## Complementing layout information with render information in SBML files

Ralph Gauges, Sven Sahle and Katja Wegner EML Research Schloss-Wolfsbrunnen Weg 33 D-69118 Heidelberg Germany

October 11, 2006

## 1 Introduction

In 2003 we proposed an extension to the SBML file format that allowed programs to include layout and render information on graphical representation of reaction networks in SBML files. It soon became evident during the discussion on the SBML mailing list that a consensus for both layout and render information would not be reached fast, therefore we split the layout and the render part and concentrated on reaching consensus concerning the inclusion of layout information into SBML files. Now two years later, we consider the layout extension to be ready for general usage and as a matter of fact, it has been accepted as an official extension to be included into SBML Level 3. There are already several implementations for it and some programs already use it to exchange layout information on reaction networks. With the growing interest for graphical representations of reaction networks, we feel that it is now time to complement the layout extension with a render extension that builds on it and allows the user to define not only where the objects are to be located, but how they are to be rendered as well.

## 2 Design decisions

The first and as we think natural decision was to base the render extension on the existing layout extension. Secondly, we tried to make the render extension as flexible as possible in order to not impose any artificial limits on how programs can display their reaction networks. Since most programs do graphical representation of reaction networks in 2D, we decided to include only 2D render information in this first version of the render extension. If the need for 3D render information should arise, we will extend the render extension to include this information as well. We want to keep the render extension independant of the SBML model as well as the layout extension, therefore the render information will be stored as one or more seperate blocks. There can be one block of render information that applies to all layouts and blocks for each layout. In the beginning this render information of a layout respectively.

The render information consists of a set of styles that are associated with objects from the layout either by a list of ids of layout objects or by roles of layout objects or their corresponding model elements. Consider as example, you can define a style that can be applied to all SpeciesReference objects that are products. The render information included in the annotation of the listOfLayouts element will only be able to define styles that associate render information with roles of elements, it can not associate styles with individual objects from a layout. In order not to reinvent the wheel we loosely based this specification on SVG.

## 3 Defining render information

The render extension provides two locations where styles can be defined. First each layout can have its own set of render information located in the annotation of the layout itself. Second, a set of global render information located in the annotation of the listOfLayouts can be defined. It is important to note that each layout can have more then one style and that it is also possible to define more then one global style. Each style can also reference another style that complements it, this way the user can create styles that are based on other styles and only make slight modifications to the style they are based on. In contrast to local styles, the global styles can not reference individual layout elements by an id, it can only define role based or type based styles.

The top level element for the per layout render information is called listOfRenderInformation which can contain a list of one or more render-Information elements of type LocalRenderInformation. The LocalRender-Information datatype is based on the SBase datatype from SBML and has five attributes. The id attribute is of type SId just like the ids used in SBML. It is used to give the renderInformation element a unique id through which it can be referenced from other LocalRenderInformation objects. The optional attribute name is there to be able to give a LocalRenderInformation object a more user friendly name that can be displayed in programs. In cases where there is more then one LocalRenderInformation object per layout, this might make it easier for a user to find the render information he or she wants to associate with a given layout. The attributes programName and programVersion are optional and can be used to store information about the program that created the render information. Another optional attribute called referenceRenderInformation can be used to specify the id of another local (or global) render information object that complements the current render information object. So if a program can find no fitting render information in the current render information object, it can go on to the one referenced and see if it can find fitting information there. In order to avoid loops, only render information objects that have already been defined before may be referenced. So local render information objects may reference any global render information object as well as any local render information object that has already been defined.

In addition to those five attributes, the LocalRenderInformation object has four elements. The first element is called listOfColorDefinitions and is used to predefine a set of color to be referenced in styles. The second element is called listOfGradientDefinitions and it is used to predefine linear and radial gradients to be referenced in a style. How colors and gradients can be defined is explained in the section called Colors and Gradients. The third is called listOfLineEndings and it is used to define a set of line endings that can be applied to path objects. This is explained in more detail in the section called Defining Line Endings. The fourth element is called listOfStyles and it can hold one or more local style objects. Each local style object is located in an element called style and is of type LocalStyle.

First, a LocalStyle has an attribute called id that uniquely identifies it. It also has an optional roleList attribute which lists all the roles the style applies to and it can have a typeList attribute which lists all the element types the style applies to. The valid types for the typeList attribute are a combination of one or more of the following values separated by whitespaces: COMPARTMENTGLYPH, SPECIESGLYPH, REACTION-GLYPH, SPECIESREFERENCEGLYPH, TEXTGLYPH, GRAPHICAL-OBJECT and ANY

The ANY keyword specifies that this styles applies to any type of glyph and would be equivalent to listing all the other keywords. Concerning the valid keywords for the **roleList** attribute we had thought about taking those from some kind of controlled vocabulary. Preferably, this would be some kind of ontology like SBO. The specifics of this will have to be discussed with other interested parties. For the time being, all layout objects derived from GraphicalObject will get an additional attribute called objectRole. This attribute can be used to specify a string that specifies the role of the given object. If the same string appears in the roleList of some render information object, the render information applies to the object, but only if there was not a render information object that is more specific (see Style resolution and Role resultion below). LocalStyle objects can have one more optional attribute which is called **idList**. This is simply a list of ids of objects from the layout the style applies to.

The only subelement of a style is a g element which specifies how the element(s) covered by the idList, roleList and typeList are to be rendered. The details of this element are described in the section about grouping below.

ListOfLocalRenderInformation inherits from SBase renderInformation : LocalRenderInformation[1..\*]

LocalRenderInformation inherits from SBase			
id	:	SId	
name	:	string {use="optional"}	
programName	:	string {use="optional"}	
programVersion	:	string {use="optional"}	
reference Render Information	:	string {use="optional"}	
listOfColorDefinitions	:	$ListOfColorDefinitions \{use="optional"\}$	
list Of Gradient Definitions	:	$ListOfGradientDefinitions \ \{use="optional"\}$	
listOfLineEndings	:	ListOfLineEndings {use="optional"}	
listOfStyles	:	ListOfLocalStyles {use="optional"}	

ListOfLocalStyles inherits from SBase

style : LocalStyle[1..\*]

LocalStyle inherits from Style idList : string[1..\*] {use="optional"}

Style inherits from SBase		
id	:	SId
roleList	:	string[1*] {use="optional"}
typeList	:	$string[1*] {use="optional"}$
g	:	Group

## example:

```
</listOfColorDefinitions>
          <listOfGradientDefinitions>
            <linearGradient ... >
                   .
            </linearGradient>
            <radialGradient ... >
            </radialGradient>
                 .
          </listOfGradientDefinitions>
          <listOfLineEndings>
                 .
                 .
          </listOfLineEndings>
          <listOfStyles>
            <style id="CompartmentGlyphStyle" typeList="COMPARTMENTGLYPH">
              <g ...>
                .
              </g>
            </style>
          </listOfStyles>
        </renderInformation>
      </listOfRenderInformation>
    </annotation>
  </layout>
</listOfLayouts>
```

Global render information is specified very similar to local render information there are only some slight differences that one has to be aware of. Global render information is stored in an element called listOfGlobalRenderInformation which contains one ore more renderInformation elements of type GlobalRenderInformation. The attribute and elements of GlobalRenderInformation objects and LocalRenderInformation objects are the same. The only difference here is the fact that GlobalRenderInformation objects in their **referenceRenderInformation** attribute may only reference ids of other GlobalRenderInformation objects that have already been defined. The **listOfStyles** element of the GlobalRenderInformation object contains one or more **style** elements but this time these are of type GlobalStyle. The GlobalStyle datatype is also very similar to the LocalStyle datatype, the only difference being that the GlobalStyle does not have an **idList** attribute since referencing individual ids from a layout does not make sense for a global render information object. Save for those few differences, global and local render information is specified in the same way.

ListOfGlobalRenderInfor	ma	tion inherits from <b>SBase</b>		
renderInformation : Glob	alR	enderInformation[1*]		
GlobalRenderInformation inherits from SBase				
id	:	SId		
name	:	string {use="optional"}		
programName	:	string {use="optional"}		
programVersion	:	string {use="optional"}		
reference Render Information	:	string {use="optional"}		
listOfColorDefinitions	:	ListOfColorDefinitions {use="optional"}		
list Of Gradient Definitions	:	$ListOfGradientDefinitions \ \{use="optional"\}$		
listOfLineEndings	:	ListOfLineEndings {use="optional"}		
listOfStyles	:	ListOfGlobalStyles {use="optional"}		

#### example:

```
<listOfLayouts xmlns="http://projects.eml.org/bcb/sbml/level2"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
<annotation>
<listOfGlobalRenderInformation
xmlns="http://projects.eml.org/bcb/sbml/render/level2">
<renderInformation id="FancyRenderer_GlobalDefault"
name="default global style"
```

```
programName="FancyRenderer"
    programVersion="0.1.1">
    <listOfColorDefinitions>
        ...
        ./listOfColorDefinitions>
        .listOfGradientDefinitions>
        .listOfGradientDefinitions>
        ...
        ./listOfGradientDefinitions>
        .listOfLineEndings>
        ...
        ./listOfStyles>
        ...
        ./listOfGlobalRenderInformation>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfLino>
        </listOfGlobalRenderInformation>
        </listOfLino>
        </listOfLino>
```

## 3.1 Defining styles

### 3.2 Specifying positions and sizes

Positions and sizes for render elements can be specified as a combination of absolute values where the default unit is pt (1/72 inch) like in the layout extension and relative values in % where the % symbol has to be added to the value. Each coordinate can have zero or one relative component and zero or on absolute component. E.g. to specify a coordinate that is 5 points from the right edge of the current viewport the user could specify - 5+100%. In order to make parsing of coordinate infomrmation easier, the absolute component has to be specified before the relative component if there is a relative component. All values are relative to the bounding box of the corresponding element

in the layout. This bounding box basically specifies a viewbox for the render elements to be drawn on.

#### 3.3 Colors and Gradients

Although, it is possible to specify the color for a graphical primitive directly, colors and especially gradients can be specified in a so called listOfColorDefinitions and listOfGradient-Definitions element which is a subelement of the RenderInformation data type. The listOfColorDefinitions element holds one or more elements called colorDefinition of type ColorDefinition. The ColorDefinition data type is derived from SBase and has two additional attributes. One id attribute which uniquely identifies the ColorDefinition object within a Render-Information object and an attribute called value which holds a color value.

Color values are specified as a 6 to 8 digit hex string which defines the RGBA value of the color. If only the first six digits for the RGB value are given, the alpha value is assumed to be 0xFF which means that the color is totally opaque. SVG only has RGB color definitions and the A value is handled by the strokeopacity and fill-opacity attribute. The way SVG handles the opacity of a color differs from other software frameworks which mostly use RGBA values to specify a color and the opacity. Since we think using RGBA values is more common, we choose to use RGBA values for the render extension as well. Instead of specifying a color value, the value 'none' can be given which is equal to no drawing at all. To specify 'none' for the stop-color of a gradient is not allowed.

${\bf Color Definition} \ {\bf inherits} \ {\bf from} \ {\bf SBase}$		
id	:	SId
value	:	string

#### example:

All graphical primitives in the render extension have a stroke attribute that is used to specify the color of the stroke that is used to draw the curve or the outline of ellipses, rectangles or polygons. This stroke attribute can either hold a color value or it can hold the id of a predefined ColorDefinition object.

The listOfGradientDefinitions element holds one or more linearGradient or radialGradient subelements of type LinearGradient or RadialGradient respectively. A linearGradient element has eight attributes. The id attribute uniquely identifies it within a RenderInformation object. The attributes x1, y1, z1, x2, y2 and z2 are all optional and define a vector on which the gradient stops are mapped. If not specified, x1, y1 and z1 default to 0% and x2,y2 and z2 default to 100%. The last attribute called **spreadMethod** is also optional and specifies the method that is used to continue the gradient pattern if the vector points do not span the whole bounding box of the object the gradient is applied to. The attribute can have three values called **pad**, **reflect** or **repeat**. A value of **pad**, which is also the default, means that the gradient color at the endpoint of the vector defines how the gradient is continued beyond that point. A value of **reflect** means the gradient continues from end to start and then from start to end again and so on. A value of **repeat** simply means that the gradient pattern is repeated from start to end over and over again.

To specify the mentioned gradient stops the linear gradient element can hold one or more subelements called **stop** which are of type GradientStop. The GradientStop datatype has two

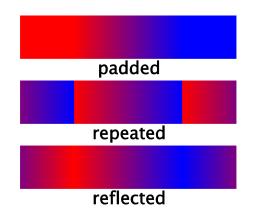


Figure 1: example of different SVG spreadMethod values

attributes. The first attribute, called offset, represents the distance from the starting point of the vector defined by x1, y1, z1, x2, y2 and z2. The value is given as a positive percentage value (usually somewhere between 0% and 100%). The other attribute is called stop-stroke and defines the color for the given gradient stop. The attributes value can either be given as a hexadecimal color value or as the id of a ColorDefinition object from the listOfColorDefinitions (see above). To specify the id of another gradient as the value of a stop-color attribute is considered an error. In case the two points that define the gradient vector are identical, the area will be painted with a single color taken from the last gradient stop element.

#### example:

```
<listOfGradientDefinitions>
<linearGradient x1="30%" y1="50%" x2="70%" y2="50%">
<stop offset="0%" stop-color="#0000A0" />
<stop offset="100%" stop-color="darkred" />
</lineaGradient>
.
.
```

</listOfGradientDefinitions>

The RadialGradient data type has 9 attributes. Just like the LinearGradient it has an id that uniquely identifies it within

LinearGradient inherits from SBase		
id	:	SId
x1	:	string {use="optional" default=" $0\%$ "}
y1	:	string {use="optional" default=" $0\%$ "}
z1	:	string {use="optional" default=" $0\%$ "}
x2	:	string {use="optional" default=" $100\%$ "}
y2	:	string {use="optional" default=" $100\%$ "}
z2	:	string {use="optional" default=" $100\%$ "}
spreadMethod	:	string {use="optional" default="pad"}
stop	:	GradientStop[1*]
GradientStop	inł	nerits from <b>SBase</b>
offset :	$\operatorname{str}$	ing

:

stop-color

string

a RenderInformation object and it also has the same spread-Method attribute with the same possible values. The attributes cx, cy and cz define the center of the radial gradient. The attributes are optional and can either be given in absolute or relative coordinates. If ommited, these three attribute values default to 50%. The r attribute defines the radius of the gradient and it can also be specified in either absolute or relative coordinates. Specifying negative values for  $\mathbf{r}$  is considered an error just like it is in SVG. The attributes fx, fy and fz specify the focal point of the gradient. The gradient will be drawn such that the 0% stop is mapped to (fx,fy,fz). The attributes fx, fy and fz are optional. If one is omitted it is considered to coincide with the value of cx, cy and cz respectively.

RadialGradient inherits from SBase		
id	:	SId
cx	:	string {use="optional" default=" $50\%$ "}
су	:	string {use="optional" default=" $50\%$ "}
cz	:	string {use="optional" default=" $50\%$ "}
r	:	string {use="optional" default=" $50\%$ "}
fx	:	string {use="optional"}
fy	:	string {use="optional"}
fz	:	string {use="optional"}
spreadMethod	:	<pre>string {use="optional" default="pad"}</pre>
stop	:	GradientStop[1*]

#### example:

```
<listOfGradientDefinitions>
<radialGradient cx="50%" cy="50%" r="20" spreadMethod="repeat">
<stop offset="10%" stop-color="#000040" />
<stop offset="90%" stop-color="#0000C0" />
</radialGradient>
.
.
.
</listOfGradientDefinitions>
```

#### 3.4 Graphical primitives

The graphical primitives polygons, rectangles and ellipses are based on the corresponding elements from SVG. For lines, arcs and general path primitives, we basically reuse the curve element from the layout extension. There is however one difference to the Curve datatype from the layout extension. Whereas Point objects in the layout extension could only contain absolute values for their coordinates, Point objects in the render extension can contain relative coordinate values. Since polygons are very similar to general path primitives, we also make use of the Curve datatype to specify polygons in the render extension.

All graphical primitives have some attributes in common that specify some drawing properties. As mentioned in the **Colors** 

and Gradients section, each graphical primitive has a stroke attribute that defines the color curves and outlines of geometric shapes are drawn. In addition to that, the stroke-width attribute specifies the width of the stroke and the stroke-dasharray is a list of numbers that specifies the lengths of dashes and gaps that are used to draw the line. The individual numbers in the list are seperated by kommas. In addition to those attributes, ellipses, polygons, ellipses, curves and rectangles have an attribute called fill that specifies the fill style of those elements. The fill style can either be a hexadecimal color value or the id of a ColorDefinition object or a GradientDefinition object. Instead of specifying a color or gradient name, 'none' can be specified. E.g. if you want to have some shape unfilled, specify a fill value of 'none'. Additionaly an attribute called fill-rule can be used to specify how the shape should be filled. Allowed values for fill-rule are nonzero which is the default, evenodd or inherit. For a detailed description on how those attributes work, we would like to refer you to the corresponding documentation in the SVG spec. As time permits we will add our own documentation eventually. Another attribute that all graphical primitives have in common is the transform attribute. This attribute can be used to specify a six element matrix which corresponds to a affine transformation matrix. The details are described in the section called "Transformations" below.

GraphicalPrimitive1D inherits from $SBase$		
stroke	:	string {use="optional"}
stroke-width	:	string {use="optional"}
stroke-dasharray	:	double[1*] {use="optional"}
transform	:	string {use="optional"}

GraphicalPrimitive2D inherits from GraphicalPrimitive1D			
fill	:	string {use="optional"}	
fill-rule	:	string {use="optional" default="nonzero"}	

#### 3.4.1 Curves

Simple lines and complex curves are represented by the curve element introduced in the layout extension. A curve has a listOfCurveSegments which can hold an arbitrary number of line segments and cubic bezier elements in any order. With this, any path (no matter how complex it is) can be represented. As mentioned above, Point objects used to specify the individual curve segments can contain relative values for their coordinates as well as absolute values. The coordinate values are always with respect to the bounding box of the layout object the render information applies to. To assign line endings to the start and end of a path object two new attributes were introduced they are called startHead and endHead and specify the id of the line ending that shall be applied to the start and the end of the curve respectively. Both attributes are optional. How line endings are defined is described in the section called **Defining** Line Endings.

#### example:

#### 3.4.2 Polygons

A polygon object is made up of a **polygon** element which contains a listOfCurveSegments with curveSegment elements that defines the edge of the polygon. The major differences to the curve object is that the individual curveSegments can only be straight lines and that last point of the curve is connected to the first, so the polygon is always closed and that

Curve inherits from GraphicalPrimitive2D		
startHead	:	SId {use="optional"}
endHead	:	SId {use="optional"}
listOfCurveSegments	:	${\it ListOfCurveSegments}$
listoreurvesegments	•	ListOlCurveSegments

ListOfCurveSegments inherits from SBase curveSegment : LineSegment[1..\*]

<b>Point</b> inherits fi	rom <b>SBase</b>
--------------------------	------------------

- id : SId {use="optional"}
- $x \quad : \quad \mathrm{double}$
- y : double
- z : double {use="optional" default="0.0"}

#### LineSegment inherits from SBase

start	:	Point
end	:	Point

# CubicBezier inherits from LineSegmentbasePoint1:Point {use="optional"}basePoint2:Point {use="optional"}

the polygon can therefore have a fill style that determines how the inside of the polygon is to be rendered.

Polygon inherits from GraphicalPrimitive2DlistOfCurveSegments:ListOfCurveSegments

#### example:

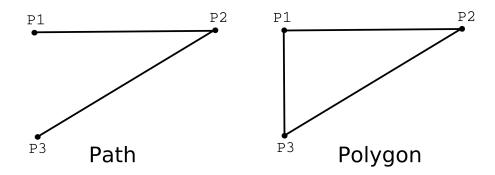


Figure 2: Rendering of a Path vs. rendering of a Polygon with the same base points

#### 3.4.3 Rectangles

The rectangle definition was taken from SVG and allows the definition of rectangles with or without rounded edges. The rectangle has the attributes  $\mathbf{x}$ ,  $\mathbf{y}$  and  $\mathbf{z}$  to specify its position within the bounding box of the enclosing layout object and a width and height attribute that specifies the width and height of the rectangle, either in absolute values or as a percentage of the width and height of the enclosing bounding box. The default value for the optional  $\mathbf{z}$  attribute is 0.0. Additionally the rectangle has two optional attributes  $\mathbf{rx}$  and  $\mathbf{ry}$  is specified, the other is presumed to have the same value. The default value for  $\mathbf{rx}$  and  $\mathbf{ry}$  is 0.0 which means that the edges are not rounded.

Rectar	ngle	e inherits from <b>GraphicalPrimitive2D</b>
x	:	string
У	:	string
z	:	string {use="optional" default=" $0.0$ "}
width	:	string
height	:	string
rx	:	string {use="optional" default=" $0.0$ "}
ry	:	string {use="optional" default=" $0.0$ "}

#### example:

#### 3.4.4 Ellipses

The definition of an ellipse was also taken directly from SVG. The ellipse has the attributes cx, cy and cz to specify the center of the ellipse and rx and ry to specify the radius of the ellipse along the x-axis and the y-axis respectively. If only rx or ry is specified, the other is presumed to have the same value. Circles are a special case of an ellipse where rx and ry are equal. Again cz is optional and its default value is 0.0.

Ellipse inherits from GraphicalPrimitive2D string :  $\mathbf{c}\mathbf{x}$ cy : string string {use="optional" default="0.0"}  $\mathbf{cz}$ : string : rx string {use="optional"} ry :

#### example:

#### 3.4.5 Text elements

In order to draw text, we use the text element from SVG with slight modifications. Like the text element in SVG, our text element has the attributes font-family to specify which font to use and font-size to specify the size of the font. Both attributes are optional. If specified, font-size must be a positive absolute or relative size.

For reasons of simplicity, we limit the display of text to normal text, outlined or filled-outlined text are not supported. Also in order to simplify text display we think it would be best practice if programs would limit the choice of the font-family attribute to the generic families serif, sansserif and monospace. But since those only apply to western languages, it make sense to use other values for font-familie in certain cases.

The horizontal alignment of text element can be specified by the text-anchor attribute. Allowed values are start, middle and end. SVG does not seem to provide any means for the vertical alignment of text, therefore in order to make it easier for implementers we don't. On the other hand if people think that this is a necessary feature, we can either extend the allowed values for the text-anchor attribute, or we can add a second attribute with the same allowed values to do vertical text alignment. Depending on the value of the text-anchor attribute, the x, y and z attributes of the text element either specify the left bottom corner, the middle bottom position or the right bottom corner of the text. As in rectangles and ellipses, the z attribute is optional and its default value is 0.0.

The text element has two more attributes. One is called font-weight and specifies wether a font is to be drawn bold. The only values allowed for font-weight are bold and normal. Likewise the font-style attribute determines wether a font is to be drawn italic or normal and consequently the only allowed values are italic and normal. Both attributes are optional.

Text inherits from GraphicalPrimitive1D				
х	:	string		
У	:	string		
z	:	string {use="optional" default=" $0.0$ "}		
font-family	:	string {use="optional"}		
font-size	:	string {use="optional"}		
font-weight	:	string {use="optional"}		
font-style	:	string {use="optional"}		
text-anchor	:	string {use="optional"}		

#### example:

```
<g ...>
<text x="50%" y="50%" text-anchor="middle" stroke="#FF0000"
font-family="serif" font-size="20.0" >This is a Text</text>
.
.
.
.
.
.
```

#### 3.4.6 Bitmaps

To include bitmaps into a graphical representation we use the image element from SVG. The image element in SVG can also be used to include complete SVG vector images which we explicitly exclude in this version of the proposal since we think it would be too complicated. If the community feels that there is the need to include vector graphics, we could integrate the according SVG specificatin without changes.

The image element has six attributes. The x, y and z attributes specify the position of the image within the bounding box and the width and height attributes specify its width and height. The z attribute is optional and its default value is 0.0. The actual image data is not embedded in the render information, but the image element has an attribute called xlink:href that references an external JPEG or PNG file. If the referenced image is larger then the given width and height, it has to be scaled to the given dimensions.

<b>Image</b> inherits from <b>SBase</b>				
x	:	string		
у	:	string		
z	:	string {use="optional" default=" $0.0$ "}		
width	:	string		
height	:	string		
href	:	string		

#### example:

```
<g ...>
<image x="10%" y="10%" width="80" height="100" href="Glucose.png" />
.
.
.
.
</g>
```

#### 3.5 Transformations

In order to be able to display text that is not aligned horizontally or vertically or to effectively compose groups of objects from primitives, transformation like rotation, translation and scaling are needed. SVG, among other options, allows the user to specify a 3x3 matrix transformation matrix:

$$\left[\begin{array}{rrrr}a & c & e \\ b & d & f \\ 0 & 0 & 1\end{array}\right]$$

Since the last row of the matrix is always 0 0 1, the matrix is specified as a six vector. Therefore, in the render extension each group or graphical primitive can have a **transform** attribute just as in SVG. The allowed value for the attribute is the form: **a**, **b**, **c**, **d**, **e**, **f**, where a-f denote the values for the transformation matrix as stated above.

#### example:

#### 3.6 Grouping

Like in SVG, several graphical primitives can be grouped inside a g element to generate more complex render information. stroke, stroke-width, stroke-dasharrays, transform, fill, font-family, font-size, font-weight, font-style and text-anchor attributes can be applied to groups. If any of those attributes is specified for a Group object, it specifies the

attribute	default value		
stroke-width	0.0		
stroke-dasharrays	empty list		
transform	1.0, 0.0, 0.0, 0.0, 1.0, 0.0		
fill	None		
font-family	sans-serif		
font-size	0		
font-weight	normal		
font-style	normal		
text-anchor	start		
startHead	none		
endHead	none		

Table 1: Attribute default values.

corresponding attribute for all graphical primitives and groups defined within this group. If a graphical primitive or a group redefines one or more of those attributes, the newly defined values take effect. If an object within the group does not redefine those values, those of the group apply. If an attribute is not defined in any object of a style, its default values take effect. These default values are listed in Table 1.

It might seem a little unusual that the default values for stroke-width and text-size are set to 0. The reason for this is that a style that only contains an empty group is meant to define that the element the style applies to is not to be rendered. Since the render information for curves in SpeciesReferenceGlyphs and ReactionGlyphs as well as the render information for TextGlyphs is defined via attributes from the outermost group element of a style (see below), the group would explicitly have to define the stroke-width or the text-size to be 0 which would be inconsistent with the implied meaning of an empty group. The outermost group can also contain information about arrow heads to be used on curves specified in the layout. This information is given via the startHead and endHead attributes just like for curve elements. These attributes only apply to curve objects from the layout, not to curve objects within the group. Since those two attributes only make sense on the outermost group of a style, they are to be ignored on all other groups. The default value for those attributes is none which means that no line ending is to be drawn.

Each group has an id through which it can be referenced. This way groups can be nested by referencing one group within another. In order not to create loops, only groups that have been defined previously in the render information can be referenced. No forward declarations as references are allowed. In addition to those attributes a Group object can contain 0 or more child elements that form the render information. These child elements can either be graphical primitives, e.g. rectangles, ellipses, curves, polygons, text elements images or groups.

Group inherits from GraphicalPrimitive1D				
fill	:	string		
font-family	:	string		
font-size	:	string {use="optional" default=" $0.0$ "}		
font-weight	:	string		
font-style	:	string		
text-anchor	:	string		
children	:	(GraphicalPrimitive1D and/or Image)[0*]		

#### example:

```
<g stroke="#000000" font-family="serif" >
    <rectangle x="0%" y="0%" width="100%" height="100%"
        fill="blueLinearGradient" />
        <text x="50%" y="50%" font-size="80%" text-anchor="middle"
            stroke="#FF0000" />
</g>
```

## 4 Defining Line Endings

In many graphs the relations between nodes are depicted by lines and often the type of relation is encoded in the line ending. For this reason, the render extension provides ways to specify a set of arbitrary line endings and means to apply those to path objects. The individual line endings are defined in an element called listOfLineEndings which comes right before the listOfStyles.

The individual line endings are defined as groups just like styles. This way arbitraryly complex line endings can be defined. Each line ending is encapsulated in an element called lineEnding and contains two subelements. The first element is called boundingBox and it specifies the the viewport that is used to draw the line ending. Just like the bounding boxes of the layout extension, this bounding box contains a position subelement and a dimensions subelement. The dimensions element works just as you would expect it, since it specifies the size of the viewport for the line ending along each of the axes. The meaning of the position element differs slightly. If the position was at P(0.0, 0.0, 0.0), the origin of the line ending would be mapped to the corresponding vertex of the line (either start or end), if any of the position components differs from 0.0, it specifies by how much the line ending has to be moved in respect to the vertex it is applied to. (For thos of you who are familier with SVG markers, this is just the opposite of how SVG is doing it. So in order to generate SVG markers refX and refY attributes, you have to multiply the corresponding position values by -1. The second child is a group element that hold the render information for the line ending

The two attributes of the lineEnding element are the id attribute which is used to specify a unique id for the line ending by which it can be referenced and an attribute called enableRotationalMapping. The enableRotationalMapping attribute specifies wether a line ending will be rotated depending on the slope of the line it is applied to or if it is drawn just the way it was specified. The default value for the attribute is **true** which means that the line ending is rotated depending on the slope of the line. A more detailed description of this mapping is given below.

In this version of the render extension, we limit the render information to 2D objects. Since the layout information on which the render information relies is in a 3D coordinate system, we need to provide some definition of how the 2D line ending objects are to be applied to the 3D path objects. First we define that the origin of the coordinate system for drawing a line ending is the endpoint of the line the line ending is to be applied to. If the enableRotationalMapping attribute is set to true, we define that the tangent to the path object at this point coincides with the positive x axis of the coordinate system for the arrow head. In order to be able to use one line ending definition for the start as well as the end of the line, we also define that the tangent vector to the path object at the endpoint points away from the line.

In order to apply a line ending which is defined using only 2D coordinates onto a line which has been defined using 3D coordinates, we need to define a kind of mapping. The first definition we make is that the origin of the line ending viewport is mapped to the end of the line to which the line ending is applied. If the enableRotationalMapping attribute is set to false, the line endings coordinate system is the same as the global coordinate system used to draw the layout, only the origin is moved to the line end the line ending is going to be applied to. If the enableRotationalMapping attribute is set to true, which is the default, we define that the x,y-plane of the line endings viewport is mapped to the the plane that results from taking the unit vector of the slope of the line and unit vector that results

from orthonormalizing the slope vector and a second vector that has no component along the z axis. If the slope of the line has a positive component along the x axis, the orthonormalized vector also has to have a positive component along the y axis. In order to retain the right handed coordinate system, the z axis of the line endings coordinate system is perpendicular to the plane created by the other two vectors and has a positive component along the global coordinate systems z-axis. Likewise if the slope has a negative component along the global coordinate systems x axis, the y component of the orthonormalized second vector has a negative component along the y axis of the global coordinate system and to retain the right handed coordinate system, the third vector which is perpendicular to the plane made by the slope and its orthonormalized vector, has a positive component along the global coordinate systems z axis.

If the slope of the line points directly along the positive z axis of the global coordinate system, the line endings coordinate system is mapped to the line ending by a  $-90^{\circ}$  rotation around the y axis of the line endings coordinate system and a translation of the origin of the line endings coordinate system to the end of the line. If the slope points directly down the negative z axis, the line endings coordinate system has to be rotated by  $+90^{\circ}$  around its y axis before translation to the position of the curves end.

This may all sound very complicated, but in the end, the calculations to be done are not difficult and straight forward. A mathematical description of the calculations necessary is given in Appendix A.

If we define  $Q = -\frac{dy_s}{dx_s}$  and  $D = "\frac{1}{\sqrt{Q^2+1}}"$  then the transformation of any point P = (x, y, z) in the line endings coordinate system to the global coordinate system depending on the slope

of the curve  $\vec{S} = \begin{pmatrix} dx_s \\ dy_s \\ dz_s \end{pmatrix}$  and the curves endpoint  $O = \begin{pmatrix} x_O \\ y_O \\ z_O \end{pmatrix}$ can be decribed by:

$$P_{new} = \begin{pmatrix} dx_s * x + SGN(dx_s) * Q * D * y - dz_s * SGN(dx_s) * D * z + x_O \\ dy_s * x + SGN(dx_s) * D * y + dz_s * SGN(dx_s) * Q * D * z + y_O \\ dz_s * x + (dx_s * SGN(dx_s) * D - dy_s * SGN(dx_s) * Q * D) * z + z_O \end{pmatrix}$$

This is for the cases where the slope vector  $\vec{S}$  does run parallel to the global coordinate systems z axis. For this species case, the new point is calculated by:

$$P_{new} = \left(\begin{array}{c} SGN(dz_s) * -z + x_O \\ y + y_O \\ SGN(dz_s) * x + z_O \end{array}\right)$$

The SGN function describes the sign of its argument. It returns 1 for positive numbers, 0 for 0 and -1 for negative numbers. For the details of how this transformation was calculated and the definition of the SGN function see Appendix Α.

The mapping of line endings to lines is done before all transformations defined for the line have been applied. Transformation defined on the line ending itself or on any of its components are to be applied before the line ending is mapped to the curve.

In order to declare that a certain line ending is to be used on a path object, the curve element has two attributes called startHead and endHead which hold the id of a line ending definition for the start and for the end of the path respectively.

LineEnding inherits from GraphicalPrimitive2D					
id	:	SId			
enable Rotational Mapping	:	boolean default=true			
boundingBox	:	BoundingBox			
g	:	Group			

#### example:

```
<lineEnding id="SimpleArrowHead">
 <boundingBox>
  <position x="-10.0" y="-4.0" />
   <dimensions width="12.0" height="8.0"/>
</boundingBox>
 <g>
```

```
<polygon>
     <curve>
       <listOfCurveSegments>
         <curveSegment xsi:type="LineSegment">
           <start x="100%" y="50%" />
           <end x="0%" y="100%" />
         </curveSegment>
         <curveSegment xsi:type="LineSegment">
           <start x="0%" y="100%" />
           <end x="0%" y="0%" />
         </curveSegment>
         <curveSegment xsi:type="LineSegment">
           <start x="0%" y="0%" />
           <end x="100%" y="50%" />
         </curveSegment>
       </listOfCurveSegments>
     </curve>
  </polygon>
</g>
</lineEnding>
```

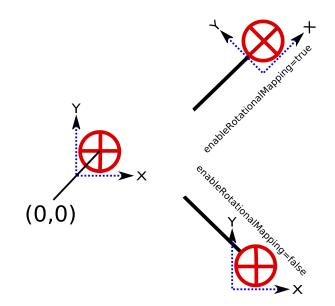


Figure 3: example of a line ending with and without rotation mapping enabled

## 5 Style resolution

When a program tries to resolve which style applies to a certain object it should follow the rule that more specific style definitions take precedence over less specific ones and that if there are several styles with the same specificity, the first one encountered in the file is to be taken. In essence this means that a program first has to search the local render information for a style that references the id of the object, if none is found it searches for a style that mentions the role of the object if it has one (see next section). If it does not find one, it searches for a style for the type of the object. If a render information references another render information object via its referenceRenderInformation attribute, the program has to go through that one as well to see if a more specific render information is present there. If the chain of referenced RenderInformation objects has been searched and no style has been found that fits, it is up to the program how the object is rendered. If a program explicitly wants to define render information that states that some objects are not to be rendered at all, it has to define a style that does nothing, i.e. has no render information but applies to the objects that are not to be rendered. If several type based styles are found that would fit, a style that applies to only one type takes precedence over a style that applies to several types.

## 6 Role resolution

This render extension explicitly provides means to write render information that renders layout objects based on certain roles those render objects or their corresponding model objects have. So far SBML models or layouts do not contain such role information or only for a limited number of objects if one would consider the role attribute of SpeciesReferenceGlyph objects to fall into this category. Although there is currently no means to specify these roles, there are already initiatives underway that try to complement SBML files with more biological information based on ontologies. One of these initiatives, the sboTerms, is about to be included into SBML Level 2 Version 2. This ontology or a similar one could provide this role information in the future. For the time being, we define an additional attribute called object-Role for all layout objects derived from GraphicalObject including GraphicalObject itself. The attribute specifies a user defined role string. render information including the same roleString in its roleList applies to the object. This is only true if no more specific render information takes precedence (see Style resolution).

A specific style can reference one or more roles to which it applies. Roles of objects could be taken from the sboTerm of the corresponding object and we expect model objects as well as layout objects to use sboTerms to specify roles for individual objects. When a program tries to determine which style applies to a specific object it might have to determine the role of the object first. If the layout object itself has a role, this will be taken, otherwise if the layout object is associated with an object in the model, the program should get the role from the associated object. If none of them has a role, no role based style can be applied to the object.

## 7 Style information for ReactionGlyphs and SpeciesReferenceGlyphs

When defining a style for a ReactionGlyph or SpeciesReferenceGlyph object, one has to distinguish wether the layout only specifies a bounding box for the object or if it specifies a curve. In the case of a bounding box, you want to define complete render information, whereas in the case of a curve, you only want to set certain attributes that determine certain aspects about how the curve is drawn, e.g. its color. To resolve this conflict, the style for such an object has to define render information for both cases. The render information for the case of a bounding box is specified just like render information for any other object within a Group. Render information for the case of a curve is defined by the appropriate attributes that are in effect in the outermost Group object itself. Those attributes include stroke, stroke-width and stroke-dasharray. Additionally startHead and endHead can be specified to define line endings for layout curve objects.. If the group does not define one or more of these attributes, the default value is used (see section on Grouping).

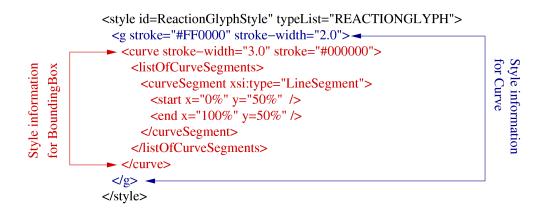


Figure 4: style with render information for objects with curve or bounding box

## 8 Style information for TextGlyphs

Just as in the case of curves in ReactionGlyphs and Species-ReferenceGlyphs, TextGlyphs already can be considered to be render information which is located in the layout because a Text-Glyph already specifies the text to be rendered and it therefore does not need additional render information in the form of a text element. On the other hand, it needs render information about the font properties the text is to be rendered with. Just as for the curve object for ReactionGlyphs and Species-ReferenceGlyphs, this render information is taken from the font related attributes of the outermost group element of the style that is used to render a TextGlyph. Any additional information within the group is ignored. If the group does not specify any of the font-family, font-size, font-weight, font-style or text-anchor attributes, the default values are to be used.

## 9 Uniqueness of IDs

Since local and global render information objects can reference other render information objects, programs creating render information need to make sure that all the IDs are unique within the reference history. In other words, a render information object that references another render information object must make sure that none of its IDs is equal to an ID in any of the directly or indirectly referenced render information objects. An exception to this rule is to create e.g. a color definition with the same ID as the color definiton in a referenced style in this case interpreting programs can assume that this color definition is supposed to override a color definition in a referenced render information object. Likewise it is also possible to override a color definition with a gradient and vice versa, line ending definitions should only be overridden with other line ending definitions however.

## 10 Appendix A

Position of line end:  $O(x_O, y_O, z_O)$ Normalized slope vector at end:  $\vec{S} = \begin{pmatrix} dx_s \\ dy_s \\ dz_s \end{pmatrix}$ 

Orthogonal vector to  $\vec{S}$  with z = 0:

$$dx_{s} * x_{2} + dy_{s} * y_{2} = 0$$
  
$$dx_{s} * x_{2} = -dy_{s} * y_{2}$$
  
$$x_{2} = -\frac{dy_{s} * y_{2}}{dx_{s}}$$

Choosing  $y_2 = 1 \Rightarrow x_2 = -\frac{dy_s}{dx_s}$  $\vec{V}_2 = (-\frac{dy_s}{dx_s}, 1, 0)$ 

Normalize  $\vec{V_2}$ : Length of  $\vec{V_2}$ :  $l_{\vec{V_2}} = \sqrt{\left(-\frac{dy_s}{dx_s}\right)^2 + 1}$ 

$$\vec{V}_{2N} = \begin{pmatrix} -\frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ 0 \end{pmatrix}$$

Retain right handed coordinate system:

$$\vec{V}_{2N} = \begin{pmatrix} SGN(dx_s) * -\frac{dy_s}{dx_s * \sqrt{\left(-\frac{dy_s}{dx_s}\right)^2 + 1}} \\ SGN(dx_s) * \frac{1}{\sqrt{\left(-\frac{dy_s}{dx_s}\right)^2 + 1}} \\ 0 \end{pmatrix}$$

SGN(x) is defined as:

$$SGN(x) = \begin{cases} 1 \text{ for } x > 0 \\ 0 \text{ for } x = 0 \\ -1 \text{ for } x < 0 \end{cases}$$

Calculation of the third vector:

$$\begin{split} \vec{V}_{3N} &= \vec{S} \times \vec{V}_{2N} \\ &= \begin{pmatrix} dx_s \\ dy_s \\ dz_s \end{pmatrix} \times \begin{pmatrix} SGN(dx_s) * - \frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} dy_s * 0 - dz_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ dz_s * SGN(dx_s) * - \frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} - dx_s * 0 \\ dx_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} - dy_s * SGN(dx_s) * - \frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \end{pmatrix} \\ &= \begin{pmatrix} -dz_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ dz_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ dz_s * SGN(dx_s) * - \frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \end{pmatrix} \end{split}$$

Now we have to map the line endings coordinate system to the coordinate system specified by  $\vec{S}$ ,  $\vec{V}_{2N}$  and  $\vec{V}_{3N}$ . This basically involves rotations around the x,y and z axis of the line endings coordinate system:

$$T \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \vec{S} \ \vec{V}_{2N} \ \vec{V}_{3N} \end{pmatrix}$$

$$T = \begin{pmatrix} dx_s & SGN(dx_s) * -\frac{dy_s}{dx_s * \sqrt{\left(-\frac{dy_s}{dx_s}\right)^2 + 1}} & -dz_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ dy_s & SGN(dx_s) * \frac{1}{\sqrt{\left(-\frac{dy_s}{dx_s}\right)^2 + 1}} & dz_s * SGN(dx_s) * -\frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \\ dz_s & 0 & dx_s * SGN(dx_s) * \frac{1}{\sqrt{-\frac{dy_s}{dx_s}^2 + 1}} - dy_s * SGN(dx_s) * -\frac{dy_s}{dx_s * \sqrt{-\frac{dy_s}{dx_s}^2 + 1}} \end{pmatrix}$$

And last but not least, we have to translate the coordinate system to the endpoint of the curve. So the overall transformation to map a point P(x, y, z) in the line endings coordinate system to the curve is:

$$P_T = (T \cdot P) + O$$

$$\begin{split} P_T &= \left( T \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right) + \begin{pmatrix} x_O \\ y_O \\ z_O \end{pmatrix} \\ \text{Let } D &= \frac{1}{\sqrt{\left( -\frac{dy_s}{dx_s} \right)^2 + 1}} \\ T &= \left( \begin{array}{ccc} dx_s & SGN(dx_s) * -\frac{dy_s}{dx_s} * D & -dz_s * SGN(dx_s) * D & x_O \\ dy_s & SGN(dx_s) * D & dz_s * SGN(dx_s) * -\frac{dy_s}{dx_s} * D & y_O \\ dz_s & 0 & dx_s * SGN(dx_s) * D - dy_s * SGN(dx_s) * -\frac{dy_s}{dx_s} * D & z_O \\ 0 & 0 & 0 & 1 \end{array} \right) \\ P_T &= \left( \begin{array}{ccc} dx_s & SGN(dx_s) * -\frac{dy_s}{dx_s} * D & -dz_s * SGN(dx_s) * D & y_O \\ dz_s & 0 & dx_s * SGN(dx_s) * -\frac{dy_s}{dx_s} * D & z_O \\ 0 & 0 & 0 & 1 \end{array} \right) \\ P_T &= \left( \begin{array}{ccc} dx_s & SGN(dx_s) * -\frac{dy_s}{dx_s} * D & -dz_s * SGN(dx_s) * D & y_O \\ dy_s & SGN(dx_s) * -\frac{dy_s}{dx_s} * D & -dz_s * SGN(dx_s) * D & y_O \\ dy_s & SGN(dx_s) * D & dz_s * SGN(dx_s) * D & y_O \\ dz_s & 0 & dx_s * SGN(dx_s) * D - dy_s * SGN(dx_s) * -\frac{dy_s}{dx_s} * D & z_O \\ 0 & 0 & 0 & 0 \end{array} \right) \cdot \left( \begin{array}{c} x \\ y \\ z \\ 1 \end{array} \right) \\ \end{split}$$