# Diffuse meaning

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**Abstract**

Explanations about the notation conventions in chemlambda, to be used with [2] and [3]. This is part of a work in progress.

## 1 Molecules

Chemlambda is a graph rewrite system, together with an algorithm for the application of rewrites. The graphs used in chemlambda are colored ribbon graphs called "molecules".

A ribbon graph[1] is a graph where a cyclic order of the incident edges is added to each node. Imagine that edges of the graph are made by two half-edges and that nodes of the graph are identified with the collection of half edges incident to it. Then a ribbon graph may be defined as the collection of half-edges, together with two permuations, one recording the cyclic order of the half-edges incident to each node, the other being used to associate to each half-edge the complementary half-edge (i.e. the other half of the edge).

Here I use open ribbon graphs.

**Definition 1.1** *An open ribbon graph is a quadruple $(H, F, \sigma, \eta)$ where $H$ is a finite, non empty set of half-edges, $F$ is a subset of $H$ and $\sigma : H \to H$ and $\eta : H \setminus F \to H \setminus F$ are permutations such that eta is involutive (i.e. $\eta^2 = id$) and without fixed points.*

*The nodes of the open ribbon graph are the orbits of the permutation $\sigma$. The valence of a node is the number of elements of the respective orbit.*

*The edges of the ribbon graph are the orbits of the permutation $\eta$. The free half-edges of the ribbon graph are the elements of $F$.*

*The half-edges of a node are called the ports of the node. The port value of a port is:*

*- the port itself if the port is free (belongs to $F$),*

*- else is the edge where the port belongs.*

*If $G$ is the graph then $F(G) = F$ is the set of free half-edges, $E(G)$ is the set of edges, $N(G)$ is the set of nodes and $Val(G) = E(G) \cup F(G)$ is the set of port values.*

Further we shall consider only open ribbon graphs with nodes having valence equal to 1, 2, or 3. The short name "open 3-ribbon graphs" will be used for those.

Let's explain now a notion of directed open 3-ribbon graphs. Take the collection of positions:

$$Pos = \{middle, left, right\} \times \{in, out\}$$

together with the two projections $(a, b) \in Pos \mapsto \pi_1(a, b) = a$ and $(a, b) \in Pos \mapsto \pi_2(a, b) = b$.

**Definition 1.2** *A directed open 3-ribbon graph $(G, pos)$ is an open 3-ribbon graph $G = (H, F, \sigma, \eta)$ and a function $pos : H \to Pos$ with the properties:*

- *for any $h \in H \setminus F$ $\pi_2(pos(\eta(h))) \neq \pi_2(pos(h))$,*
- *for any node $N \in N(G)$ which is not 1 valent, there are two ports $h, g \in N$ such that $\pi_2(pos(h)) \neq \pi_2(pos(g))$,*
- *for any 1-valent or 2-valent node $N \in N)G)$ and for any port $h \in N$ we have $\pi_1(h) = middle$,*
- *from the previous conditions it follows that for any 3-valent node $N \in N(G)$ there are two ports $g, f \in N$ such that $\pi_2(pos(g)) = \pi_2(pos(f)$; the remaining port $h \in N$ is called the mark of the 3-valent node $N$. The mark $h$ has the property $\pi_1(h) = middle$.*
- *for any 3-valent node $N \in N(G)$ with mark $k \in N$ the following happens: if $\pi_2(pos(h)) = in$ then $pos(\sigma(h)) = (right, out)$ and $pos(\sigma^2(h)) = (left, out)$, else $pos(\sigma(h)) = (left, in)$ and $pos(\sigma^2(h)) = (right, in)$.*

*For any edge $e \in E(G)$, the source of the edge is $s(e) \in H \setminus F$ such that $\pi_2(pos(s(e))) = out$ and the target of the edge is $t(e) \in H \setminus F$ such that $\pi_2(pos(s(e))) = in$.*
*A free half-edge $h \in F(G)$ is a source if $\pi_2(pos(h)) = in$ and a sink if $\pi_2(pos(h)) = out$.*

Finally, a molecule is a directed open 3-ribbon graph with colored nodes and half-edges. Take the collection of colors

$$Col = \{R, G, Y, in, out\}$$

where $in, out$ are the same as those from the definition of the set $Pos$. We call $R$ the red color, $G$ the green color and $Y$ the yellow color.

**Definition 1.3** *A molecule $(G, pos, col)$ is a directed open 3-ribbon graph $(G, pos)$ with a function $col : N(G) \cup H \to Col$ such that:*

- *for any half-edge $h \in H$ we have $col(h) = \pi_2(pos(h))$*
- *for any 1-valent node $N \in N(G)$ let $h \in N$ be the unique port; if $col(h) = in$ then $col(N) = out$ and the node is called a FROUT (free-out node) or $col(N) = R$ and the node is called a T (terminal node), else $col(h) = out$, in which case $col(N) = in$ and the node is called a FRIN (free-in node),*
- *any 2-valent node has the color Y and is called an Arrow (arrow node),*
- *for any 3-valent node $N \in N(G)$, with mark $h \in N$, if $col(h) = in$ then either $col(N) = G$ and the node is called a FO (fanout node), or $col(N) = Y$ and the node is call a FOE (external fanout node), or $col(N) = R$ and the node is called an L (lambda node), else $col(h) = out$, in which case either $col(N) = G$ and the node is called an A (application node) or $col(N) = R$ and the node is called a FI (fanin node).*

**Remark.** In [2], [3] I use a black color for the node T and a white color for the node Arrow. They are not strictly needed, as this definition shows.

One may add supplementary nodes and half-edges to any molecule with free half-edges, so that the resulting molecule has no free half-edges. This is the reason for the existence of FRIN and FROUT nodes in the formalism.

Let $(G, pos, col)$ be a molecule with the set $F(G)$ of free half-edges nonempty. For any $h \in F(G)$:

- if $h$ is a source, i.e. $\pi_2(pos(h)) = in$ then introduce a new half-edge $h' \notin H$ and extend the permutation $\sigma$ with $\sigma(h') = h'$ which creates a new node $N$. Extend the position function with $pos(h') = (middle, out)$ and the coloring with $col(h') = out$ and $col(N) = in$, thus defining the new node as a FRIN node. Extend the permtuation $\eta$ by $\eta(h) = h'$ and $\eta(h') = h$.

- if $h$ is a sink, i.e. $\pi_2(pos(h)) = out$ then introduce a new half-edge $h' \notin H$ and extend the permutation $\sigma$ with $\sigma(h') = h'$ which creates a new node $N$. Extend the position function with $pos(h') = (middle, in)$ and the coloring with $col(h') = in$ and $col(N) = out$, thus defining the new node as a FROUT node. Extend the permutation $\eta$ by $\eta(h) = h'$ and $\eta(h') = h$.

THis is called the completion of the molecule.

## 2 Notations for molecules, decorations and triangulations

It is useful to have manageable notations for molecules, and also to have a more visual description of them. That is why I introduce the mol notation and the graph description of a molecule.

Let $(G, pos, col)$ be a molecule and $\phi : E(G) \to X$ be an injective function which associate to any edge of the molecule an unique identifier from a (big enough) set $X$ of names. Take also $\mu : N(G) \to \mathbb{N}$ be a numbering of the nodes of the molecule, i.e. an injective function from 1 to the cardinal of $N(G)$ (or from 0 to the prdecessor of the cardinal of N(G), according to the numbering convention preferred by the reader).

Let $N$ be the node with $\mu(N) = n$ and $h \in N$ any of the ports of the node. The port $h$ has a port variable $e$, which is the edge where it belongs, $h \in e$. The port $h$ is uniquely determined among the ports of $N$ by the value of $pos(h) = (u, v)$. I shall use in the next definition the notation

$$u.v \; = \; \phi(e)$$

i.e. if the position of the port $h$ is $(u, v)$ then $u.v$ denotes the name of the port variable of the port $h$.

**Definition 2.1** *We associate to the molecule (and implicitly up to the function $\phi$ and $\mu$) a list of lines, where the n-th line describes n-th node according to the numbering $\mu$. The structure of the line $n$ is the following. Each line is a list of strings separated by a separation character (say a blank).*

- *If the node $N$ is 1-valent, let $h \in N$ be it's unique port. If $col(h) = in$ and $col(N) = out$ then the line has two fields: "FROUT middle.in". If $col(h) = in$ and $col(N) = R$ then the line is: "T middle.in". If $col(h) = out$ then the line has two fields: "FRIN middle.out".*

- *If the node is 2-valent: "Arrow middle.in middle.out".*

- *If the node is 3-valent, then let $f, h, g$ be the three ports. There are two possiblities. The first is that $pos(f) = (middle, in)$, $pos(h) = (left, out)$ and $pos(g) = (right, out)$. Let $col(N)$ be the color of the node. The line which describes this node is "L middle.in left.out right.out" if $col(N) = R$, "FO middle.in left.out right.out" if $col(N) = G$, or "FOE middle.in left.out right.out" if $col(N) = Y$.*

  *The second possibility is that $pos(f) = (left, in)$, $pos(h) = (right, in)$ and $pos(g) = (middle, out)$. Let $col(N)$ be the color of the node. The line which describes this node is "A left.in right.in middle.out" if $col(N) = G$, "FI left.in right.in middle.out" if $col(N) = R$.*

*The list associated to the molecule is called a mol file.*

A mol file is therefore a finite list of lines, each line having 2, 3, or 4 fields. The color of the node is determined by the first field. The other fields contain names of port variables. A mol file has the

property that any name of a port variable can appear once or twice, not more. If the name of a port variable appears once then it correspond to a free port.

We can recover back the molecule, from the associated mol file, in the following way.

We produce an auxiliary list from the mol file, by rewriting each line of the mol file like this (the algorithm supposes that this is a mol file for a molecule, so it does not check for correctness, but such ckecks are trivial to add).

- read the line, let $s_0$, ..., $s_k$ be the fields, where $k = 1, 2$ or 3
- if $k = 1$ then: if $s_0 = FRIN$ then rewrite $s_1$ into $(s_1, middle, out)$, else rewrite $s_1$ into $(s_1, middle, in)$
- if $k = 2$ then rewrite $s_1$ into $(s_1, middle, in)$ and $s_2$ into $(s_2, middle, out)$
- if $k = 3$ then: if $s_0 = A$ or $s_0 = FI$ then rewrite $s_1$ into $(s_1, left, in)$, $s_2$ into $(s_2, right, in)$ and $s_3$ into $(s_3, middle, out)$, else rewrite $s_1$ into $(s_1, middle, in)$, $s_2$ into $(s_2, left, in)$ and $s_3$ into $(s_3, right, out)$.

The set $V(M)$ of variables of a mol file $M$ are the strings which appear in the rewriten mol file, but not in the first position in a line. This is the set of half-edges. Each variable has a first component, called name, and second and third component, called the type. The set $F$ of free half-edges is the subset of $V(M)$ of variables which have names which appear only once in the mol file. The function *pos* is the projection on the 2nd and 3rd components. This gives also the function *col* for the ports, it is left to find it for the nodes.

The permutation $\eta$ is defined by looking at the 1st and 3rd component of a half-edge: $\eta((e, a, in)) = (e, b, out)$ and $\eta(e, b, out) = (e, a, in)$, for any $e \in V(M) \setminus F$.

The permutation $\sigma$ is defined in a similar way, by noticing that each line gives an orbit of the permutation. Also the color of the nodes can be defined, easily, from the color conventions explained in definition 2.1. If the line starts with:

- FRIN, FROUT or T then $\sigma(h) = h$ where $h$ is the second field of that line in the rewritten list,
- Arrow then $\sigma(h) = g$ and $\sigma(g) = h$ where $h$ and $h$ are the other two fields of that line in the rewritten list,
- A, L, FI, FO, FOE then let f,g,h be and the next 3 fields are, in order. If the first field is A or FI then $\sigma(h) = f$, $\sigma(f) = g$ and $\sigma(g) = h$, else $\sigma(f) = h$, $\sigma(h) = g$ and $\sigma(g) = f$.

To a molecule which does not have free half-edges we can also associate a undirected graph, with nodes and edges having type, nodes being also colored. We can imagine the nodes of the graph as colored disks, where the type of the node is encoded in the radius of the disk and the color is the one of the node. Likewise, we may imagine the edges as having the thickness according to its type.

The set of nodes of this graph is the union of the half-edges and nodes. The molecule nodes have the type "main" and the color given by the function *col*. The ports have the the type "port" and the color

The set of edges of this graph is the union of two sets:

- the set of pairs of ports $(h, \eta(h))$ for any $h \in H$ with $col(h) = out$; any such pair has the type "ext".
- the set of pairs $(N, h)$ with $h$ a port of $N$, any such pair has the type "int".

Even simpler, we may associate to a molecule which does not have free half-edges a directed multigraph, with the nodes decorated with one of the names A, L, FI, FO, FOE, Arrow, FRIN, FROUT,

T. Each node has ports and the ports are connected by directed edges, where the direction is from a port with color "out" to a port with color "in". In depictions of such graphs we use the convention to represent them in the plane, such that the permutation $\sigma$ appear as the usual orientation in the trigonometric convention. Of course that these graphs are not planar, therefore the edges may intersect in such a depiction. This the convention used in [4] and [5].

## References


[1] K. Igusa, Higher Franz-Reidemeister torsion, v. 31, Amer. Math. Soc. (2002)

[2] M. Buliga, Chemlambda moves,
http://chorasimilarity.github.io/chemlambda-gui/dynamic/moves.html

[3] M. Buliga, Molecular computers,
http://chorasimilarity.github.io/chemlambda-gui/dynamic/molecular.html

[4] M. Buliga, Graphic lambda calculus. Complex Systems 22, 4 (2013), 311-360,
http://arxiv.org/abs/1305.5786

[5] M. Buliga, Chemical concrete machine,
http://arxiv.org/abs/1309.6914