CellML Specification Documentation Release

The CelIML Editorial Board

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CONTENTS

1	Definitions	3				
2	General matters2.1CellML and XML2.2Equivalent CellML infosets2.3Character information items2.4Use of namespaces2.5Extension information items2.6Identifiers2.7Specific information items2.8RDF element information items	5 5 5 6 6 7 7				
3	Data representation formats in CellML					
4	The model element information item 4.1 Top-level of CellML infosets	11 11 11				
5	The import element information item 5.1 Specific information items	13 13				
6	The import units element information item 6.1 Specific information items	15 15				
7	The import component element information item 7.1 Specific information items	17 17				
8	The units element information item 8.1 Specific information items	19 19				
9	The unit element information item 9.1 Specific information items	21 21				
10	The component element information item 10.1 Specific information items	23 23				
11	The variable element information item 11.1 Specific information items	25 25				
12	The group element information item 12.1 Specific information items	27 27				

13	The relationship_ref element information item 13.1 Specific information items	29 29
14	The component_ref element information item 14.1 Specific information items	31 31
15	The connection element information item 15.1 Specific information items	33 33
16	The map_components element information item 16.1 Specific information items	35 35
17	The map_variables element information item 17.1 Specific information items	37 37
18	Interpretation of CellML models	39
	18.1 Interpretation of imports	39
	18.2 Units reference	39
	18.3 Interpretation of units	41
	18.4 Component reference	42
	18.5 Variable reference	43
	18.6 Interpretation of initial values	43
	18.7 Effect of units on variables	43
	18.8 Interpretation of mathematics	44
	18.9 Interpretation of grouping	44
	18.10 Variable equivalence networks	45
19	References	47
20	Summary of all TODO's	49

This document is an unofficial working draft. The below describes the intended status of the specification, and not its current status.

This document specifies version 1.2 of CellML, an XML-based language for describing and exchanging mathematical models.

This is the *normative* specification of CellML. It is intended to provide the minimum amount of information needed to describe CellML. An *informative* specification is available which is annotated with much more explanatory material.

Todo

Provide a 'proper' URL for the informative version of the specification.

DEFINITIONS

The key words "MUST", "MUST NOT", "REQUIRED", "SHALL", "SHALL NOT", "SHOULD", "SHOULD NOT", "RECOMMENDED", "MAY", and "OPTIONAL" in this document are to be interpreted as described in RFC 2119.

The key phrase "information item", as well as any specific type of information item such as an "element information item", are to be interpreted as described in XML Information Set.

- **CellML infoset** An XML information set containing a hierarchy of information items conforming to the rules described in this document.
- **CellML model** A mathematical model represented by a hierarchy of one or more CellML infosets, according to the rules described in this document.
- CellML processing software Software which processes CellML in accordance with the rules of this document.

Namespace An XML namespace, as defined in Namespaces in XML.

- CellML namespace Any namespace starting with http://www.cellml.org/cellml/.
- CellML 1.0 namespace The namespace http://www.cellml.org/cellml/1.0#.
- CellML 1.1 namespace The namespace http://www.cellml.org/cellml/1.1#.
- CellML 1.2 namespace The namespace http://www.cellml.org/cellml/1.2#.
- MathML namespace The namespace http://www.w3.org/1998/Math/MathML.
- RDF namespace The namespace http://www.w3.org/1999/02/22-rdf-syntax-ns#.
- CellML metadata namespace The namespace http://www.cellml.org/metadata/1.0#.
- Extension namespace Any namespace which is not a CellML namespace, and is not the RDF
 namespace, the MathML namespace, http://www.w3.org/XML/1998/namespace,
 http://www.w3.org/2000/xmlns/, http://www.w3.org/1999/xlink, or the empty namespace.
- CellML information item Any information item in a CellML namespace.
- **Basic Latin alphabetic character** A Unicode character in the range U+0041 to U+005A or in the range U+0061 to U+007A.
- European numeric character A Unicode character in the range U+0030 to U+0039.
- **Basic Latin alphanumeric character** A Unicode character which is either a basic Latin alphabetic character or a European numeric character.
- Basic Latin underscore The Unicode character U+005F.
- Whitespace character Any one of the Unicode characters U+0020, U+0009, U+000D or U+000A.
- RDF triple As defined in RDF Concepts and Abstract Syntax.

GENERAL MATTERS

2.1 CelIML and XML

- 1. Every CellML infoset SHALL be represented in an XML document which conforms with the well-formedness requirements of the XML 1.0.
- 2. In this document, the remaining provisions relating to CellML infosets shall be interpreted as being constraints on the XML information set represented by that CellML infoset.

2.2 Equivalent CelIML infosets

- 1. Two CellML infosets shall be equivalent if one can be transformed to another by making zero or more of the following changes:
 - (a) Changing the representation of the XML file in ways which do not change the XML information set represented.
 - (b) Adding, removing, and/or modifying comment information items.
 - (c) Changing (inserting, removing, and/or modifying) one or more namespace information items, and/or modifying the prefix of one or more information items, without changing the namespace that any information item is in.
 - (d) The following paragraph applies only to character information items which are the direct child of an element information item in a CellML namespace, or in the MathML or RDF namespace.

Inserting or removing character information items that consist entirely of whitespace characters, changing the number of whitespace characters in such an information item, or changing the number of whitespace characters at the beginning or end of a character information item.

2. CellML processing software MUST treat CellML infosets which are equivalent according to the above rules in an identical fashion.

2.3 Character information items

An element information item in the CellML namespace MUST NOT contain any character information items, except for character information items which consist entirely of whitespace characters.

2.4 Use of namespaces

- 1. CellML infosets MUST NOT contain any element or attribute information items, except as permitted in this specification.
- 2. CellML infosets MUST NOT contain any character information items which are children of element information items in a CellML namespace, except as permitted in this specification.
- 3. CellML processing software SHOULD NOT attempt to process CellML infosets which contain information items in a CellML namespace other than the CellML 1.0, CellML 1.1 and CellML 1.2 namespaces.
- 4. CellML infosets MUST NOT contain any element information items in the RDF namespace, unless:
 - (a) The element information item or one of its ancestors is an element information item in the RDF namespace, with local name RDF (the RDF element information item); and
 - (b) The RDF element information item forms the top-level of a valid RDF/XML tree, per production 7.2.9 in RDF/XML Syntax Specification.
- 5. CellML infosets MUST NOT contain any element information items in the MathML namespace, unless:
 - (a) The element information item or one of its ancestors is an element information item in the MathML namespace, with local name math (the math element information item); and
 - (b) The math element information item forms the top-level of a valid MathML tree, as described in MathML 2.0.

2.5 Extension information items

- 1. CellML infosets MAY contain zero or more element or attribute information items in an extension namespace (extension information items), as children of CellML information items.
- 2. Information items in the empty namespace, which appear as children of extension element information items, SHALL also be treated as extension information items.
- 3. Extension information items MAY contain extension information items as their children. In addition, extension elements MAY contain presentation MathML children. For the avoidance of doubt, it is noted that extension information items MAY also contain any other information items not disallowed by this specification or a referenced normative specification.
- 4. CellML processing software MUST NOT raise an error solely because it encounters an unrecognised extension element.
- 5. CellML processing software which reads CellML and then writes a modified version back out SHOULD preserve unrecognised extension information items when the parent information item is not modified.
- 6. CellML processing software MUST NOT allow the mathematical interpretation of a CellML model to be altered by any information present in extension information items.
- 7. For the avoidance of doubt, extension information items MUST NOT contain CellML information items as descendents.

2.6 Identifiers

1. Any element information item in the CellML namespace MAY contain an attribute information item with local name id, in the CellML metadata namespace. This attribute information item SHALL be treated as having attribute type ID, as defined in section 3.3.1 of XML 1.0.

2.7 Specific information items

- 1. A specific information item is an information item which is not:
 - (a) A comment information item;
 - (b) A character information item;
 - (c) An extension information item or a descendant of such an information item; or
 - (d) A namespace information item.
- 2. Specific information items MUST NOT appear in a CellML infoset except where explicitly allowed by this specification, or where allowed by a normative specification referenced by this specification.
- 3. The order in which specific information items appear as children of an element information item defined in this specification SHALL NOT affect the interpretation of the CellML model.

2.8 RDF element information items

- 1. Every element information item in the CellML namespace MAY contain zero or more RDF element information item children.
- 2. An RDF element information item SHALL be an element item in the RDF namespace, with local name RDF (the RDF element information item), and MUST form the top-level of a valid RDF/XML tree, per production 7.2.9 in RDF/XML Syntax Specification.
- 3. An RDF element information item MUST NOT appear in a CellML infoset except as allowed by rule 1 above.

Todo

Find out which rule 1 we are we talking about here. Andre: it is the rule 1 just here (2.8.1 currently) but need to work out how to properly reference other rules. Probably shouldn't rely on section numbers being consistent.

- 4. CellML processing software MUST NOT allow the mathematical interpretation of a CellML model to be altered by any information present in RDF data.
- 5. The set of all RDF triples associated with a CellML infoset SHALL refer to the union of all sets of RDF triples produced by parsing all the RDF element information items according to the RDF/XML Syntax Specification.
- 6. Two CellML infosets which differ only by the addition, removal, or modification of RDF element information items (or information items descended from them), but which have the same set of all RDF triples, SHALL be termed RDF-equivalent CellML infosets.
- 7. CellML processing software MUST NOT treat RDF-equivalent CellML infosets differently.

DATA REPRESENTATION FORMATS IN CELLML

The following data representation formats are defined for use in this specification:

- 1. A CellML identifier:
 - (a) SHALL be a sequence of Unicode characters.
 - (b) SHALL NOT contain any characters except basic Latin alphanumeric characters and basic Latin underscores.
 - (c) SHALL contain one or more basic Latin alphabetic characters.
 - (d) SHALL NOT begin with a European numeric character.
 - (e) SHALL, when comparing two identifiers, be considered identical to another identifier if and only if both identifiers have identical sequences of Unicode character codes.
- 2. A non-negative integer string:
 - (a) SHALL be a base 10 representation of a non-negative integer.
 - (b) SHALL consist entirely of European numeric characters.
- 3. An integer string:
 - (a) SHALL be a base 10 representation of an integer.
 - (b) SHALL, when the integer being represented is negative, consist of the basic Latin hyphen-minus character U+002D, followed by the non-negative integer string representation of the absolute value of the integer.
 - (c) SHALL, when the integer being represented is non-negative, consist of the non-negative integer string representation of the integer.
- 4. A basic real number string:
 - (a) SHALL be a base 10 representation of a real number.
 - (b) SHALL, when the basic real number being represented is negative, begin with the basic Latin hyphenminus character U+002D as the sign indicator.
 - (c) MAY contain a single decimal point separator, which SHALL be the basic Latin full stop character U+002E.
 - (d) SHALL, other than the sign indicator and the decimal point separator, consist only of European numeric characters.
- 5. A real number string:

- (a) SHALL be a base 10 representation of a real number $r = s \cdot 10^e$, where s is the significand, a real number, and e is the exponent, an integer.
- (b) The representation of the number SHALL be the representation of the significand followed immediately by the representation of the exponent.
- (c) The significand SHALL be represented as a basic real number string.
- (d) If the exponent is zero, the exponent MAY be represented by an empty string, or MAY be represented according to the following rule. If the exponent is non-zero, it MUST be represented according to the following rule.
- (e) An exponent SHALL be represented by an exponent separator character, followed by the integer string representation of the value of the exponent. The exponent separator character SHALL be either the basic Latin 'E' character U+0045 or the basic Latin 'e' character U+0065.

THE MODEL ELEMENT INFORMATION ITEM

4.1 Top-level of CelIML infosets

The top-level element information item in a CellML infoset MUST be an element information item in the CellML namespace, with local name model. This element information item is referred to in this specification as the model element.

- 1. Every model element MUST contain a name attribute in the empty namespace. The value of the name attribute MUST be a valid CellML identifier, and SHALL be interpreted as a unique identifier for the CellML infoset.
- 2. A model element MAY contain zero or more additional specific information item children, each of which MUST be of one of the following types:
 - (a) A component element;
 - (b) A connection element;
 - (c) A group element;
 - (d) An import element; or
 - (e) A units element.

THE IMPORT ELEMENT INFORMATION ITEM

import element information items (referred to in this specification as import elements) are element information items in the CellML namespace with local name equal to import.

- 1. Every import element MUST contain an attribute information item in the namespace http://www.w3.org/1999/xlink, and with local name href. The value of this attribute SHALL be a valid locator href, as defined in section 5.4 of the XLink specification. The href attribute SHALL be treated according to the XLink specification, by applying the rules for simple-type elements. When describing an import element or one of its children, the phrase "imported CellML infoset" SHALL refer to the CellML infoset obtained by parsing the XML document referenced by the href attribute.
- 2. Every import element MAY contain zero or more specific information children, each of which MUST be of one of the following types:
 - (a) An import units element; or
 - (b) An import component element.
- 3. The imported CellML infoset SHALL NOT be equivalent to this CellML infoset. Any CellML infoset imported, directly or indirectly, by the imported CellML infoset SHALL NOT be equivalent to this CellML infoset.

THE IMPORT UNITS ELEMENT INFORMATION ITEM

import units element information items (referred to in this specification as import units elements) are element information items in the CellML namespace with local name equal to units, which appear as children of import elements.

- 1. Every import units element MUST contain a name attribute in the empty namespace. The value of the name attribute MUST be a valid CellML identifier. The value of the name attribute MUST NOT be identical to the name attribute of any other units element or import units element in the CellML infoset.
- 2. Every import units element MUST contain a units_ref attribute in the empty namespace. The value of the units_ref attribute MUST be a valid CellML identifier. The value of the units_ref attribute MUST match the value of the name attribute on a units element or import units element in the imported CellML infoset. The value of the units_ref attribute MUST NOT match the value of the units_ref attribute on any sibling import units element.

THE IMPORT COMPONENT ELEMENT INFORMATION ITEM

import component element information items (referred to in this specification as import component elements) are element information items in the CellML namespace with local name equal to component, which appear as children of import elements.

- 1. Every import component element MUST contain a name attribute in the empty namespace. The value of the name attribute MUST be a valid CellML identifier. The value of the name attribute MUST NOT be identical to the name attribute of any other component element or import component element in the CellML infoset.
- 2. Every import component element MUST contain a component_ref attribute in the empty namespace. The value of the component_ref attribute MUST be a valid CellML identifier. The value of the component_ref attribute MUST match the value of the name attribute on a component element or import component element in the imported CellML infoset. The value of the component_ref attribute MUST NOT match the value of the component_ref attribute on any sibling import component element.

THE UNITS ELEMENT INFORMATION ITEM

units element information items (referred to in this specification as units elements) are element information items in the CellML namespace with local name equal to units, and with either a model element or a component element as their parent.

- 1. Every units element MUST contain a name attribute in the empty namespace. The value of the name attribute MUST be a valid CellML identifier.
 - (a) Where the parent of the units element is a model element, the value of the name attribute MUST NOT be identical to the name attribute of any other units element child of that model element, or of any import units element in the CellML infoset.
 - (b) Where the parent of the units element is a component element, the value of the name attribute MUST NOT be identical to the name attribute of any other units element child of that component element.
 - (c) In any case, the value of the name attribute MUST NOT be equal to a cell in the name column of the *Built-in units* table.
- 2. A units element MAY contain a base_units attribute in the empty namespace. If present, the value of the base_units attribute MUST be equal to either yes or no. If the attribute is present and equal to yes, then the following paragraph does not apply.
- 3. A units element MAY contain one or more unit element children.

NINE

THE UNIT ELEMENT INFORMATION ITEM

unit element information items (referred to in this specification as unit elements) are element information items in the CellML namespace with local name equal to unit, and with a units element as their parent.

- 1. Every unit element MUST contain a units attribute information item in the empty namespace. The value of the units attribute MUST be a valid units reference, as defined in the *Units reference* section.
 - (a) The units element inclusion digraph SHALL be a conceptual digraph defined for the purpose of the constraint in the next paragraph, and SHALL contain one node for every units element in the CellML model. The units element inclusion digraph SHALL contain an arc from units element A to units element B if and only if units element A contains a unit element with units attribute value that is a units reference to units element B.
 - (b) The value of the units attribute MUST NOT be such that the units element inclusion digraph contains one or more cycles.
- 2. A unit element MAY contain any of the following attribute information items in the empty namespace:
 - (a) The prefix attribute. If present, the value of the attribute MUST meet the constraints specified in the *Interpretation of units* section.
 - (b) The offset attribute. If present, the value of the attribute MUST be a real number string. If the attribute is present and has value other than a real number string representing 0, then this unit element MUST NOT have any sibling unit elements, and the value of the exponent attribute, if present, MUST be a real number string representing 1.
 - (c) The multiplier attribute. If present, the value of the attribute MUST be a real number string.
 - (d) The exponent attribute. If present, the value of the attribute MUST be a real number string.

THE COMPONENT ELEMENT INFORMATION ITEM

component element information items (referred to in this specification as component elements) are element information items in the CellML namespace with local name component, and which appear as a child of a model element.

- 1. Every component element MUST contain a name attribute in the empty namespace. The value of the name attribute MUST be a valid CellML identifier. The value of the name attribute MUST NOT be identical to the name attribute on any other component element or import component element in the CellML infoset.
- 2. A component element MAY contain zero or more specific information item children, each of which MUST be of one of the following types:
 - (a) A units element;
 - (b) A variable element; or
 - (c) An element information item in the MathML namespace, and with local name math, which MUST be the top-level of a content MathML tree, as described in MathML 2.0.

THE VARIABLE ELEMENT INFORMATION ITEM

variable element information items (referred to in this specification as variable elements) are element information items in the CellML namespace with local name equal to variable, and which appear as a child of a component element.

11.1 Specific information items

- 1. Every variable element MUST have each of the following attribute information items in the empty namespace:
 - (a) The name attribute. The value of the name attribute MUST be a valid CellML Identifier. The value of the name attribute MUST NOT be identical to the name attribute on any sibling variable element.
 - (b) The units attribute. The value of the units attribute MUST be a valid CellML Identifier, and MUST meet the constraints described in the *Effect of units on variables* section.
- 2. Every variable element MAY contain one or more of the following attribute information items in the empty namespace:
 - (a) The public_interface attribute. If the attribute is present, it MUST have value in, out, or none.
 - (b) The private_interface attribute. If the attribute is present, it MUST have value in, out, or none. It MUST NOT have value in if the public_interface attribute also has the value in.
 - (c) The initial_value attribute. If the attribute is present, it MUST meet the requirements described **HERE**.

Todo

Need to provide a link to where the requirements for the initial_value attribute are.

CHAPTER

TWELVE

THE GROUP ELEMENT INFORMATION ITEM

group element information items (referred to in this specification as group elements) are element information items in the CellML namespace with local name equal to group.

- 1. Every group element MUST contain one or more relationship_ref elements.
- 2. Every group element MUST contain one or more component_ref elements.

CHAPTER THIRTEEN

THE RELATIONSHIP_REF ELEMENT INFORMATION ITEM

relationship_ref element information items (referred to in this specification as relationship_ref elements) are element information items in the CellML namespace with local name equal to relationship_ref.

- 1. Every relationship_ref element MUST contain exactly one attribute information item with local name relationship. This limit of one attribute information item SHALL apply without regard to the namespace in which the attribute information item is, and SHALL, to the extent that it conflicts, override the ordinary rules for extension information items.
- 2. In the event that the relationship attribute is in the empty namespace, it MUST either take the value encapsulation or containment.
- 3. There MUST NOT exist a sibling relationship_ref element such that the namespace of the relationship attribute on the sibling element is identical to the namespace of the relationship attribute on this element, and the value of the relationship attribute on the sibling element is identical to the value of the relationship attribute on this element.
- 4. A relationship_ref element MAY contain an attribute in the empty namespace with local name name. In this case, it MUST NOT have a relationship attribute in the empty namespace with value encapsulation. The value of the name attribute MUST be a valid CellML identifier.

CHAPTER FOURTEEN

THE COMPONENT_REF ELEMENT INFORMATION ITEM

component_ref element information items (referred to in this specification as component_ref elements) are element information items in the CellML namespace with local name equal to component_ref.

- 1. Every component_ref element MUST contain an attribute information item in the empty namespace and with local name component. The value of this attribute MUST be a valid CellML identifier, and MUST match the name attribute on a component element or an import component element in the CellML infoset.
- 2. Every component_ref element MAY in turn contain zero or more component_ref element children.
- 3. In addition, component_ref elements which are children of group elements MUST contain at least one component_ref element child.

CHAPTER

FIFTEEN

THE CONNECTION ELEMENT INFORMATION ITEM

connection element information items (referred to in this specification as connection elements) are element information items in the CellML namespace with local name equal to connection.

- 1. Every connection element MUST contain exactly one map_components element.
- 2. Every connection element MUST contain one or more map_variables elements.

CHAPTER SIXTEEN

THE MAP_COMPONENTS ELEMENT INFORMATION ITEM

map_components element information items (referred to in this specification as map_components elements) are element information items in the CellML namespace with local name equal to map_components, and which appear as a child of a connection element.

- 1. Each map_components element MUST contain a component_1 attribute in the empty namespace. The value of the component_1 attribute MUST be a valid CellML identifier. The value of this attribute MUST be equal to the name attribute on a component or import component element in the CellML infoset.
- 2. Each map_components element MUST contain a component_2 attribute in the empty namespace. The value of the component_2 attribute MUST be a valid CellML identifier. The value of this attribute MUST be equal to the name attribute on a component or import component element in the CellML infoset. It MUST NOT be equal to the value of the component_1 attribute.

CHAPTER SEVENTEEN

THE MAP_VARIABLES ELEMENT INFORMATION ITEM

map_variables element information items (referred to in this specification as map_variables elements) are element information items in the CellML namespace with local name equal to map_variables, and which appear as a child of a connection element.

- 1. Each map_variables element MUST contain a variable_1 attribute in the empty namespace. The value of the variable_1 attribute MUST be a valid CellML identifier. The value of this attribute MUST be equal to the name attribute on a variable element child of the component element referenced by the component_1 attribute on the map_components element which is a sibling of this element.
- 2. Each map_variables element MUST contain a variable_2 attribute in the empty namespace. The value of the variable_2 attribute MUST be a valid CellML identifier. The value of this attribute MUST be equal to the name attribute on a variable element child of the component element referenced by the component_2 attribute on the map_components element which is a sibling of this element.

INTERPRETATION OF CELLML MODELS

18.1 Interpretation of imports

- 1. Each import element present in a CellML infoset (the importing infoset) SHALL define a new and separate instance of the CellML infoset referenced by the href attribute (the imported infoset).
- 2. The following component elements SHALL be "pertinent component elements":
 - (a) All component elements in the top-level CellML infoset for the CellML model;
 - (b) All component elements referenced by import component elements in the top-level CellML infoset; and
 - (c) All component elements which are descendants in the encapsulation digraph of a pertinent component element.

18.2 Units reference

- 1. A units reference SHALL be a CellML identifier, and SHALL be interpreted based on the context within the CellML model in which it occurs.
- 2. A CellML infoset MUST NOT contain a units reference to which all scoping rules are inapplicable.
- 3. Where more than one of the units scoping rules apply, the applicable rule which appears first in this specification SHALL be used.
- 4. The units scoping rules are as follows:
 - (a) Where a units reference appears in an information item which is descended from a component element, and there is a units element child of that component element with a name attribute identical to the units reference, then the units reference SHALL refer to that units element.
 - (b) Where a units reference appears in an information item which is descended from the model element, and there is a units element child of that model element with a name attribute identical to the units reference, then the units reference SHALL refer to that units element.
 - (c) Where there is an import units element in the CellML infoset, such that the import units element has a name attribute identical to the units reference, then the units reference SHALL be treated as if the units reference appeared in the imported model, and referred to the name specified in the units_ref attribute of the import units element.

(d) Where the units reference is equal to a cell in the name column of the *Built-in units* table, then the units reference SHALL be a reference to the built-in unit corresponding to that row of the table.

Name	Base unit?	Multiplier and dimensions in terms of base units	Offset from base units
ampere	yes	-	-
becquerel	no	$1 \cdot second^{-1}$	0
candela	yes	-	-
celsius	no	$1 \cdot kelvin$	273.15
coulomb	no	$1 \cdot second \cdot ampere$	0
dimensionless	no	1	0
farad	no	$1 \cdot metre^{-2} \cdot kilogram^{-1} \cdot second^4 \cdot ampere^2$	0
gram	no	$10^{-3} \cdot kilogram$	0
gray	no	$1 \cdot metre^2 \cdot second^{-2}$	0
henry	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-2} \cdot ampere^{-2}$	0
hertz	no	$1 \cdot second^{-1}$	0
joule	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-2}$	0
katal	no	$1 \cdot second^{-1} \cdot mole$	0
kelvin	yes	-	-
kilogram	yes	-	-
liter	no	$10^{-3} \cdot metre^3$	0
litre	no	$10^{-3} \cdot metre^3$	0
lumen	no	$1 \cdot candela$	0
lux	no	$1 \cdot metre^{-2} \cdot candela$	0
meter	no	$1 \cdot metre$	0
metre	yes	-	-
mole	yes	-	-
newton	no	$1 \cdot metre \cdot kilogram \cdot second^{-2}$	0
ohm	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-3} \cdot ampere^{-2}$	0
pascal	no	$1 \cdot metre^{-1} \cdot kilogram \cdot second^{-2}$	0
radian	no	1	0
second	yes	-	-
siemens	no	$1 \cdot metre^{-2} \cdot kilogram^{-1} \cdot second^3 \cdot ampere^2$	0
sievert	no	$1 \cdot metre^2 \cdot second^{-2}$	0
steradian	no	1	0
tesla	no	$1 \cdot kilogram \cdot second^{-2} \cdot ampere^{-1}$	0
volt	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-3} \cdot ampere^{-1}$	0
watt	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-3}$	0
weber	no	$1 \cdot metre^2 \cdot kilogram \cdot second^{-2} \cdot ampere^{-1}$	0

Table 18.1: Built-in units

Name	Value
yotta	24
zetta	21
exa	18
peta	15
tera	12
giga	9
mega	6
kilo	3
hecto	2
deka	1
deci	-1
centi	-2
milli	-3
micro	-6
nano	-9
pico	-12
femto	-15
atto	-18
zepto	-21
yocto	-24

Table 18.2: Prefix values

18.3 Interpretation of units

- 1. The base units SHALL consist of the user defined base units, and the built-in base units (those units defined in rows of the *Built-in units* table having 'yes' in the 'Base unit?' column).
- 2. There SHALL be one user defined base unit for every units element in the CellML model which has a base_units attribute in the empty namespace, having value yes.
- 3. The base unit reduction of a units reference SHALL consist of a real valued offset, a real valued multiplier, and a set of tuples each consisting of a base unit and a real valued exponent. The base unit reduction of a units reference SHALL be determined as follows:
 - (a) Where the units reference is to a unit which is a base unit, then the base unit reduction of the units reference SHALL have offset 0.0, multiplier 1.0, and the set of tuples SHALL have a single member, which SHALL consist of the base units being referenced and the exponent 1.0.
 - (b) Where the units reference is to built-in units other than a base unit, then the base unit reduction SHALL be derived from the row of ? for which the value in the 'Name' column matches the name of the units reference. The offset of the base unit reduction SHALL be equal to the number in the 'Offset from base units' column of the row, and the multiplier SHALL be equal to the number at the start of the 'Multiplier and dimensions in terms of base units' column of the row. The set of tuples SHALL contain one member for every built-in base unit named in the 'Multiplier and dimensions in terms of base units' column of the built-in unit referenced, and the exponent appearing in superscript immediately after the units name in the table cell.
 - (c) Where the units reference is to a unit which is neither built-in, nor a base unit, the resultant base unit reduction SHALL be defined as a composition of the base unit reductions referenced from the unit element information items (the operand base unit reductions), in accordance with the following rules:

- i. The prefix term is a conceptual property of unit elements, defined here for later use. If the unit element does not have a prefix attribute information item, the prefix term SHALL have value 0.0. If the prefix attribute information item has a value which is a real number string, then the prefix term SHALL have the corresponding numerical value. Otherwise, the prefix attribute information item MUST have a value taken from the 'Name' column of the *Prefix values* table, and the prefix term SHALL have the value taken from the 'Value' column of the same row.
- ii. The exponent term is a conceptual property of unit elements, defined here for later use. If a unit element has no exponent attribute information item, the exponent term SHALL have value 1.0. Otherwise, the value of the exponent attribute information item MUST be a real number string, and the value of the exponent term SHALL be the numerical value of that string.
- iii. The multiplier term is a conceptual property of unit elements, defined here for later use. The multiplier term SHALL be the real number value of the multiplier attribute information item on the units element (or 1.0 in the absence of such an attribute information item), multiplied by 10.0 raised to the power of the product of the prefix term and the exponent term.
- iv. The offset term is a conceptual property of unit elements, defined here for later use. If a unit element has no offset attribute information item, the offset term SHALL have value 0.0. Otherwise, the value of the offset attribute information item MUST be a real number string, and the value of the offset term SHALL be the numerical value of that string.
- v. Where the units reference is to a units element with a single unit child element, then the resultant base unit reduction SHALL have multiplier equal to the product of the multiplier of the operand base unit reduction and the multiplier term of the unit element. It SHALL have offset equal to the sum of the offset of the operand base unit reduction and the offset term of the unit element.
- vi. Where the units reference is to a units element with a number of unit child elements not equal to 1.0, then the resultant base unit reduction SHALL have multiplier equal to the product of the multipliers of each operand base unit reduction, and the multiplier term of each unit element. It SHALL have offset equal to 0.0.
- vii. The set of tuples on the resultant base unit reduction SHALL have one member for every distinct base unit present in the set of tuples for any of the operand base unit reductions. The exponent alongside each of these base units in the resultant base unit reduction SHALL be the sum, across all tuples for the base unit from operand base unit reductions, of pairwise products of the exponent term on the corresponding unit element and the exponent from the tuple.

18.4 Component reference

- 1. A component reference SHALL be the name of a component, and SHALL be interpreted based on the context within the CellML model in which it occurs.
- 2. A component reference present in an information item which is a descendant of a model element SHALL be identical to either the name attribute on a component element or to the name attribute on an import component element.
- 3. A component reference which is identical to the name attribute on a component element SHALL be treated as a reference to that component element.
- 4. A component reference which is identical to the name attribute on an import component element SHALL be treated as if the component reference appeared in the imported model, and referred to the name specified in the component_ref attribute of the import component element.
- 5. It is noted, for the avoidance of doubt, that CellML models MAY apply the previous rule recursively, to reference an import component element which in turn references another import component element.

18.5 Variable reference

- 1. When present in an information item which is a descendant of a component element, a variable reference SHALL be the name of a variable, and SHALL refer to the variable element in the same component with a name attribute identical to the variable reference.
- 2. In all other cases, a variable reference SHALL consist of a component reference and a variable name. In this case, the variable reference SHALL be treated as if it was present in the component element referenced by the component reference.

18.6 Interpretation of initial values

- 1. This section applies to the interpretation of the initial_value attribute, when it appears as an attribute information item on a variable element.
- 2. The initial_value attribute MUST either be a real number string, or a variable reference.
- 3. Where the initial_value attribute has a real number value, it SHALL be interpreted as a statement that the variable on which the attribute appears is equal to that real number value, under the conditions when the initial value holds.
- 4. Where the initial_value attribute is a variable reference, it SHALL be interpreted as a statement that the variable on which the attribute appears is equal to the referenced variable under the conditions when the initial value holds.

Todo

Need a reasonable definition of the conditions when the initial value holds, because we can't really use the 1.1 version because it is problematic for a number of reasons.

18.7 Effect of units on variables

- 1. The units attribute on a variable element MUST be a valid units reference. The target of this units reference is referred to as the variable units, and the corresponding base units reduction is referred to as the variable base unit reduction.
- 2. The variable base unit reduction of a variable element MUST have an identical set of tuples to the set of tuples on the source variable base element units reduction. Two sets of tuples SHALL be considered identical if and only if neither set contains any tuple not present in the other. Two tuples are considered identical if both the base units and exponent on the tuple are the same.
- 3. The following symbols are defined for the purposes of the formulae in the *Interpretation of mathematics* section:
 - (a) m_V is the multiplier on the variable base unit reduction.
 - (b) o_V is the offset on the variable base unit reduction.
 - (c) m_S is the multiplier on the source variable base unit reduction.
 - (d) o_S is the offset on the source variable base unit reduction.

18.8 Interpretation of mathematics

- 1. Every MathML element in the CellML model, which appears as a direct child information item of the MathML math element information item, which in turn appears as a child information item of a pertinent component element, SHALL be treated as a statement which holds true unconditionally.
- 2. Every MathML element which appears as a direct child information item of the MathML math element information item SHALL be treated as a statement which holds true unconditionally.
- 3. Every variable name given using the MathML ci element SHALL be treated as a variable reference within the component element ancestor the MathML is contained within.
- 4. Every such variable reference SHALL be treated as a linear expression $\frac{m_V}{m_S} \cdot x o_V + \frac{m_S}{m_V} \cdot o_S$. In this equation, x represents the variable in the mathematical model, in the units of the source variable element, while the remaining variables SHALL be interpreted as specified in the *Effect of units on variables* section.
- 5. Every MathML cn element MUST have an attribute information item in the CellML namespace, with local name units. The value of this attribute information item MUST be a valid units reference. The referenced units SHALL NOT affect the mathematical interpretation of the CellML model. However, CellML processing software MAY use this information to assist the user in the detection and correction of units errors in the CellML model.

18.9 Interpretation of grouping

- 1. Two relationship_ref elements SHALL be considered to refer to the same relationship if and only if all of the following conditions hold:
 - (a) The attribute information item with local name relationship is in an identical namespace on both element information items;
 - (b) The attribute information item with local name relationship has identical values on each of the element information items; and
 - (c) Either the attribute information item in the empty namespace and with local name name is absent on both element information items, or, it is present on both element information items and has identical value.
- 2. For every distinct relationship referred to by a relationship_ref element in the CellML model, there SHALL be a conceptual relationship digraph in which there is one node for every component in the CellML model.
- 3. Where a component_ref element appears as a child of another component_ref element, then for all relationship_ref elements which are children of the ancestral group element, there SHALL be an arc in the relationship digraph corresponding to the relationship referenced by the relationship_ref element, and that arc SHALL be from the component referenced by the parent component_ref element and to the component referenced by the child component_ref element.
- 4. The term encapsulation digraph SHALL refer to the relationship digraph for the relationship corresponding to the relationship_ref attribute in the empty namespace and with value encapsulation (and with no name attribute).
- 5. The encapsulation digraph MUST NOT contain any loops, and MUST NOT contain any cycles in the underlying graph (that is, it must be a tree).
- 6. The encapsulated set for a component *A* SHALL be the set of all components to which there exists an arc in the encapsulation digraph from the node corresponding to *A*.
- 7. The encapsulation parent for a component *A* SHALL be the component corresponding to the node which is the parent node in the encapsulation digraph of the node corresponding to *A*.

- 8. The sibling set for a component *A* SHALL be the set of all components which have the same encapsulation parent as *A*, or in the case that *A* has no encapsulation parent, SHALL be the set of all components which do not have an encapsulation parent.
- 9. The hidden set for a component *A* SHALL be the set of all components *B* where component *B* is not in the encapsulated set for component *A*, and component *B* is not the encapsulation parent of component *A*, and component *B* is not in the sibling set for component *A*.
- 10. CellML models MUST NOT contain map_components elements such that the component referenced by the component_1 attribute is in the hidden set of the component referenced by the component_2 attribute.

18.10 Variable equivalence networks

- 1. A variable equivalence network SHALL be a directed graph with one node for every variable element in the CellML model.
- 2. For every map_variables element present in the CellML model, there SHALL be an arc in the variable equivalence network.
- 3. One endpoint of the arc in the variable equivalence network SHALL be the node corresponding to the variable A referenced by the component_1 and variable_1 attributes.
- 4. One endpoint of the arc in the variable equivalence network SHALL be the node corresponding to the variable *B* referenced by the component_2 and variable_2 attributes.
- 5. CellML models MUST NOT contain any pair of map_variables elements which each make reference to the same sets of variables (without regard to whether the variable_1 attribute of one map_variables element references the variable referenced by the variable_1 or variable_2 attribute of the other).
- 6. When the component parent element of variable *A* is in the sibling set of the component parent element of variable *B*, the applicable interface for variables *A* and *B* SHALL be the public interface.
- 7. Where the component parent element of variable A is in the encapsulated set of the component parent element of variable B, the applicable interface for variable A SHALL be the public interface, and the applicable interface for variable B SHALL be the private interface.
- 8. Where the component parent element of variable *B* is in the encapsulated set of the component parent element of variable *A*, the applicable interface for variable *A* SHALL be the private interface, and the applicable interface for variable *B* SHALL be the public interface.
- 9. For a given variable, if the applicable interface is the public interface, the applicable interface attribute SHALL be the public_interface attribute information item on the corresponding variable element. If the applicable interface is the private interface, the applicable interface attribute SHALL be the private_interface attribute information item on the corresponding variable element.
- 10. In any case, if the applicable interface attribute is absent, the following rules in this section SHALL still apply as if the applicable interface attribute was present, and had the value none.
- 11. CellML models MUST NOT contain map_variables elements unless the value of the applicable interface attributes on variables A and B are both either in or out, and those two attribute values are different from each other.
- 12. The direction of the arc SHALL be from the node corresponding to the variable with the applicable interface attribute equal to in, and SHALL be to the node corresponding to the variable with the applicable interface attribute equal to out.
- 13. For the purposes of this specification, the variable elements in a CellML model SHALL be treated as belonging to one of several disjoint sets of connected variables. Each set of connected variables is the set of all

variable elements for which the corresponding nodes in the variable equivalence network form a weakly connected subgraph. Each set of connected variables represents one variable in the mathematical model.

14. In every set of connected variables, there MUST be exactly one variable element which has neither a public interface of in nor a private interface of in. This variable element is referred to as the source variable element. Within this specification, the variable in the mathematical model is described as if it was in the units specified on the source variable element.

CHAPTER

NINETEEN

REFERENCES

RFC 2119: Key words for use in RFCs to Indicate Requirement Levels (March 1997) Extensible Markup Language (XML) 1.0 (Fourth Edition) (16 August 2006) XML Information Set (Second Edition) (4 February 2004) Namespaces in XML (Second Edition) (16 August 2006) Resource Description Framework (RDF): Concepts and Abstract Syntax (10 February 2004) RDF/XML Syntax Specification (Revised) (10 February 2004) Mathematical Markup Language (MathML) Version 2.0 (Second Edition) (21 October 2003) XML Linking Language (XLink) Version 1.0 (27 June 2001)

CHAPTER

TWENTY

SUMMARY OF ALL TODO'S

Todo

Provide a 'proper' URL for the informative version of the specification.

(The original entry is located in abstract.rst, line 16.)

Todo

Need a reasonable definition of the conditions when the initial value holds, because we can't really use the 1.1 version because it is problematic for a number of reasons.

(The *original entry* is located in /var/build/user_builds/cellml-specifications-sphinx-testing/checkouts/latest/source/model-interpretation.rst, line 345.)

Todo

Need to provide a link to where the requirements for the initial_value attribute are.

(The *original entry* is located in /var/build/user_builds/cellml-specifications-sphinx-testing/checkouts/latest/source/variable-element-item.rst, line 37.)

Todo

Find out which rule 1 we are we talking about here. Andre: it is the rule 1 just here (2.8.1 currently) but need to work out how to properly reference other rules. Probably shouldn't rely on section numbers being consistent.

(The *original entry* is located in /var/build/user_builds/cellml-specifications-sphinx-testing/checkouts/latest/source/general-matters.rst, line 162.)