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Units Definition and Examples

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1 Introduction

Throughout January and February 2001, one of the biggest headaches for Warren was the specification of a units system for CellML. The problem was that he needed to completely define how a units definition should be recursively expanded in order that the conversion of variable values from one set of units to another would be consistent across all applications. Warren tried to pass his problems on to as many other people as possible, but few really cared. It was not until 20 March 2001 that some real progress was made, with the help of Poul Nielsen.

In this document, a range of test units definitions are expanded to demonstrate thoroughly how the proposed expansion technique should be applied.

2 Simple Units Definitions

2.1 What the spec says

To quote from the 2001-03-02 draft of the CellML specification:

A 'simple units' definition occurs when units are defined as a linear function of some previously defined simple units or base units. This occurs when a `<units>` element contains only a single child `<unit>` element, that `<unit>` element has an `exponent` attribute value of "1.0", and the units definition referenced by the `units` attribute is one of the SI or user-defined base units or is itself a simple units definition. These are the only conditions under which a `<unit>` element may define an `offset` attribute. The formula that expresses how the old units (referenced by the value of the `units` attribute on the `<unit>` element) are transformed into the new units (defined by the value of the `name` attribute on the parent `<units>` element) is given below:

$$x_{new} [Units] = \left(multiplier \left[\frac{Units}{units} \right] prefix \right) x_{old} [units] + offset [Units] \quad (1)$$

Terms in square brackets represent the units associated with a term in the expression, x_{old} is the value to be transformed from the old units, x_{new} is the resulting value in the new units, `Units` are the units being defined, and `multiplier`, `prefix`, `units`, and `offset` correspond to the values of the appropriate attributes on the `<unit>` element.

2.2 What the spec should say

The formula is wrong. The prefix is just another multiplier, and the units previously associated with the multiplier should really be associated with the product of the prefix and multiplier. The correct formula follows.

$$x_{new} [Units] = (multiplier prefix) \left[\frac{Units}{units} \right] x_{old} [units] + offset [Units] \quad (2)$$

A proposal for the complete discussion of user-defined simple and complex units is given in Section 4.

2.3 Examples

Simple units definitions are fairly easy to deal with, because the units of the variables in the equations never feature any products. We will look at an expansion of the units definition for degrees fahrenheit given below.

```
<units name="fahrenheit">
  <unit multiplier="1.8" units="celsius" offset="32.0" />
</units>
```

The expansion follows, where we have abbreviated the name of the units being defined (**fahrenheit**) to *fnht* to save space.

$$\begin{aligned} x_f [fnht] &= 1.8 \left[\frac{fnht}{celsius} \right] x_c [celsius] + 32.0 [fnht] \\ &= 1.8 \left[\frac{fnht}{celsius} \right] \left(1.0 \left[\frac{celsius}{kelvin} \right] x_k [kelvin] - 273.15 [celsius] \right) + 32.0 [fnht] \\ &= 1.8 \left[\frac{fnht}{kelvin} \right] x_k [kelvin] - 491.67 [fnht] + 32.0 [fnht] \\ &= 1.8 \left[\frac{fnht}{kelvin} \right] x_k [kelvin] - 459.67 [fnht] \end{aligned} \quad (3)$$

3 Complex Units Definition

3.1 What the spec said

Quoting from the 2001-03-02 draft of the CellML specification:

‘Complex units’ are the product of multiple base quantities, and are created by placing several **<unit>** elements inside a single **<units>** element, or by defining an **exponent** attribute with a value other than "1.0" on any **<unit>** element. The conversion between the new units and the product of the constituent units is given by the formula below.

$$x_{new} [Units] = x_{old} [u_1^{e_1} \dots u_n^{e_n}] m_1 \left[\frac{Units^{\frac{1}{n}}}{u_1^{e_1}} \right] p_1^{e_1} \dots m_n \left[\frac{Units^{\frac{1}{n}}}{u_n^{e_n}} \right] p_n^{e_n} \quad (4)$$

The m_n , p_n , u_n , and e_n terms refer to the values of the **multiplier**, **prefix**, **units**, and **exponent** attributes on the n -th **<unit>** element respectively. Note that this specification forbids **offset** attributes from being defined on any unit elements that occur inside a complex units definition.

It is very important to note that when a complex units definition references a simple units definition, any offset associated with the simple units definition is removed. This means that the conversions such as the one between degrees Fahrenheit per inch and degrees Celsius per centimetre involve only a scale factor.

3.2 What the spec should say

The formula should be re-arranged so that the prefixes and multipliers are all lumped into a single term which has units representing the entire conversion from the units being defined to the products of all of the constituent units, as shown below.

$$x_{new} [Units] = (m_1 \dots m_n p_1^{e_1} \dots p_n^{e_n}) \left[\frac{Units}{u_1^{e_1} \dots u_n^{e_n}} \right] x_{old} [u_1^{e_1} \dots u_n^{e_n}] \quad (5)$$

A proposal for the complete discussion of user-defined simple and complex units is given in Section 4.

3.3 Examples

First of all we will revisit the definitions of the convenience units defined in the CellML specification. The CellML versions of these units definitions and the associated equations are.

```
<units name="celsius">
  <unit units="kelvin" offset="-273.15" />
</units>
```

$$x_{new} [celsius] = 1.0 \left[\frac{celsius}{kelvin} \right] x_{old} [kelvin] - 273.15 [celsius] \quad (6)$$

```
<units name="gram">
  <unit multiplier="0.001" units="kilogram" />
</units>
```

$$x_{new} [gram] = 0.001 \left[\frac{gram}{kilogram} \right] x_{old} [kilogram] \quad (7)$$

```
<units name="litre">
  <unit multiplier="1000" prefix="centi" units="metre" exponent="3" />
</units>
```

$$\begin{aligned} x_{new} [litre] &= \left(1000 (10^{-2})^3 \right) \left[\frac{litre}{metre^3} \right] x_{old} [metre^3] \\ &= 0.001 \left[\frac{litre}{metre^3} \right] x_{old} [metre^3] \end{aligned} \quad (8)$$

Now we'll work through some other examples to thoroughly demonstrate the expansion of units definitions into their constituent base units. First we define an **inch**.

```
<units name="inch">
  <unit multiplier="2.54" prefix="centi" units="metre" />
</units>
```

$$\begin{aligned}
 x_{new} [inch] &= (2.54 \cdot 10^{-2}) \left[\frac{inch}{metre} \right] x_{old} [metre] \\
 &= 0.0254 \left[\frac{inch}{metre} \right] x_{old} [metre]
 \end{aligned}
 \tag{9}$$

Next we define the units of **celsius_per_centimetre**, which we will abbreviate to *cpcm* in the mathematics, in order to save space. Note that the definition of **celsius** given in Equation (6) involves an offset. This offset is ignored when the definition is substituted into the complex units definition.

```

<units name="celsius_per_centimetre">
  <unit units="celsius" />
  <unit prefix="centi" units="metre" exponent="-1" />
</units>

```

$$\begin{aligned}
 x_{new} [cpcm] &= (10^{-2})^{-1} \left[\frac{cpcm}{celsius\ metre^{-1}} \right] x_{old} [celsius\ metre^{-1}] \\
 &= 100 \left[\frac{cpcm}{celsius\ metre^{-1}} \right] x_{old} [celsius\ metre^{-1}]
 \end{aligned}
 \tag{10}$$

Now things we get more interesting: we expand the definition of **fahrenheit_per_inch**, which we will abbreviate to *fpi* to save space. This expansion is handled in steps.

```

<units name="fahrenheit_per_inch">
  <unit units="fahrenheit" />
  <unit units="inch" exponent="-1" />
</units>

```

$$x_{new} [fpi] = 1.0 \left[\frac{fpi}{fahrenheit\ inch^{-1}} \right] x_{old} [fahrenheit\ inch^{-1}]
 \tag{11}$$

In Equation (11), there is no obvious substitution for the x_{old} term, which has units that are the product of two non-base units definitions. We must expand this term to continue. In order to do this, let's invert the definition of **inch** given in Equation (9). We introduce the variables y_{new} and y_{old} here to represent the unknown values with inverted units.

$$y_{new} [inch^{-1}] = 39.370 \left[\frac{inch^{-1}}{metre^{-1}} \right] y_{old} [metre^{-1}]
 \tag{12}$$

Now let's consider the multiplication of the definition of **fahrenheit** given in Equation (3) and the inverted inch definition given in Equation (12), where we abbreviate **fahrenheit** and **inch** to *f* and *i* respectively. Note that the offset from the definition of **fahrenheit** has been dropped. The variables v_{new} and v_{old} are introduced to represent the unknown temperature values.

$$v_{new} [f] y_{new} [i^{-1}] = 1.8 \left[\frac{f}{kelvin} \right] v_{old} [kelvin] 39.370 \left[\frac{i^{-1}}{metre^{-1}} \right] y_{old} [metre^{-1}]
 \tag{13}$$

The v_{new} and y_{new} variables can be multiplied together to produce a new unknown z_{new} which has units which are the product of the units on v_{new} and y_{new} . Similarly z_{old} is the product of v_{old} and y_{old} .

$$z_{new} [f\ i^{-1}] = 70.866 \left[\frac{f\ i^{-1}}{kelvin\ metre^{-1}} \right] z_{old} [kelvin\ metre^{-1}]
 \tag{14}$$

Now we can substitute z_{new} from Equation (14) into Equation (11) in place of x_{old} and simplify the result to give a complete expansion of **fahrenheit_per_inch**.

$$\begin{aligned}
 x_{new} [fpi] &= 1.0 \left[\frac{fpi}{fahrenheit\ inch^{-1}} \right] x_{old} [fahrenheit\ inch^{-1}] \\
 &= 1.0 \left[\frac{fpi}{fahrenheit\ inch^{-1}} \right] 70.866 \left[\frac{fahrenheit\ inch^{-1}}{kelvin\ metre^{-1}} \right] z_{old} [kelvin\ metre^{-1}] \quad (15) \\
 &= 70.866 \left[\frac{fpi}{kelvin\ metre^{-1}} \right] z_{old} [kelvin\ metre^{-1}]
 \end{aligned}$$

In the last example, we'll look at the expansion of the units definition for **millimolar**, which will be found in the majority of models defined using CellML. A CellML definition is given below.

```

<units name="millimolar">
  <unit prefix="milli" units="mole" />
  <unit units="litre" exponent="-1" />
</units>

```

The initial expansion is shown below.

$$x_{new} [millimolar] = 10^{-3} \left[\frac{millimolar}{mole\ litre^{-1}} \right] x_{old} [mole\ litre^{-1}] \quad (16)$$

We can create an expansion for x_{old} by inverting the definition for litre given in Equation (8), and multiplying each side of the equation by 1.0 mole. These terms are absorbed into the variables, and the conversion factor is multiplied by 1.0 mole/mole to keep the units consistent.

$$x_{new} [litre^{-1}] = 1000 \left[\frac{litre^{-1}}{metre^{-3}} \right] x_{old} [metre^{-3}] \quad (17)$$

$$y_{new} [mole\ litre^{-1}] = 1000 \left[\frac{mole\ litre^{-1}}{mole\ metre^{-3}} \right] y_{old} [mole\ metre^{-3}] \quad (18)$$

Substituting Equation (18) into Equation (16) gives the result below.

$$\begin{aligned}
 x_{new} [millimolar] &= 10^{-3} \left[\frac{millimolar}{mole\ litre^{-1}} \right] 1000 \left[\frac{mole\ litre^{-1}}{mole\ metre^{-3}} \right] y_{old} [mole\ metre^{-3}] \\
 &= 1.0 \left[\frac{millimolar}{mole\ metre^{-3}} \right] y_{old} [mole\ metre^{-3}] \quad (19)
 \end{aligned}$$

4 New Units Discussion

The full introduction of simple and complex units definitions at the end of Section 5.2.3 in the 2001-03-02 draft of the specification should read:

A *simple units* definition occurs when units are defined as a linear function of some previously defined simple units or base units. In a simple units definition, a **<units>** element contains only a single child **<unit>** element, that **<unit>** element has an **exponent** attribute value of "1.0", and the units definition referenced by the **units** attribute is one of the SI or user-defined base units or is itself a simple units definition. These are the only conditions under which a **<unit>** element may define an **offset** attribute with a value other than "0.0". The formula that expresses how the old units (referenced by the value of

the **units** attribute on the **<unit>** element) are transformed into the new units (defined by the value of the **name** attribute on the parent **<units>** element) is given below.

$$x_{new} [Units] = (multiplier\ prefix) \left[\frac{Units}{units} \right] x_{old} [units] + offset [Units] \quad (20)$$

Terms in square brackets represent the units associated with values in the expression, which are italicized. x_{old} is the value to be transformed from the old units, and x_{new} is the resulting value in the new units. $Units$ are the units being defined, and $multiplier$, $prefix$, $units$ and $offset$ correspond to the values of the appropriate attributes on the **<unit>** element.

Complex units are the product of multiple units. In a complex units definition, a units element contains multiple child unit elements, or some unit element defines an exponent attribute with a value other than 1.0. The conversion between the new units and the product of the constituent units is given by the formula below.

$$x_{new} [Units] = (m_1 \dots m_n p_1^{e_1} \dots p_n^{e_n}) \left[\frac{Units}{u_1^{e_1} \dots u_n^{e_n}} \right] x_{old} [u_1^{e_1} \dots u_n^{e_n}] \quad (21)$$

The m_i , p_i , u_i , and e_i terms refer to the values of the **multiplier**, **prefix**, **units** and **exponent** attributes on the i -th **<unit>** element respectively.

The **offset** attribute may not be defined on any **<unit>** elements that occur inside a complex units definition. When a complex units definition references a simple units definition, any offset associated with the simple units definition is removed. This means that conversions such as the one between degrees Fahrenheit per inch and degrees Celsius per centimetre involve only a scale factor.