Including Layout Information in SBML Files Version 1.2

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Introduction

With SBML there now is a common standard for the exchange of dynamical systems data which has already been adopted by many applications in this field [1, 2, 3]. Since SBML had no means of storing layout information for reaction networks, we developed an extension to SBML that would allow us to store this layout information in SBML files. There already exists an extension to SBML by Herbert M. Sauro that deals with layout information in SBML files [5] well tailored to his program JDesigner [4]. However, in order to provide generality, our specification tries to limit the extensions to just specifying information that concerns the placement of the objects and leaves the rendering to the application.

Design principles and general structure

The overall structure of this proposal reflects some design decisions that will be explained in this paragraph. These decisions are mainly based on the discussion on the mailing list.

First it was requested that it should be possible to have several layouts in one sbml file. This leads to the obvious choice to have a **listOfLayouts** outside the **model** part of the sbml file instead of direct annotations to the model elements.

The next question is how tight the relation between the model and the layout should be. It was requested that there should be no strict one-to-one connection between model elements and layout elements. Therefore the layout part of the sbml file cannot just duplicate the structure of the model part. This leads to a structure where a layout contains several lists of layout elements (compartmentGlyphs, speciesGlyphs, ...) There seems to be consensus that one model element can be represented by several layout elements. For example it can be useful to have several representations of one species in the layout to avoid lots of crossing arrows. This can be accomplished if every layout element has a field that refers to the id of a model element.

We also think that there are cases where a layout element does not correspondent to exactly one model element. This could occur if the layout shows a simplified version of the model where one reaction in the layout correspondents to several reactions and intermediate species in the model. This is the reason why the field in the layout elements that refers to the model elements is optional.

Further on we think that the layout should be described in biochemical terms (species, reactions, ...) and not in terms of graph theory (nodes, edges).

Otherwise an existing language for graph layouts could be used.

The result of all this is a way to describe a graphical layout of a reaction network in biochemical terms. This layout can be closely tied to the biochemical model. A graphical model editor for example would typically create a layout that is closely connected (by a one-to-several relation from the model elements to the layout elements) to the model. A more general layout design program could also create a layout that is not so closely tied to the model, for example it could create a layout that shows a simplified version of the model.

Last but not least we decided to separate between layout information and render information. By layout information we mean the position and size of all the layout elements and their relations. Render information would be colors, line widths, bitmaps, ... While every program dealing with layouts should be able to read and write the layout information the render information could be ignored or could have program specific extensions. This proposal concentrates on the layout part because we thought it would be easier to reach an agreement on the overall structure of the layout without the rendering details. The rendering detail are described in another document for now, but we expect the documents to be merged eventually.

All size information given for layout objects are understood to be pt, which is defined to be 1/72 of an inch. This will be consistent with the way font sizes will be specified in the render part of the diagram.

Nomenclature

The UML diagrams in this document show the name of the class on top. Below are the attributes specific to that class. Optional attributes have some default value which may be NULL. Arrays are written in square brackets where with the valid array length within those brackets. So a array [2..] would mean that it can hold from 2 to ∞ number of objects (assuming that you have some very large harddisk).

Inheritance tree

Namespace

For the extensions we use a separate namespace of the following form xmlns:sl2="http://projects.eml.org/bcb/sbml/level2". A SBML file that would utilize the extension could have the following form:

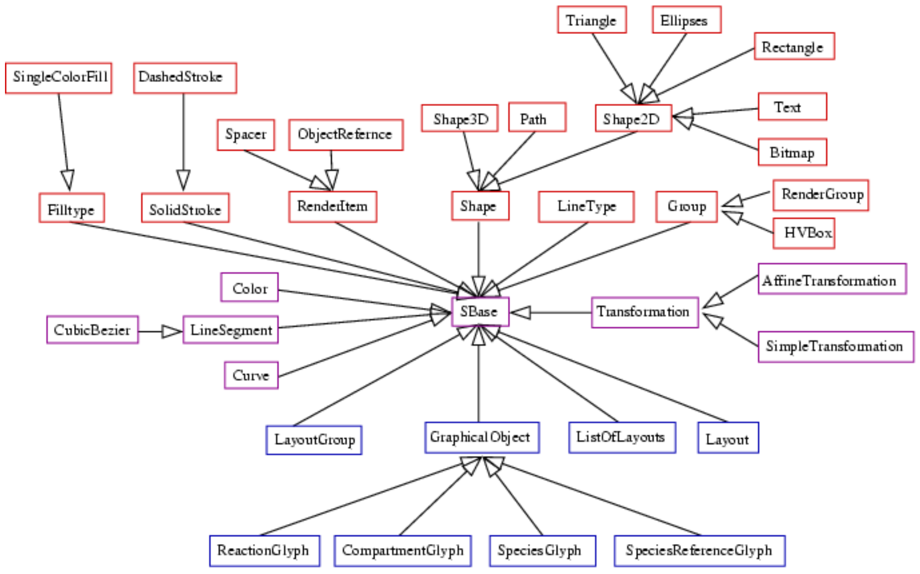
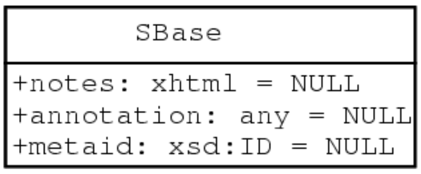


Figure 1: Inheritance tree for the layout and render classes

```
<?xml version="1.0" encoding="UTF-8"?>
   <sbml xmlns:sbml="http://www.sbml.org/sbml/level2" level="2" \\
         version="1"
         xmlns:sl2="http://projects.eml.org/bcb/sbml/level2"
         xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
         xsi:schemaLocation="http://projects.eml.org/bcb/sbml/level2
         http://projects.eml.org/bcb/sbml/level2/layout2.xsd">
```

Metainformation

All the layout classes below are now derived from a class called SBase which was taken from the SBML Level 2 schema specification (http://www.sbml.org/sbml/level2/version1/). This enables programs to store metainformation with the layout objects.



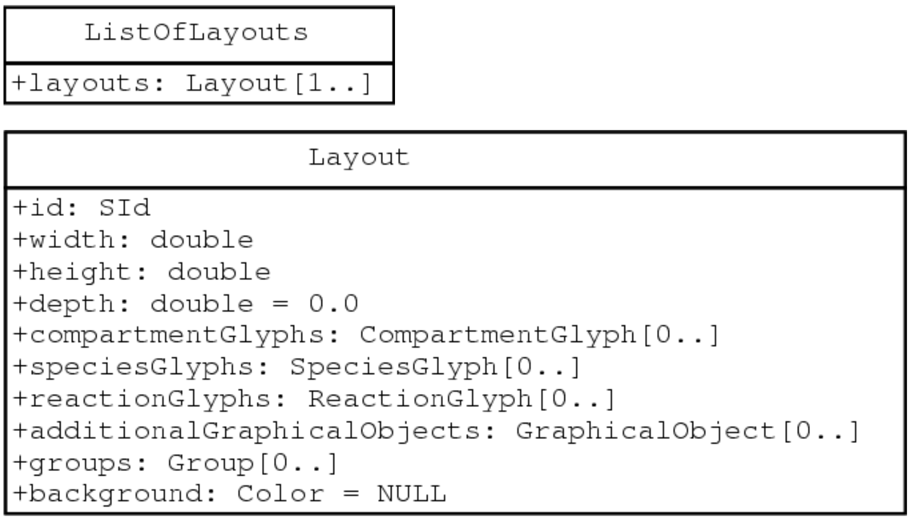
XML Schema representation:

```
<xsd:complexType name="SBase" abstract="true">
 <xsd:sequence>
  <xsd:element name="notes" minOccurs="0">
   <xsd:complexType>
    <xsd:sequence>
     <xsd:any namespace="http://www.w3.org/1999/xhtml"
              processContents="skip"
              maxOccurs="unbounded"/>
    </xsd:sequence>
   </xsd:complexType>
  </xsd:element>
  <xsd:element name="annotation" minOccurs="0">
   <xsd:complexType>
    <xsd:sequence>
     <xsd:any processContents="skip" maxOccurs="unbounded"/>
    </xsd:sequence>
   </xsd:complexType>
  </xsd:element>
 </xsd:sequence>
 <xsd:attribute name="metaid" type="xsd:ID" use="optional"/>
</xsd:complexType>
```

<listOfLayouts > and <layout >

Due to the discussion on the sbml mailing list, we took the layout information out of the actual model into a separate tag called listOfLayouts which is placed within the annotation tag of the sbml tag. This list can hold one or more layout objects which in turn hold layout information for some or all elements of the sbml model plus additional objects that need not be connected to the model. The only attribute added to the ones from SBase for the <layout > tag is an id which uniquely identifies the layout object and the dimensions of the bounding box for the layout. The dimensions of the bounding box are given by a width, height and an optional depth attribute, all of type double. If not specified, the depth value defaults to 0.0. Ids are defined to be the same as SId in SBML Level 2.

XML Schema representation:


ListOfLayouts
+layouts: Layout[1..]
Layout
+id: SId
+width: double
+height: double
+depth: double = 0.0
+compartmentGlyphs: CompartmentGlyph[0..]
+speciesGlyphs: SpeciesGlyph[0..]
+reactionGlyphs: ReactionGlyph[0..]
+additionalGraphicalObjects: GraphicalObject[0..]
+groups: Group[0..]
+background: Color = NULL

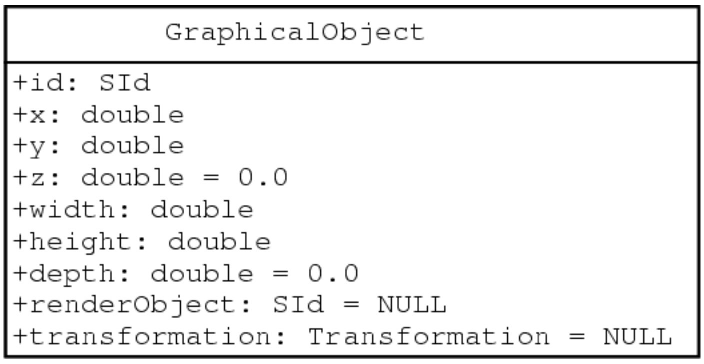
```
<xsd:simpleType name="SId">
 <xsd:restriction base="xsd:string">
  <xsd:pattern value="(_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*"/>
 </xsd:restriction>
</xsd:simpleType>


<xsd:complexType name="ListOfCompartmentGlyphs">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:sequence>
    <xsd:element name="compartmentGlyph" type="sl2:CompartmentGlyph"
                 maxOccurs="unbounded"/>
   </xsd:sequence>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="ListOfSpeciesGlyphs">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:sequence>
    <xsd:element name="speciesGlyph" type="sl2:SpeciesGlyph" maxOccurs="unbounded"/>
   </xsd:sequence>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="ListOfReactionGlyphs">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
```

```
    <xsd:sequence>
     <xsd:element name="reactionGlyph" type="sl2:ReactionGlyph" maxOccurs="unbounded"/>
    </xsd:sequence>
   </xsd:extension>
  </xsd:complexContent>
 </xsd:complexType>

 <xsd:complexType name="ListOfAdditionalGraphicalObjects">
  <xsd:complexContent>
   <xsd:extension base="sl2:SBase">
    <xsd:sequence>
     <xsd:any namespace="##other" processContents="skip"
       minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
   </xsd:extension>
  </xsd:complexContent>
 </xsd:complexType>

 <xsd:complexType name="ListOfGroups">
  <xsd:complexContent>
   <xsd:extension base="sl2:SBase">
    <xsd:sequence>
     <xsd:element name="group" type="sl2:LayoutGroup" maxOccurs="unbounded"/>
    </xsd:sequence>
   </xsd:extension>
  </xsd:complexContent>
 </xsd:complexType>

 <xsd:complexType name="Layout">
   <xsd:complexContent>
     <xsd:extension base="sl2:SBase">
       <xsd:sequence>
         <xsd:element name="listOfCompartmentGlyphs"
                      type="sl2:ListOfCompartmentGlyphs" minOccurs="0"/>
         <xsd:element name="listOfSpeciesGlyphs" type="sl2:ListOfSpeciesGlyphs"
                      minOccurs="0"/>
         <xsd:element name="listOfReactionGlyphs" type="sl2:ListOfReactionGlyphs"
                      minOccurs="0"/>
         <xsd:element name="listOfAdditionalGraphicalObjects"
                      type="sl2:ListOfAdditionalGraphicalObjects" minOccurs="0"/>
         <xsd:element name="listOfGroups" type="sl2:ListOfGroups" minOccurs="0"/>
       </xsd:sequence>
       <xsd:attribute name="id" type="sl2:SId"/>
       <xsd:attribute name="width"  type="xsd:double"/>
       <xsd:attribute name="height" type="xsd:double"/>
       <xsd:attribute name="depth"  type="xsd:double" use="optional" default="0.0"/>
     </xsd:extension>
   </xsd:complexContent>
 </xsd:complexType>
```

```
<xsd:complexType name="ListOfLayouts">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:sequence>
    <xsd:element name="layout" type="sl2:Layout" maxOccurs="unbounded"/>
   </xsd:sequence>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>

<xsd:element name="listOfLayouts" type="sl2:ListOfLayouts"/>
```

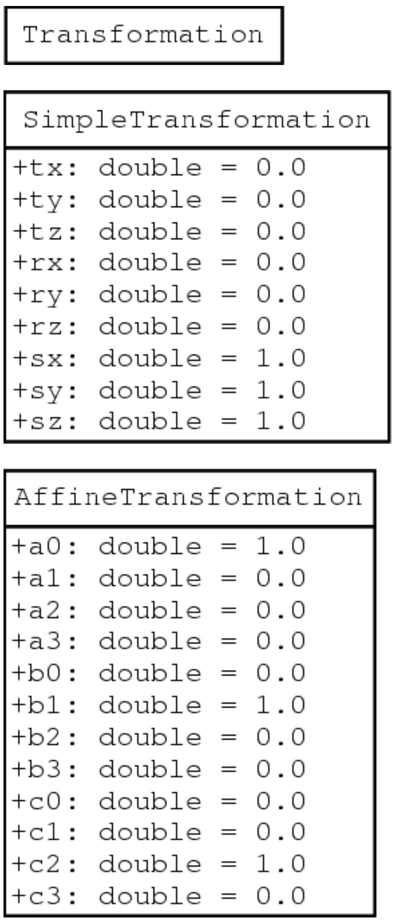
<GraphicalObject> and <Transformation>

Most objects for which layout information is to be included in an SBML file have a corresponding object in the SBML model. As there might be cases where the user wants to include objects in the layout that are not part of the model, we include a listOfAdditionalGraphicalObjects in each layout object. This list holds one or more GraphicalObject elements. The GraphicalObject has an id attribute of type SId through which it can be identified, it has x, y and z attributes of type double to specify its position. And it has width, height and depth attributes of type double for the size of the bounding box of the object. The z and depth attributes are optional and default to 0.0. The GraphicalObject class also has an attribute called renderObject of type SId to specify the render object associated with this layout object and last but not least, an optional Transformation object can be specified. This transformation is to be executed on the render object prior to rendering. This way several layout objects may reference the same render object, but draw it in a different size or angle. All other layout Objects (CompartmentGlyph, SpeciesGlyph, ReactionGlyph and SpeciesReferenceGlyph) are derived from GraphicalObject.



```
GraphicalObject
+id: SId
+x: double
+y: double
+z: double = 0.0
+width: double
+height: double
+depth: double = 0.0
+renderObject: SId = NULL
+transformation: Transformation = NULL
```

Right now, our proposal contains two types of transformation which are both derived from an abstract base class called Transformation which in turn is derived from SBase. The Transformation class does not add any new attributes to SBase. From Transformation we derive a class SimpleTransformation which has some attributes to specify translational (tx,ty,tz), rotational (rx,ry,rz) and scaling (sy,sy,sz) transformations for all three axes. All attributes are double values and optional. The default values are 1.0 for the three scaling attributes and 0.0 for the other six attributes. The SimpleTransformation will probably cover 99% of what users need, but in case this is not enough, we have a second type of transformation, the AffineTransformation. The AffineTransformation specifies a 4x3 transformation matrix. The parameters are aligned in rows with 4 parameters each. The parameters are called a0,a1,a2,a3 for row one b0,b1,b2,b3 for row 2 and c0,c1,c2,c3 for row 3. All parameters are optional and the defaults are such that the identity matrix results.

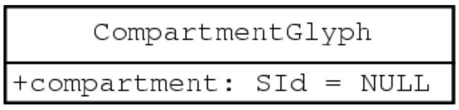


```
<xsd:complexType>
  <xsd:complexContent>
    <xsd:extension base="sl2:SBase">
      <xsd:sequence>
        <xsd:element name="transformation" type="sl2:Transformation" minOccurs="
      </xsd:sequence>
      <xsd:attribute name="id" type="sl2:SId"/>
      <xsd:attribute name="x" type="xsd:double"/>
      <xsd:attribute name="y" type="xsd:double"/>
      <xsd:attribute name="z" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="width" type="xsd:double"/>
      <xsd:attribute name="height" type="xsd:double"/>
      <xsd:attribute name="depth" type="xsd:double" use="optional" default="0.0"
      <xsd:attribute name="renderObject" type="sl2:SId"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:complexType>
  <xsd:complexContent>
    <xsd:extension base="sl2:SBase">
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="SimpleTransformation">
  <xsd:complexContent>
    <xsd:extension base="sl2:Transformation">
      <xsd:attribute name="tx" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="ty" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="tz" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="rx" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="ry" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="rz" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="sx" type="xsd:double" use="optional" default="1.0"/>
      <xsd:attribute name="sy" type="xsd:double" use="optional" default="1.0"/>
      <xsd:attribute name="sz" type="xsd:double" use="optional" default="1.0"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
```

```
<xsd:complexType name="AffineTransformation">
  <xsd:complexContent>
    <xsd:extension base="sl2:Transformation">
      <xsd:attribute name="a0" type="xsd:double" use="optional" default="1.0"/>
      <xsd:attribute name="a1" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="a2" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="a3" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="b0" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="b1" type="xsd:double" use="optional" default="1.0"/>
      <xsd:attribute name="b2" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="b3" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="c0" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="c1" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="c2" type="xsd:double" use="optional" default="1.0"/>
      <xsd:attribute name="c3" type="xsd:double" use="optional" default="0.0"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
```

<Compartment> Layout Information

The CompartmentGlyph class is derived from GraphicalObject and has the same attributes. Additionally it has an optional reference to the id of the corresponding compartment in the model. Since the compartment id is optional, the user can specify compartments in the layout that are not part of the model.



XML Schema representation:

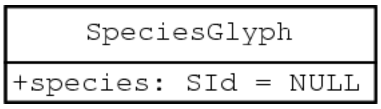
```
<xsd:complexType name="CompartmentGlyph">
 <xsd:complexContent>
  <xsd:extension base="sl2:GraphicalObject">
   <xsd:attribute name="compartment" type="sl2:SId" use="optional"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>
```

example:

```
.
.
.
<compartment id="compartment" volume="1"/>
.
.
.
<sl2:listOfCompartmentGlyphs>
    <sl2:compartmentGlyph id="cGlyph" compartment="compartment"
                          x="10.0" y="10.0" w="60" h="50"/>
</sl2:listOfCompartmentGlyphs>
.
.
.
```

<Species> Layout Information

Since an sbml document can contain species that don't appear in any reaction a species can have zero or more representations on screen which are represented by <speciesGlyph> and are grouped in a <listOfSpeciesGlyphs> tag. In addition to the attributes from GraphicalObject, the speciesGlyph object has a **species** attribute which is the id of the corresponding species object in the model. The **species** attribute is optional to allow the program to specify species representations that do not have a direct correspondence in the model. This might be useful if some pathway has been collapsed, but is still treated by layout programs.



XML Schema representation:

```
<xsd:complexType name="SpeciesGlyph">
 <xsd:complexContent>
  <xsd:extension base="sl2:GraphicalObject">
   <xsd:attribute name="species" type="sl2:SId" use="optional"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>
```

example:

```
.
```

```
    .
    .
    <species id="ATP" compartment="compartment" initialAmount="0">
    .
    .
    .
    <sl2:listOfSpeciesGlyphs>
      <sl2:speciesGlyph id="ATP_Glyph" species="ATP" x="295.0" y="123.0" w="16.0"/>
              .
              .
              .
    </sl2:listOfSpeciesGlyphs>
    .
    .
    .
```

<Reaction> Layout Information

The reaction layout is now also a subclass of GraphicalObject, therefore it has a defualt bounding box attribute. This differs from the last versions of this document, where the reaction layout consisted of two pseudo nodes. Actually this is only a renaming of attributes to make it more consistent with compartment and species layout information. The two points given by the bounding box can still be interpreted as being the two pseudo nodes of a reaction. The **reaction** attribute specifies the id of the corresponding reaction in the model. Again, this reference is optional. The ReactionGlyph also holds a listOfSpeciesReferenceGlyphs (see below) which correspond to the layout representations of the reactants of the reaction in the model.

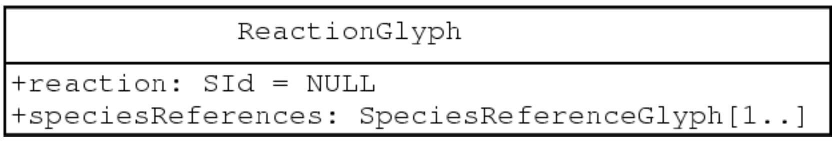


Figure 2: Inheritance tree for the layout and render classes

XML Schema representation:

```
<xsd:complexType name="ListOfSpeciesReferenceGlyphs">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:sequence>
    <xsd:element name="speciesReferenceGlyph" type="sl2:SpeciesReferenceGlyph"
                 minOccurs="1" maxOccurs="unbounded"/>
   </xsd:sequence>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="ReactionGlyph">
 <xsd:complexContent>
  <xsd:extension base="sl2:GraphicalObject">
   <xsd:sequence>
    <xsd:element name="listOfSpeciesReferenceGlyphs"
                 type="sl2:ListOfSpeciesReferenceGlyphs"
                 minOccurs="1" maxOccurs="1"/>
   </xsd:sequence>
   <xsd:attribute name="reaction" type="sl2:SId" use="optional"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>
```

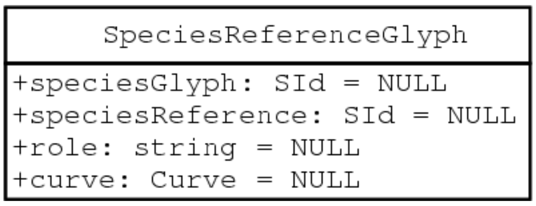
example:

```
    .
    .
    .
    <reaction id="reaction_0" reversible="false">
      <listOfReactants>
         <speciesReference species="P_i" stoichiometry="1"/>
             .
             .
             .
    </reaction>
    .
    .
    .
    <sl2:listOfReactionGlyphs>
      <sl2:reactionGlyph id="reaction_0_Glyph" reaction="reaction_0"
                        x1="119.0" y1="166.0" x2="120.0" y2="183.0"/>
            .
            .
            .
    </sl2:listOfReactionGlyphs>
    .
    .
    .
```

<SpeciesReference> Layout Information

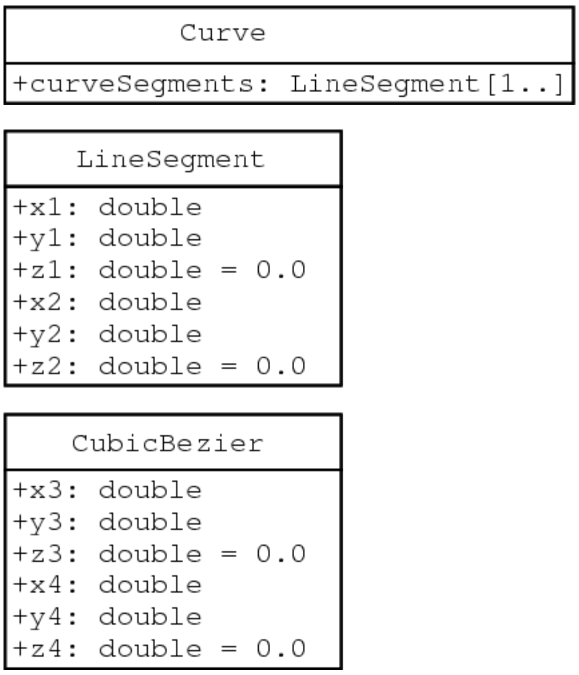
The graphical connection between a speciesGlyph and a reactionGlyph (which would be an arrow or some curve in most cases) is represented by the **species-**

ReferenceGlyph object. A **listOfSpeciesReferenceGlyphs** is contained in a **reactionGlyph**.



The **speciesReferenceGlyph** has a **speciesGlyph** attribute that contains the id of the graphical object that is to be connected to the reactionGlyph. This can be the id of a graphical representation of a species (as defined in the <listOfSpeciesGlyphs>) or the id of a group (see below). The **speciesReference** attribute refers to a speciesReference in the model and is optional. Since species references in sbml level 1 as well as level 2 do not have ids, we chose to put a new tag called id which has an attribute called id that is of type sl2:SId into the annotation part of the corresponding SpeciesReference element. This tag has to be unique within the global namespace of the SBML model and can thus be used to reference a given species reference. The **role** attribute is used to specify how the species reference should be displayed. Allowed values are substrate, product, sidesubstrate, sideproduct, modifier, activator and inhibitor. This attribute is optional and should only be necessary if the optional speciesReference attribute is not given or if the respective information from the model needs to be overridden. The values *substrate* and *product* are used if the species reference is a main product or substrate in the reaction. **sidesubstrate** and **sideproduct** are used for stuff like ATP, NAD+, etc. that some renderers might choose to display as side reactants. **activator** and **inhibitor** are modifiers where their influence on the reaction is known and **modifier** is a more general term if the influence is unknown or changes during the course of the simulation. This list is probably not exhaustive and will be updated as needed. Future version of SBML may very well have an id for the SpeciesReference objects as well as some kind of role attribute. If this is the case, we will drop both attributes here since they are no longer necessary.

So far we have defined which graphical objects should be connected to the reaction glyph in which way. This is the minimum information that a render program with biochemical knowledge needs to render the reaction layout. For generality two alternative ways to specify more detailed layout information are provided. In most cases the relation of a species to a reaction will be graphically represented by a curve. In this case a **curve** tag that contains a **listOfCurveSegments** can be used. The **listOfCurveSegments** contains an arbitrary number of curve segments. For now we provide the definitions for two types of curve segments (**LineSegment** and **CubicBezier**) but leave it open if this should in future be restricted to only one type or even generalized to more different line types. All segment types, which is just CubicBezier so far, are derived from the LineSegment type. The type of the curve segment has to be specified with a **xsi:type** attribute in the **curveSegment** tag. The LineSegment just specifies the start and the end point of a line segment which should be a common feature of all types of curve segments, the CubicBezier additionally defines two control points needed to specify a cubic Bezier curve segment. If the curve attribute is specified this takes precedence over the bounding box defined by the attributes of the GraphicalObject from which SpeciesReferenceGlyph inherits.



XML Schema representation:

```
<xsd:complexType name="LineSegment">
  <xsd:complexContent>
    <xsd:extension base="sl2:SBase">
      <xsd:attribute name="x1" type="xsd:double"/>
      <xsd:attribute name="y1" type="xsd:double"/>
      <xsd:attribute name="z1" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="x2" type="xsd:double"/>
      <xsd:attribute name="y2" type="xsd:double"/>
      <xsd:attribute name="z2" type="xsd:double" use="optional" default="0.0"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="CubicBezier">
  <xsd:complexContent>
    <xsd:extension base="sl2:LineSegment">
      <xsd:attribute name="x3" type="xsd:double"/>
      <xsd:attribute name="y3" type="xsd:double"/>
      <xsd:attribute name="z3" type="xsd:double" use="optional" default="0.0"/>
      <xsd:attribute name="x4" type="xsd:double"/>
      <xsd:attribute name="y4" type="xsd:double"/>
      <xsd:attribute name="z4" type="xsd:double" use="optional" default="0.0"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="ListOfCurveSegments">
  <xsd:complexContent>
    <xsd:extension base="sl2:SBase">
      <xsd:sequence>
        <xsd:element name="curveSegment" type="sl2:LineSegment"
                          minOccurs="1" maxOccurs="unbounded"/>
      </xsd:sequence>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="Curve">
  <xsd:complexContent>
    <xsd:extension base="sl2:SBase">
      <xsd:sequence>
        <xsd:element name="listOfCurceSegments" type="sl2:ListOfCurveSegments"/>
      </xsd:sequence>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>

<xsd:simpleType name="RoleString">
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="substrate"/>
    <xsd:enumeration value="product"/>
    <xsd:enumeration value="sidesubstrate"/>
    <xsd:enumeration value="sideproduct"/>
    <xsd:enumeration value="modifier"/>
    <xsd:enumeration value="activator"/>
    <xsd:enumeration value="inhibitor)"/>
  </xsd:restriction>
</xsd:simpleType>
```

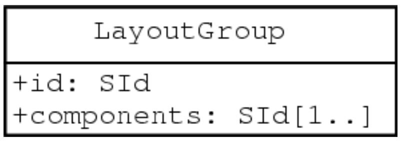
```
<xsd:complexType name="SpeciesReferenceGlyph">
 <xsd:complexContent>
  <xsd:extension base="sl2:GraphicalObject">
   <xsd:sequence>
     <xsd:element name="curve" type="sl2:Curve" minOccurs="0" maxOccurs="1"/>
   </xsd:sequence>
   <xsd:attribute name="speciesGlyph" type="sl2:SId" use="optional"/>
   <xsd:attribute name="speciesReference" type="sl2:SId" use="optional"/>
   <xsd:attribute name="role" type="sl2:RoleString" use="optional"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>
```

example:

```
        .
        .
        .
    <sl2:speciesGlyph id="P_iGlyph" species="P_i_s1" x="0.0" y="1.8"
                      w="1.0" h="1.0"/>
        .
        .
        .
    <sl2:reactionGlyph id="reaction_0_Glyph" reaction="reaction_0"
                      x1="2.3" y1="1.0" x2="3.0" y2="1.0">
      <sl2:listOfSpeciesReferenceGlyphs>
        <sl2:speciesReferenceGlyph id="SP1_Glyph" speciesGlyph="P_iGlyph"
                                  speciesReference="P_i_sr1">
          <sl2:curve>
            <sl2:listOfCurveSegments>
              <sl2:curveSegment xsi:type="sl2:CubicBezier" x1="0.0" y1="1.8"
                              x2="0.3" y2="0.8"
                              cx1="0.1" cy1="1.9" cx2="0.3" cy2="0.7"/>
              <sl2:curveSegment xsi:type="sl2:LineSegment" x1="0.3" y1="0.8"
                              x2="2.3" y2="1.0" />
            <sl2:/listOfCurveSegments>
          <sl2:/curve>
        </sl2:speciesReferenceGlyph>
            .
            .
            .
      </sl2:listOfSpeciesReferenceGlyphs>
    </sl2:reactionGlyph>
        .
        .
```

Grouping Information

In this specification, we added the possibility to group several representation objects. This is useful for editors that need to know which objects should be moved together when doing drags. Another possibility one gets with grouping is to group several objects together and have just one relationGlyph object for the whole group. E.g. someone want to display a reaction as A+B —> C+D in this case, he would group the species reference representations for the substrates and the additional graphical object that represents the '+' sign and adds the layoutGlyph for the connection to the reaction. Likewise he would do for the products. Each group object has an id which can be referenced in a reaction representation as a species reference representation. Each group consists of two or more components which have an attribute called **ref** that is a reference to the graphical object that is to be added to the group. Examples will follow. The Component class does not need to be implemented as a class since it can be implemented as a list of SIds in the LayoutGroup class. Therefore Component is missing from the UML diagram.



XML Schema representation:

```
<xsd:complexType name="Component">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:attribute name="ref" type="sl2:SId"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>

<xsd:complexType name="LayoutGroup">
 <xsd:complexContent>
  <xsd:extension base="sl2:SBase">
   <xsd:sequence>
    <xsd:element name="component" type="sl2:Component" minOccurs="2"
                 maxOccurs="unbounded"/>
   </xsd:sequence>
   <xsd:attribute name="id" type="sl2:SId"/>
  </xsd:extension>
 </xsd:complexContent>
</xsd:complexType>
```

Further Plans

We already started on the definition of the render part of this proposal. Until is has reached a certain level of maturity we will keep those two documents separate. Eventually though, they will end up in one common proposal document. This document is a work in progress and can be subject to changes any time. We are glad for any suggestions, corrections or hints to further improve these extensions. Hopefully with some help we could come up with a set of extensions that would suite the needs of many applications developed in this area. This specification was intended for the use with sbml level 2. With some slight changes it can also be used with sbml level 1 documents. Actually the only major changes that would have to be made is to change all references to SId to be references to SNames.

Example File

Last but not least, we include a small sample file to illustrate and complement the paragraphs above. Note that both the picture and the example code were manually modified. There does not exist an actual implementation of this latest version of our proposal yet. The model consists of two reactions. Which are the first reaction of glycolysis where glucose is converted to glucose-6-phosphate (G6P) and the reverse reaction of gluconeogenesis where glucose-6-phosphate is hydrolyzed to glucose. We did not include any coordinates in the third dimension, since we are only working in 2D space so far. As can be seen in the screenshot, the glucose SpeciesReference has two representational objects on screen whereas glucose-6-phosphate only has one. This difference is reflected in the file where the glucose species has two nodes in the listOfNodes whereas G6P only has one. This example show not all but only the main features of our proposal.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1"
      xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
      xmlns:sl2="http://projects.eml.org/bcb/sbml/level2"
      xsi:schemaLocation="http://projects.eml.org/bcb/sbml/level2
              http://projects.eml.org/bcb/sbml/level2/layout2.xsd">
  <model name="Untitled">
    <listOfCompartments>
      <compartment id="compartment" volume="1"/>
    </listOfCompartments>
    <listOfSpecies>
      <species id="ATP" compartment="compartment" initialAmount="0"/>
      <species id="P_i" compartment="compartment" initialAmount="0"/>
```

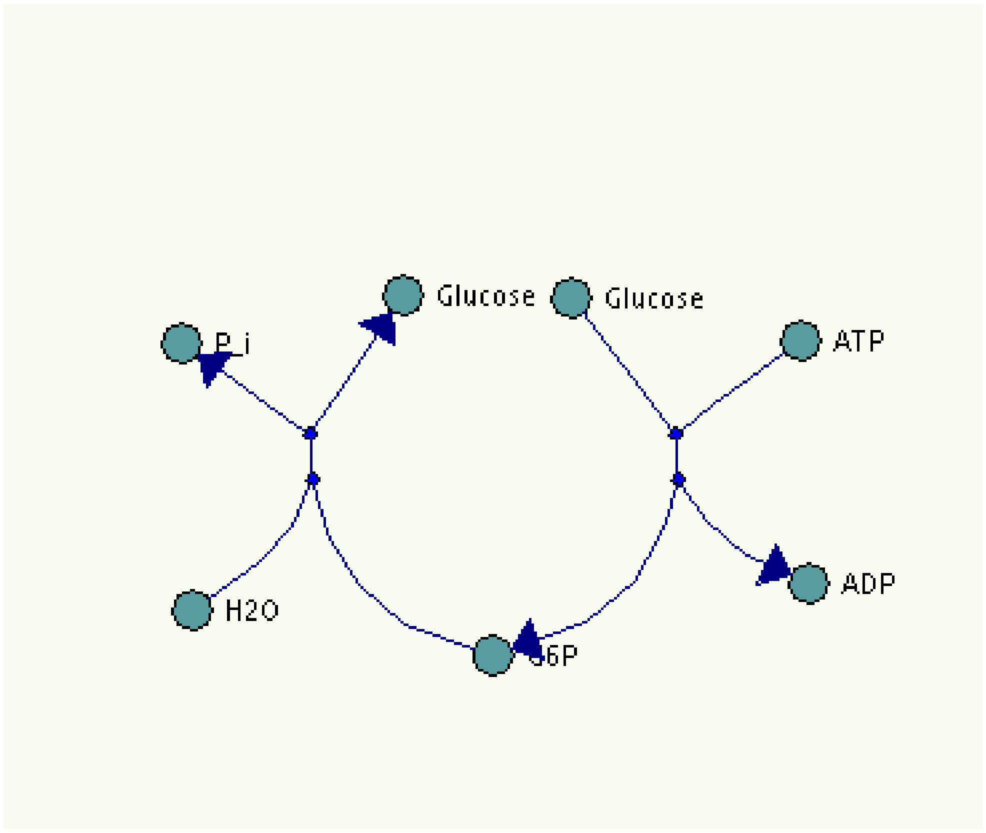


Figure 3: One possible rendering of the example layout. This is somewhat modified by hand because we do not have a working implementation of the last version of our proposal.

```
    <species id="Glucose" compartment="compartment" initialAmount="0"/>
    <species id="ADP" compartment="compartment" initialAmount="0"/>
    <species id="H2O" compartment="compartment" initialAmount="0"/>
    <species id="G6P" compartment="compartment" initialAmount="0"/>
  </listOfSpecies>
  <listOfReactions>
    <reaction id="reaction_0" reversible="false">
      <listOfReactants>
        <speciesReference species="H2O" stoichiometry="1">
          <annotation>
           <sl2:id id="H2O"/>
          </annotation>
        </speciesReference>
        <speciesReference species="G6P" stoichiometry="1">
          <annotation>
           <sl2:id id="G6P_1"/>
          </annotation>
        </speciesReference>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="P_i" stoichiometry="1">
          <annotation>
           <sl2:id id="P_i_sr1"/>
          </annotation>
        </speciesReference>
        <speciesReference species="Glucose" stoichiometry="1">
          <annotation>
           <sl2:id id="Glucose_1"/>
          </annotation>
        </speciesReference>
      </listOfProducts>
    </reaction>
    <reaction id="reaction_1" reversible="false">
      <listOfReactants>
        <speciesReference species="ATP" stoichiometry="1">
          <annotation>
           <sl2:id id="ATP"/>
          </annotation>
        </speciesReference>
        <speciesReference species="Glucose" stoichiometry="1">
          <annotation>
           <sl2:id id="Glucose_2"/>
          </annotation>
        </speciesReference>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="ADP" stoichiometry="1">
          <annotation>
           <sl2:id id="ADP"/>
          </annotation>
        </speciesReference>
        <speciesReference species="G6P" stoichiometry="1">
          <annotation>
           <sl2:id id="G6P_2"/>
          </annotation>
        </speciesReference>
      </listOfProducts>
    </reaction>
  </listOfReactions>
</model>
<annotation>
  <sl2:listOfLayouts xmlns:sl2="http://projects.eml.org/bcb/sbml/level2"
                     xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
                     xsi:schemaLocation="http://projects.eml.org/bcb/sbml/level2\
                     http://projects.eml.org/bcb/sbml/level2/layout2.xsd">
    <sl2:layout id="layout1" width="320" height="270">
```

```
<sl2:listOfCompartmentGlyphs>
  <sl2:compartmentGlyph id="compGlyph" compartment="compartment"
                x="10.0" y="10.0" w="60" h="50"/>
</sl2:listOfCompartmentGlyphs>
<sl2:listOfSpeciesGlyphs>
  <sl2:speciesGlyph id="ATP_Glyph" species="ATP" x="295.0" y="123.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="P_iGlyph" species="P_i" x="63.0" y="124.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="Glucose_Glyph1" species="Glucose" x="146.0" y="106.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="Glucose_Glyph2" species="Glucose" x="209.0" y="107.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="ADP_Glyph" species="ADP" x="298.0" y="214.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="H2O_Glyph" species="H2O" x="67.0" y="224.0"
                w="16.0" h="16.0"/>
  <sl2:speciesGlyph id="G6P_Glyph" species="G6P" x="180.0" y="241.0"
                w="15.0" h="16.0"/>
</sl2:listOfSpeciesGlyphs>
<sl2:listOfReactionGlyphs>
  <sl2:reactionGlyph id="reaction_0_Glyph" reaction="reaction_0"
                x="120.0" y="183.0" width="119.0" height="166.0">
    <sl2:listOfSpeciesReferenceGlyphs>
      <sl2:speciesReferenceGlyph id="SP1_Glyph" speciesGlyph="P_i_Glyph"
                              speciesReference="P_i_sr1"/>
      <sl2:speciesReferenceGlyph id="SP2_Glyph" speciesGlyph="Glucose_Glyph1"
                              speciesReference="Glucose_1" role="substrate"/>
      <sl2:speciesReferenceGlyph id="SP3_Glyph" speciesGlyph="H2O_Glyph"
                              speciesReference="H2O"/>
      <sl2:speciesReferenceGlyph id="SP4_Glyph" speciesGlyph="G6P_Glyph"
                              speciesReference="G6P_1">
        <sl2:curve>
          <sl2:listOfCurveSegments>
            <sl2:curveSegment xsi:type="sl2:CubicBezier" x1="180" y1="241"
                            x2="120" y2="183"
                            cx1="155" cy1="230" cx2="120" cy2="200"/>
          <sl2:/listOfCurveSegments>
        <sl2:/curve>
      </sl2:speciesReferenceGlyph>
    </sl2:listOfSpeciesReferenceGlyphs>
  </sl2:reactionGlyph>
  <sl2:reactionGlyph id="reaction_1_Glyph" reaction="reaction_1"
                x1="256.0" y1="166.0" x2="257.0" y2="183.0">
    <sl2:listOfSpeciesReferenceGlyphs>
      <sl2:speciesReferenceGlyph id="SP5_Glyph" speciesGlyph="ATP_Glyph"
                              speciesReference="ATP"/>
      <sl2:speciesReferenceGlyph id="SP6_Glyph" speciesGlyph="Glucose_Glyph2"
                              speciesReference="Glucose_2"/>
            <sl2:speciesReferenceGlyph id="SP7_Glyph" speciesGlyph="ADP_Glyph"
                                       speciesReference="ADP"/>
            <sl2:speciesReferenceGlyph id="SP8_Glyph" speciesGlyph="G6P_Glyph"
                                       speciesReference="G6P_2">
              <sl2:curve>
                <sl2:listOfCurveSegments>
                  <sl2:curveSegment xsi:type="sl2:CubicBezier" x1="257" y1="183"
                                    x2="180" y2="241"
                                    cx1="257" cy1="200" cx2="210" cy2="230"/>
                <sl2:/listOfCurveSegments>
              <sl2:/curve>
            </sl2:speciesReferenceGlyph>
          </sl2:listOfSpeciesReferenceGlyphs>
        </sl2:reactionGlyph>
      </sl2:listOfReactionGlyphs>
      <sl2:listOfAdditionalGraphicalObjects>
        <textLabel id="label1" x="100.0" y="85.0"
                   w="180.0" h="25.0">Reaction Layout</textLabel>
      </sl2:listOfAdditionalGraphicalObjects>
    </sl2:layout>
  </sl2:listOfLayouts>
 </annotation>
</sbml>
```

Contact Information

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Todo

- We need many more examples with nice pictures to go with them. This probably has to wait until the implementation is finished.
- Implement this proposal on top of libsbml with wrappers for Java, Python and C++

List Of Changes

Version 1.2

- Group class has been renamed to LayoutGroup to avoid future conflict with the abstract Group class of the render part
- This documents contains some new attributes to objects that are needed to connect this layout information part to the actual render information. All Glyph objects are now derived from GraphicalObject. GraphicalObject has the information for a bounding box and the reference to the id of the connected render object. A transformation to transform the render object prior to rendering can be given as well. GraphicalObject is also used in the listOfAdditionalGraphicalObjects to specify objects to include in the layout that have nothing to do with a chemical model. It could for example be used to draw some legend.
- We took the Transformation, SimpleTransformation and AffineTransformation from the render document and included them here as well since they are needed for GraphicalObject (see last point.)
- Since ReactionGlyph is now derived from GraphicalObject, the two points specified now have the notation of a bounding box and they can be seen as such. On the other hand, programs can still interpret them as two pseudo nodes as was the default so far. Maybe there should be a tag that specifies which it is.
- SpeciesReferenceGlyph, derived from GraphicalObject now includes all the attributes to specify a bounding box. Additionally it can hold a Curve object which overrides the information on the bounding box.

Version 1.1b

- Document now states that the default unit for the diagram is pt.
- Layout object gets three attributes width, height and depth.

Version 1.1a

- Curve Segments can now hold 3D information.

Version 1.1

- Added new edge information to the speciesRefernceGlyph. Edges can now be build from lists of straight lines and cubic bezier segments.
- Added the possibility of grouping of several graphical representations. These groups can then be used in the graphical representation instead of a SpeciesReferenceGlyph.
- Changed all tag names ending with GR(s) to to names ending with Glyph(s)
- Dropped refRole attribute from SpeciesReferenceGlyph in favor of an id in the annotations of the SpeciesReference.
- Changed refSpeciesGlyph attribute to ref so it is more consistent with the rest of the layout objects.
- Fixed the screenshot and corresponding example to correct the error in the pathway. Sample included does still not fully represent the screenshot with this new specification.
- speciesReferences can now be referenced by the speciesReference attribute of the speciesReferenceGlyph. The species reference id that is needed for this is added into the annotations tag of the speciesReference tag in the model.
- The naming of references is now more sbml like since the attributes are called after the object they reference.

References

[1] System Biology Markup Language Level 1 Website (*http://www.sbml.org/sbml/docs/index.html*)

[2] Michael Hucka, Andrew Finney, Herbert Sauro, Hamid Bolouri: Systems Biology Markup Language (SBML) Level 1: Structures and Facilities for Basic Model Definitions (*http://www.sbml.org/sbml/docs/papers/sbml-level-1/html/sbml-level-1.html*)

[3] Hucka M., Finney A., Sauro H.M., Bolouri H., Doyle J.C., Kitano H., Arkin A.P., Bornstein B.J., Bray D., Cornish-Bowden A., Cuellar A.A., Dronov S., Gilles E.D., Ginkel M., Gor V., Goryanin I.I., Hedley W.J.,

Hodgman T.C., Hofmeyr J.H., Hunter P.J., Juty N.S., Kasberger J.L., Kremling A., Kummer U., Le Novere N., Loew L.M., Lucio D., Mendes P., Minch E., Mjolsness E.D., Nakayama Y., Nelson M.R., Nielsen P.F., Sakurada T., Schaff J.C., Shapiro B.E., Shimizu T.S., Spence H.D., Stelling J., Takahashi K., Tomita M., Wagner J., Wang J. (2003) The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models, *Bioinformatics*, **19**, 524-31.

[4] JDesigner Website (*http://www.cds.caltech.edu/ hsauro/JDesigner.htm*)

[5] Herbert Sauro: JDesigner SBML Annotation (*http://www.cds.caltech.edu/ hsauro/JDSBMLEx.pdf*)