A Notation for Describing Data Representations Intended for XML Encoding

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1 Introduction

One component of the ERATO Kitano Systems Biology Project is the creation of a workbench that provides interoperability between a number of simulation packages. Developing a framework for database storage and inter-program exchange requires defining a language for communicating data. Defining this language requires first establishing a notation that humans can use to describe the data structures involved.

I propose a simple notation to be used for describing data structures that are intended to be encoded using XML, the Extensible Markup Language (Bosak and Bray, 1999; Bray, Paoli and Sperberg-McQueen, 1998; Fallside, 2000). The notation is based in part on a small subset of UML, the Unified Modeling Language (Eriksson, 1998; Oestereich, 1999), a visual language for specifying software systems. There are three main advantages to using UML class diagrams as a basis for defining data structures. First, compared to using other notations or a programming language, the UML visual representations are generally easier to read and understand by readers who are not computer scientists. Second, the visual notation is implementation-neutral—the defined structures can be encoded in any concrete implementation language, not just XML but other formats as well, making the UML-based definitions more useful and flexible. Third, UML is a de facto industry standard (OMG, 2000), documented in many books and available in many software tools including mainstream development environments (such as Microsoft Visual Basic 5 Enterprise Edition). Readers are therefore more likely to be familiar with it than other notations.

Readers do not need to know UML in advance; this document provides descriptions of all the constructs used. The notation presented here can be expressed not only in graphical diagram form (which is what UML is all about) but also in textual form, allowing descriptions to be easily written in a text editor and sent as plain-text email.

The scope of the notation is limited to classes and their attributes, not class methods or operations. One of the goals of this effort has been to develop a consistent, systematic method for translating UML-based class diagrams into XML Schemas. Another goal has been to maintain a reasonably simple notation and UML-to-XML mapping. An important side-effect of this is that the vocabulary of the notation is purposefully limited to only a handful of constructs. It is explicitly *not* intended to cover the full power of UML or XML. This limited vocabulary has nevertheless been sufficient for the applications to which it has been applied so far in the Systems Biology workbench project.

2 Representing Object Structures in XML

XML provides the ability to define hierarchically-nested structures; this works well for representing object-oriented data because objects are basically nested field-value structures. An XML data stream or document consists of a series of descriptions of data objects. The structure of the data stream, meaning the permitted vocabulary and organization of entities in the stream, can be optionally predefined in the form of either a *Document Type Definition* or an *XML Schema*.

An *XML Schema* (Biron and Malhotra, 2000; Fallside, 2000; Thompson et al., 2000) is used to specify the kinds of objects allowed in an XML data stream, as well as how the objects and their properties are to be organized and the types of values that can be assigned to the object attributes. It provides more expressive power than the alternative mechanism for defining XML structures, the document type definition (DTD).

The following is an example XML Schema definition for a simple kind of data object:

```
<xs:schema xmlns:xs="http://www.w3.org/1999/XMLSchema">

  <xs:complexType name="ObjectClass">
    <xs:attribute name="attributeA" type="xs:string"/>
    <xs:attribute name="attributeB" type="xs:integer"/>
  </xs:complexType>

  <xs:element name="Object" type="ObjectClass"/>

</xs:schema>
```

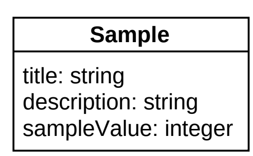
This definition begins with a qualified element, xs:schema, that tells an XML parser that the rest of the stream is an XML Schema definition. The symbols that belong to the XML Schema standard are prefixed with the characters "xs:". The use of xs: in particular, rather than some other prefix, is set by the xmlns:xs="..." portion of the first line. This is a *namespace* specification that communicates to the parser that the prefixed symbols belong to the space of symbols defined for XML Schema. The rest of the Schema defines an object class unimaginatively called ObjectClass having two attributes attributeA and attributeB. The second-to-last line states that an instance of an XML data stream based on this Schema definition can contain one top-level object, called Object, constructed according to the class ObjectClass.

Attribute types and other characteristics are defined in the following sections, along with principles for combining them and defining object classes. For brevity, in the rest of this document, only the relevant XML Schema definitions are given, without enclosing <xs:schema ...> ... </xs:schema> wrappers and without explicit definition of top-level objects that use the object classes defined.

Although it is extremely powerful, the XML Schema language (and for that matter, the DTD language) is complicated and not suitable as a descriptive specification language for humans communicating about data structures used in a software project. A more suitable language is UML, but there does not exist an agreed-upon approach for translating object classes represented in UML class diagrams into XML Schemas. The rest of this document presents one viable approach.

2.1 Basis of the Approach

An instance of a data object is always constructed according to a blueprint or *class* definition that specifies the internal structure of the object. The "structure" is its attributes and the types of data values that are permitted to be stored in the attributes. In UML notation, a class is represented as a box with a title and a list of attributes below it, as in the example shown at right. The example shows an object class named Sample having three attributes: title, description, and sampleValue. A full class definition would also include a list of operations or methods that an object understands, but the scope of the present effort is limited to data attributes only.



In XML, objects in a document or data stream are referred to as *elements*. Elements can contain values that may themselves be other elements, and elements can have annotations in the form of attributes. The following snippet of XML illustrates the different parts of an XML representation:

```
<element1 attributeA="attributeA-value">element1-value</element1>
<element2 attributeB="attributeB-value" attributeC="attributeC-value">
  <element3>element3-value</element3>
  <element4 attributeD="attributeD-value">element4-value</element4>
</element2>
```

The example above shows four separate elements. Some of the elements have attributes (element1, element2, element4), while others do not (element3). Some of the elements have simple values (element1, element3, element4), while the other one (element2) contains two other elements (element3, element4) as its value.

XML element attributes are name-value pairs that can only be used to hold simple (scalar) values. Storing a value that is more structured (e.g., another object) requires the use of a subelement. When encoding a UML data structure in XML, an attribute in the UML structure may or may not be made into an XML element attribute. Indeed, one of the first questions that needs to be answered when developing an XML format is: what should be stored as element attributes, and what should be stored as element values?

There is no agreed-upon rule to answer this question. Some authors lean towards using element values to store content and attributes to store annotations about the elements (Box, Skonnard and Lam, 2000; St. Laurent, 2000). But this is not universally accepted (Cover, 2000), and in fact, one of the original architects of XML has stated that "I've never heard a convincing universal decision procedure for what should be an element and what an attribute" (Bray, 1998). Instead of representing data object attributes as separate XML elements, it is also valid to represent them as a collection of attributes on a single element. To put this into concrete terms, here are two XML samples that can both be taken to express the same data:

```
<Sample>
  <title>My title</title>
  <description>My description</description>
  <sampleValue>42</sampleValue>
</Sample>
```

Approach 1

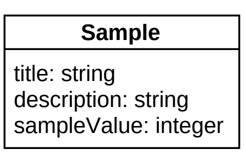
```
<Sample title="My title"
        description="My description"
        sampleValue="42"/>
```

Approach 2

The second approach is a more compact encoding, in part because it can be written using a short format, <tag .../>, instead of the full nested tag pair <tag ...></tag>; the shorter format is allowed when an XML element does not have a value. The approach also leads to a direct correspondence between object attributes and XML element attributes: when we speak about an "attribute" of an object, the corresponding XML construct is usually an attribute on an element, as in the example on the right above. For these reasons, the notation presented here is based on the second approach.

3 The UML-Based Notation and Its Textual and XML Forms

The following example presents an object class definition in the UML-style notation adopted here, along with its representation in a textual form and in XML Schema syntax:



UML Form

```
Sample
_________________________
title:        string
description:  string
sampleValue:  integer
```

Textual Form

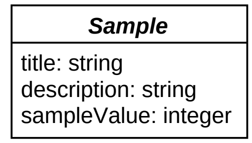
```
<xs:complexType name="Sample">
  <xs:attribute name="title" type="xs:string"/>
  <xs:attribute name="description" type="xs:string"/>
  <xs:attribute name="sampleValue" type="xs:integer"/>
</xs:complexType>
```

XML Schema Form

All three forms define the same data structure: a class Sample of objects having three attributes title, description and sampleValue. The components are named according to a particular naming convention. First, the name of the class must begin with an uppercase letter, can contain letters, numerals and underscore characters, and (due to limitations in the software tools we are using) cannot contain other types of characters. Words within the names should each be capitalized. Second, attribute names generally begin with a lowercase letter but otherwise follow the convention for class names; for example, an attribute might be named `sampleValue`. An exception to this rule can be made when the attribute name begins with a word that is normally capitalized, such as an acronym or symbolic name (e.g., "`Q10Scaling`").

Attributes are typed. There are a number of possible datatypes, as explained in Sections 3.1–3.5. The type specifier is written after the name of the attribute, as in, for example, `title: string`. This convention is commonly used in UML textbooks (e.g., Eriksson and Penker, 1998) and software tools. An alternative UML style puts the type specifier before the attribute name, as in, for instance, `string title`.

It is sometimes useful to specify that an object class is *abstract*, meaning that it is only intended to serve as a basis for defining other classes and not to be instantiated directly into objects. In such cases, the class name is written in an italic or slanted typeface, as in the example shown at right. In XML, abstract classes are defined by adding `abstract="true"` to the type definition:




```
<xs:complexType name="Sample" abstract="true">
  ...
</xs:complexType>
```

To express in the textual form of this notation that a class is abstract, the name of the class should be followed by the annotation {`abstract`} following the name of the class, as in `Sample` {`abstract`}.

3.1 Simple Attributes

A simple attribute is one having a simple data value, for instance a number or a string. All three of the attributes shown in the `Sample` example above are simple attributes. The set of simple types that are permitted is the set defined by the XML Schema Datatypes standard (Biron and Malhotra, 2000) plus simple types derived from the built-in ones. Figure 1 lists the simple types built into XML Schema.

Type	Example(s)
binary	`100010`
boolean	`true, false, 1, 0`
byte	`-1, 126`
century	`19`
date	`1999-05-31, ---05`
decimal	`-1.23, 0, 123.4, 1000.00`
double	`-INF, -0, 0, 1.7E-2, 3, INF, NaN`
ENTITIES	
ENTITY	
float	`-INF, -0, 0, 1.7E-2, 3, INF, NaN`
ID	`m32`
IDREF	`m32`
IDREFS	`m32 m33 m34 m35`
int	`-1, 126789675`
integer	`-126789, -1, 0, 1, 126789`
language	
long	`-1, 12678967543233`
month	`1999-05`
Name	`shipTo`
NCName	`Address`
negativeInteger	`-126789, -1`

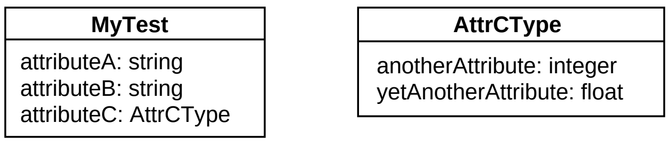
Type	Example(s)
NMTOKEN	`US`
NMTOKENS	`US UK`
nonNegativeInteger	`0, 1, 126789`
nonPositiveInteger	`-126789, -1, 0`
NOTATION	
positiveInteger	`1, 126789`
QName	`po:Address`
recurringDate	`--05-31`
recurringDay	`----31`
recurringDuration	`--05-31T13:20:00`
short	`-1, 12678`
string	`This is a string`
time	`13:20:00.000-05:00`
timeDuration	`P1Y2M3DT10H30M12.3S`
timeInstant	`1999-05-31T13:20:0.0-05:00`
timePeriod	`1999-05-31T13:20`
unsignedByte	`0, 126`
unsignedInt	`0, 1267896754`
unsignedLong	`0, 12678967543233`
unsignedShort	`0, 12678`
uriReference	`http://www.me.com/x.html#id5`
year	`1999`

Figure 1: *Simple types built into XML Schema, according to the W3C Working Draft of 7 April 2000. Detailed definitions of these types are available at* `http://www.w3.org/TR/xmlschema-2/`.

3.2 Complex Attributes

An attribute in an object can be a container for a collection of attributes under a common heading. In that case, the attribute is said to be *complex* because its value is not a simple scalar. This is roughly equivalent to a "struct" in the language C.

In UML, a complex type is defined as a separate class. The following is an example of a class, `MyTest`, having three attributes, `attributeA`, `attributeB` and `attributeC`. The first two attributes have simple types, and the third attribute's type is a newly-defined class, `AttrCType`, itself containing two more attributes.



In a programming language, given an object `obj` of class `MyTest`, the attributes might be accessed as

```
obj.attributeA
obj.attributeB
obj.attributeC.anotherAttribute
obj.attributeC.yetAnotherAttribute
```

As explained in Section 2.1, simple attributes in UML class definitions are translated into element attributes in XML. Complex types translate directly into the `complexType` element in XML Schemas. However, in XML, an element attribute cannot have a complex type, which means that a complex attribute in the present notation must be made into an XML *subelement* within the containing XML element. This leads to the question of how to name and structure the subelement. The approach taken here is to name the subelement after the attribute, as illustrated in the following example of an object instance based on `MyTest`:

```
<MyTest attributeA="foo" attributeB="bar">
  <attributeC anotherAttribute="2" yetAnotherAttribute="4.3"/>
</MyTest>
```

Note how the attribute `attributeC` is written out as a separate XML subelement, but the type of `attributeC` is not explicitly stated in the data object. This is in parallel to how the type also ends up hidden in the programming language example involving object `obj` given above. Only the label `attributeC` and the attributes `anotherAttribute` and `yetAnotherAttribute` appear.

Here is the XML Schema definition corresponding to the class diagram above:

```
<xs:complexType name="AttrCType">
  <xs:attribute name="anotherAttribute" type="xs:integer"/>
  <xs:attribute name="yetAnotherAttribute" type="xs:float"/>
</xs:complexType>

<xs:complexType name="MyTest">
  <xs:attribute name="attributeA" type="xs:string"/>
  <xs:attribute name="attributeB" type="xs:string"/>
  <xs:element   name="attributeC" type="AttrCType"/>
</xs:complexType>
```

The only naming convention defined here for complex types is that the names should begin with a capital letter. However, it is a good idea to make the name of a complex type reflect the attribute to which it is connected. (E.g., for an attribute named `version`, the complex type might be named `Version`.)

3.3 Links

A link is a reference to another part of the same database object or to a completely separate database object. It is a way of referring or pointing to part of an object, or to a whole other object, by name, without incorporating the actual physical object itself. Two different approaches apply in the two cases, one for intra-object links and one for inter-object links. They have parallels in XML, and the present notation reflects the approach used in XML.

3.3.1 Intra-Object Links

In XML, links between elements within the same object can be handled using a particular set of data types that are treated specially by XML parsers. The basic idea is the following. The attribute that contains the link itself must have the type `IDREF`; the referenced component (the target) must have an attribute of type `ID`. Components of an object or a particular XML data stream are given unique identifiers assigned to attributes of type `ID`. Uniqueness of identifiers is enforced by XML parsers, which are required to collect all attribute values of type `ID` and verify their uniqueness within an XML document or data stream. An `IDREF` value is required by the XML standard to match *some* `ID` attribute within a given data stream or document, or else the XML parser must generate an error (Biron and Malhotra, 2000). The effect of this is that XML parsers enforce the rule that a link to a component in an object or data stream does in fact refer to a component that is actually present.

The type `ID` is defined as being a token beginning with a letter or one of two possible punctuation characters (specifically, underscore or colon), and continuing with letters, digits, hyphens, underscores, colons, or full stops, collectively known as *name characters* (Thompson et al., 2000). There is also a list version of `IDREF` called `IDREFS` that is not necessary in the present context because of how lists are handled in this notation; see Section 3.5.

In order to use this XML facility, the notation described here follows the XML approach in using attributes of type `ID` and `IDREF` to effectuate linking. The convention adhered to here is that objects that can be targets of links need to have an attribute named `id` of type `ID`. References to these objects or object components must be made using attributes of type `IDREF`.

The following is a example of a class definition that uses intra-object linking:

ReferenceExample
attributeA: string attributeB: string attributeC[0..*]: CType whichCToUse: IDREF

CType
id: ID someValue: integer

Here is the XML Schema corresponding to the definition above:

```
<xs:complexType name="CType">
  <xs:attribute name="id"        type="xs:ID"/>
  <xs:attribute name="someValue" type="xs:integer"/>
</xs:complexType>

<xs:complexType name="ReferenceExample">
  <xs:attribute name="attributeA" type="xs:string"/>
  <xs:attribute name="attributeB" type="xs:string"/>
  <xs:element   name="listOfAttributeCs">
    <xs:complexType>
      <xs:element name="attributeC" type="CType" minOccurs="0" maxOccurs="unbounded"/>
    </xs:complexType>
  </xs:element>
  <xs:attribute name="whichCToUse" type="xs:IDREF"/>
</xs:complexType>
```

And the following is an example XML stream that makes use of the definition above:

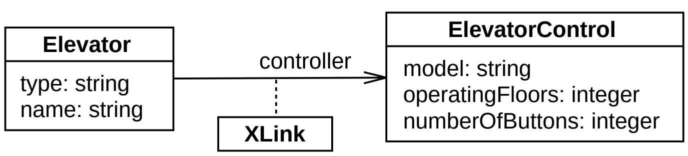
```
<ReferenceExample attributeA="something" attributeB="something else" whichCToUse="c2">
  <listOfAttributeCs>
    <attributeC id="c1" someValue="42"/>
    <attributeC id="c2" someValue="24"/>
    <attributeC id="c3" someValue="99"/>
  </listOfAttributeCs>
</ReferenceExample>
```

In the example above, each item in the `listOfAttributeCs` element has a different value in the `id` attribute, and the attribute `whichCToUse` refers to one of the items in the list by its `id` value.

It is worth noting in passing that this approach can be used to represent graph structures in XML. By assigning `ID` type identifiers to different elements in a data structure, it is possible to have elements link to each other and thereby allow full graph-structured data to be represented.

3.3.2 Inter-Object Links

Links may be established between separate objects (i.e., objects in separate XML data streams or documents). In UML, a link between two conceptually separate object classes is indicated by drawing a line between them. Such an *association line* can be directed (i.e., an arrow) when the connection is always from one particular class to the other, and a third class can be associated with the connection to define additional properties. To handle inter-object links in the present framework, all three of these features need to be invoked. The following example illustrates these ideas:



The meaning of the above is: `Elevator` consists of all the attributes within the box of the class definition, *plus* the attribute `controller`, which is a link of type `XLink` to an object of class `ElevatorControl`. By UML convention, the attribute `controller` does not appear in the `Elevator` box itself. In reading UML diagrams containing associations between classes, it is therefore important to count *both* the attributes within the class box as well as the attributes shown on association lines.

Here is the same example in textual form:

```
Elevator                                           ElevatorControl
__________________________________________         __________________________
type:        string                                model:            string
name:        string                                operatingFloors:  integer
controller:  XLink {link to ElevatorControl}       numberOfButtons:  integer
```

A link in the present notation is implemented by using a specific complex type, `XLink`, and then defining attributes that serve as links to be of this type. The type `XLink` is meant to signify the use of the *XML Linking Language*, XLink (DeRose et al., 2000; St. Laurent, 200). `XLink` uses the two essential attributes that define an XML link, namely `xlink:type` and `xlink:href`. The former can be given a default value, so only `xlink:href` needs to be set in actual use. The form of the value of the `xlink:href` reference target will depend on the particular server storing the database, but the form will generally be a `uriReference` (see Figure 1). Unfortunately, there is no method for indicating the intended type of the target object in a simple XLink link; consistency between the desired type and the actual type of the target referenced by the link must be handled by the program.

The following XML Schema defines the classes `Elevator` and `XLink` used in the example above; the class `ElevatorControl` is assumed to be defined in a separate Schema:

```
<xs:complexType name="XLink">
  <xs:attribute name="xlink:type" type="string" use="default" value="simple"/>
  <xs:attribute name="xlink:href" type="xs:uriReference"/>
</xs:complexType>

<xs:complexType name="Elevator">
  <xs:attribute name="type" type="xs:string"/>
  <xs:attribute name="name" type="xs:string"/>
  <xs:element   name="controller" type="XLink"/>
</xs:complexType>
```

The following is an example of a portion of XML data that uses the Schema:

```
<Elevator type="Argo K21" name="Main">
  <controller xlink:href="http://www.myserver.net/db/controllers/kc9"/>
</Elevator>
```

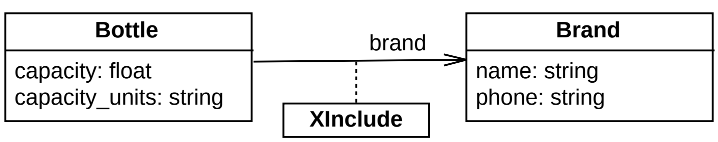
For the limited applications that are the domain of the present document, only the “simple” XLink type is required (DeRose et al., 2000); more elaborate versions of XLink also exist, but are not used here.

3.4 Inclusion

The kinds of links described in the previous section point to other structures without actually including the structures at the point where the reference occurs. In some limited situations, it is also useful to include one data object directly inside another. For example, programs communicating data structures in the absence of database facilities may need to package up entire objects and send them without leaving links that the recipient may not be able to dereference. Expressing object inclusion of this kind requires a variation of the link notation defined in the previous section.

Inclusion of objects in this fashion is most appropriately handled in XML using *XInclude*, the XML Inclusions definition (Marsh and Orchard, 2000). There are currently significant limitations to using XInclude. It is a work in progress and not yet a standard, so the actual syntax of XInclude described here may vary in the future; moreover, no XML processors support XInclude yet. Nevertheless, XInclude is used in the present notation in anticipation of its eventual standardization. The XInclude features used here are extremely limited, so implementing support for XInclude in application programs should not be difficult.

Here is an example of an object inclusion:



The following XML Schema defines the class `Bottle` used in the example above; the class `Brand` is assumed to be defined elsewhere in a separate Schema:

```
<xs:complexType name="XInclude">
  <xs:attribute name="xinclude:href" type="xs:uriReference"/>
</xs:complexType>

<xs:complexType name="Bottle">
  <xs:attribute name="capacity"       type="xs:float"/>
  <xs:attribute name="capacity_units" type="xs:string"/>
  <xs:element   name="brand"          type="XInclude"/>
</xs:complexType>
```

The following is an example of XML using the Schema:

```
<Bottle capacity="5.0" capacity_units="gallon">
  <brand xinclude:href="http://www.myserver.net/bottledb/maker52"/>
</Bottle>
```

3.5 Lists

An attribute can be a list of simple types, or a list of complex types, or a list of link or inclusion types. All items in the list must have the same type. In some programming languages such as Java or C, a list might be represented as a vector or array.

In the diagrammatic and textual forms of the current notation, lists are expressed using a style loosely based on C and Java-style array notation, with a multiplicity specifier enclosed in square brackets. The multiplicity specifier consists of numerals or the asterisk character, optionally separated by commas or '..' (the last to indicate a range). Asterisk means "zero or more". For example, "`somevar[10]: integer`" means that `somevar` is a list of exactly ten integers. Similarly, "`author[1..*]: string`" means that attribute `author` is a list of one or more strings. The table at the right gives a number of other examples of multiplicity specifications.

1	exactly one
0,1	zero or one
0..4	between zero and four
3,7	either three or seven
0..*	zero or more
*	zero or more
1..*	one or more

Regardless of whether the type of an attribute is simple, complex, or a link, the approach used here to translate from a list form into XML is the same: create a subelement named `listOf____s`, where the blank indicates the capitalized name of the attribute, and then put a list of elements named after the attribute as the content of the `listOf____s` element. Small variations need to be introduced for coping with various details of different data types, and these are explained in the following paragraphs.

3.5.1 Lists of Simple Types

Perhaps the most natural way of representing a list of simple attributes would be to have multiple instances of the same attribute on an object, such as `<Object somevar="value1" somevar="value2" ...>` However, XML does not allow more than one element attribute of the same name, therefore an attribute that is a list of simple types must be translated into a sequence of subelements. The approach adopted here is to use a series of subelements named after the attribute, each having a single element attribute named `value` used to store the actual value of the item. Here is an example:

SomeThing
attributeA: integer attributeB[0..*]: string

UML Form

```
<xs:complexType name="SomeThing">
  <xs:attribute name="attributeA" type="xs:string"/>
  <xs:element   name="listOfAttributeBs">
    <xs:complexType>
      <xs:element name="attributeB" type="xs:string"
                  minOccurs="0" maxOccurs="unbounded"/>
    </xs:complexType>
  </xs:element>
</xs:complexType>
```

XML Schema Form

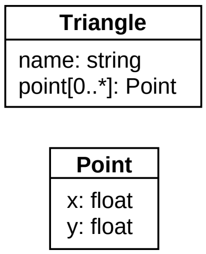
The definitions above would allow product XML data objects such as the following; note how the values of the `attributeB` strings are recorded on the `value` attributes in the elements of the list:

```
<SomeThing attributeA="123">
  <listOfAttributeBs>
    <attributeB value="first string"/>
    <attributeB value="second string"/>
    <attributeB value="third string"/>
  </listOfAttributeBs>
</SomeThing>
```

3.5.2 Lists of Complex Types

The approach to encoding a complex attribute described in Section 3.2 involves translating it into a subelement. The approach to encoding a list of complex types parallels the one for encoding simple types, but without the need for an additional `value` attribute. The elements in the list are each identical to the element that would be present if there were no list and only a single complex attribute.

The following example definition illustrates the idea:




```
<xs:complexType name="Point">
  <xs:attribute name="x" type="xs:float"/>
  <xs:attribute name="y" type="xs:float"/>
</xs:complexType>

<xs:complexType name="Triangle">
  <xs:attribute name="name" type="xs:string"/>
  <xs:element   name="listOfPoints">
    <xs:complexType>
      <xs:element name="point" type="Point"
                  minOccurs="0" maxOccurs="unbounded"/>
    </xs:complexType>
  </xs:element>
</xs:complexType>
```

UML Form *XML Schema Form*

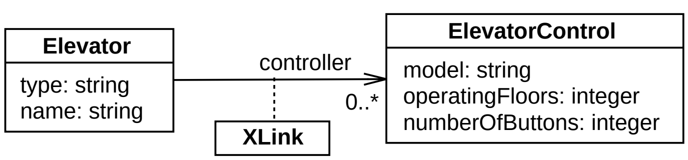
The definitions above would allow product XML data objects such as the following:

```
<Triangle name="t1">
  <listOfPoints>
    <point x="2.2" y="1.4"/>
    <point x="0.1" y="4.0"/>
    <point x="0.1" y="1.4"/>
  </listOfPoints>
</Triangle>
```

3.5.3 Lists of Links and Inclusions

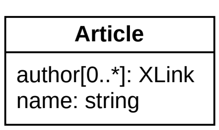
The case of intra-object links is identical to the case of a list of simple attributes discussed above. Intra-object links (Section 3.3.1) are implemented simply by using the XML type `IDREF`, so a list of links defined as, for example, `itemRef[0..*]: IDREF`, turn into a list of elements of the form `<itemRef value="..."/>`.

In the case of inter-object links or inclusions, multiplicity involving separate objects is expressed in UML with numerals on the links joining two object classes together. For example, if in the `Elevator` example of Section 3.3, `controller` had actually been a list of zero or more links to `ElevatorControl` class objects, then the corresponding UML diagram would be:



By convention, if the relationship is 1-to-1, the two numeral 1's are normally omitted from the association line in a UML diagram; see the example diagrams in Sections 3.3.2 and 3.4. The absence of any numerals on either end of an association line implies 1.

As in the case of lists of complex types, the elements used in the list of links or list of inclusions do not need any additional attributes; each list item has the same form as a single element constructed from a link attribute as described in Section 3.3. Here is an example definition:




```
<xs:complexType name="Article">
  <xs:attribute name="name" type="xs:string"/>
  <xs:element   name="listOfAuthors">
    <xs:complexType>
      <xs:element name="author" type="XLink"
                  minOccurs="0" maxOccurs="unbounded"/>
    </xs:complexType>
  </xs:element>
</xs:complexType>
```

UML Form *XML Schema Form*

The following is an XML data object based on the definitions above:

```
<Article name="t1">
  <listOfAuthors>
    <author xlink:href="http://www.myserver.net/db/author24"/>
    <author xlink:href="http://www.myserver.net/db/author54"/>
  </listOfPoints>
</Article>
```

Although the examples above were given in terms of `XLink` links, the same approach also applies to `XInclude` inclusions.

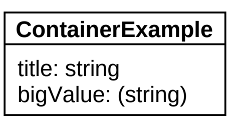
3.6 Element Values

In the present approach to translating UML to XML, most object class attributes are encoded as attributes on an XML element, and subelements are likewise used to store information using attributes. But in addition to the way that simple and complex types are used here, XML also allows elements to have content values. Consider the following example:

```
<ContainerExample title="This is a title">
  <bigValue>
    This is some long value, something really long, like a big block
    of text that might be too awkward to put inside an attribute value.
  </bigValue>
</ContainerExample>
```

The element `bigValue` above has no attributes, but does have a value. Expressing this in UML requires a notation that is not part of UML proper, so it is necessary to introduce two minor extensions to UML for this purpose. The two extensions apply to two different cases:

1. *An attribute representing a container.* This is the case of `ContainerExample` illustrated above, where an object's attribute is a container for a value in the sense that XML elements can have values. The modified UML notation adopted here is to place the type in parentheses. The parentheses signify that the attribute is special, with not actually represented as an attribute in XML but rather as an element whose value is significant. Here follows the definition corresponding to the example given above:

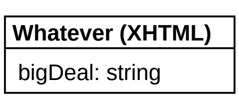



```
<xs:complexType name="ContainerExample">
  <xs:attribute name="title" type="xs:string"/>
  <xs:element   name="bigValue" type="xs:string"/>
</xs:complexType>
```

UML Form *XML Schema Form*

Restriction: The type of the container attribute in the definition must be simple; it cannot be another a complex type. (If the type were allowed to be complex, the situation would simply be identical to an ordinary complex attribute.)

2. *A class containing a value.* For this case, the modified UML notation adopted here is to place the type of the container in parentheses following the class name. For example,




```
<xs:complexType name="Whatever" content="textOnly">
  <xs:attribute name="bigDeal" type="xs:string"/>
  <xs:attribute name="type" use="fixed" value="XHTML"/>
</xs:complexType>
```

UML Form *XML Schema Form*

This allows the following kind of XML data object:

```
<Whatever bigDeal="This is an attribute">
  This has a value, but no subelements.
</Whatever>
```

The XML Schema for this case uses the special property `content="textOnly"`, which indicates that the XML element value can only contain data, not subelements. This unfortunately imposes a limitation on the resulting representation: XML parsers will not check the datatype of the content in instance objects, treating it simply as text. In order to avoid losing the type information altogether, the original type is recorded on an attribute called `type`, using a fixed value corresponding to the type stated in parentheses next to the class definition. Although XML parsers will not check the content in instance objects, programs that receive objects of this class can use the type information to perform their own checking.

Restrictions: (1) The type of the container attribute must be a simple type; it cannot be a complex type. (2) None of the attributes in the rest of the object class definition can be complex; all must have simple types.

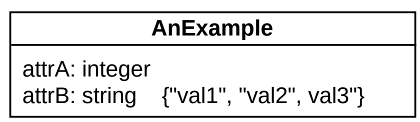
3.7 Constraints on Attribute Values

It is important to be able to express constraints on the values of attributes. A constraint refers to a limitation or restriction on the possible content or state of an attribute. For example, it may be useful to specify that a given integer attribute cannot have a value less than zero, or that a given string attribute can only take on values from a limited vocabulary.

There are two standard ways in UML to express constraints. One approach consists of adding a constraint expression in curly braces following the definition of an attribute, as in the UML shown in the following example:

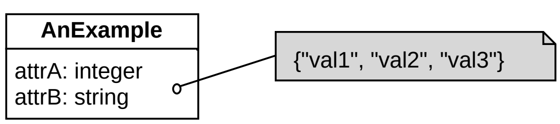
```
AnExample
-----------------------------------------
attrA: integer
attrB: string  {"val1", "val2", "val3"}
```

Textual form



UML form

Alternatively, in a UML diagram, the constraints can be placed in an external text box and a line can be drawn from the box to the attribute in question, as in the following:

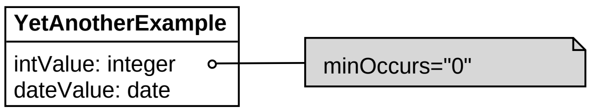


For defining constraints in UML, some authors use Object Constraint Language, a declarative language based on set theory (Oestereich, 1999). For the goals of the present notation, it is more convenient to express constraints either in a simple stylized form (as in the immediately-preceding examples) or using XML Schema language. The following are some examples that have arisen in practice:

- *String value chosen from a strictly limited vocabulary.* XML Schema defines several mechanisms for constraining values of attributes. A particularly useful one is the `enumeration` component. Here is an example of an XML Schema constraining the values of an attribute to a limited set of three specific strings for the class `AnExample` defined above:

```
<xs:complexType name="AnExample">
  <xs:attribute name="attrA" type="xs:integer"/>
  <xs:attribute name="attrB">
    <xs:simpleType base="xs:string">
      <xs:enumeration value="val1"/>
      <xs:enumeration value="val2"/>
      <xs:enumeration value="val3"/>
    </xs:simpleType>
  </xs:attribute>
</xs:complexType>
```

- *Optional attribute.* Sometimes an attribute in a class should be considered optional. For these situations, the attribute should be given the XML Schema property `minOccurs="0"`. (The default value of `minOccurs` is 1.)

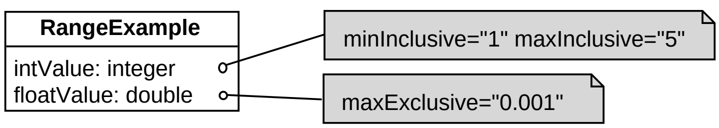
  

  UML Form

```
<xs:complexType name="YetAnotherExample">
  <xs:attribute name="intValue"  type="xs:integer" minOccurs="0"/>
  <xs:attribute name="dateValue" type="xs:date"/>
</xs:complexType>
```

  XML Schema Form

- *Minimum and maximum range values on numeric attributes.* The upper and lower value boundaries for an attribute having a numeric value can be defined using the XML Schema `minExclusive`, `minInclusive`, `maxInclusive`, and `maxExclusive` properties. For instance:

  UML Form

```
<xs:complexType name="RangeExample">
  <xs:attribute name="intValue"   type="xs:integer" minInclusive="1" maxInclusive="10"/>
  <xs:attribute name="floatValue" type="xs:double"  maxExclusive="0.001"/>
</xs:complexType>
```

  XML Schema Form

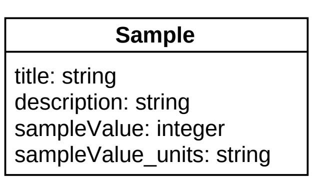
  The first attribute is limited to integer values from 1 to 10, inclusive; the second attribute is constrained to values no less than 0.001, exclusive.

There are many more situations that call for the use of constraints and that are not covered by the examples above. For such other cases, it is up to users of the present notation to devise appropriate expressions of constraints using XML Schema terms or other simple expressions. The constraint terms available in XML Schema are defined in the XML Schema specification (Biron and Malhotra, 2000; Thompson et al. 2000).

3.8 Specifying Units

It is often important to provide information about the units associated with a numerical attribute. In the approach to XML representations used here, there are two alternatives for specifying units conveniently.

The first approach is to define, for each relevant attribute, another attribute whose name has the suffix `_units` and whose type is a string, to represent the units being used for the value stored in the attribute. The following is an example:



UML Form

```
<xs:complexType name="Sample">
  <xs:attribute name="title" type="xs:string"/>
  <xs:attribute name="description" type="xs:string"/>
  <xs:attribute name="sampleValue" type="xs:integer"/>
  <xs:attribute name="sampleValue_units" type="xs:string"/>
</xs:complexType>
```

XML Schema

The second approach is suitable for groups of attributes or substructures that all use the same unit. In that case, it may be simpler to define an attribute at the class level that sets the units for a whole object.

In order to maximize the utility of having unit specifications, a given project should define a specific XML type for the units it needs to use. This specification should take the form of a datatype (perhaps called `Units`), defined in a separate XML Schema, consisting of an enumeration of strings. Here is a partial example of such an XML Schema:

```
<xs:simpleType name="Units" base="xs:string">
  <xs:enumeration value="m"/>
  <xs:enumeration value="cm"/>
  <xs:enumeration value="mm"/>

  <!-- and so on ... -->

</xs:simpleType>
```

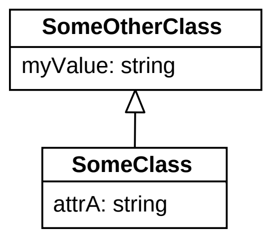
3.9 Inheritance

Inheritance allows an object class to be defined as an extension or derivation of another class. In textual form, the inheritance relationship can be written on the same line as the name of the class definition; in graphical UML form, inheritance is expressed using an open-ended arrow drawn from an inheriting class to the inherited-from class. The following illustrates both forms:

```
SomeOtherClass
______________
myValue: string

SomeClass extends SomeOtherClass
________________________________
attrA:   string
```

Textual form



UML form

The meaning of the above is that `SomeClass` inherits from `SomeOtherClass` and augments the latter type's definition by adding an attribute of its own. `SomeClass` therefore has as attributes *both* `attrA` and `myValue`, even though the box defining `SomeClass` itself does not mention the second one. `SomeOtherClass` has only one attribute, `myValue`.

In XML, inheritance can be implemented using the `base` and `derivedBy` mechanisms on a type definition. This allows an XML element/class definition to be based on another element. The following is an XML Schema for the example above:

```
<xs:complexType name="SomeOtherClass">
  <xs:attribute name="myValue" type="xs:string"/>
</xs:complexType>

<xs:complexType name="SomeClass" base="SomeOtherClass" derivedBy="extension">
  <xs:attribute name="attrA" type="xs:string"/>
</xs:complexType>
```

4 Summary

The notation proposed in this document is based on a subset of what could be used and what UML provides. It is not intended to cover the full scope of UML or XML. The subset was chosen to be as simple as possible yet allow the expression of the kinds of data structures that need to be encoded in XML for the ERATO Kitano Systems Biology workbench.

The notation proposed here is not carved in stone, and will undoubtedly continue to evolve. Please send your feedback about any aspect of this document to the author.

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