Further integration of the KISAO ontology into simulation descriptions

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Aim of the proposal

In SED-ML level 1 version 1, there is currently no mechanism to parameterize a particular simulation algorithm, for example with tolerances or algorithm-specific arguments. This proposal aims to develop the **Algorithm** class to support such parameterization.

New elements

Currently there is no way to set tolerances or other parameters for a particular simulation algorithm, yet this is often important in order to be able to reproduce a set of results. This proposal extends the Algorithm element to include an optional subelement **listOfAlgorithmParameters**. This new element contains zero or more **algorithmParameter** elements which have two mandatory attributes:

1. 'kisaoID' :the KiSAO identifier to define algorithm parameters, type **string** .

2. 'value' : a value for the parameter. This is of type **String** in this schema, but software can obtain the correct data-type by interrogating the KISAO ontology.

and one optional attribute:

1. 'name' : a human readable label for the algorithm parameter.

An example would look like this:

```
1 <algorithm kisaoID="KISAO:0000032">
2 <listOfAlgorithmParameters>
3 <algorithmParameter kisaoID="KISAO:0000211" value="23"/>
4 </listOfAlgorithmParameters>
5 </algorithm>
```

Listing 1: Example algorithm parameter

Since elements are optional, and in addition to the current elements, there are no backward compatibility issues with L1V1. All existing SED-ML documents that are valid against the L1V1 schema will continue to be valid.

Both new elements extend SEDBase so can hold annotations and notes.

Suggested text for the specification

Here is some draft text for inclusion in the 'Algorithm' section (2.4.3.2) if this proposal is adopted:

Optionally, an Algorithm element can contain a single *listOfAlgorithmParameters* element, which in turn can hold zero or more *algorithmParameter* elements. An algorithmParameter provides

configuration for how the simulation algorithm should be run, and holds two mandatory attributes - *kisaoID* and *value*. The KisaoID should be a valid Kisao identifier [descending from the root parameter node KISAO_0000201] and the value should be a String representation of the parameter's definition that appears in the Kisao ontology. Optionally, *algorithmParameter* can hold a third attribute, *name*, providing a human readable label for the algorithm parameter.

XML schema

Here are the proposed new additions and modifications to the schema:

```
1  <xs:element name="algorithm">
2  <xs:complexType>
3  <xs:complexContent>
4  <xs:extension base="SEDBase">
5  <xs:attribute name="kisaoID" type="KisaoType" use="required" />
6  <xs:sequence>
7  <xs:element ref="listOfAlgorithmParameters" minOccurs="0"
8  maxOccurs="1" />
9  </xs:sequence>
10 </xs:extension>
11 </xs:complexContent>
12 </xs:complexType>
13 </xs:element>
14
15 <xs:element name="listOfAlgorithmParameters">
16 <xs:complexType>
17 <xs:complexContent>
18 <xs:extension base="SEDBase">
19 <xs:sequence>
20 <xs:element ref="algorithmParameter" minOccurs="0"
21 maxOccurs="unbounded" />
22 </xs:sequence>
23 </xs:extension>
24 </xs:complexContent>
25 </xs:complexType>
26 </xs:element>
27
28 <xs:element algorithmParameter>
29 <xs:complexType>
30 <xs:complexContent>
31 <xs:extension base="SEDBase">
32 <xs:attribute name="kisaoID" type="KisaoType" use="required" />
33 <xs:attribute name="value" type="xs:string" use="required" />
34 <xs:attribute name="name" type="xs:string" use="optional" />
35 </xs:extension>
36 </xs:complexContent>
37 </xs:complexType>
38 </xs:element>
```

Listing 2: New and modified schema elements