CellML 2.0 Specification [May 2017 Draft]

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1. Definitions

The keywords "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 <u>XML Information Set</u>.

CellML infoset

An XML information set containing a hierarchy of information items conforming to the rules described in this document. In this specification such infosets are assumed to be CellML 2.0 infosets.

CellML model

A mathematical model represented by a hierarchy of one or more CellML infosets, according to the rules described in this document. In this specification, the topmost CellML infoset in this hierarchy is referred to as the top-level CellML infoset.

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 1.1.

CellML namespace

The CellML 2.0 namespace.

CellML 2.0 namespace

The namespace http://www.cellml.org/cellml/2.0#.

MathML namespace

The namespace http://www.w3.org/1998/Math/MathML.

CellML information item

Any information item in the CellML namespace.

Basic Latin alphabetic character

A Unicode character in the range $\underline{U+0041}$ to $\underline{U+005A}$ or in the range $\underline{U+0061}$ to $\underline{U+007A}$.

European numeric character

A Unicode character in the range $\underline{\text{U+0030}}$ to $\underline{\text{U+0039}}$.

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 $\underline{U+005F}$.

Whitespace character

Any one of the Unicode characters <u>U+0020</u>, <u>U+0009</u>, <u>U+000D</u> or <u>U+000A</u>.

2. General matters

2.1. CellML and XML

- 1. Every CellML infoset SHALL be represented in an XML document which conforms with the well-formedness requirements of <u>XML 1.1</u>.
- 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. Semantically equivalent CellML infosets

- 1. Two CellML infosets SHALL be deemed semantically equivalent in terms of model content if one can be transformed into the other by making zero or more of the following changes:
 - 1. Changing the representation of the XML file in ways which do not change the XML information set represented.
 - 2. Adding, removing, and/or modifying comment information items.
 - 3. 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.
 - 4. 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 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.

2.3. 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. Element and attribute information items in a CellML infoset MUST belong to one of the following namespaces, unless explicitly indicated otherwise:
 - 1. The CellML namespace
 - 2. MathML 2.0, where:
 - 1. The element information item or one of its ancestors is an element information item in the MathML namespace, with a local name equal to math (the math element information item); and

2. The math element information item forms the top-level of a valid MathML 2.0 tree

2.5. XML Document Identifiers

1. Any element information item in the CellML namespace MAY contain an unprefixed attribute information item with local name id. This attribute information item SHALL be treated as having attribute type ID, as defined in section 3.3.1 of XML 1.1.

- 1. For the purposes of this specification, a specific information item is one of the following (see https://www.w3.org/TR/xml-infoset/#infoitem for definitions):
 - 1. A document information item;
 - 2. An element information item:
 - 3. An attribute information item;
 - 4. A processing instruction information item;
 - 5. An unexpanded entity reference information item;
 - 6. A document type declaration information item;
 - 7. An unparsed entity information item;
 - 8. A notational 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 semantic interpretation of the CellML model.

3. Data representation formats in CellML

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

1. A CellML identifier:

- 1. SHALL be a sequence of Unicode characters.
- 2. SHALL NOT contain any characters except basic Latin alphanumeric characters and basic Latin underscores.
- 3. SHALL contain one or more basic Latin alphabetic characters.
- 4. SHALL NOT begin with a European numeric character.
- 5. SHALL, when comparing two identifiers, be considered identical to another identifier if and only if both identifiers have identical sequences of Unicode characters.

2. A non-negative integer string:

- 1. SHALL be a base 10 representation of a non-negative integer.
- 2. SHALL consist entirely of European numeric characters.

3. An integer string:

- 1. SHALL be a base 10 representation of an integer.
- 2. SHALL, when the integer being represented is negative, consist of the basic Latin hyphen-minus character <u>U+002D</u>, followed by the non-negative integer string representation of the absolute value of the integer.
- 3. 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:

- 1. SHALL be a base 10 representation of a real number.
- 2. SHALL, when the basic real number being represented is negative, begin with the basic Latin hyphen-minus character <u>U+002D</u> as the sign indicator.
- 3. MAY contain a single decimal point separator, which SHALL be the basic Latin full stop character <u>U+002E</u>.
- 4. SHALL, other than the sign indicator and the decimal point separator, consist only of European numeric characters.

5. A real number string:

- 1. SHALL be a base 10 representation of a real number *r*=s · 10^e, where s is the significand, a real number, and e is the exponent, an integer.
- 2. The representation of the number SHALL be the representation of the significand followed immediately by the representation of the exponent.
- 3. The significand SHALL be represented as a basic real number string.
- 4. A non-zero 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.
- 5. If the exponent is zero, the exponent MAY be represented by an empty string, or MAY be represented according to the rule for non-zero exponent.

4. The model element information item

4.1. Top-level of CellML infosets

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

- 1. Every model element MUST contain an unprefixed name attribute. The value of the name attribute MUST be a valid CellML identifier.
- 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:
 - 1. A component element; or
 - 2. A connection element; or
 - 3. An encapsulation element; or
 - 4. An import element; or
 - 5. A units element;
- 3. A model element MUST NOT contain more than one encapsulation element.

5. The import element information item

An import element information item (referred to in this specification as an import element) is an element information item in the CellML namespace with a 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 a local name equal to 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 document referenced by the href attribute.
- 2. Every import element MAY contain zero or more specific information item children, each of which MUST be of one of the following types:
 - 1. An import units element; or
 - 2. An import component element.
- 3. The imported CellML infoset MUST NOT be semantically equivalent (see <u>Semantically equivalent CellML infosets</u>) to the importing CellML infoset. Any CellML infoset imported, directly or indirectly, by the imported CellML infoset MUST NOT be semantically equivalent to the importing CellML infoset.

6. The import units element information item

An import units element information item (referred to in this specification as an import units element) is an element information item in the CellML namespace with a local name equal to units, which appears as a child of an import element.

- 1. Every import units element MUST contain an unprefixed 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 of any other units element that appears as the direct child of a model element or import units element in the CellML infoset.
- 2. Every import units element MUST contain an unprefixed units_ref attribute. 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.

7. The import component element information item

An import component element information item (referred to in this specification as an import component element) is an element information item in the CellML namespace with a local name equal to component, which appears as a child of an import element.

- 1. Every import component element MUST contain an unprefixed 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 of any other component element or import component element in the CellML infoset.
- 2. Every import component element MUST contain an unprefixed component_ref attribute. 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. See also the Component reference section.

8. The units element information item

A units element information item (referred to in this specification as a units element) is an element information item in the CellML namespace with a local name equal to units, and with a model element as its parent.

- 1. Every units element MUST contain an unprefixed name attribute. The value of the name attribute MUST be a valid CellML identifier.
- 2. 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.
- 3. The value of the name attribute MUST NOT be equal to the name of any of the units listed in the <u>Built-in units</u> table.
- 4. A units element MAY contain one or more unit element children.

9. The unit element information item

A unit element information item (referred to in this specification as a unit element) is an element information item in the CellML namespace with a local name equal to unit, and with a units element as its parent.

- 1. Every unit element MUST contain an unprefixed units attribute information item. The value of the units attribute MUST be a valid units reference, as defined in the Units reference section.
 - 1. For the purpose of the constraint in the next paragraph, the units element inclusion digraph SHALL be defined as a conceptual digraph which 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.
 - 2. The value of the units attribute MUST NOT be such that the units element inclusion digraph contains one or more cycles (in other words, units definitions must not be circular).
- 2. A unit element MAY contain any of the following unprefixed attribute information items:
 - 1. The prefix attribute. If present, the value of the attribute MUST meet the constraints specified in the <u>Interpretation of units</u> section.
 - 2. The multiplier attribute. If present, the value of the attribute MUST be a real number string.
 - 3. The exponent attribute. If present, the value of the attribute MUST be a real number string.

10. The component element information item

A component element information item (referred to in this specification as a component element) is an element information item in the CellML namespace with a local name equal to component, and which appears as a child of a model element.

- 1. Every component element MUST contain an unprefixed 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 other component element or import component element in the CellML infoset.
- 2. A component element MAY contain one or more specific information item children, each of which MUST be of one of the following types:
 - 1. A variable element; or
 - 2. A reset element; or
 - 3. A math element

11. The variable element information item

A variable element information item (referred to in this specification as a variable element) is an element information item in the CellML namespace with a local name equal to variable, and which appears as a child of a component element.

- 1. Every variable element MUST have each of the following unprefixed attribute information items:
 - 1. 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.
 - 2. 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 unprefixed attribute information items:
 - 1. The interface attribute. If the attribute is present, it MUST have one of the values public, private, public and private, or none.
 - 2. The initial_value attribute. If the attribute is present, it MUST meet the requirements described by the <u>Interpretation of initial values</u> section.

12. The reset element information item

A reset element information item (referred to in this specification as a reset element) is an element information item in the CellML namespace with a local name equal to reset, and which appears as a child of a component element.

- 1. Every reset element MUST have each of the following unprefixed attribute information items:
 - 1. The variable attribute. The value of the variable attribute MUST be a variable reference to a variable defined within the component element parent of the reset element.
 - 2. The order attribute. The value of the order attribute MUST be an integer string. The value of the order attribute MUST be unique for all reset elements for variables that are in the same connected variable set (see <u>Interpretation of map_variables</u>).
 - 3. A reset element MUST contain one or more specific information item children, each of which MUST be a when element.

13. The when element information item

A when element information item (referred to in this specification as a when element) is an element information item in the CellML namespace with a local name equal to when, and which appears as a child of a reset element.

- 1. Every when element MUST contain an unprefixed order attribute. The value of the order attribute MUST be an integer string. All sibling when elements MUST have a unique value for order.
- 2. A when element MUST contain two specific information item children, each of which MUST be math elements.

14. The math element information item

A math element information item (referred to in this specification as a math element) is an element information item in the MathML namespace that appears as a direct child of a component element, or as a direct child of a when element.

14.1. Specific information items

- 1. A math element MUST be the top-level of a content MathML tree, as described in MathML 2.0.
- 2. Each element information item child of a math element MUST have an element-type name that is listed in the <u>Supported MathML Elements</u> table, and where allowable types are listed in that table the element MUST exhibit one of those types.
- 3. Every variable name given using the MathML ci element MUST be a variable reference to a variable within the component element that the math element is contained within.
- 4. Any MathML on elements MUST each have an attribute information item in the CellML namespace, with a local name equal to units. The value of this attribute information item MUST be a valid units reference.

Table: Supported MathML Elements

Element Category	Element List
Simple Operands	<ci>, <cn> (allowable types: real (default), e-notation), <sep></sep></cn></ci>
Basic Structural	<apply>, <piecewise>, <piece>, <otherwise></otherwise></piece></piecewise></apply>
Relational and Logical Operators	<eq>, <neq>, <gt>, <lt>, <geq>, <leq>, <and>, <or>, <xor>, <not></not></xor></or></and></leq></geq></lt></gt></neq></eq>
Arithmetic Operators	<pre><plus>, <minus>, <times>, <divide>, <power>, <root>, <abs>, <exp>, <ln>, <log>, <floor>, <ceiling>, <min>, <max>, <rem>,</rem></max></min></ceiling></floor></log></ln></exp></abs></root></power></divide></times></minus></plus></pre>
Calculus Elements	<diff></diff>
Qualifier Elements	 /sour>, <logbase>, <degree> (child of <root> or <diff>)</diff></root></degree></logbase>
Trigonometric Operators	<pre><sin>, <cos>, <tan>, <sec>, <cot>,</cot></sec></tan></cos></sin></pre>
Mathematical and Logical Constants	<pi><pi><pi><pi><pi><exponentiale>, <notanumber>, <infinity>, <true>, <false></false></true></infinity></notanumber></exponentiale></pi></pi></pi></pi></pi>

15. The encapsulation element information item

An encapsulation element information item (referred to in this specification as an encapsulation element) is an element information item in the CellML namespace with a local name equal to encapsulation, and which appears as a child of a model element.

15.1. Specific information items

1. Every encapsulation element MUST contain one or more component ref elements.

16. The component_ref element information item

A component_ref element information item (referred to in this specification as a component_ref element) is an element information item in the CellML namespace with a local name equal to component_ref, and which appears as a child of an encapsulation element.

- 1. Every component_ref element MUST contain an unprefixed component attribute information item. 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. component_ref elements which are immediate children of encapsulation elements MUST each contain at least one component ref element child.

17. The connection element information item

A connection element information item (referred to in this specification as a connection element) is an element information item in the CellML namespace with a local name equal to connection, and which appears as a child of a model element.

- 1. Each connection element MUST contain an unprefixed component_1 attribute. 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 (see Component reference).
- 2. Each connection element MUST contain an unprefixed component_2 attribute. 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 (see Component reference). It MUST NOT be equal to the value of the component 1 attribute.
- 3. A CellML infoset MUST NOT contain more than one connection element with a given pair of components referenced by the component_1 and component_2 attribute values, in any order.
- 4. Every connection element MUST contain one or more map variables elements.

18. The map_variables element information item

A map_variables element information item (referred to in this specification as a map_variables element) is an element information item in the CellML namespace with a local name equal to map_variables, and which appears as a child of a connection element.

- 1. Each map_variables element MUST contain an unprefixed variable_1 attribute. 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 or import component element referenced by the component 1 attribute on the connection element which is the parent of this element.
- 2. Each map_variables element MUST contain an unprefixed variable_2 attribute. 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 or import component element referenced by the component_2 attribute on the connection element which is the parent of this element.
- 3. A connection element MUST NOT contain more than one map_variables element with a given variable_1 attribute value and variable_2 attribute value pair.

19. Interpretation of CellML models

19.1. 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). See <u>Units reference</u> and <u>Component reference</u> for the specifics of importing units and components.

19.2. Units reference

- 1. A units reference SHALL be a CellML identifier, and in terms of the semantics of the model content SHALL be interpreted dependent on the context of the CellML model in which it occurs, according to the units referencing rules defined later in this section.
- 2. A CellML infoset MUST NOT contain a units reference for which no referencing rule can be held to have been followed.
- 3. The units referencing rules are:
 - 1. Where there is a units element with a name attribute identical to the units reference, then the units reference SHALL refer to that units element.
 - 2. 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 with respect to referencing rules as if the units reference appeared in the imported infoset, in an information item descended from the imported infoset's model element, and referred to the name specified in the units ref attribute of the import units element.
 - 3. Where the units reference is equal to the value in the 'Name' column of the <u>Built-in units</u> table, then the units reference SHALL be a reference to the built-in unit corresponding to that row of the table.

Table: Built-in units

Name	Multiplier(s)	Unit reduction tuple (dimension, exponent) set
ampere	-	-
becquerel	1	(second, -1)
candela	-	-
coulomb	1, 1	(second, 1), (ampere,1)
dimensionless	-	-
farad	1, 1, 1, 1	(metre, -2), (kilogram, -1), (second, -4), (ampere,2)
gram	0.001	(kilogram,1)
gray	1, 1	(metre, 2), (second, -2)
henry	1, 1, 1, 1	(metre, 2), (kilogram, 1), (second, -2), (ampere, -2)
hertz	1	(second, -1)
joule	1, 1, 1	(metre, 2), (kilogram, 1), (second, -2)

katal	1, 1	(second, -1), (mole, 1)
kelvin	-	-
kilogram	-	-
liter	0.001	(metre, 3)
litre	0.001	(metre, 3)
lumen	1	(candela, 1)
lux	1, 1	(metre, -2), (candela, 1)
meter	1	(metre, 1)
metre	-	-
mole	-	-
newton	1, 1, 1	(metre, 1), (kilogram, 1), (second, -2)
ohm	1, 1, 1, 1	(metre, 2), (kilogram, 1), (second, -3), (ampere, -2)
pascal	1, 1, 1	(metre, -1), (kilogram, 1), (second, -2)
radian	1, 1	(metre, 1), (metre, -1)
second	-	-
siemens	1, 1, 1, 1	(metre, -2), (kilogram -1), (second, 3), (ampere, 2)
sievert	1, 1	(metre, 2), (second, -2)
steradian	1, 1	(metre, 2), (metre, -2)
tesla	1, 1, 1	(kilogram, 1), (second, -2), (ampere, -1)
volt	1, 1, 1, 1	(metre, 2), (kilogram, 1), (second , -3), (ampere, -1)
watt	1, 1, 1	(metre, 2), (kilogram, 1), (second, -3)
weber	1, 1, 1, 1	(metre, 2), (kilogram, 1), (second, -2), (ampere, -1)

19.3. Interpretation of units

- 1. The units element SHALL be interpreted as the product of its unit element children, according to the following rules:
 - 1. The prefix term is a conceptual property of unit elements. 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 an integer string, then the value of the prefix term SHALL be the numerical value of that string. 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.
 - 2. The exponent term is a conceptual property of unit elements. 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.

- 3. The multiplier term is a conceptual property of unit elements. If a unit element has no multiplier attribute information item, the multiplier term SHALL have value 1.0. Otherwise, the value of the multiplier attribute information item MUST be a real number string, and the value of the multiplier term SHALL be the numerical value of that string.
- 4. The relationship between the product, *P*, of numerical values given in each and every child unit element units, to a numerical value, *x*, with units given by the encompassing units element, SHALL be

$$x[u_x] = \frac{1}{(10^{p_1^{e_1}} ... 10^{p_n^{e_n}} m_1 ... m_n)} \left[\frac{u_x}{u_1^{e_1} ... u_n^{e_n}} \right] P[u_1^{e_1} ... u_n^{e_n}]$$

where: u_x denotes the units of the units element; p_i , e_i , m_i , and u_i refer to the prefix, exponent and multiplier terms and units of the *i*th unit child element, respectively. Square brackets encompass the units of numerical values.

- 2. For the purposes of this specification, the "irreducible units" of a model SHALL consist of 1) the units defined in a model that are not defined in terms of other units (i.e. the set of units elements in the CellML model which have no unit child elements), and 2) built-in irreducible units (those built-in units with '-' in the 'Unit Reduction...' column of the <u>Built-in units</u> Table) referenced by variables or other units in the model.
- 3. The "unit reduction" is a conceptual property of units elements. It consists of a set of tuples where each tuple is composed of a) a unit name and b) a real-valued exponent. Tuples SHALL be determined as follows:
 - 1. If the units element has no unit child elements, then the set of tuples SHALL have a single member, which SHALL consist of the name of the units element and the exponent 1.0.
 - 2. If the units element has one or more unit child elements, then the set of tuples SHALL consist of the entire collection of tuples given by all unit child elements. Tuples for each unit child element SHALL be determined as follows:
 - 1. Where the units reference of the unit child element is to a single unit which is an irreducible unit, then the set of tuples SHALL have a single member, which SHALL consist of the name of the irreducible unit being referenced and the exponent 1.0.
 - 2. Where the units reference of the unit child element is to built-in units other than an irreducible unit, then the tuples SHALL be derived directly from the <u>Built-in units</u> table. Specifically, the set of tuples SHALL consist of the tuples given in the 'Unit reduction tuple ... set' column of the row for which the value in the 'Name' column matches the name of the units reference.
 - 3. Where the units reference of the unit child element is to a unit which is neither built-in, nor an irreducible unit, the set of tuples SHALL be defined recursively as the set of tuples for the units element so referenced.

- 4. The exponents of each tuple in the set for the current unit element, as derived by following rule 3.2.1, 3.2.2 or 3.2.3 above, SHALL be multiplied by the exponent term of the current, referencing, unit element.
- 3. Tuples which have the name element of 'dimensionless' SHALL be removed from the set of tuples. Note that this can result in the set of tuples being empty.
- 4. Where the set of tuples consists of tuples which have the same name element, those tuples SHALL be combined into a single tuple with that name element and an exponent being the sum of the combined tuples' exponents. If the resulting tuple's exponent term is zero, the tuple SHALL be removed from the set of tuples. Note that this can result in the set of tuples being empty.

Table: Prefix values

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

19.4. 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 for the purposes of referencing as if the component reference appeared in the imported model, and referred to element with 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.

19.5. 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 that 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 just the variable name present in the component element referenced by the component reference.

19.6. Interpretation of initial values

- 1. The initial_value attribute of a variable element MUST either be a real number string, or a variable reference.
- 2. The conditions when initial values hold are (by design) not defined in a CellML model document. It is intended that those conditions be supplied by CellML processing software where appropriate.
- 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.

19.7. Effect of units on variables

1. The value of the units attribute on every variable element MUST be a valid units reference. The target of this units reference is referred to as the variable units, and the corresponding unit reduction (see <u>Interpretation of units</u>) is referred to as the variable unit reduction.

19.8. Interpretation of mathematics

1. The following component elements SHALL, for the purposes of this specification, be "pertinent component elements":

- 1. All component elements in the top-level CellML infoset for the CellML model;
- 2. All component elements referenced by import component elements (see <u>The import component element information item</u>) in the top-level CellML infoset; and
- 3. All component elements which are descendants in the encapsulation digraph (see <u>Interpretation of encapsulation</u>) of a pertinent component element.
- 2. Every MathML element in the CellML model which appears as a direct child information item of a MathML math element information item, which in turn appears as a child information item of a pertinent component element, SHALL be treated, in terms of the semantics of the mathematical model, as a statement which holds true unconditionally.
- 3. Units referenced by a units attribute information item 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.

19.9. Interpretation of encapsulation

- 1. For the purposes of this specification, there SHALL be a "conceptual encapsulation digraph" in which there is one node for every component in the CellML model.
- 2. Where a component_ref element appears as a child of another component_ref element, there SHALL be an arc in the encapsulation digraph, and that arc SHALL be from the node corresponding to the component referenced by the parent component_ref element, and to the node corresponding to the component referenced by the child component ref element.
- 3. The encapsulation digraph MUST NOT contain any loops, and MUST NOT contain any directed cycles.
- 4. The encapsulated set for a component A SHALL be the set of all components B such that there exists an arc in the encapsulation digraph from the node corresponding to A to the node corresponding to B.
- 5. 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.
- 6. 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.
- 7. 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.
- 8. There MUST NOT be a connection element such that the component referenced by the component_1 attribute is in the hidden set of the component referenced by the component 2 attribute, nor vice versa.

19.10. Interpretation of map_variables

- 1. For the purposes of this specification, a variable equivalence (conceptual) network SHALL be a graph with one node for every variable element in the CellML model.
- 2. For each map_variables element present in the CellML model, we define variables *A* and *B* for use in the rules in this section as follows.
 - 1. Variable A SHALL be the variable referenced by the encompassing connection element's component_1 and this map_variables element's variable 1 attributes.
 - 2. Variable *B* SHALL be the variable referenced by the encompassing connection element's component_2 and this map_variables element's variable 2 attributes.
- 3. For every map_variables element present in the CellML model, there SHALL be an arc in the variable equivalence network.
 - 1. One endpoint of the arc in the variable equivalence network SHALL be the node corresponding to variable *A*.
 - 2. One endpoint of the arc in the variable equivalence network SHALL be the node corresponding to variable *B*.
- 4. CellML models MUST NOT contain any pair of map_variables elements which define the same arc in the variable equivalence network (according to the previous paragraph).
- 5. The variable equivalence network MUST NOT contain any cycles (that is, it must be a tree).
- 6. For each map_variables element present in the CellML model, the variable unit reduction (see Effect of units on variables) of variable *A* MUST have an identical set of tuples to the variable unit reduction of variable *B*. Two sets of tuples SHALL be considered identical if all of the tuples from each set are present in the other, or if both sets are empty. Two tuples are considered identical if and only if both the name and exponent value of each tuple are equivalent.
- 7. Processing software concerned with providing numerical solutions to the mathematical model MAY provide automatic numerical conversion between variables which have the same variable unit reduction but different multipliers (see <u>Interpretation of units</u>) by employment of conversion factors.
- 8. For a given variable, the available interfaces SHALL be determined by the interface attribute information item on the corresponding variable element as follows.
 - 1. A value of public specifies that the variable has a public interface.
 - 2. A value of private specifies that the variable has a private interface.
 - 3. A value of public_and_private specifies that the variable has both a public and a private interface.
 - 4. A value of none specifies that the variable has no interface.
 - 5. If the interface attribute information item is absent, then the variable has no interface.

- 9. The applicable interfaces for variables A and B SHALL be defined as follows.
 - 1. When the parent component element of variable A is in the sibling set of the parent component element of variable B, the applicable interface for both variables A and B SHALL be the public interface.
 - 2. When the parent component element of variable *A* is in the encapsulated set of the parent component 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.
 - 3. When the parent component element of variable *B* is in the encapsulated set of the parent component 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.
- 10. CellML models MUST NOT contain a map_variables element where the applicable interface of variable A or B is not defined or is not an available interface.
- 11. For the purposes of this specification, the variable elements in a CellML model SHALL be treated as belonging to one of one or more disjoint "connected variable sets". 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 underlying mathematical model.

19.11. Interpretation of variable resets

- 1. Each reset element describes a change to be applied to the variable referenced by the variable attribute when specified conditions are met during the simulation of the model.
- 2. All reset elements SHALL be considered sequentially for the connected variable set (see <u>Interpretation of map_variables</u>) to which the referenced variable belongs. The sequence SHALL be determined by the value of the reset element's order attribute, lowest (least positive) having priority.
- 3. The change, and conditions for the change, to a variable for a given reset element SHALL be defined by the evaluation of that element's when child elements.
 - a. A when element SHALL be deemed to be true when the evaluation of the MathML expression encoded in first child element of the when element changes from the boolean expression false to true.
 - b. If a when element is deemed to be true, then false, then true again during the same 'instant' or interval of integration, it SHALL nevertheless be held to be false.
 - c. The second child element of a when element SHALL define the MathML expression to be evaluated and assigned to the parent reset element's referenced variable when the when element is deemed to be true.
 - d. Consideration of the set of when child elements of a given reset element SHALL stop at the first occurrence of a when deemed to be true.

e. The order of consideration of the set of when child elements SHALL be based on the value of the when element's order attribute, lowest having priority.

20. References

RFC 2119: Key words for use in RFCs to Indicate Requirement Levels (March 1997)

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