that this identifier carries no mathematical interpretation and cannot be used in mathematical formulas in a model. **ChangedMath** also has an optional `name` attribute, of type `string`. The `name` attribute may be used in the same manner as other `name` attributes on SBML Level 3 Version 1 Core objects; please see Section 3.3.2 of the SBML Level 3 Version 1 Core specification for more information.

3.5.2   The `changedBy` attribute

The `changedBy` attribute is required, and is of type `string`. The attribute must be set to the namespace URI of the SBML Level 3 package (or to the namespace URI of a custom annotation) that redefines or alters the mathematical semantics of the parent object. In other words, if the mathematical semantics of a given component C in a model is changed by the use of a Level 3 package P, then C can be given a **ChangedMath** child, and its attribute `changedBy` should be P's namespace URI. The examples below will make this more clear.

Valid values for the `changedBy` token include the namespace URIs for any SBML L3 package flagged `required` ="`true`", and namespace URIs for any custom annotation in an SBML model. Namespace URIs for any SBML L3 package flagged `required`="`false`" are not valid values for the `changedBy` token, as the package in question by definition cannot change the mathematical meaning of any element in the model.

No two child **ChangedMath** elements of any single **SBase** object may have the same `changedBy` value.

3.5.3   The `viableWithoutChange` attribute

The `viableWithoutChange` attribute is required, and is of type `boolean`. The attribute should be used to indicate whether an interpreter that does not understand the package or custom anntoation from the `changedBy` attribute would have an interpretable version of the mathematics for the given component in a model. This can be established using two criteria: "Complete" and "Workable". Obviously, if the math being interpreted is incomplete, the `viableWithoutChange` attribute must be "`false`". If the math is complete, then whether the solution is "workable" requires a judgement call on the part of the modeler: if the modeler feels that the alternative version makes sense in an alternative context, they may set the attribute value to "`true`"; conversely, if they feel that the resulting model component makes no sense, even if technically "complete", then they should set the attribute value to "`false`".

When two different packages or annotations alter the mathematical interpretation of an **SBase** object in different ways, and two corresponding **ChangedMath** elements are added, each should consider whether the aspect of the change that package is responsible for has an alternative, irrespective of how the other package affects the element. In our above example where both the Spatial Processes and the Hierarchical Model Composition package affected the same **Species**, the **ChangedMath** element for the Spatial Processes package may have its `viableWithoutChange` attribute set to "`true`" if an alternate framework without Spatial Processes constructs is present (even if spread

across multiple **Submodel** elements from the Hierarchical Model Composition package). Conversely, if the **Reaction**   1
that affects the **Species** is in a **Submodel**, the corresponding `viableWithoutChange` for that package should be set   2
to "`false`" if that **Reaction** is considered vital to the understanding and interpertation of the model.   3

3.6   Additional considerations   4

The Required Elements package is not, itself, required (that is, models that use it must set `required`="`false`" for its   5
namespace when using it) because it cannot change any mathematical semantics. However, it is intended to be   6
used by other required packages, which may in turn make the use of this package in certain contexts defined in   7
those package specifications.   8

4 Examples

This section contains examples employing the Required Elements package for SBML Level 3.

4.1 Function whose interpretation is reasonable in the absence of a package

In this example, there is a **FunctionDefinition** object that has had its mathematics changed by an (as-yet hypothetical) Distributions package.

```
<listOfFunctionDefinitions>
  <functionDefinition id="unitGaussian">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <lambda>
        <bvar>
          <ci> mean </ci>
        </bvar>
        <bvar>
          <ci> variance </ci>
        </bvar>
        <ci> mean </ci>
      </lambda>
    </math>
    <distrib:drawFromDistribution>
      <listOfDistribInputs>
        <distribInput id="mean" index="0"/>
        <distribInput id="var" index="1"/>
      </listOfDistribInputs>
      <uncertml xmlns="http://uncertml.org/3.0">
        <NormalDistribution>
          <mean>mean</mean>
          <variance>var</variance>
        </NormalDistribution>
      </uncertml>
    </distrib:drawFromDistribution>
    <req:listOfChangedMaths>
      <req:changedMath changedBy="http://www.sbml.org/sbml/level3/version1/distrib/version1"
                       viableWithoutChange="true" />
    </req:listOfChangedMaths>
  </functionDefinition>
</listOfFunctionDefinitions>
```

The function `unitGaussian` above has both a straight SBML Level 3 Core definition (whose MathML formula has the effect of returning "`mean`", unchanged), and a package-defined version (in effect, "select a random number from a Gaussian distribution with mean "`mean`" and variance "`var`""). The modeler has elected to claim that the SBML Core definition's version of the function is adequate for the model in which it is being used, although different results are to be expected.

4.2 Function whose interpretation is *not* reasonable in the absence of a package

In this example, the modeler has decided that the plain SBML Level 3 Core version of the mathematics will not make an adequate substitution for using the mathematics defined by the Distributions package, as it returns '0' instead of something more reasonable:

```
<listOfFunctionDefinitions>
  <functionDefinition id="unitGaussian">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <lambda>
```

```
        <bvar>                                                                          1
          <ci> mean </ci>                                                               2
        </bvar>                                                                          3
        <bvar>                                                                          4
          <ci> var </ci>                                                                5
        </bvar>                                                                          6
        <cn> 0 </cn>                                                                     7
      </lambda>                                                                          8
    </math>                                                                             9
    <distrib:drawFromDistribution>                                                      10
      <listOfDistribInputs>                                                             11
        <distribInput id="mean" index="0"/>                                             12
        <distribInput id="var" index="1"/>                                              13
      </listOfDistribInputs>                                                            14
      <uncertml xmlns="http://uncertml.org/3.0">                                        15
         <NormalDistribution>                                                           16
           <mean>mean</mean>                                                            17
           <variance>var</variance>                                                     18
         </NormalDistribution>                                                          19
      </uncertml>                                                                       20
    </distrib:drawFromDistribution>                                                     21
    <req:listOfChangedMaths>                                                            22
      <req:changedMath changedBy="http://www.sbml.org/sbml/level3/version1/distrib/version1"  23
                   viableWithoutChange="false" />                                        24
    </req:listOfChangedMaths>                                                           25
  </functionDefinition>                                                                 26
</listOfFunctionDefinitions>                                                            27
                                                                                        28
```

4.3   Function whose definition is incomplete

In the following example, the function definition is marked as having `viableWithoutChange`="`false`" because the lambda function is actually incomplete, and returns nothing at all.

```
<listOfFunctionDefinitions>                                                             33
  <functionDefinition id="unitGaussian">                                                34
    <math xmlns="http://www.w3.org/1998/Math/MathML">                                   35
      <lambda>                                                                          36
        <bvar>                                                                          37
          <ci> mean </ci>                                                               38
        </bvar>                                                                          39
        <bvar>                                                                          40
          <ci> variance </ci>                                                           41
        </bvar>                                                                          42
      </lambda>                                                                         43
    </math>                                                                             44
    <distrib:drawFromDistribution>                                                      45
      <listOfDistribInputs>                                                             46
        <distribInput id="mean" index="0"/>                                             47
        <distribInput id="var" index="1"/>                                              48
      </listOfDistribInputs>                                                            49
      <uncertml xmlns="http://uncertml.org/3.0">                                        50
         <NormalDistribution>                                                           51
           <mean>mean</mean>                                                            52
           <variance>var</variance>                                                     53
         </NormalDistribution>                                                          54
      </uncertml>                                                                       55
    </distrib:drawFromDistribution>                                                     56
    <req:listOfChangedMaths>                                                            57
      <req:changedMath changedBy="http://www.sbml.org/sbml/level3/version1/distrib/version1"  58
                   viableWithoutChange="false" />                                        59
    </req:listOfChangedMaths>                                                           60
  </functionDefinition>                                                                 61
</listOfFunctionDefinitions>                                                            62
                                                                                        63
```

5 Relationship with other packages

Each package that can be set `required`="`true`" has the potential to interact with the Required Elements package. For packages that have already been finalized, we present validation rules that, if followed, would allow a software package that did not understand the package in question to know what math was changed from what would have been expected, had those package constructs not been present. For packages that have not yet been finalized, hypothetical validation rules are proposed based on the current version of the specification, but to fully ensure that all the appropriate **ChangedMath** elements were added to a document with that package, a full set of validation rules that matched the final package specification would have to be produced, either as a part of that other package's specification, or as part of a future version of this specification.

It is important to note that a package that *can* be used to change the mathematical interpretation of a core element *must* be set `required`="`true`", regardless of whether or not it actually does so within the SBML Document in which it appears. For that reason, a document may have a required package present that nevertheless will not have any corresponding **ChangedMath** elements.

Determining whether a model follows the given validation rules will require understanding of that package, which presents a sort of catch-22 for any software tool: the only reason to use Required Elements constructs in the first place is to mitigate situations where a package is *not* understood. We propose that any software in this situation use an external validator that understands all packages in a technical sense, but has no need to actually interpret the models mathematically, to ensure that a model is valid, and then proceed from there. If the model is valid, all mathematically-modified elements from SBML packages will be guaranteed to have **ChangedMath** children. The same is obviously not true of custom annotations; in that case, one must trust the original modeler or software package to have introduced **ChangedMath** elements where appropriate.

It is important to note that all the validation rules presented only take effect if the Required Elements package namespace is present in an SBML document. In effect, by adding the package to your model, you agree to abide by the validation rules herein. However, it is perfectly possible to use the packages without 'Required Elements'; you then simply revert to the standard global required/not required package information, which may be perfectly acceptable.

5.1 The Hierarchical Model Composition package

The URI "`http://www.sbml.org/sbml/level3/version1/comp/version1`" is used to refer to the Hierarchical Model Composition package. This must be the string used for any `changedBy` attribute that refers to this package.

The Hierarchical Model Composition package allows modelers to compose models hierarchically, by adding a list of **Model** objects to the document, allowing them to be imported into other models via the **Submodel** construct, and then connecting elements of those models together with **ReplacedElement** and **ReplacedBy** constructs.

It is only the last of those three abilities that can directly change the mathematical interpretation of an element of the main **Model** object in an SBML Document. Defining a new **Model** will not change the interpretation of anything in the original **Model**, nor will incorporating submodels into the original **Model**.

All elements with mathematical meaning which have been given a **ReplacedBy** child have had their meaning changed, by definition. Therefore, any **Compartment**, **Parameter**, **Reaction**, **Species**, **Constraint**, **Event**, **FunctionDefinition**, **InitialAssignment**, or **Rule** with a **ReplacedBy** child must be given a **ChangedMath** child. (Other elements with mathematical meaning exist in SBML Level 3 Core, but are not on this list because they may not have **ReplacedBy** children.) The value of the `viableWithoutChange` may be set to be "`true`" if the original element is completely defined (or if it is *at least as* defined as its replacement), and must be set "`false`" otherwise. The attribute may also be set "`false`" if the original element differs from its replacement, and/or if their mathematical interpretation is changed by some other element in the replacement (such as by a **Rule** or **Reaction**; see below).

Compartment, **Parameter**, **Reaction**, **Species**, and **SpeciesReference** elements all have the ability to have their mathematical interpretation changed by **InitialAssignment**, **Rule**, and **Event** constructs. If any of these three elements

are present in a **Submodel**, and their target is an element in the main model (because their 'local' target has been replaced by the main model element), that element in the main model must be given a **ChangedMath** child referencing this package. The value of the `viableWithoutChange` may be set to be "`true`" if the modeler determines that the absence of the **InitialAssignment**, **Rule**, or **Event** creates an alternate model scenario that is nonetheless workable.

Any element that does not fall under the above two situations will not have its math changed, and must therefore not have a **ChangedMath** child targeting this package.

Modelers that wish to use **ChangedMath** elements in **Model** elements that are *not* the direct child of the `sbml` element may do so, but this only facilitates the translation of those tertiary models to their own SBML Documents: any software that could read and understand a tertiary model must, by definition, be able to understand the Hierarchical Model Composition package, and therefore has no need of any **ChangedMath** element that targets this package.

5.2   The Qualitative Models package

In the first release of Version 1 of the Qualitative Models package, the specification claims that the `required` attribute may be set to be "`true`", but the SBML Editors have recently clarified the interpretation of the `required` flag such that, because the constructs added by the package cannot affect core constructs, it should instead always be set to be "`false`". Therefore, there is no need to create any **ChangedMath** elements that target this package: any such elements are illegal.

5.3   The Distributions package

The URI "`http://www.sbml.org/sbml/level3/version1/distrib/version1`" is used to refer to the Distributions package. This must be the string used for any `changedBy` attribute that refers to this package.

The Distrubtions package has not yet been finalized, but in its current (draft) form, it can be used to annotate SBML elements with information about the error or uncertainty in their values, which does not affect the mathematics of the model, and to modify **FunctionDefinition** elements to produce draws from distributions, which does. Any **FunctionDefinition** so modified must be given a **ChangedMath** referring to this package; the `viableWithoutChange` element must be set "`false`" if the original **Math** child is incomplete, and may be set "`true`" if the deterministic value it produces results in a workable, though non-random, model. No other element may be given a **ChangedMath** child that targets this package.

5.4   The Multistate and Multicomponent Species package

The URI "`http://www.sbml.org/sbml/level3/version1/multi/version1`" is used to refer to the Multistate and Multicomponent Species package. This must be the string used for any `changedBy` attribute that refers to this package.

The Multistate and Multicomponent Species package has not yet been finalized, but in its current (draft) form, it allows the redefinition of **Species** and **Compartment** elements as types which might be instantiated in a number of ways. Any such 'prototype'-style elements would need **ChangedMath** children. Furthermore, as currently written, no such **Species** or **Compartment** may be instantiated or changed, whether by attribute, **InitialAssignment**, or **Rule**, and the value of the `viableWithoutChange` attribute would always be required to be set "`false`".

5.5   The Spatial Processes package

The URI "`http://www.sbml.org/sbml/level3/version1/spatial/version1`" is used to refer to the Spatial Processes package. This must be the string used for any `changedBy` attribute that refers to this package.

The Spatial Processes package has not yet been finalized, but in its current (draft) form, it modifies **Species**, **Compartment**, and **Reaction** elements such that they can be modeled spatially, with partial differential equations. All such modified elements must therefore be given **ChangedMath** children–the specification itself details how this

is to be done, and what values for `viableWithoutChange` are appropriate.

5.6   The Arrays package

The URI "`http://www.sbml.org/sbml/level3/version1/arrays/version1`" is used to refer to the Arrays package. This must be the string used for any `changedBy` attribute that refers to this package.

The Arrays package has not yet been finalized, but in its current (draft) form, it has the ability to modify any element with mathematical meaning to represent an array instead of a single value. All such modified elements must therefore be given **ChangedMath** children, with more details to follow as the package is developed.

5.7   The Dynamic Structures package

The URI "`http://www.sbml.org/sbml/level3/version1/dyn/version1`" is used to refer to the Dynamic Structures package. This must be the string used for any `changedBy` attribute that refers to this package.

The Dynamic Structurs package has not yet been finalized, and is not, as of this writing, undergoing active development. Any structures it sets in place to create or destroy elements with mathematical meaning would clearly affect the mathematics of the model, and any elements so affected would be appropriate targets for **ChangedMath** children.

5.8   Non-required packages

The Annotations, Flux Balance Constraints, Layout, Render, Groups, and this Required Elements package all explicitly do not affect the mathematics of a model, and must be set `required`="`false`". No **ChangedMath** element may therefore reference these packages.

5.9   Future packages

It is hoped that, should this Required Elements package prove useful, packages defined in the future will explicitly mention what elements it defines that must be given **ChangedMath** children, and what values to give its attributes.

A Validation of SBML documents using Required Elements constructs

This section summarizes all the conditions that must (or in some cases, at least *should*) be true of an SBML Level 3 Version 1 model that uses the Required Elements package. We use the same conventions that are used in the SBML Level 3 Version 1 Core specification document. In particular, there are different degrees of rule strictness. Formally, the differences are expressed in the statement of a rule: either a rule states that a condition *must* be true, or a rule states that it *should* be true. Rules of the former kind are strict SBML validation rules—a model encoded in SBML must conform to all of them in order to be considered valid. Rules of the latter kind are consistency rules. To help highlight these differences, we use the following three symbols next to the rule numbers:

☑ A checked box indicates a *requirement* for SBML conformance. If a model does not follow this rule, it does not conform to the Required Elements package specification. (Mnemonic intention behind the choice of symbol: "This must be checked.")

▲ A triangle indicates a *recommendation* for model consistency. If a model does not follow this rule, it is not considered strictly invalid as far as the Required Elements package specification is concerned; however, it indicates that the model contains a physical or conceptual inconsistency. (Mnemonic intention behind the choice of symbol: "This is a cause for warning.")

★ A star indicates a strong recommendation for good modeling practice. This rule is not strictly a matter of SBML encoding, but the recommendation comes from logical reasoning. As in the previous case, if a model does not follow this rule, it is not considered an invalid SBML encoding. (Mnemonic intention behind the choice of symbol: "You're a star if you heed this.")

The validation rules listed in the following subsections are all stated or implied in the rest of this specification document. They are enumerated here for convenience. Unless explicitly stated, all validation rules concern objects and attributes specifically defined in the Required Elements package.

☞ For convenience and brievity, we use the shorthand "`req:x`" to stand for an attribute or element name `x` in the namespace for the Required Elements package, using the namespace prefix `req`. In reality, the prefix string may be different from the literal "`req`" used here (and indeed, it can be any valid XML namespace prefix that the modeler or software chooses). We use "`req:x`" because it is shorter than to write a full explanation everywhere we refer to an attribute or element in the Required Elements package namespace.

General rules about the Required Elements package

req-10101 ☑ To conform to Version 1 of the Required Elements package specification for SBML Level 3, an SBML document must declare the use of the following XML Namespace: "`http://www.sbml.org/sbml/level3/version1/req/version1`". (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.1 on page 5.)

req-10102 ☑ Wherever they appear in an SBML document, elements and attributes from the Required Elements package must be declared either implicitly or explicitly to be in the XML namespace "`http://www.sbml.org/sbml/level3/version1/req/version1`". (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.1 on page 5.)

req-10103 ☑ The value of attribute `req:required` on the **SBML** object must be set to "`false`". (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.1 on page 5.)

General rules about identifiers

req-10201 ☑ (Extends validation rule #10301 in the SBML Level 3 Version 1 Core specification.) Within a **Model** object, the values of the attributes `id` and `req:id` on every instance of the following classes of objects must be unique across the set of all `id` and `req:id` attribute values of all

such objects in a model: the **Model** itself, plus all contained **FunctionDefinition**, **Compartment**, **Species**, **Reaction**, **SpeciesReference**, **ModifierSpeciesReference**, **Event**, and **Parameter** objects, plus any **ChangedMath** objects defined by the Required Elements package, plus any objects defined by any other package with `package:id` attributes defined as falling in the 'SId' namespace. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.1 on page 5.)

req-10202 ☑ The value of a `req:id` attribute must always conform to the syntax of the SBML data type `SId`. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5.1 on page 7.)

req-10203 ☑ The value of a `req:name` attribute must always conform to the syntax of type `string`. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5.1 on page 7.)

req-10204 ☑ The value of a `req:changedBy` attribute must always conform to the syntax of type `string`. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5.2 on page 7.)

req-10205 ☑ The value of a `req:viableWithoutChange` attribute must always conform to the syntax of type `boolean`. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5.3 on page 7.)

Rules for the SBase abstract class

req-20101 ☑ Any object derived from the *SBase* class (defined in SBML Level 3 Version 1 Core) may contain at most one instance of a **ListOfChangedMaths** subobject. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.3 on page 5.)

req-20102 ☑ Apart from the general notes and annotation subobjects permitted on all SBML objects, a **ListOfChangedMaths** container object may only contain **ChangedMath** objects. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.3 on page 5.)

req-20103 ☑ A **ListOfChangedMaths** object may have the optional attributes `metaid` and `sboTerm` defined by SBML Level 3 Core. No other attributes from the SBML Level 3 Core namespace or the Required Elements namespace are permitted on a **ListOfChangedMaths** object. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.3 on page 5.)

req-20104 ☑ The **ListOfChangedMaths** in an *SBase* object is optional, but if present, must not be empty. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.4 on page 6.)

Rules for ChangedMath objects

req-20201 ☑ A **ChangedMath** object may have the optional SBML Level 3 Core attributes `metaid` and `sboTerm`. No other attributes from the SBML Level 3 Core namespace are permitted on a **ChangedMath** object. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5 on page 6)

req-20202 ☑ A **ChangedMath** object may have the optional SBML Level 3 Core subobjects for notes and annotation. No other subobjects from the SBML Level 3 Core namespace or the Required Elements namespace are permitted in a **ChangedMath** object. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5 on page 6)

req-20203 ☑ A **ChangedMath** object may have the optional attributes `req:id` and `req:name`, and must have the required attributes `req:changedBy` and `req:viableWithoutChange`. No other attributes

from the Required Elements namespace are permitted on a **ChangedMath** object. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5 on page 6)

req-20204 ☑ The value of the `req:changedBy` attribute on a **ChangedMath** object must reference the URI of an SBML Level 3 Version 1 package namespace, or the URI of a custom annotation namespace. (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5 on page 6)

req-20205 ☑ The value of the `req:changedBy` attribute on a **ChangedMath** object may not reference the URI of an SBML Level 3 Version 1 package namespace if the value of that package's `required` attribute is "`false`". (References: SBML Level 3 Package Specification for Required Elements, Version 1, Section 3.5 on page 6)

Acknowledgments

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