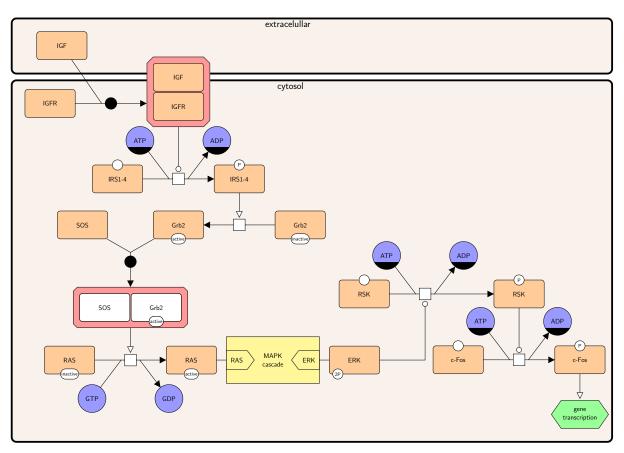
# sbgntikz

# manual for version 1.1.0

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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 Introduction

#### 1.1 About

sbgntikz is a TikZ [?] library to draw SBGN PD, AF or ER maps [?] 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 ?? references all glyphs and their associated keywords, whereas section ?? 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 ??, and might have different (and maybe better) solutions to the issues presented in section ??.

#### 1.2 Installation and usage

The directory tikz-sbgn/ should be copied to a directory where it can be found by the T<sub>E</sub>X engine:

- in the directory of your LATEX source file
- in your local texmf directory. This directory is usually /home/<user>/texmf/ under Linux, /Users/Library/texmf/ under MacOS, and C:/Users/<user>/texmf under Windows, but it can depend on your OS version and TEX distribution. Your texmf directory can be found using the kpsewhich -var-value=TEXMFHOME command.

Usually, TikZ is installed within your TEX distribution, so TikZ and sbgntikz can be imported directly into your IATEX source file with no further installation 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);
```

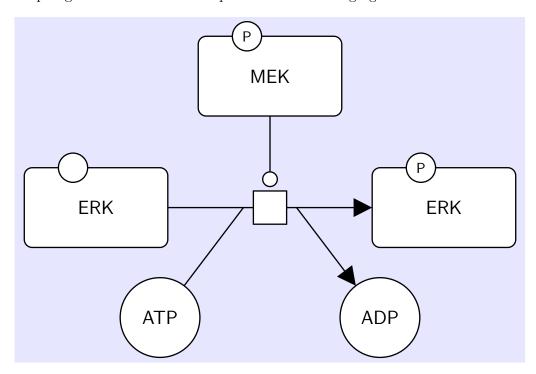
where

- <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 ?? 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
\hookrightarrow of 120 deg
\node[generic process, connectors = horizontal, right = of erk] (p) {}; % we add connectors, and
\hookrightarrow 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
\hookrightarrow \quad \textit{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}
```

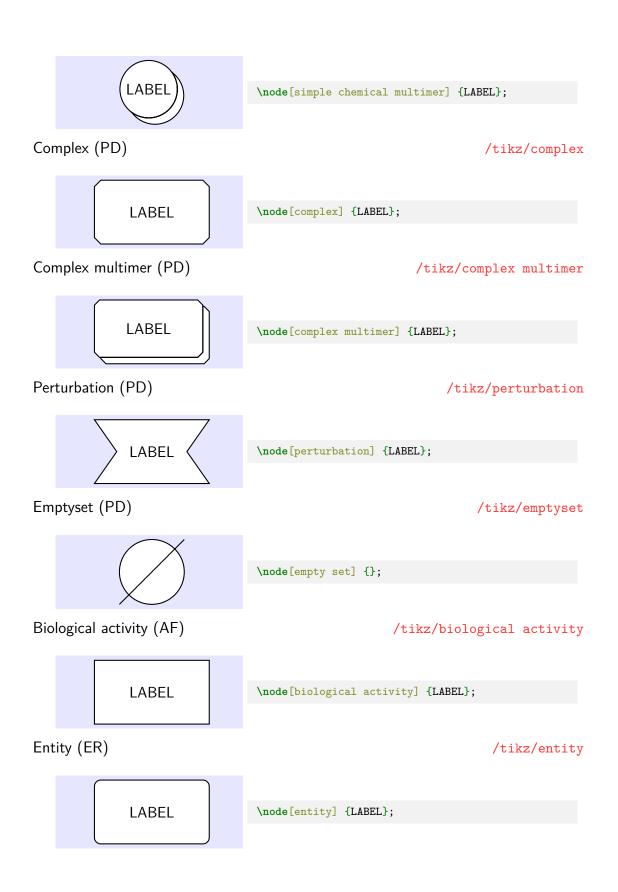
Compiling the above code would produce the following figure:



# 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 **LABEL** \node[simple chemical] {LABEL}; Simple chemical multimer (PD) /tikz/simple chemical multimer



Outcome (ER)

\[ \lambda \text{node[outcome] \{\};} \]

Value (ER)

\[ \lambda \text{value} \text{value} \]

\[ \lambda \text{node[value] \{\val\};} \]

Compartment (PD, AF, ER)

\[ \lambda \text{tikz/compartment} \]



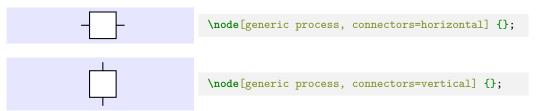
\node[compartment, shape=rectangle, minimum

 width=85pt, minimum height=70pt, rounded
 corners=10pt] {LABEL};

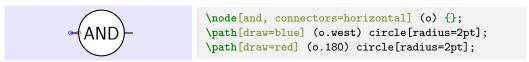
# Connectors (PD)

/tikz/connectors={vertical, horizontal}

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



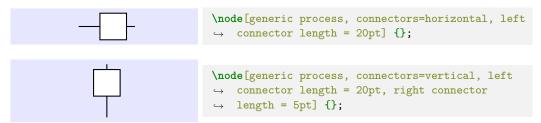
Cardinal anchors are set to the tip of the connectors. Other border anchors are not changed.



#### Connector length (PD)

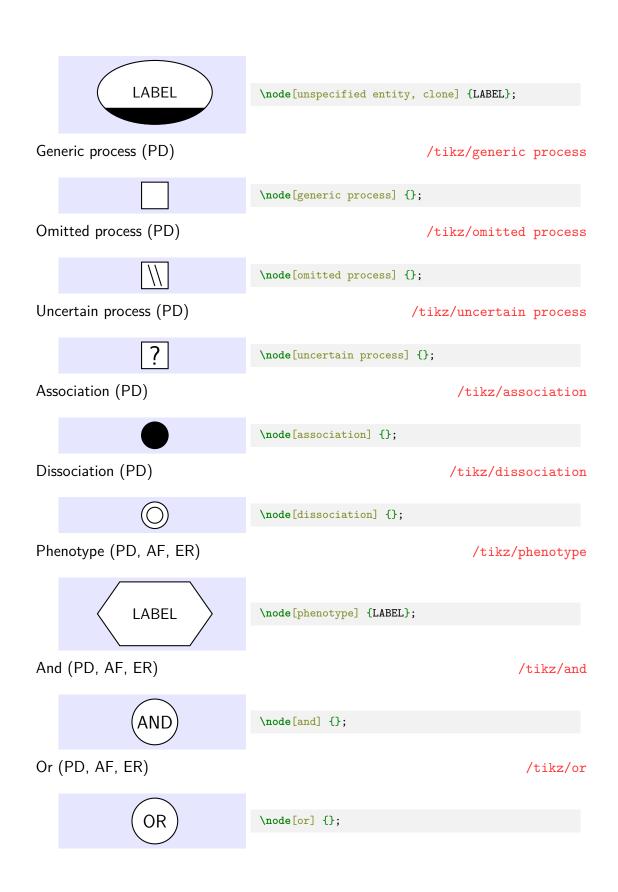
/tikz/{left, right} connector length=<dimension>

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.



The default connector length is 10pt.

Clone (PD) /tikz/clone



```
Not (PD, AF, ER)
                                                                       /tikz/not
                                 \node[not] {};
Delay (PD, AF, ER)
                                                                     /tikz/delay
                                 \node[delay] {};
Submap (PD)
                                                                    /tikz/submap
                                 \node[submap, minimum width=85pt, minimum
              LABEL
                                 → height=70pt] {LABEL};
Tag (PD)
                                                                       /tikz/tag
             LABEL
                                 \node[tag] {LABEL};
2.2 Arcs
Logic arc (PD, AF, ER)
                                                                /tikz/logic arc
                                 \draw[logic arc] (0,0) -- (3cm,0);
Equivalence arc (PD)
                                                          /tikz/equivalence arc
                                 \draw[equivalence arc] (0,0) -- (3cm,0);
Consumption (PD)
                                                              /tikz/consumption
                                 \draw[consumption] (0,0) -- (3cm,0);
Production (PD)
                                                                /tikz/production
                                 \draw[production] (0,0) -- (3cm,0);
Reversible (PD)
                                                                /tikz/reversible
```

```
\draw[reversible] (0,0) -- (3cm,0);
Modulation (PD, AF, ER)
                                                           /tikz/modulation=<color>
                                    \draw[modulation] (0,0) -- (3cm,0);
   The optional argument <color> can be used to set the fill color of the arc's tip:
                                    \draw[modulation=red!30] (0,0) -- (3cm,0);
Stimulation (PD, AF, ER)
                                                          /tikz/stimulation=<color>
                                    \draw[stimulation] (0,0) -- (3cm,0);
   The optional argument <color> can be used to set the fill color of the arc's tip:
                                    \draw[stimulation=red!30] (0,0) -- (3cm,0);
                       \triangleright
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) --
                       \downarrow \triangleright
                                    \hookrightarrow (3cm,0);
Catalysis (PD)
                                                             /tikz/catalysis=<color>
                                    \draw[catalysis] (0,0) -- (3cm,0);
   The optional argument <color> can be used to set the fill color of the arc's tip:
                        \bigcirc
                                    \draw[catalysis=red!30] (0,0) -- (3cm,0);
Absolute stimulation (ER)
                                               /tikz/absolute stimulation=<color>
                     \Rightarrow
                                    \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) --
                                       (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);
```

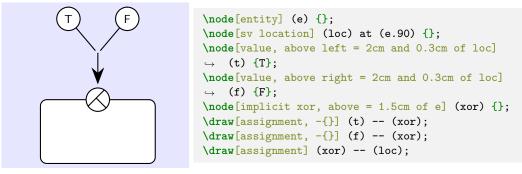
Assignment (ER)

/tikz/assignment

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

Implicit XOR (ER)

/tikz/imlicit xor



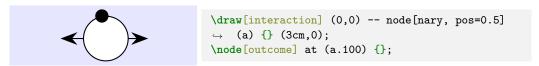
To keep the style defined for the assignment arc while removing the arrowhead when drawing an assignment arc from a value to an implicit xor, we use the option -{}.

Interaction (ER)

/tikz/interaction

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

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



Anchor point (ER)

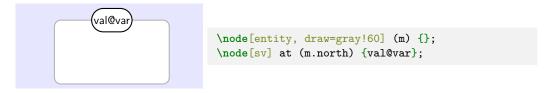
/tikz/anchor point



#### 2.3 Nodes' and arcs' attributes

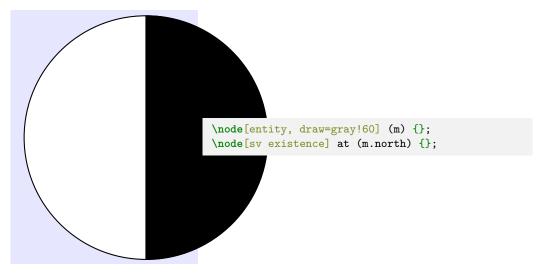
State variable (PD, ER)

/tikz/sv



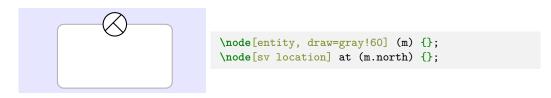
Existence state variable (ER)

/tikz/sv existence



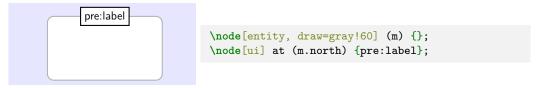
Location state variable (ER)

/tikz/sv location

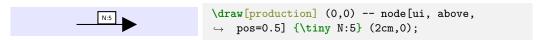


Unit of information (PD, ER)

/tikz/ui

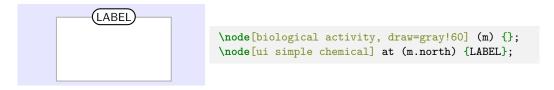


In PD, stoichiometry can be drawn using a unit of information along an arc:



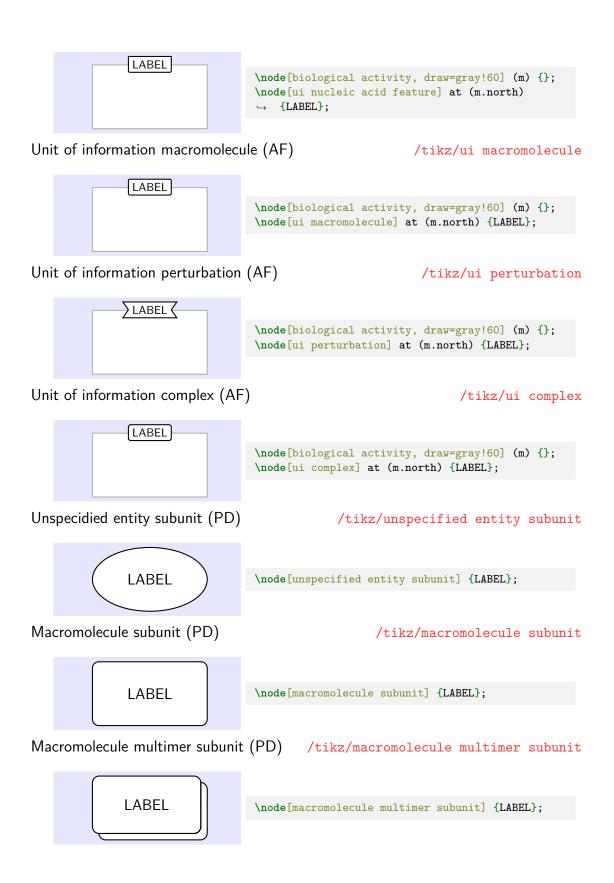
Unit of information simple chemical (AF)

/tikz/ui simple chemical



Unit of information nucleic acid feature (AF)

/tikz/ui nucleic acid feature

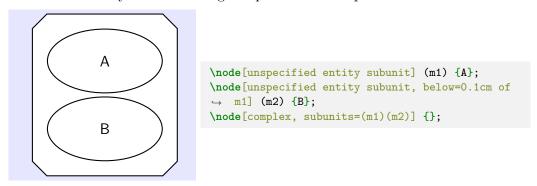


Nucleic acid feature subunit (PD) /tikz/nucleic acid feature subunit \node[nucleic acid feature subunit] {LABEL}; LABEL Nucleic acid feature multimer subunit (PD)/tikz/nucleic acid feature multimer subunit \node[nucleic acid feature multimer subunit] **LABEL** Simple chemical subunit (PD) /tikz/simple chemical subunit \node[simple chemical subunit] {LABEL}; LABEL Simple chemical multimer (PD) /tikz/simple chemical multimer subunit LABEL \node[simple chemical multimer subunit] {LABEL}; Complex subunit (PD) /tikz/complex subunit LABEL \node[complex subunit] {LABEL}; Complex multimer subunit (PD) /tikz/complex multimer subunit LABEL \node[complex multimer subunit] {LABEL};

/tikz/subunits=<(node\_1)(node\_2)..(node\_n)>

Subunits (PD)

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>

/node[biological activity, minimum width = 0,

/minimum height = 0, align=center] {\tiny

/mode[node layer=background]

/tikz/draw layer=<layer>

/tikz/draw layer=<layer>

/draw[stimulation, draw layer=background] (0,-1)

/mode[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:

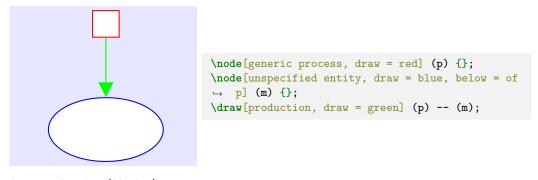
# 3 Customizing and drawing maps effectively

## 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.

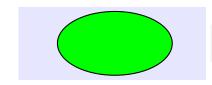
Foreground color (Nodes, Arcs)

/tikz/draw=<color>



Background color (Nodes)

/tikz/fill=<color>



Background shading (Nodes)

/tikz/shade



\node[unspecified entity, shade, top color =
 green!120, bottom color = red!120] (m) {};

Arc tip background color (Arcs)

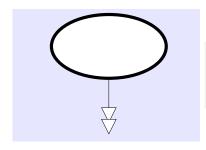
/tikz/<sbgn arc>=<color>



\draw[modulation=red!20] (0,0) -- (2,0);

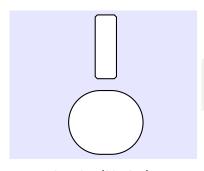
Line width (Nodes, Arcs)

/tikz/line width=<dimension>



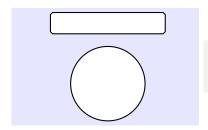
Minimum width (Nodes)

/tikz/minimum width=<dimension>



Minimum height (Nodes)

/tikz/minimum height=<dimension>



#### 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:

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

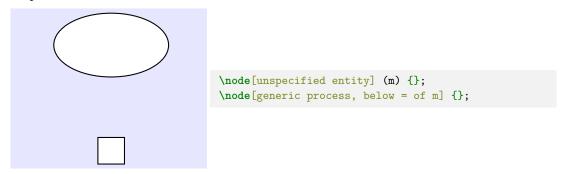
Here, we decided to place the state variable at an angle of 140° on the border of the entity pool node. Now, if we want to change the position of the entity pool node, we don't have to change the position of the state variable:

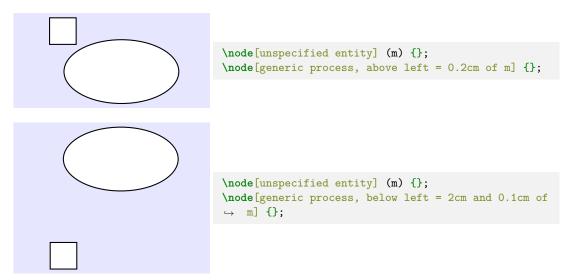
```
\node[macromolecule] at (0,2) (m) {};
\node[sv] at (m.140) {val@var};
```

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:

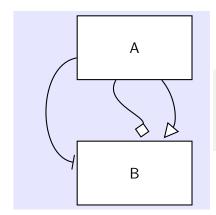
```
\draw (a) to [in=<in_angle>, out=<out_angle>] (b);
```

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:

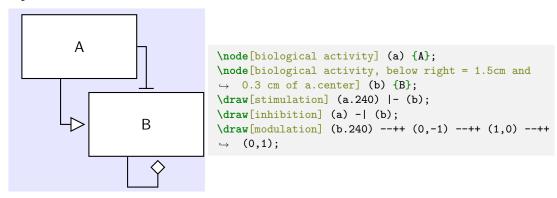
```
\draw (a) to [bend <direction>=<angle>] (b);
```

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.



```
\node[biological activity] (a) {A};
\node[biological activity, below = of a] (b) {B};
\draw[modulation] (a) to [out=-120, in=80] (b);
\draw[stimulation] (a) to [bend left=40] (b);
\draw[inhibition] (a) to [bend right=80] (b);
```

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.



#### 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] (0) \{\};
```

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 2pt) 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, that is the anchor point's default radius):

```
\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:

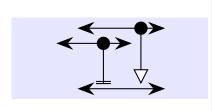
```
\draw[interaction] (0,0) -- (3,0) node[outcome, pos =

→ 0.7] (o1) {};
\draw[interaction] let \p1=(o1) in (0,-2) -- (3,-2)

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

→ node[outcome, pos = 0.3] (o2) {};
\draw[stimulation] (o1) -- (a);
```

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  $\n1$  to place the anchor point. More coordinates can be defined and accessed using the let command, always using the syntax  $\p1$  and  $\n1$ ;



```
\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 ships with an SBGN-ML [?] to TikZ converter, written in Python 3.

### 4.1 Installation

The converter depends on Matthias König's libsbgnpy library [?] 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  $\mathrm{Ti}k\mathbf{Z}$  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
- --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.
- --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).