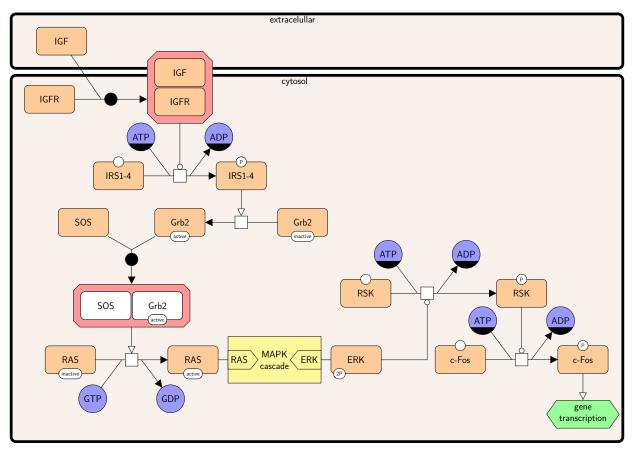
sbgntikz

manual for version 1.1.*

Adrien Rougny

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 ${\it Map\ adapted\ from\ SBGN\ PD\ language\ L1V1.3,\ Journal\ of\ Integrative\ Bioinformatics,\ 2015\ Sep\ 4;12(2):263}$

Contents

1	Intr	Introduction		
	1.1	About		
		Installation and usage		
		A first map		
2	Drawing glyphs			
	2.1	Nodes		
	2.2	Arcs		
	2.3	Nodes' and arcs' attributes		
	2.4	Layers		
3	Customizing and drawing maps effectively 1			
	3.1	Useful options for nodes and arcs		
	3.2	Positioning of nodes, arcs, and their attributes		
	3.3	Bended arcs, multi-part arcs		
	3.4	Nodes along paths for ER maps		
4	SBGN-ML to TikZ converter			
	4.1	Installation		
		Usage		

1 Introduction

1.1 About

sbgntikz is a TikZ [1] library to draw SBGN PD, AF or ER maps [2] directly into LATEX documents. It basically encodes SBGN glyphs into TikZ shapes and arrowheads named by keywords, making them straightforwardly drawable within a TikZ picture. Drawing a specific glyph is then as simple as specifying its corresponding keyword in some TikZ command.

The present manual is intended for an audience that knows SBGN but not particularly TikZ. The rest of the present section is dedicated to the first steps in using sbgntikz: installing the library and drawing a first map (while introducing some basic TikZ syntax). Section 2 references all glyphs and their associated keywords, whereas section 3 gives some TikZ options and syntaxes that I find most useful to draw SBGN maps. I believe users already familiar with TikZ will mostly be interested in reading section 2, and might have different (and maybe better) solutions to the issues presented in section 3.

1.2 Installation and usage

The directory tikz-sbgn should be copied to a directory where it can be found by your TFX engine:

- to the directory of your TEX source file or
- to a local texmf directory, whose location depends on the OS you are using:
 - Linux: to /home/<user>/texmf/tex/generic/pgf/. The index must then be updated using the texhash /home/<user>/texmf command.
 - MacOs: to /Users/Library/texmf/tex/generic/pgf/.
 - Windows: to C:\Users\<user>\texmf\tex\generic\pgf\backslash.

In all cases, the texmf directory has to be created if it does not already exist. In the case you are using MikTeX, you will need to add this directory to the TEXMF root directories in the Directories tab of the Settings page.

TikZ should already be installed within your TeX distribution. If not, you may install it via your TeX distribution, or download the latest build here. Once installed, TikZ and sbgntikz can be imported into your IATeX by adding the following two commands to your preamble:

```
\usepackage{tikz}
\usetikzlibrary{sbgn}
```

An SBGN map can then be drawn within a TikZ picture using the sbgn key:

```
\begin{tikzpicture}[sbgn]
% tikz code to draw an SBGN map
\end{tikzpicture}
```

1.3 A first map

SBGN is all about drawing nodes with specific shapes and arcs with specific arrow heads. Fortunately, drawing TikZ pictures is not different, making it pretty straightforward to draw SBGN maps using sbgntikz: the \node command is used to draw nodes, while the \draw command is used to draw arcs. The code to draw an SBGN node (or an attribute) will usually look like the following:

```
\node[<sbgn node>, ...] (name) at (point) {LABEL};
```

where

- <sbgn node> is a keyword corresponding to the type of node to be drawn (e.g. simple chemical for a simple chemical);
- ... is a list of other options for the node (e.g. its relative positioning towards another node, color, line width ...);
- (name) specifies the name of the node (optional);

- at (point) specifies the point on the canvas where to draw the node (optional, by default (0,0) if no relative positioning is specified in the nodes' options);
- {LABEL} specifies the label of the node that will be displayed (mandatory but can be empty).

As for arcs, they can be drawn using the following piece of code:

```
\draw[<sbgn arc>, ...] (a) -- (b);
```

where

- <sbgn arc> is a keyword corresponding to the type of arc to be drawn (e.g. necessary stimulation for a necessary stimulation);
- ... is a list of other options for the arc (e.g. its color, line width ...);
- (a) is a point on the canvas or the name of a node from which the arc will depart;
- (b) is a point on the canvas or the name of a node on which the arc will arrive.

Knowing those two basic syntaxes, one can draw pretty much any desired SBGN map. Following is an example of code to draw a simple PD map. It relies on relative positioning provided by TikZ's positioning library, as positioning all nodes with absolute coordinates would be too cumbersome (see section 3 for few more details, or the PGF/TikZ manual for lot more details).

```
\documentclass{standalone}
\usepackage{tikz}
\usetikzlibrary{positioning, sbgn}
\begin{document}
\begin{tikzpicture}[sbgn]
\node[macromolecule] (erk) {ERK};
                                    % this node has no absolute nor relative positioning, so it
\hookrightarrow is placed at (0,0) by default
\node[sv] at (erk.120) {}; % the state variable is placed on the border of the node, at an angle

→ of 120 deg

\node[generic process, connectors = horizontal, right = of erk] (p) {}; % we add connectors, and

→ use relative positioning

\node[macromolecule, right = of p] (perk) {ERK};
\node[sv] at (perk.120) {P};
\node[simple chemical, below left = of p] (atp) {ATP};
\node[simple chemical, below right = of p] (adp) {ADP};
\node[macromolecule, above = 2cm of p] (pmek) {MEK};
\node[sv] at (pmek.120) {P};
\draw[consumption] (erk) -- (p.west); % p being the name of the process node, p.west is the tip

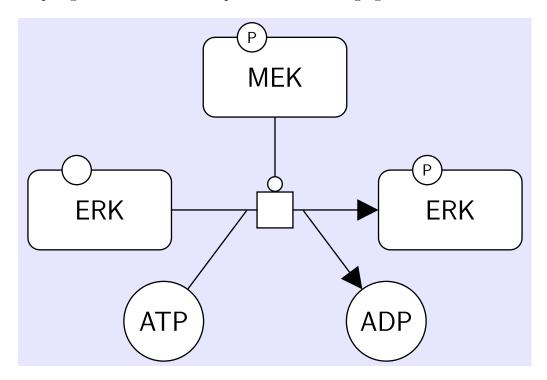
→ of its left connector

\draw[consumption] (atp) -- (p.west);
\draw[production] (p.east) -- (perk);
\draw[production] (p.east) -- (adp);
\draw[catalysis] (pmek) -- (p);
```

\end{tikzpicture}

\end{document}

Compiling the above code would produce the following figure:

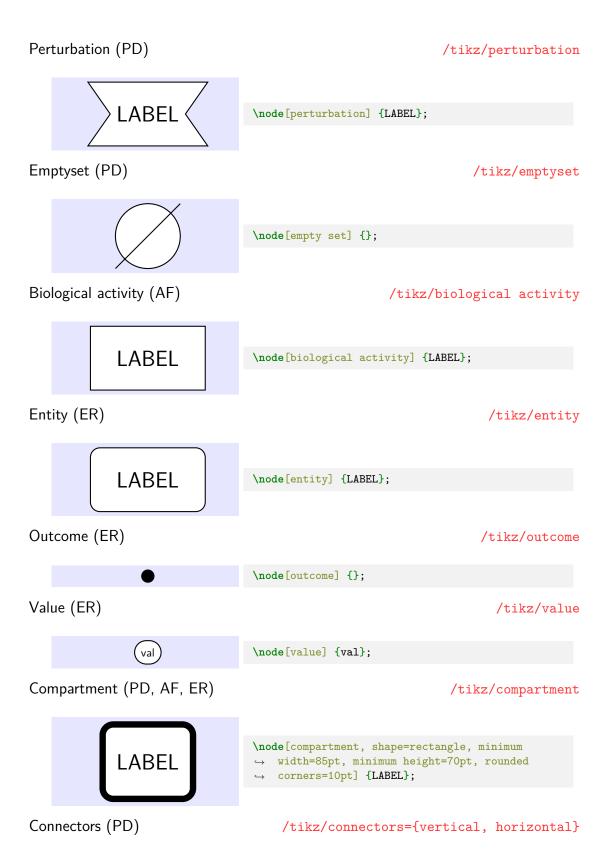


2 Drawing glyphs

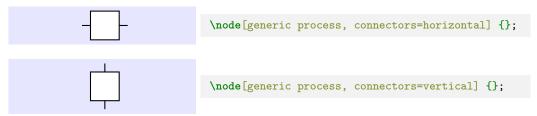
2.1 Nodes

Macromolecule (PD) /tikz/macromolecule **LABEL** \node[macromolecule] {LABEL}; Macromolecule multimer (PD) /tikz/macromolecule multimer **LABEL** \node[macromolecule multimer] {LABEL};

Nucleic acid feature (PD) /tikz/nucleic acid feature **LABEL** \node[nucleic acid feature] {LABEL}; Nucleic acid feature multimer (PD) /tikz/nucleic acid feature multimer **LABEL** \node[nucleic acid feature multimer] {LABEL}; Unspecified entity (PD) /tikz/unspecified entity **LABEL** \node[unspecified entity] {LABEL}; Simple chemical (PD) /tikz/simple chemical .ABEL \node[simple chemical] {LABEL}; Simple chemical multimer (PD) /tikz/simple chemical multimer LABEI \node[simple chemical multimer] {LABEL}; Complex (PD) /tikz/complex **LABEL** \node[complex] {LABEL}; Complex multimer (PD) /tikz/complex multimer **LABEL** \node[complex multimer] {LABEL};



Vertical or horizontal connectors can be added to process nodes and logical operators.



Cardinal anchors are set to the tip of the connectors. Other border anchors are not changed.



Connector length (PD) /tikz/{

/tikz/{left, right} connector length=<dimension>

These options allow setting the length of the connectors. left corresponds to the left and the upper connectors, and right to the right and the above connectors.

```
\node[generic process, connectors=horizontal, left

→ connector length = 20pt] {};

\node[generic process, connectors=vertical, left

→ connector length = 20pt, right connector

→ length = 5pt] {};
```

The default connector length is 10pt.

Clone (PD) /tikz/clone



Generic process (PD)

/tikz/generic process



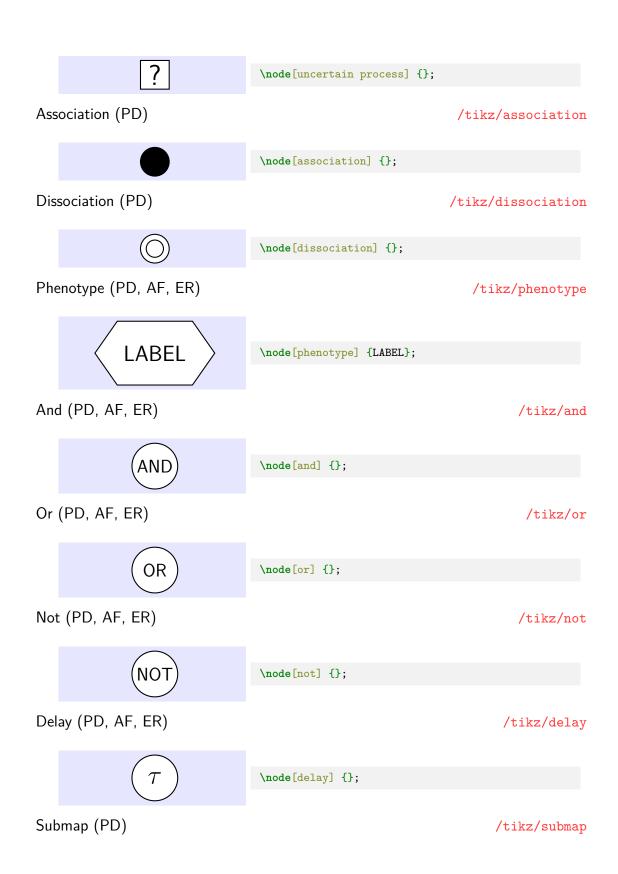
Omitted process (PD)

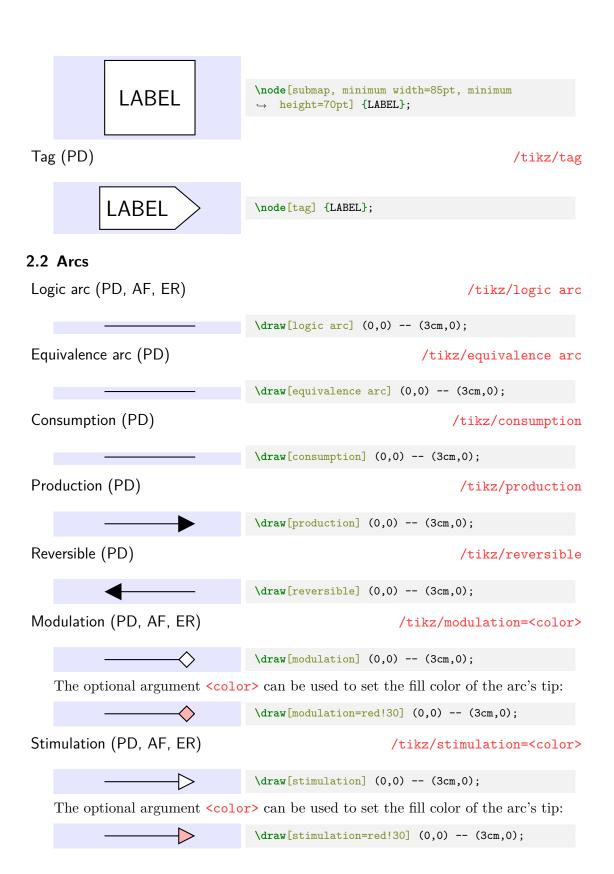
/tikz/omitted process

```
\mode[omitted process] {};
```

Uncertain process (PD)

/tikz/uncertain process





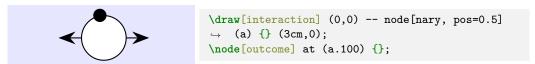
```
Necessary stimulation (PD, AF, ER)
                                             /tikz/necessary stimulation=<color>
                                    \draw[necessary stimulation] (0,0) -- (3cm,0);
   The optional argument <color> can be used to set the fill color of the arc's tip:
                                    \draw[necessary stimulation=red!30] (0,0) --
                       ₽
                                    \hookrightarrow (3cm,0);
Catalysis (PD)
                                                             /tikz/catalysis=<color>
                                    \draw[catalysis] (0,0) -- (3cm,0);
                        \odot
   The optional argument <color> can be used to set the fill color of the arc's tip:
                                    \draw[catalysis=red!30] (0,0) -- (3cm,0);
Absolute stimulation (ER)
                                               /tikz/absolute stimulation=<color>
                                    \draw[absolute stimulation] (0,0) -- (3cm,0);
   The optional argument <color> can be used to set the fill color of the arc's tip:
                                    \draw[absolute stimulation=red!30] (0,0) --
                                    \hookrightarrow (3cm,0);
Inhibition (PD, AF, ER)
                                                                     /tikz/inhibition
                                    \draw[inhibition] (0,0) -- (3cm,0);
Absolute inhibition (ER)
                                                          /tikz/absolute inhibition
                                    \draw[absolute inhibition] (0,0) -- (3cm,0);
Assignment (ER)
                                                                     /tikz/assignment
                                    \draw[assignment] (0,0) -- (3cm,0);
Implicit XOR (ER)
                                                                    /tikz/imlicit xor
                                    \node[entity] (e) {};
                                    \node[sv location] (loc) at (e.90) {};
                                    \node[value, above left = 2cm and 0.3cm of loc]
                                    \hookrightarrow (t) \{T\};
                                    \node[value, above right = 2cm and 0.3cm of loc]
                                    \hookrightarrow (f) {F};
                                    \node[implicit xor, above = 1.5cm of e] (xor) {};
                                    \draw[assignment, -{}] (t) -- (xor);
                                    \draw[assignment, -{}] (f) -- (xor);
                                    \draw[assignment] (xor) -- (loc);
```

To keep the style defined for the assignment arc while removing the arrowhead when drawing an assignment arc from a value to an implicit xor, we use the option -{}.

Interaction (ER) /tikz/interaction

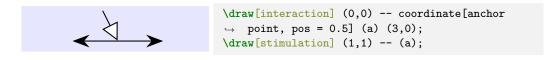
```
\draw[interaction] (0,0) -- (3cm,0);
```

N-ary interactions can be drawn using the nary node:



Anchor point (ER)

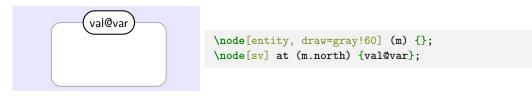
/tikz/anchor point



2.3 Nodes' and arcs' attributes

State variable (PD, ER)

/tikz/sv



Existence state variable (ER)

/tikz/sv existence



Location state variable (ER)

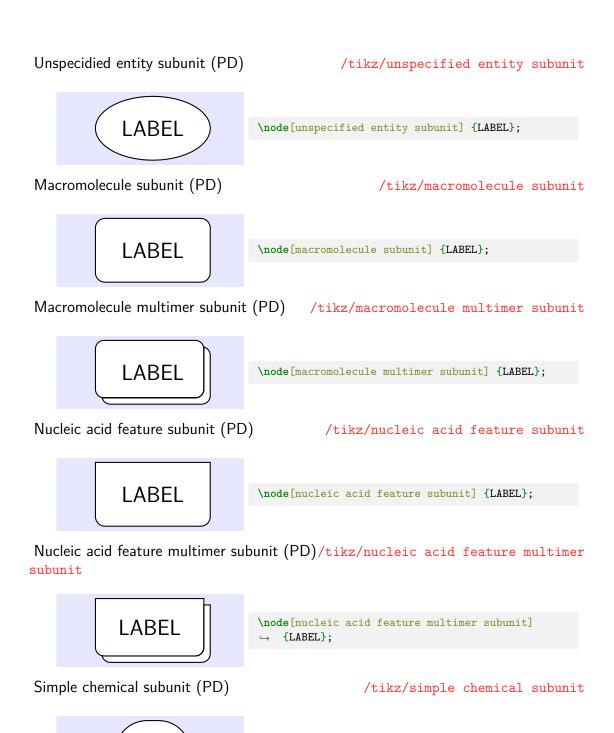
/tikz/sv location



Unit of information (PD, ER)

/tikz/ui

```
pre:label
                                  \node[entity, draw=gray!60] (m) {};
                                  \node[ui] at (m.north) {pre:label};
   In PD, stoichiometry can be drawn using a unit of information along an arc:
                                  \draw[production] (0,0) -- node[ui, above,
                 N:5
                                   \rightarrow pos=0.5] {\tiny N:5} (2cm,0);
Unit of information simple chemical (AF)
                                                         /tikz/ui simple chemical
               LABEL
                                  \node[biological activity, draw=gray!60] (m) {};
                                  \node[ui simple chemical] at (m.north) {LABEL};
Unit of information nucleic acid feature (AF)
                                                  /tikz/ui nucleic acid feature
               LABEL
                                  \node[biological activity, draw=gray!60] (m) {};
                                  \node[ui nucleic acid feature] at (m.north)
                                   Unit of information macromolecule (AF)
                                                           /tikz/ui macromolecule
               LABEL
                                  \node[biological activity, draw=gray!60] (m) {};
                                  \node[ui macromolecule] at (m.north) {LABEL};
Unit of information perturbation (AF)
                                                            /tikz/ui perturbation
              LABEL (
                                  \node[biological activity, draw=gray!60] (m) {};
                                  \node[ui perturbation] at (m.north) {LABEL};
Unit of information complex (AF)
                                                                  /tikz/ui complex
               LABEL
                                  \node[biological activity, draw=gray!60] (m) {};
                                  \node[ui complex] at (m.north) {LABEL};
```

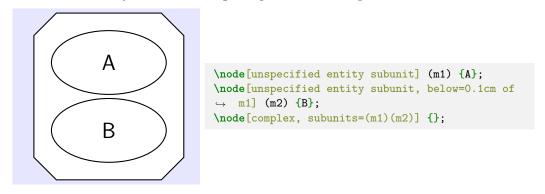


\node[simple chemical subunit] {LABEL};

Simple chemical multimer (PD) /tikz/simple chemical multimer subunit



The subunits key allows drawing complexes around specified subunits:



2.4 Layers

TikZ works with layers. By default, everything is drawn on the main layer, in the order whith which the paths to draw are declared. Adopting this default behavior within SBGNTikZ would bring some issues, for example when drawing complexes around subunits using the subunits option (the complex would be drawn on top of the subunits, masking them). Hence, SBGNTikZ defines and orders eight layers: background, compartments, nodes, arcs, subcomplexes, subunits, attributes and main (default layer). All compartments are drawn on the compartments layer, the nodes (except for narys and outcomes) on the nodes layer, the arcs on the arcs layer, the complex subunits on the subcomplexes layer, the subunits on the subunits layer, the attributes (and outcomes and narys) on the attributes, and the rest on the main layer.

One can draw a node or an arc on a specific layer using the **node layer** and **draw layer** options, respectively (big thanks to Loop Space of the tex.stackexchange.com forum for the code!).

Node on layer (PD, AF, ER)

/tikz/node layer=<layer>

```
\text{\lambda} \node[biological activity, minimum width = 0, \to minimum height = 0, align=center] {\tiny \to gene\\\tiny expression}; \node[node layer=background] \to {\tincludegraphics[scale=0.22]{images/nucleus.pdf}};

Arc on layer (PD, AF, ER)

\text{\draw[stimulation, draw layer=background] (0,-1)} \to -- (0,1); \node[biological activity] {};
```

Because SBGNTikZ uses a finite number of layers, one must be careful when drawing compartments and (sub)complexes. For example, it is by default not possible to draw a compartment inside another compartment if this latter has been drawn first. However, it is possible to achieve that by manually adding layers:

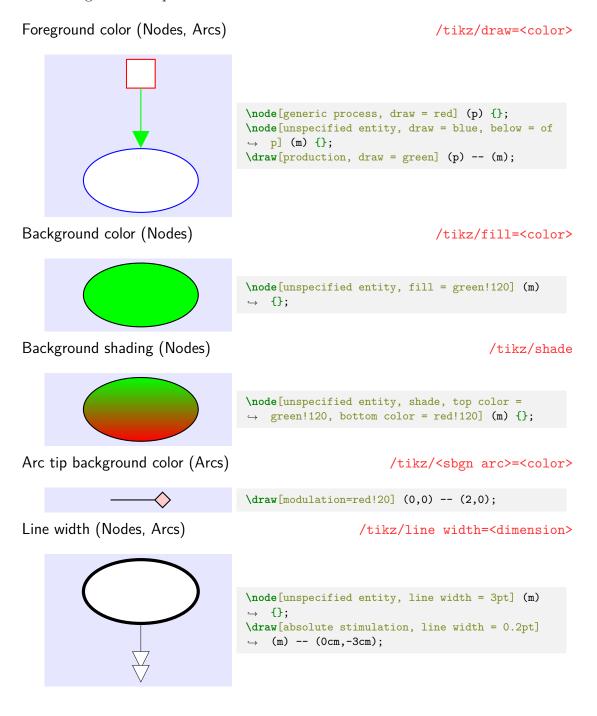
Here we added a new layer includedcompartments just after the layer compartments. Layer names should not contain any spaces. Note that we redefined the total order as it was defined previously, just adding the new layer. Missing one of the previously defined layer, or changing the order, could lead to compilation or drawing issues.

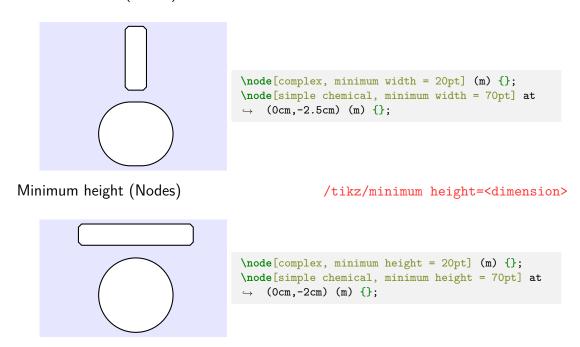
Now we can draw compartments inside other compartments, drawing the latter afterwards:

3 Customizing and drawing maps effectively

3.1 Useful options for nodes and arcs

The style of nodes and arcs (and their attributes) can be customized at will using the numerous options offered by TikZ. Following are a few options that might be useful for customizing SBGN maps.





3.2 Positioning of nodes, arcs, and their attributes

TikZ offers two ways of positioning nodes: with absolute coordinates and relatively to other nodes. We discourage using absolute coordinates as those cannot be changed easily through the drawing process. Drawing maps is far easier using relative positioning. For example, state variables can be placed using the border anchor of the entity pool node they decorate:

```
val@var

\node[macromolecule] at (0,0) (m) {};
\node[sv] at (m.140) {val@var};
```

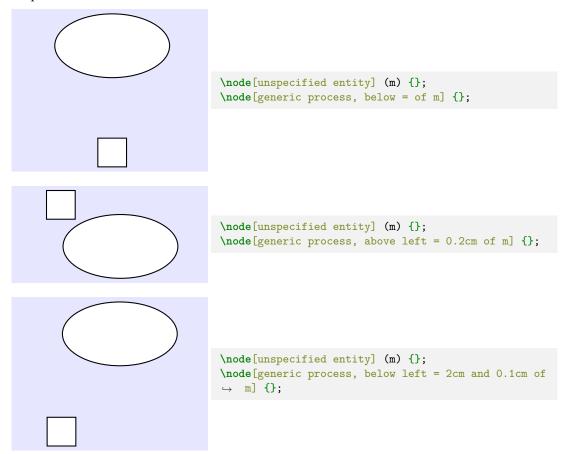
Here, we decided to place the state variable at an angle of 140° on the border of the entity pool node. Now, if we want to change the position of the entity pool node, we don't have to change the position of the state variable:

```
\node[macromolecule] at (0,2) (m) {};
\node[sv] at (m.140) {val@var};
```

Nodes can also be easily be placed relatively to other nodes using the positioning TikZ library, with the following syntax:

```
\node[<sbgn_node>, <direction> = <distance> of <node_name>] ...;
```

Here, <direction> defines in what direction the node should be place relatively to a previously defined node named <node_name>. This direction can be unitary (left, right, above, below) or composed of two values (vertical direction first, e.g. above left). The node will be placed in that direction at the distance <distance> of the border of node <node_name>. In case of a composed direction, one can define a distance for each sub-direction: <distance1> and <distance2>. If no distance is provided, the node will be placed at a distance of 1.5cm (default in sbgntikz). Following are some usage examples:



To make the node closer to the other one, a negative distance can be defined:

3.3 Bended arcs, multi-part arcs

TikZ offers a simple way to bend arcs with the following syntax:

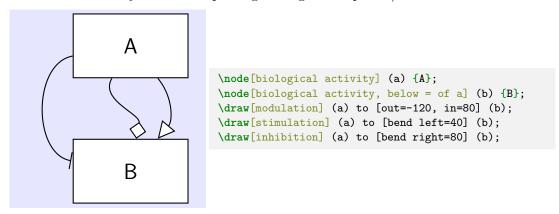
```
\draw (a) to [in=<in_angle>, out=<out_angle>] (b);
```

where <in_angle> specifies the angle at which the arc leaves the source point or node and <out_angle> the angle at which the arc arrives on the target point or node. Both angles are defined relatively to the picture's coordinate.

One can also use the following shortcut:

```
\draw (a) to [bend <direction>=<angle>] (b);
```

where <direction>={left, right} specifies the direction where to bend the arc and <angle> the angle at which the arc leaves the source point or node. The angle is this time defined relatively to the line passing through both points/nodes.



It is often necessary to break arcs into muliple parts for improved readability. TikZ offers very simple operations to break arcs into horizontal and vertical sub-parts, that replace the default -- operation. The |- operation will produce an horizontal sub-part followed by a vertical one, and the -| a vertical sub-part followed by a horizontal one. It can also be convenient to use the --+ and --++ to draw arcs with more than two sub-parts.

```
A \| \node[biological activity] (a) {A}; \| \node[biological activity, below right = 1.5cm and \| \to 0.3 cm of a.center] (b) {B}; \| \draw[stimulation] (a.240) |- (b); \| \draw[inhibition] (a) -| (b); \| \draw[modulation] (b.240) --++ (0,-1) --++ (1,0) --++ \| \to (0,1); \| \end{area}
```

3.4 Nodes along paths for ER maps

In ER maps, outcomes should be drawn along interaction or assignment arcs. TikZ provides a handy syntax to do so:

```
\\draw[interaction] (0,0) -- (3,0) node[outcome, pos = \( \to \) 0.7] (o) \{\};
```

Here, the outcome is added along the path using the node command (with no \), as if it was a normal node. The pos option allows defining the distance of the node from the source of the arc relatively to the length of the arc. Here, we placed the outcome at a distance of 70%. More than one outcome can be placed along an arc, by repeating the node syntax:

```
\draw[interaction] (0,0) -- (3,0) node[outcome, pos =

→ 0.3] (o1) {} node[outcome, pos = 0.5] (o2) {}

→ node[outcome, pos = 0.7] (o3) {};
```

One other particularity of drawing ER maps is that one might have to draw arcs targeting other arcs. This is not straightforwardly possible in TikZ, as arcs must target points or nodes. One solution provided by sbgntikz is to draw anchor point coordinates along arcs, as in the following example:

```
\draw[interaction] (0,0) -- (3,0) coordinate[anchor

→ point, pos = 0.5] (a);
\draw[stimulation] (1,1) -- (a);
```

Here, the anchor point coordinate (which is a circle with no drawing, no label and a radius of 0pt) is placed halfway along the interaction arc.

Often in ER maps, one wants to draw horizontal or vertical modulation arcs departing from outcomes. These particular cases, on the other hand, can be easily achieved using TikZ's \mid - syntax:

```
\draw[interaction] (0,0) -- (3,0);
\draw[stimulation] (1,1) -- (1,1 |- 3,0);
```

Additional space between the tip of the modulation arc and the target arc can be added (here 2pt):

```
\draw[interaction] (0,0) -- (3,0);
\draw[inhibition] (1,1) -- ($(1,1 |- 3,0)+(0,2pt)$);
```

Drawing vertical or horizontal modulation arcs can also be achieved using anchor points and TikZ's let syntax, which allows to place the anchor point at the X-coordinate (for a vertical arc) or Y-coordinate (for an horizontal arc) of the outcome. Following is an example:

In the second interaction, we define the point \p1 as being the outcome of the second interaction, and we use its X-coordinate defined as \x1 to place the anchor point. More coordinates can be defined and accessed using the let command, always using the syntax \pi and \xi,\yi:

```
\draw[interaction] (0,0) -- (3,0) node[outcome, pos =

→ 0.7] (o1) {};

\draw[interaction] (-0.7,-0.5) -- (1.9,-0.5)

→ node[outcome, pos = 0.6] (o2) {};

\draw[interaction] let \p1=(o1), \p2=(o2) in (0,-2)

→ -- (3,-2) coordinate[anchor point] (a1) at

→ (\x1,-2) coordinate[anchor point] (a2) at

→ (\x2,-2);

\draw[stimulation] (o1) -- (a1);

\draw[absolute inhibition] (o2) -- (a2);
```

4 SBGN-ML to TikZ converter

SBGNTikZ includes an SBGN-ML [3] to TikZ converter, written in Python 3.

4.1 Installation

The converter depends on Matthias König's libsbgnpy library [4] to read SBGN-ML files. This library can be installed using pip:

```
pip install libsbgnpy
```

To install the development version, please visit libsbgnpy's webpage.

4.2 Usage

By default, the converter reads an input SBGN-ML file, and outputs a TikZ picture. It's usage is as follows:

```
./sbgnml2tikz [options] INPUT FILE
```

If no option is supplied, the TikZ picture will be output as text on the terminal's STDOUT.

Options are the following:

• --tex=<OUTPUT FILE>: writes the output TikZ picture to a TeX file.

- --tex-standalone=<0UTPUT FILE>: writes the output TikZ picture to a standalone TEX file. This option necessitates the installation of the python package PyLaTeX to output the TEX file.
- --pdf=<0UTPUT FILE>: renders the output TikZ picture in a PDF file. This option necessitates the installation of the python package PyLaTeX to compile the TikZ picture into a PDF file.
- --png=<0UTPUT FILE>: renders the output TikZ picture in a PNG file. This option necessitates the installation of the python package PyLaTeX to compile the TikZ picture, and of the ImageMagick package to convert the output PDF to a PNG image.
- --no-tidy: desactivates relative positioning. Arcs and attributes are drawn using their absolute coordinates.
- --unit=<dimension unit>: the length unit to use. Default is "pt" (points). Other available units are "cm" (centimeters), "in" (inches), "px" (pixels).

References

- [1] Till Tantau. The TikZ and PGF Packages.
- [2] Nicolas Le Novere, Michael Hucka, Huaiyu Mi, Stuart Moodie, Falk Schreiber, Anatoly Sorokin, Emek Demir, Katja Wegner, Mirit I Aladjem, Sarala M Wimalaratne, et al. The systems biology graphical notation. *Nature biotechnology*, 27(8):735, 2009.
- [3] Martijn P Van Iersel, Alice C Villéger, Tobias Czauderna, Sarah E Boyd, Frank T Bergmann, Augustin Luna, Emek Demir, Anatoly Sorokin, Ugur Dogrusoz, Yukiko Matsuoka, et al. Software support for sbgn maps: Sbgn-ml and libsbgn. *Bioinformatics*, 28(15):2016–2021, 2012.
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Index

absolute inhibition, 11 absolute stimulation, 11 anchor point, 12 and, 9 arc on layer, 16 arc tip background color, 17 assignment, 11 association, 9 background color, 17 background shading, 17 biological activity, 7 catalysis, 11 clone, 8 compartment, 7 complex, 6 complex multimer, 6 complex multimer subunit, 15 connector length, 8 connectors, 7 consumption, 10 delay, 9 dissociation, 9 emptyset, 7 entity, 7 equivalence arc, 10 existence state variable, 12 foreground color, 17 generic process, 8 implicit XOR, 11 inhibition, 11 interaction, 12 line width, 17 location state variable, 12 logic arc, 10 macromolecule, 5	modulation, 10 necessary stimulation, 11 node on layer, 16 not, 9 nucleic acid feature, 6 nucleic acid feature multimer, 6 nucleic acid feature multimer subunit, 14 nucleic acid feature subunit, 14 omitted process, 8 or, 9 outcome, 7 perturbation, 7 phenotype, 9 production, 10 reversible, 10 simple chemical multimer, 6, 14 simple chemical subunit, 14 state variable, 12 stimulation, 10 submap, 9 subunits, 15 tag, 10 uncertain process, 8 unit of information, 12 unit of information complex, 13 unit of information nucleic acid feature, 13 unit of information perturbation, 13 unit of information simple chemical, 13 unspecidied entity subunit, 14 unspecified entity, 6 value, 7 bended arc, 20
macromolecule multimer, 5 macromolecule multimer subunit, 14 macromolecule subunit, 14	multi-part arc, 20
minimum height, 18 minimum width, 18	
,	