Combinatorics of higher-categorical diagrams

Amar Hadzihasanovic

Tallinn University of Technology
& Quantinuum, Compositional Intelligence

Abstract. A collection of results and proofs about pasting diagrams.

Current version: 15th November 2022

Contents

Introduction

START TENTATIVE STRUCTURE

1. Constructions
   - Pasting at submolecule
   - Suspension, Gray, join
2. Special shapes
   - Simplices, globes, cubes, opetopes
   - Proof of full subcategories
   - Constructible shapes
3. Acyclicity results
   - Flow graph and topological sorts
   - Sufficient conditions
   - Low-dimensional proofs
4. Presented ω-categories
   - The ω-category of molecules
   - Sufficient conditions for freeness
5. Algebraic classes of diagrams
   - Subdivisions
   - Basic results
6. Steiner's theory
   - Definitions and comparison
7. Geometric realisation
   - Proof of CW poset, constructibility
   - Comparison with Power?

8. Computational aspects
   - Deciding isomorphism
   - Searching for subdiagrams
9. Other formalisms
   - Comparison with Street, Johnson, Forest?

Also search through Crans, Steiner–Crans, etc for other useful results?

END TENTATIVE STRUCTURE

1. Oriented graded posets

1.1. *Some basic definitions of order theory*

1.1.1 (Covering relation)**.** Let P be a finite poset with order relation $\leq$. Given elements $x, y \in P$, we say that y *covers* x if $x < y$ and, for all $y' \in X$, if $x < y' \leq y$ then $y' = y$.

1.1.2 (Hasse diagram)**.** Let P be a finite poset. The *Hasse diagram* of P is the directed acyclic graph $\mathscr{H}P$ whose

- set of vertices is the underlying set of P, and
- for all vertices x, y, there is an edge from y to x if and only if y covers x.

1.1.3 (Closure of a subset)**.** Let P be a poset and $U \subseteq P$. The *closure of* U is the subset $\mathrm{cl}\, U \coloneqq \{x \in P \mid \exists y \in U\, x \leq y\}$.

1.1.4 (Closed subset)**.** Let U be a subset of a poset. We say that U is *closed* if $U = \mathrm{cl}\, U$.

Lemma 1.1.5 — *Let U, V be subsets of a poset. If $U \subseteq V$ then $\mathrm{cl}\, U \subseteq \mathrm{cl}\, V$. In particular, if $U \subseteq V$ and V is closed then $\mathrm{cl}\, U \subseteq V$.*

Proof. Let $x \in \mathrm{cl}\, U$. Then there exists $y \in U$ such that $x \leq y$. Since $U \subseteq V$, $y \in V$. It follows that $x \in \mathrm{cl}\, V$. ∎

Lemma 1.1.6 — *Let $(U_i)_{i \in I}$ be a family of subsets of a poset. Then*

$$\mathrm{cl} \bigcup_{i \in I} U_i = \bigcup_{i \in I} \mathrm{cl}\, U_i.$$

In particular, if all the U_i are closed, so is their union.

Proof. Straightforward. ∎

1.1.7 (Maximal element)**.** Let U be a closed subset of a poset, and $x \in U$. We say that x is *maximal in* U if it is not covered by any element in U. We write $\mathscr{M}\!ax\, U$ for the set of maximal elements in U.

Lemma 1.1.8 — *Let U be a finite closed subset of a poset. Then U is the closure of its set of maximal elements, that is, $U = \mathrm{cl}\, \mathscr{M}\!ax\, U$.*

Proof. Since $\mathscr{M}\!ax\, U \subseteq U$, by Lemma 1.1.5 we have $\mathrm{cl}\, \mathscr{M}\!ax\, U \subseteq \mathrm{cl}\, U = U$.

Conversely, let $x \in U$. We construct a sequence of elements $x_i \in U$ such that $i < j$ implies $x_i < x_j$. Let $x_0 := x$. For each $i \geq 0$, if x_i is maximal in U, then stop. Otherwise, pick an element x_{i+1} in U such that x_{i+1} covers x_i. Since U is finite, this procedure must stop at some finite n. Then $x \leq x_n$ and x_n is maximal in U, so $x \in \mathrm{cl}\, \mathscr{M}\!ax\, U$. ∎

1.1.9 (Graded poset)**.** Let P be a finite poset. We say that P is *graded* if, for all $x \in P$, all maximal paths starting from x in $\mathscr{H}P$ have the same length.

1.1.10 (Dimension of an element)**.** Let P be a graded poset and $x \in P$. The *dimension* of x is the length $\dim x$ of a maximal path starting from x in $\mathscr{H}P$.

Comment 1.1.11. The dimension is also known as the *rank* or *degree* of an element.

Lemma 1.1.12 — *Let P be a graded poset and $x, y \in P$. If $x \leq y$, then* $\dim x \leq \dim y$.

Proof. Take a maximal path starting from x in $\mathscr{H}P$. Since $x \leq y$, there is a path going from y to x in $\mathscr{H}P$. Concatenating the two paths gives a maximal path from y, whose length is greater than the length of the path from x. ∎

1.1.13 (Grading of a subset)**.** Let U be a subset of a graded poset. For each $n \in \mathbb{N}$, we write $U_n := \{x \in U \mid \dim x = n\}$. We have $U = \bigcup_{n \in \mathbb{N}} U_n$.

1.1.14 (Dimension of a subset)**.** Let U be a closed subset of a graded poset. The *dimension* of U is the integer

$$\dim U := \begin{cases} \max\{\dim x \mid x \in U\} & \text{if } U \text{ is non-empty,} \\ -1 & \text{if } U \text{ is empty.} \end{cases}$$

Remark 1.1.15. In particular, $\dim \mathrm{cl}\, \{x\} = \dim x$.

1.1.16 (Codimension of an element)**.** Let U be a closed subset of a graded poset. The *codimension* of x in U is the integer $\mathrm{codim}_U(x) := \dim U - \dim x$.

1.1.17 (Pure subset)**.** Let U be a closed subset of a graded poset. We say that U is *pure* if all the maximal elements of U have dimension $\dim U$, that is, $\mathscr{M}\!ax\, U = (\mathscr{M}\!ax\, U)_{\dim U}$.

1.2. Orientation and boundaries

1.2.1 (Orientation on a graded poset)**.** Let P be a graded poset. An *orientation* on P is an edge-labelling of $\mathscr{H}P$ with values in $\{+,-\}$.

Comment 1.2.2. We will use $\alpha, \beta, \ldots$ for variables ranging over $\{+,-\}$. We let $-\alpha$ be $-$ if $\alpha = +$ and $+$ if $\alpha = -$.

1.2.3 (Oriented graded poset)**.** An *oriented graded poset* is a graded poset P together with an orientation on P.

Remark 1.2.4. Every closed subset of an oriented graded poset inherits by restriction a structure of oriented graded poset.

1.2.5 (Faces and cofaces)**.** Let P be an oriented graded poset and $x \in P$. The set of *input faces* of x is

$$\Delta^- x := \{y \in P \mid x \text{ covers } y \text{ with orientation } -\}$$

and the set of *output faces* of x is

$$\Delta^+ x := \{y \in P \mid x \text{ covers } y \text{ with orientation } +\}.$$

Dually, the set of *input cofaces* of x is

$$\nabla^- x := \{y \in P \mid y \text{ covers } x \text{ with orientation } -\}$$

and the set of *output cofaces* of x is

$$\nabla^+ x := \{y \in P \mid y \text{ covers } x \text{ with orientation } +\}.$$

1.2.6 (Input and output boundaries)**.** Let U be a closed subset of an oriented graded poset. For all $\alpha \in \{+,-\}$ and $n \in \mathbb{N}$, let

$$\Delta^\alpha_n U := \{x \in U_n \mid \nabla^{-\alpha} x \cap U = \varnothing\}.$$

For each $n \in \mathbb{N}$, the *input n-boundary* of U is the closed subset

$$\partial^-_n U := \mathrm{cl}\,(\Delta^-_n U) \cup \bigcup_{k<n} \mathrm{cl}\,(\mathscr{M}ax\, U)_k$$

and the *output n-boundary* of U is the closed subset

$$\partial^+_n U := \mathrm{cl}\,(\Delta^+_n U) \cup \bigcup_{k<n} \mathrm{cl}\,(\mathscr{M}ax\, U)_k.$$

We omit the subscript when $n = \dim U - 1$ and let $\partial^\alpha_{-1} U = \partial^\alpha_{-2} U := \varnothing$.

1.2.7. We will use the following notations, for x an element in an oriented graded poset, U a closed subset, $n \in \mathbb{N}$, and $\alpha \in \{+,-\}$:

$$\partial_n^\alpha x \coloneqq \partial_n^\alpha \mathrm{cl}\,\{x\}, \qquad \partial_n U \coloneqq \partial_n^- U \cup \partial_n^+ U, \qquad \Delta_n U \coloneqq \Delta_n^- U \cup \Delta_n^+ U.$$

Remark 1.2.8. We have already that $\Delta^\alpha x = \Delta^\alpha \mathrm{cl}\,\{x\}$.

Lemma 1.2.9 — *Let U be a closed subset of an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+,-\}$. Then* $\dim \partial_n^\alpha U \leq n$.

Proof. Let $x \in \partial_n^\alpha U$. By definition there exists y such that $x \leq y$ and either $y \in \Delta_n^\alpha U$, so $\dim y = n$, or $y \in (\mathscr{M}ax\, U)_k$, and $\dim y = k < n$. In either case, by Lemma 1.1.12, $\dim x \leq \dim y \leq n$. ∎

Lemma 1.2.10 — *Let U be a closed subset of an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+,-\}$. Then*

1. $(\partial_n^\alpha U)_n = \Delta_n^\alpha U$,
2. $(\mathscr{M}ax\,(\partial_n^\alpha U))_k = (\mathscr{M}ax\, U)_k$ *for all* $k < n$.

Proof. Let $x \in \partial_n^\alpha U$. Then by definition there exists y such that $x \leq y$ and either $y \in \Delta_n^\alpha U$ or $y \in (\mathscr{M}ax\, U)_k$ for some $k < n$. If x is maximal, necessarily $x = y$, and we obtain one inclusion. The converse inclusions are evident. ∎

Lemma 1.2.11 — *Let U be a closed subset in an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+,-\}$. Then*

1. $(\mathscr{M}ax\, U)_n = \Delta_n^+ U \cap \Delta_n^- U$,
2. *if* $n = \dim U$ *then* $(\mathscr{M}ax\, U)_n = \Delta_n^\alpha U = U_n$.

Proof. Let $x \in U$, $\dim x = n$. Then x is maximal if and only if it has no cofaces in U, if and only if $\nabla^{-\alpha} x \cap U = \nabla^\alpha x \cap U = \varnothing$, if and only if $x \in \Delta_n^+ U \cap \Delta_n^- U$. If $n = \dim U$, then every element of U_n is maximal in U, so

$$U_n = (\mathscr{M}ax\, U)_n \subseteq \Delta_n^\alpha U \subseteq U_n$$

using the first part of the proof, and we conclude that they are all equal. ∎

Lemma 1.2.12 — *Let U be a closed subset of an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+,-\}$. Then*

1. $\partial_n^\alpha U \subseteq U$,
2. $\partial_n^\alpha U = U$ *if and only if* $n \geq \dim U$.

Proof. By definition, $\Delta_n^\alpha U \subseteq U$ and $(\mathscr{M}ax\, U)_k \subseteq U$ for all $k < n$. Because U is closed, by Lemma 1.1.5 it also contains their closures. This proves that $\partial_n^\alpha U \subseteq U$.

Suppose $n < \dim U$. By Lemma 1.2.9, $\dim \partial_n^\alpha U \leq n < \dim U$, so $U \neq \partial_n^\alpha U$. Conversely, suppose $n \geq \dim U$. By Lemma 1.1.8 and Lemma 1.1.6,

$$U = \mathrm{cl}\, \mathscr{M}ax\, U = \bigcup_{k \leq \dim U} \mathrm{cl}\, (\mathscr{M}ax\, U)_k.$$

If $n > \dim U$, this is included in (hence equal to) $\partial_n^\alpha U$. If $n = \dim U$, we use Lemma 1.2.11 to rewrite this as

$$\mathrm{cl}\, (\Delta_n^\alpha U) \cup \bigcup_{k<n} \mathrm{cl}\, (\mathscr{M}ax\, U)_k,$$

which is equal to $\partial_n^\alpha U$. ∎

Corollary 1.2.13 — *Let U be a non-empty closed subset of an oriented graded poset. Then*

$$\dim U = \min\{n \in \mathbb{N} \mid \partial_n^+ U = \partial_n^- U = U\}.$$

Lemma 1.2.14 — *Let U, V be closed subsets of an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+, -\}$. Then*

1. $\mathscr{M}ax\, (U \cup V) = (\mathscr{M}ax\, U \cap \mathscr{M}ax\, V) + (\mathscr{M}ax\, U \setminus V) + (\mathscr{M}ax\, V \setminus U)$,
2. $\Delta_n^\alpha (U \cup V) = (\Delta_n^\alpha U \cap \Delta_n^\alpha V) + (\Delta_n^\alpha U \setminus V) + (\Delta_n^\alpha V \setminus U)$.

Proof. Follows straightforwardly from the definitions using the decomposition $U \cup V = (U \cap V) + (U \setminus V) + (V \setminus U)$. ∎

Corollary 1.2.15 — *Let U, V be closed subsets of an oriented graded poset, $n \in \mathbb{N}$, and $\alpha \in \{+, -\}$. Then $\partial_n^\alpha (U \cup V) \subseteq \partial_n^\alpha U \cup \partial_n^\alpha V$.*

1.3. Maps of oriented graded posets

1.3.1 (Map of oriented graded posets)**.** Let P, Q be oriented graded posets. A *map* $f \colon P \to Q$ is a function of their underlying sets that satisfies

$$f(\partial_n^\alpha x) = \partial_n^\alpha f(x) \tag{1.1}$$

for all $x \in P$, $n \in \mathbb{N}$, and $\alpha \in \{+, -\}$.

Lemma 1.3.2 — *Let $f \colon P \to Q$ be a map of oriented graded posets. Then*

1. *f is closed, that is, if $U \subseteq P$ is closed, then $f(U) \subseteq Q$ is closed;*

2. *f is order-preserving, that is, if $x \leq y$ then $f(x) \leq f(y)$;*
3. *f does not increase dimension, that is,* $\dim f(x) \leq \dim x$ *for all $x \in P$.*

Proof. Let $x \in P$, and fix $m \geq \max\{\dim x, \dim f(x)\}$. By Lemma 1.2.12, for all $\alpha \in \{+, -\}$,

$$\mathrm{cl}\,\{f(x)\} = \partial_m^\alpha f(x) = f(\partial_m^\alpha x) = f(\mathrm{cl}\,\{x\}).$$

Since every closed subset U is a union of subsets of the form $\mathrm{cl}\,\{x\}$, and the image of a union is the union of the images, we conclude that f is closed. Since $y \leq x$ if and only if $y \in \mathrm{cl}\,\{x\}$, this also implies that f is order-preserving.

Finally, if $\dim x = n$, then for all $\alpha \in \{+, -\}$

$$\partial_n^\alpha f(x) = f(\partial_n^\alpha x) = f(\mathrm{cl}\,\{x\}) = \mathrm{cl}\,\{f(x)\},$$

and from Corollary 1.2.13 we deduce that $\dim f(x) \leq n$. ∎

1.3.3 (Inclusion of oriented graded posets)**.** An *inclusion* is an injective map of oriented graded posets.

Lemma 1.3.4 — *Let $\imath \colon P \hookrightarrow Q$ be an inclusion of oriented graded posets. Then*

1. *$\imath$ is order-reflecting, that is, if $\imath(x) \leq \imath(y)$, then $x \leq y$;*
2. *$\imath$ preserves dimensions, that is,* $\dim \imath(x) = \dim x$ *for all $x \in P$;*
3. *$\imath$ preserves the covering relation and orientations, that is, if y covers x in P with orientation α, then $\imath(y)$ covers $\imath(x)$ in Q with orientation α.*

Proof. Let $x, y \in P$ be such that $\imath(x) \leq \imath(y)$ in Q. Then $\imath(x) \in \mathrm{cl}\,\{\imath(y)\}$ which is equal to $\imath(\mathrm{cl}\,\{y\})$, so there exists $x' \leq y$ in P such that $\imath(x) = \imath(x')$. Because $\imath$ is injective, $x = x'$, so $x \leq y$.

Suppose y covers x. Then $\imath(x) < \imath(y)$. If $\imath(x) < z' \leq \imath(y)$, since $\imath$ is closed, $z' = \imath(z)$ for some $z \in P$, and because $\imath$ is order-reflecting, $x < z \leq y$. It follows that $z = y$, hence $z' = \imath(y)$, so $\imath(y)$ covers $\imath(x)$. This proves that $\imath$ preserves the covering relation. In particular, $\imath$ takes a path of length n from x in $\mathscr{H}P$ to a path of length n from $\imath(x)$ in $\mathscr{H}Q$. Since $\imath$ does not increase dimensions, it must preserve them.

Finally, suppose y covers x with orientation α. Then $x \in \Delta^\alpha y \subseteq \partial^\alpha y$, so $\imath(x) \in \partial^\alpha \imath(y)$. Because $\imath$ preserves dimensions, this is only possible if $\imath(x) \in \Delta^\alpha \imath(y)$, that is, if $\imath(y)$ covers $\imath(x)$ with orientation α. ∎

Corollary 1.3.5 — *Let $\imath \colon P \hookrightarrow Q$ be an inclusion of oriented graded posets and $U \subseteq P$ a closed subset. For all $n \in \mathbb{N}$ and $\alpha \in \{+, -\}$, the restriction of $\imath$ to $\partial_n^\alpha U$ is an isomorphism with image $\partial_n^\alpha \imath(U)$.*

1.3.6. There is a category **ogPos** whose objects are oriented graded posets and morphisms are maps of oriented graded posets. Let **Pos** be the category of posets and order-preserving maps. Lemma 1.3.2 implies that forgetting the orientation determines a functor

$$\mathsf{U}\colon \mathbf{ogPos} \to \mathbf{Pos}.$$

In addition, Lemma 1.3.4 implies that the underlying map of an inclusion is a closed embedding of posets, that is, a closed map that is both order-preserving and order-reflecting.

Proposition 1.3.7 — *The category* **ogPos** *has*

1. *a terminal object* 1,
2. *an initial object* $\varnothing$,
3. *pushouts of inclusions,*

all created by the forgetful functor to **Pos**.

Proof. All of these limits and colimits exist in **Pos**, so we only need to show that they can be lifted to **ogPos**.

The terminal poset is the poset with a single element, and the initial poset is the empty poset. Both of them admit a unique orientation. Let P be an oriented graded poset. Both the unique map from $\mathsf{U}P$ to the terminal poset and the unique map from the initial poset trivially satisfy (1.1), so they lift to maps of oriented graded posets.

Let $\imath_1\colon Q \hookrightarrow P_1$ and $\imath_2\colon Q \hookrightarrow P_2$ be inclusions of oriented graded posets. Computing their pushout in **Pos** determines two order-preserving maps

$$\jmath_1\colon \mathsf{U}P_1 \to \mathsf{U}P_1 \cup \mathsf{U}P_2, \qquad \jmath_2\colon \mathsf{U}P_2 \to \mathsf{U}P_1 \cup \mathsf{U}P_2.$$

Since $\mathsf{U}\imath_1$ and $\mathsf{U}\imath_2$ are closed embeddings, it is an exercise to show that $\jmath_1$ and $\jmath_2$ are also closed embeddings, and deduce that $\mathsf{U}P_1 \cup \mathsf{U}P_2$ is a graded poset. Since $\jmath_1$ and $\jmath_2$ preserve the covering relation and are jointly surjective, we can put a unique orientation on $\mathsf{U}P_1 \cup \mathsf{U}P_2$ in such a way that $\jmath_1$ and $\jmath_2$ both preserve orientations; overlaps are resolved by the fact that $(\mathsf{U}\imath_1);\jmath_1 = (\mathsf{U}\imath_2);\jmath_2$ and $\imath_1$ and $\imath_2$ preserve orientations. This choice of orientation determines a unique lift of the pushout to **ogPos**. ■

Corollary 1.3.8 — *Every oriented graded poset P is the colimit of the diagram of inclusions*

$$\mathsf{U}P \to \mathbf{ogPos}, \qquad (x \leq y) \mapsto (\mathrm{cl}\,\{x\} \hookrightarrow \mathrm{cl}\,\{y\}).$$

Proof. This is true of the underlying posets, and the colimit can be constructed with pushouts and the initial object. ∎

Proposition 1.3.9 — *Every map $f\colon P \to Q$ of oriented graded posets factors as a surjective map $P \twoheadrightarrow \widehat{P}$ followed by an inclusion $\widehat{P} \hookrightarrow Q$. This factorisation is unique up to isomorphism.*

Proof. The underlying map of posets admits an essentially unique factorisation as a surjective map followed by a closed embedding. Given a closed embedding $\widehat{P} \hookrightarrow Q$, there is a unique orientation on $\widehat{P}$ which makes it an inclusion of oriented graded posets. Thus the factorisation lifts uniquely to **ogPos**. ∎

2. Regular molecules

2.1. Pastings and globularity

2.1.1 (Pasting construction)**.** Let U, V be oriented graded posets, $k \in \mathbb{N}$, and let $\varphi\colon \partial_k^+ U \overset{\sim}{\hookrightarrow} \partial_k^- V$ be an isomorphism. The *pasting of U and V at the k-boundary along φ* is the oriented graded poset $U \#_k^\varphi V$ obtained as the pushout

$$\begin{tikzcd}
\partial_k^+ U \arrow[r, hook, "\varphi"] \arrow[d, hook] & \partial_k^- V \arrow[r, hook] & V \arrow[d, hook] \\
U \arrow[rr, hook] & & U \#_k^\varphi V \arrow[ul, phantom, "\ulcorner", very near start]
\end{tikzcd}$$

in **ogPos**.

Comment 2.1.2. By Corollary 1.3.5, we can identify U and V with their isomorphic images in the pasting, in such a way that $U \#_k^\varphi V$ splits as $U \cup V$ with $U \cap V = \partial_k^+ U = \partial_k^- V$. We will regularly make such an identification.

Lemma 2.1.3 — *Let U, V be oriented graded posets, $k \in \mathbb{N}$, and suppose $U \#_k^\varphi V$ is defined. Then*

1. $\partial_k^-(U \#_k^\varphi V) = \partial_k^- U$,
2. $\partial_k^+(U \#_k^\varphi V) = \partial_k^+ V$.

Proof. Since $\partial_k^- V = U \cap V \subseteq U$, we have $\Delta_k^- V \subseteq U$ and $(\mathscr{M}ax\, V)_j \subseteq U$ for all $j < k$. It follows from Lemma 1.2.14 that

$$(\mathscr{M}ax\,(U \cup V))_j \subseteq (\mathscr{M}ax\, U)_j, \qquad \Delta_k^-(U \cup V) \subseteq \Delta_k^- U,$$

so $\partial_k^-(U \cup V) \subseteq \partial_k^- U$.

Conversely, suppose $x \in \partial_k^- U$. Then there exists y such that $x \leq y$ and $y \in \Delta_k^- U$ or $y \in (\mathscr{M}ax\, U)_j$ for some $j < k$.

Suppose that $y \in \Delta_k^- U$. If $y \notin V$ then $y \in \Delta_k^-(U \cup V)$ by Lemma 1.2.14. If $y \in V$ then $y \in (U \cap V)_k$ which by Lemma 1.2.10 is equal to $\Delta_k^- V$. It follows that $y \in \Delta_k^- U \cap \Delta_k^- V$, and by Lemma 1.2.14 $y \in \Delta_k^-(U \cup V)$.

Suppose that $y \in (\mathscr{M}ax\, U)_j$ with $j < k$. By Lemma 1.2.10,

$$(\mathscr{M}ax\, U)_j = (\mathscr{M}ax\,(\partial_k^+ U))_j = (\mathscr{M}ax\,(\partial_k^- V))_j = (\mathscr{M}ax\, V)_j,$$

and by Lemma 1.2.14 $y \in (\mathscr{M}ax\,(U \cup V))_j$. In either case $x, y \in \partial_k^-(U \cup V)$, so $\partial_k^-(U \cup V) = \partial_k^- U$. The proof that $\partial_k^+(U \cup V) = \partial_k^+ V$ is dual. ∎

2.1.4 (Globularity)**.** Let U be an oriented graded poset. We say that U is *globular* if, for all $k, n \in \mathbb{N}$ and $\alpha, \beta \in \{+, -\}$, if $k < n$ then

$$\partial_k^\alpha(\partial_n^\beta U) = \partial_k^\alpha U.$$

Remark 2.1.5. By Lemma 1.2.12, this equation is only non-trivial when $n < \dim U$.

Lemma 2.1.6 — *Let U be a globular oriented graded poset, $n \in \mathbb{N}$, and $\beta \in \{+, -\}$. Then $\partial_n^\alpha U$ is globular.*

Proof. Let $k < m$ be natural numbers and $\alpha, \gamma \in \{+, -\}$. If $m < n$, using globularity of U twice,

$$\partial_k^\alpha(\partial_m^\gamma(\partial_n^\beta U)) = \partial_k^\alpha(\partial_m^\gamma U) = \partial_k^\alpha U = \partial_k^\alpha(\partial_n^\beta U).$$

If $m \geq n$, by Lemma 1.2.12 we have $\partial_m^\gamma(\partial_n^\beta U) = \partial_n^\beta U$, so

$$\partial_k^\alpha(\partial_m^\gamma(\partial_n^\beta U)) = \partial_k^\alpha(\partial_n^\beta U).$$ ∎

Lemma 2.1.7 — *Let U, V be globular oriented graded posets, $k \in \mathbb{N}$, and suppose $U \#_k^\varphi V$ is defined. For all $j < k$ and $\alpha \in \{+, -\}$,*

$$\partial_j^\alpha U = \partial_j^\alpha V = \partial_j^\alpha(U \#_k^\varphi V).$$

Proof. The first equality follows from globularity by

$$\partial_j^\alpha U = \partial_j^\alpha(\partial_k^+ U) = \partial_j^\alpha(\partial_k^- V) = \partial_j^\alpha V.$$

From Corollary 1.2.15, we also have $\partial_j^\alpha(U \cup V) \subseteq \partial_j^\alpha U = \partial_j^\alpha V$, so it suffices to prove the converse inclusion.

Let $x \in \partial_j^\alpha U$. Then there exists y such that $x \leq y$ and $y \in \Delta_j^\alpha U$ or $y \in (\mathscr{M}ax\, U)_\ell$ for some $\ell < j$. Using Lemma 1.2.10 together with the fact that $\partial_j^\alpha U = \partial_j^\alpha V$, we get in the first case that $y \in \Delta_j^\alpha V$ and in the second case that $y \in (\mathscr{M}ax\, V)_\ell$. We conclude by Lemma 1.2.14. ∎

Lemma 2.1.8 — *Let U, V be globular oriented graded posets, $k \in \mathbb{N}$, and suppose $U \#_k^\varphi V$ is defined. For all $n > k$ and $\alpha \in \{+, -\}$, the pasting $\partial_n^\alpha U \#_k^\varphi \partial_n^\alpha V$ is well-defined, and maps isomorphically to $\partial_n^\alpha(U \#_k^\varphi V)$.*

Proof. By globularity, $\partial_k^+(\partial_n^\alpha U) = \partial_k^+ U$ and $\partial_k^-(\partial_n^\alpha V) = \partial_k^- V$, so φ has the correct type to determine the pasting $\partial_n^\alpha U \#_k^\varphi \partial_n^\alpha V$.

By Corollary 1.3.5, the inclusions of U and V into $U \#_k^\varphi V$ preserve boundaries, so by the universal property of $\partial_n^\alpha U \#_k^\varphi \partial_n^\alpha V$ we get an inclusion

$$\partial_n^\alpha U \#_k^\varphi \partial_n^\alpha V \hookrightarrow U \#_k^\varphi V.$$

It suffices then to show that its image is $\partial_n^\alpha(U \#_k^\varphi V)$. If we identify U and V with their isomorphic images in $U \#_k^\varphi V$, this is equivalent to proving

$$\partial_n^\alpha U \cup \partial_n^\alpha V \subseteq \partial_n^\alpha(U \cup V);$$

the converse inclusion is given by Corollary 1.2.15.

Let $x \in \partial_n^\alpha U$. Then there exists y such that $x \leq y$ and $y \in \Delta_n^\alpha U$ or $y \in (\mathscr{M}ax\, U)_j$ for some $j < n$. If $y \in \Delta_n^\alpha U$, since $U \cap V = \partial_k^+ U = \partial_k^- V$ is at most k-dimensional, by Lemma 1.2.14

$$\Delta_n^\alpha(U \cup V) = \Delta_n^\alpha U + \Delta_n^\alpha V,$$

so $y \in \Delta_n^\alpha(U \cup V)$. Similarly, if $y \in (\mathscr{M}ax\, U)_j$ and $k < j < n$,

$$(\mathscr{M}ax\,(U \cup V))_j = (\mathscr{M}ax\, U)_j + (\mathscr{M}ax\, V)_j,$$

so $y \in (\mathscr{M}ax\,(U \cup V))_j$. In either case $x, y \in \partial_n^\alpha(U \cup V)$.

Suppose then that $y \in (\mathscr{M}ax\, U)_j$ with $j \leq k$. By Lemma 1.2.11 we have $(\mathscr{M}ax\, U)_k \subseteq \Delta_k^+ U$, so from Lemma 1.2.10 and $\partial_k^+ U = \partial_k^- V$ we deduce that $y \in \Delta_k^- V$ if $j = k$ and $y \in (\mathscr{M}ax\, V)_j$ if $j < k$. Applying Lemma 1.2.14 once more, we deduce in the first case that $y \in \Delta_k^-(U \cup V)$ and in the second case that $z \in (\mathscr{M}ax\,(U \cup V))_j$. In either case, $x, y \in \partial_n^\alpha(U \cup V)$.

This proves that $\partial_n^\alpha U \subseteq \partial_n^\alpha(U \cup V)$; the proof that $\partial_n^\alpha V \subseteq \partial_n^\alpha(U \cup V)$ is symmetrical. ∎

Lemma 2.1.9 — *Let U, V be globular oriented graded posets, $k \in \mathbb{N}$, and suppose $U \#_k^\varphi V$ is defined. Then $U \#_k^\varphi V$ is globular.*

Proof. Let $m, n \in \mathbb{N}$ such that $m < n$, and $\alpha, \beta \in \{+, -\}$. If $n < k$, by Lemma 2.1.7

$$\partial_m^\alpha(\partial_n^\beta(U \#_k^\varphi V)) = \partial_m^\alpha(\partial_n^\beta U) = \partial_m^\alpha(U) = \partial_m^\alpha(U \#_k^\varphi V).$$

If $n = k$, by Lemma 2.1.3 and Lemma 2.1.7,

$$\partial_m^\alpha(\partial_n^-(U \#_k^\varphi V)) = \partial_m^\alpha(\partial_n^- U) = \partial_m^\alpha(U) = \partial_m^\alpha(U \#_k^\varphi V)$$

and

$$\partial_m^\alpha(\partial_n^+(U \#_k^\varphi V)) = \partial_m^\alpha(\partial_n^+ V) = \partial_m^\alpha(V) = \partial_m^\alpha(U \#_k^\varphi V).$$

Finally, if $n > k$, by Lemma 2.1.8 we have

$$\partial_m^\alpha(\partial_n^\beta(U \#_k^\varphi V)) = \partial_m^\alpha(\partial_n^\beta U \#_k^\varphi \partial_n^\beta V),$$

and by Lemma 2.1.6 $\partial_n^\beta U$ and $\partial_n^\beta V$ are globular. If $m < k$ we use Lemma 2.1.7 to obtain

$$\partial_m^\alpha(\partial_n^\beta U \#_k^\varphi \partial_n^\beta V) = \partial_m^\alpha(\partial_n^\beta U) = \partial_m^\alpha U = \partial_m^\alpha(U \#_k^\varphi V).$$

If $m = k$ we use Lemma 2.1.3 instead to obtain

$$\partial_m^-(\partial_n^\beta U \#_k^\varphi \partial_n^\beta V) = \partial_m^-(\partial_n^\beta U) = \partial_m^- U = \partial_m^-(U \#_k^\varphi V)$$

and similarly

$$\partial_m^+(\partial_n^\beta U \#_k^\varphi \partial_n^\beta V) = \partial_m^+(\partial_n^\beta V) = \partial_m^+ V = \partial_m^+(U \#_k^\varphi V).$$

Finally, if $m > k$ we use Lemma 2.1.8 once more to obtain

$$\partial_m^\alpha(\partial_n^\beta U \#_k^\varphi \partial_n^\beta V) = \partial_m^\alpha(\partial_n^\beta U) \#_k^\varphi \partial_m^\alpha(\partial_n^\beta V) = \partial_m^\alpha U \#_k^\varphi \partial_m^\alpha V$$

and once more to obtain

$$\partial_m^\alpha U \#_k^\varphi \partial_m^\alpha V = \partial_m^\alpha(U \#_k^\varphi V). \qquad \blacksquare$$

2.2. Rewrites and roundness

2.2.1 (Rewrite construction)**.** Let U, V be oriented graded poset of the same dimension n, and suppose $\varphi\colon \partial U \xrightarrow{\sim} \partial V$ is an isomorphism restricting to isomorphisms $\varphi^\alpha\colon \partial^\alpha U \xrightarrow{\sim} \partial^\alpha V$ for each $\alpha \in \{+, -\}$. Construct the pushout

$$\begin{tikzcd}
\partial U \arrow[r, hook, "\varphi"] \arrow[d, hook] & \partial V \arrow[r, hook] & V \arrow[d, hook] \\
U \arrow[rr, hook] & \arrow[ur, phantom, "\ulcorner"] & \partial(U \Rightarrow^\varphi V)
\end{tikzcd}$$

in **ogPos**. The *rewrite of U into V along* φ is the oriented graded poset $U \Rightarrow^\varphi V$ obtained by adjoining a single $(n+1)$-dimensional element $\top$ to $\partial(U \Rightarrow^\varphi V)$, with

$$\Delta^-\top := U_n, \qquad \Delta^+\top := V_n.$$

Comment 2.2.2. By Corollary 1.3.5, we can identify U and V with their isomorphic images in $U \Rightarrow^\varphi V$, in such a way that $U \Rightarrow^\varphi V$ splits as $(U \cup V) + \{\top\}$, with $U \cap V = \partial U = \partial V$.

Lemma 2.2.3 — *Let U, V be oriented graded posets and suppose $U \Rightarrow^{\varphi} V$ is defined. Then*

1. $\partial^{-}(U \Rightarrow^{\varphi} V) = U$,
2. $\partial^{+}(U \Rightarrow^{\varphi} V) = V$.

Proof. Identifying U and V with their isomorphic images, we will prove that $\partial^{-}(U \Rightarrow^{\varphi} V) = U$ and $\partial^{+}(U \Rightarrow^{\varphi} V) = V$. Let $n \coloneqq \dim U = \dim V$. By construction, we have $\Delta_n^{-}(U \Rightarrow^{\varphi} V) = U_n$ and $\Delta_n^{+}(U \Rightarrow^{\varphi} V) = V_n$.

For all $k < n$, we have $(\mathscr{M}ax\,(U \Rightarrow^{\varphi} V))_k = (\mathscr{M}ax\,(U \cup V))_k$. We claim that this is equal to both $(\mathscr{M}ax\, U)_k$ and $(\mathscr{M}ax\, V)_k$. For $k < n-1$,

$$(\mathscr{M}ax\, U)_k = (\mathscr{M}ax\, \partial^{\alpha} U)_k = (\mathscr{M}ax\, \partial^{\alpha} V)_k = (\mathscr{M}ax\, V)_k$$

by Lemma 1.2.10. For $k = n-1$, by Lemma 1.2.11

$$(\mathscr{M}ax\, U)_{n-1} = \Delta^{-}U \cap \Delta^{+}U = \Delta^{-}V \cap \Delta V = (\mathscr{M}ax\, V)_{n-1}.$$

We then conclude by Lemma 1.2.14. ∎

Lemma 2.2.4 — *Let U, V be globular oriented graded posets and suppose $U \Rightarrow^{\varphi} V$ is defined. Then $U \Rightarrow^{\varphi} V$ is globular.*

Proof. For all $k < \dim U = \dim V$ and $\alpha \in \{+, -\}$, we have

$$\partial_k^{\alpha} U = \partial_k^{\alpha}(\partial^{\beta} U) = \partial_k^{\alpha}(\partial^{\beta} V) = \partial_k^{\alpha} V$$

since $\partial^{\beta} U = \partial^{\beta} V$ and U, V are globular. It then suffices to show that, for all $k < \dim U$ and $\alpha \in \{+, -\}$,

$$\partial_k^{\alpha}(U \Rightarrow^{\varphi} V) = \partial_k^{\alpha} U.$$

Indeed, suppose this holds, and let $k < n < \dim\,(U \Rightarrow^{\varphi} V)$ and $\alpha, \beta \in \{+, -\}$. If $n = \dim U$, then by Lemma 2.2.3

$$\partial_k^{\alpha}(\partial_n^{-}(U \Rightarrow^{\varphi} V)) = \partial_k^{\alpha} U = \partial_k^{\alpha}(U \Rightarrow^{\varphi} V)$$

and similarly

$$\partial_k^{\alpha}(\partial_n^{+}(U \Rightarrow^{\varphi} V)) = \partial_k^{\alpha} V = \partial_k^{\alpha} U = \partial_k^{\alpha}(U \Rightarrow^{\varphi} V).$$

If $n < \dim U$, then

$$\partial_k^{\alpha}(\partial_n^{\beta}(U \Rightarrow^{\varphi} V)) = \partial_k^{\alpha}(\partial_n^{\beta} U) = \partial_k^{\alpha} U = \partial_k^{\alpha}(U \Rightarrow^{\varphi} V)$$

using the globularity of U.

Let then $k < \dim U$ and $\alpha \in \{+, -\}$. We have $\Delta_k^{\alpha}(U \Rightarrow^{\varphi} V) = \Delta_k^{\alpha}(U \cup V)$. Since $\Delta_k^{\alpha} U = \Delta_k^{\alpha} V$, by Lemma 1.2.15 we have $\Delta_k^{\alpha}(U \cup V) = \Delta_k^{\alpha} U$. Similarly, we prove that for all $j < k$ we have $(\mathscr{M}ax\,(U \cup V))_j = (\mathscr{M}ax\, U)_j$. It follows that $\partial_k^{\alpha}(U \Rightarrow^{\varphi} V) = \partial_k^{\alpha} U$. ∎

2.2.5 (Roundness)**.** Let U be an oriented graded poset. We say that U is *round* if, for all $n < \dim U$,

$$\partial_n^- U \cap \partial_n^+ U = \partial_{n-1} U.$$

Lemma 2.2.6 — *Let U be round. Then U is pure.*

Proof. We will prove the contrapositive. Suppose that U is not pure. Then there exists a maximal element x in U with $k := \dim x < \dim U$. By Lemma 1.2.11, $x \in \partial_k^- U \cap \partial_k^+ U$. Then $\partial_k^- U \cap \partial_k^+ U$ is k-dimensional and cannot be equal to $\partial_{k-1} U$, which is $(k-1)$-dimensional. It follows that U is not round. ∎

Lemma 2.2.7 — *Let U be round and globular, $n \in \mathbb{N}$, and $\alpha \in \{+, -\}$. Then $\partial_n^\alpha U$ is round and globular.*

Proof. If $n \geq \dim U$ there is nothing to prove, so suppose $n < \dim U$. By Lemma 2.1.6, $\partial_n^\alpha U$ is globular. Let $k < \dim(\partial_n^\alpha U) \leq n$. Then

$$\partial_k^-(\partial_n^\alpha U) \cap \partial_k^+(\partial_n^\alpha U) = \partial_k^- U \cap \partial_k^+ U = \partial_{k-1} U = \partial_{k-1}(\partial_n^\alpha U)$$

using globularity and roundness of U. ∎

Lemma 2.2.8 — *Let U, V be round and globular and suppose $U \Rightarrow^\varphi V$ is defined. Then $U \Rightarrow^\varphi V$ is round and globular.*

Proof. Globularity follows from Lemma 2.2.4, so we only need to prove roundness. Let $n := \dim U = \dim V$. By Lemma 2.2.3

$$\partial^-(U \Rightarrow^\varphi V) \cap \partial^+(U \Rightarrow^\varphi V) = U \cap V = \partial U = \partial V,$$

and by globularity $\partial U = \partial(\partial^-(U \Rightarrow^\varphi V)) = \partial_{n-1}(U \Rightarrow^\varphi V)$. Finally, for $k < n$

$$\partial_k^-(U \Rightarrow^\varphi V) \cap \partial_k^+(U \Rightarrow^\varphi V) = \partial_k^- U \cap \partial_k^+ U = \partial_{k-1} U = \partial_{k-1}(U \Rightarrow^\varphi V)$$

by globularity of $U \Rightarrow^\varphi V$ and roundness of U. ∎

2.3. The inductive construction of molecules

2.3.1 (Regular molecule)**.** The class of *regular molecules* is the inductive subclass of oriented graded posets generated by the following clauses.

1. (*Point*). The terminal oriented graded poset 1 is a regular molecule.
2. (*Paste*). If U, V are regular molecules, $k < \min\{\dim U, \dim V\}$, and $\varphi\colon \partial_k^+ U \overset{\sim}{\hookrightarrow} \partial_k^- V$ is an isomorphism, then $U \#_k^\varphi V$ is a regular molecule.

3. (*Atom*). If U, V are *round* regular molecules of the same dimension and $\varphi\colon \partial U \overset{\sim}{\hookrightarrow} \partial V$ is an isomorphism restricting to $\varphi^\alpha\colon \partial^\alpha U \overset{\sim}{\hookrightarrow} \partial^\alpha V$ for each $\alpha \in \{+,-\}$, then $U \Rightarrow^\varphi V$ is a regular molecule.

Lemma 2.3.2 — *Let U be a regular molecule. If $\dim U = 0$, then $U = 1$.*

Proof. By induction on the construction of U. If U was produced by (*Point*), then $U = 1$ and $\dim U = 0$. If U was produced by (*Paste*), then it splits as $U_1 \#_k^\varphi U_2$ where U_1, U_2 are regular molecules with $k < \min\{\dim U_1, \dim U_2\}$. Then $\dim U = \max\{\dim U_1, \dim U_2\} > k \geq 0$. If U was produced by (*Atom*), then it is of the form $U_1 \Rightarrow^\varphi U_2$, and $\dim U = \dim U_1 + 1 = \dim U_2 + 1 > 0$. ■

Lemma 2.3.3 — *Let U be a regular molecule, $n \in \mathbb{N}$, $\alpha \in \{+,-\}$. Then*

1. *U is globular,*
2. *$\partial_n^\alpha U$ is a regular molecule,*
3. *if $n < \dim U$, then $\dim \partial_n^\alpha U = n$.*

Proof. By induction on the construction of U. Suppose U was produced by (*Point*). Then U is the terminal oriented graded poset, it has no non-trivial boundaries, and is trivially globular.

Suppose U was produced by (*Paste*). Then $U = U_1 \#_k^\varphi U_2$ for some regular molecules U_1, U_2. By the inductive hypothesis, U_1 and U_2 are globular, and by Lemma 2.1.9 so is U. We have $k < \min\{\dim U_1, \dim U_2\}$. If $n = k$, then by Lemma 2.1.3 $\partial_n^- U$ is equal to $\partial_n^- U_1$ and $\partial_n^+ U$ to $\partial_n^+ U_2$. By the inductive hypothesis, both of these are n-dimensional regular molecules. If $n < k$, then by Lemma 2.1.7 $\partial_n^\alpha U$ is equal to $\partial_n^\alpha U_1$, and again the inductive hypothesis applies. If $n > k$, then by Lemma 2.1.8 $\partial_n^\alpha U$ is equal to $\partial_n^\alpha U_1 \#_k^\varphi \partial_n^\alpha U_2$. By the inductive hypothesis, $\partial_n^\alpha U_1$ and $\partial_n^\alpha U_2$ are regular molecules, and if $n < \dim U = \max\{\dim U_1, \dim U_2\}$, at least one of them is n-dimensional.

Finally, suppose U was produced by (*Atom*). Then $U = U_1 \Rightarrow^\varphi U_2$ for some round regular molecules U_1, U_2 of the same dimension. By the inductive hypothesis, U_1 and U_2 are globular, and by Lemma 2.2.4 so is U. If $n \geq \dim U$, then $\partial_n^\alpha U = U$ is by assumption a regular molecule. If $n = \dim U - 1$, then by Lemma 2.2.3 $\partial^- U$ is equal to U_1 and $\partial^+ U$ to U_2, both regular molecules of dimension n. If $n < \dim U - 1$, then $\partial_n^\alpha U = \partial_n^\alpha U_1 = \partial_n^\alpha U_2$ by globularity, and the inductive hypothesis applies. ■

2.3.4 (Atom). An *atom* is a regular molecule with a greatest element.

Lemma 2.3.5 — *Let U be a regular molecule. The following are equivalent:*

1. *U is an atom;*

2. the final inductive step producing U is (Point) or (Atom).

Proof. If U was produced by (*Point*), then U is the terminal oriented graded poset, which trivially has a greatest element.

If U was produced by (*Paste*), then U splits as a union $U_1 \cup U_2$, where $U_1 \cap U_2 = \partial_k^+ U_1 = \partial_k^- U_2$ and $k < \max\{\dim U_1, \dim U_2\}$. Then there exist elements $x_1 \in U_1$ and $x_2 \in U_2$ such that

1. x_1 is maximal in U_1 and x_2 is maximal in U_2,
2. $\dim x_1 > k$ and $\dim x_2 > k$.

By Lemma 1.2.9, $\dim(U_1 \cap U_2) \le k$, so neither x_1 nor x_2 are contained in $U_1 \cap U_2$. It follows that x_1 and x_2 are distinct maximal elements of U, so U does not have a greatest element.

If U was produced by (*Atom*), then U splits as $(U_- \cup U_+) + \{\top\}$, where U_- and U_+ are round regular molecules of dimension n, and $\Delta^\alpha \top = (U_\alpha)_n$ for each $\alpha \in \{+, -\}$. By Lemma 2.2.6, we have $U_\alpha = \mathrm{cl}\,(U_\alpha)_n$, so $U_\alpha = \partial^\alpha \top \subseteq \mathrm{cl}\,\{\top\}$. It follows that all elements of U are in the closure of x, that is, x is the greatest element of U. ■

Corollary 2.3.6 — *All atoms are round.*

Proof. Let U be an atom. If it was produced by (*Point*), it is trivially round. If it was produced by (*Atom*), it is round by Lemma 2.2.8. ■

Lemma 2.3.7 — *Let U be a regular molecule, $x \in U$. Then $\mathrm{cl}\,\{x\}$ is an atom.*

Proof. By induction on the construction of U. If U was produced by (*Point*), then x must be the unique element of U whose closure is U itself. If U was produced by (*Paste*), it splits as $U_1 \cup U_2$, and $x \in U_1$ or $x \in U_2$; the inductive hypothesis applies. If U was produced by (*Atom*), it splits as $(U_1 \cup U_2) + \{\top\}$, and either $x \in U_1$ or $x \in U_2$, in which case the inductive hypothesis applies, or $x = \top$, and $\mathrm{cl}\,\{x\} = U$ is an atom by Lemma 2.3.5. ■

2.4. The graph of a regular molecule

2.4.1 (Directed graph with open edges). A *directed graph with open edges* is a directed graph

$$\mathcal{G} := \; E_\mathcal{G} \underset{t}{\overset{s}{\rightrightarrows}} N_\mathcal{G} + W_\mathcal{G}$$

with set of vertices bipartite into a set $N_\mathcal{G}$ of *node vertices* and a set $W_\mathcal{G}$ of *wire vertices*, satisfying the following properties:

1. the bipartition $N_\mathcal{G} + W_\mathcal{G}$ exhibits $\mathcal{G}$ as a bipartite graph, that is, every edge connects a node vertex to a wire vertex or vice versa;
2. each wire vertex is the source of at most one edge and the target of at most one edge.

Comment 2.4.2. This is equivalent to the structure called an *open graph* in [DK13] and simply a *graph* in [Koc16].

2.4.3 (Boundary of a directed graph with open edges)**.** Let $\mathcal{G}$ be a directed graph with open edges. The *input boundary* of $\mathcal{G}$ is the set

$$\Delta^-\mathcal{G} := \{x \in W_\mathcal{G} \mid t^{-1}(x) = \varnothing\}$$

and the *output boundary* of $\mathcal{G}$ is the set

$$\Delta^+\mathcal{G} := \{x \in W_\mathcal{G} \mid s^{-1}(x) = \varnothing\}.$$

2.4.4 (Graph of a regular molecule)**.** Let U be a regular molecule, $n := \dim U$. The *graph of* U is the directed graph

$$\mathcal{G}U := \quad E_{\mathcal{G}U} \underset{t}{\overset{s}{\rightrightarrows}} N_{\mathcal{G}U} + W_{\mathcal{G}U},$$

where

- $E_{\mathcal{G}U} := \{(x, y) \mid x \in U_n, y \in \Delta^+x\} + \{(x, y) \mid y \in U_n, x \in \Delta^-y\}$,
- $N_{\mathcal{G}U} := U_n$,
- $W_{\mathcal{G}U} := U_{n-1}$,
- $s\colon (x, y) \mapsto x$,
- $t\colon (x, y) \mapsto y$.

Proposition 2.4.5 — *Let U be a regular molecule. Then*

1. *$\mathcal{G}U$ is a directed graph with open edges,*
2. *$\mathcal{G}U$ is acyclic,*
3. *$\Delta^\alpha\mathcal{G}U = \Delta^\alpha U$ for all $\alpha \in \{+, -\}$.*

Proof. The fact that $\Delta^\alpha\mathcal{G}U = \Delta^\alpha U$ for all $\alpha \in \{+, -\}$ is immediate from the definitions. Moreover, $\mathcal{G}U$ is bipartite by construction, so it suffices to check the other conditions.

We proceed by induction on the construction of U. If U was produced by (*Point*) or by (*Atom*), then by Lemma 2.3.5 it has a greatest element $\top$. In this case, $\mathcal{G}U$ has a single edge $(x, \top)$ for each $x \in \Delta^-\top$ and a single edge $(\top, x)$ for each $x \in \Delta^+\top$. Since $\Delta^-\top \cap \Delta^+\top = \varnothing$, the graph is acyclic.

If U was produced by (*Paste*), it is of the form $U_1 \#_k^\varphi U_2$. Let $n := \dim U$. If $k < n-1$, then $\mathcal{G}U$ splits into the disjoint union of its restriction to U_1 and to U_2. If $n = \dim U_1 = \dim U_2$ we can conclude by the inductive hypothesis. Otherwise, the inductive hypothesis applies to one of the components, while the other is a discrete graph with no node vertices, trivially satisfying the conditions of an acyclic directed graph with open edges.

If $k = n-1$, observe first that necessarily $\dim U_1 = \dim U_2 = n$. Then $\mathcal{G}U$ is the union of $\mathcal{G}U_1$ and $\mathcal{G}U_2$, and their intersection consists of the wire vertices in $\Delta^+_{n-1}U_1 = \Delta^-_{n-1}U_2$. Let x be a wire vertex. If $x \in U_1 \setminus U_2$ or $x \in U_1 \setminus U_2$, it is the source of at most one edge and the target of at most one edge by the inductive hypothesis applied to $\mathcal{G}U_1$ and $\mathcal{G}U_2$. If $x \in U_1 \cap U_2$, then $x \in \Delta^+\mathcal{G}U_1$, so it is the source of no edge of $\mathcal{G}U_1$ and at most one edge of $\mathcal{G}U_2$, and $x \in \Delta^-\mathcal{G}U_2$, so it is the target of no edge of $\mathcal{G}U_2$ and the source of at most one edge of $\mathcal{G}U_1$.

Finally, suppose there is a cycle in $\mathcal{G}U$. Because $\mathcal{G}U_1$ and $\mathcal{G}U_2$ are separately acyclic, such a cycle needs to cross from U_1 to $U_2 \setminus U_1$ and back. However, a path entering U_1 from $U_2 \setminus U_1$ must enter a wire vertex y from a node vertex $x \in U_2$ such that $y \in \Delta^+x$. But $(U_1 \cap U_2)_{n-1} = \Delta^-U_2$, so this is impossible. We conclude that $\mathcal{G}U$ is acyclic. ∎

Lemma 2.4.6 — *Let U be a regular molecule, $n := \dim U > 0$, and $x \in U_n$. Then there exist $y_- \in \Delta^-U$ and $y_+ \in \Delta^+U$ such that there is a path from y_- to y_+ passing through x in $\mathcal{G}U$.*

Proof. We construct a path $x = x_0 \to y_0 \to \ldots \to x_m \to y_+$ by successive extensions; the construction of a path from y_- to x is dual. Suppose we have reached x_i. By Lemma 2.3.7 $\mathrm{cl}\,\{x_i\}$ is an atom, so ∂^+x_i is $(n-1)$-dimensional and Δ^+x_i is non-empty. Pick y_i in Δ^+x_i. If y_i has no input cofaces, then $y_i \in \Delta^+U$, so we can let $m := i$ and $y_+ := y_i$. Otherwise, pick $x_{i+1} \in \nabla^-y_i$. Since $\mathcal{G}U$ is finite and acyclic by Proposition 2.4.5, this procedure must terminate after a finite number of steps. ∎

Proposition 2.4.7 — *Let U be a regular molecule and $\imath\colon U \overset{\sim}{\hookrightarrow} U$ an automorphism. Then $\imath$ is the identity.*

Proof. We proceed by induction on $n := \dim U$. If $n = 0$, then $U = 1$ by Lemma 2.3.2. Since 1 is terminal, its only automorphism is the identity.

Suppose $n > 0$ and let $\alpha \in \{+,-\}$. By Proposition 2.3.3, $\partial^\alpha U$ is a regular molecule of dimension $n-1$, and $\imath(\partial^\alpha U) = \partial^\alpha U$. By the inductive hypothesis, the restriction of $\imath$ to $\partial^\alpha U$ is the identity.

Let $x \in \mathscr{M}ax\, U$, and suppose $\imath(x) = x$. Then $\imath(\partial^\alpha x) = \partial^\alpha x$. By Lemma 2.3.7, $\mathrm{cl}\,\{x\}$ is an atom, so $\partial^\alpha x$ is a regular molecule of dimension strictly lower than n. By the inductive hypothesis the restriction of $\imath$ to $\partial^\alpha x$ is the identity. Since $\mathrm{cl}\,\{x\} = (\partial^- x \cup \partial^+ x) + \{x\}$, it follows that $\imath$ restricts to the identity on $\mathrm{cl}\,\{x\}$. Therefore, it suffices to prove that $\imath$ fixes all $x \in \mathscr{M}ax\, U$.

If $\dim x < n$, then $x \in \partial^\alpha U$, and we have already proved $\imath(x) = x$. Suppose then $\dim x = n$, and construct a path $y_- = y_0 \to x_0 \to \ldots \to y_m \to x_m = x$ in $\mathcal{G}U$ as in Lemma 2.4.6. Since $\imath$ preserves the covering relation and orientations, it maps this path to another path in $\mathcal{G}U$. We have $y_0 \in \partial^- U$, so $\imath(y_0) = y_0$. Suppose $\imath(y_i) = y_i$. Since y_i is a wire vertex in a directed graph with open edges, x_i is the only node vertex with an edge from y_i, so necessarily $\imath(x_i) = x_i$. If $i < m$, then $\imath$ is the identity on $\mathrm{cl}\,\{x_i\}$, so $\imath(y_{i+1}) = y_{i+1}$. Iterating until we reach m, we conclude. ■

Corollary 2.4.8 — *Let U, V be regular molecules. If U and V are isomorphic, there exists a unique isomorphism $\varphi\colon U \xrightarrow{\sim} V$.*

Comment 2.4.9. It follows that, if U, V are regular molecules, there is at most *one* isomorphism $\varphi\colon \partial_k^+ U \xrightarrow{\sim} \partial_k^- V$, so we can write

$$U \#_k V := U \#_k^\varphi V,$$

and speak simply of *the pasting of U and V at the k-boundary.*

Corollary 2.4.10 — *Let U, V be round regular molecules, and suppose $\partial^\alpha U$ and $\partial^\alpha V$ are isomorphic for all $\alpha \in \{+, -\}$. Then there exists a unique isomorphism $\varphi\colon \partial U \xrightarrow{\sim} \partial V$ restricting to isomorphisms $\varphi^\alpha\colon \partial^\alpha U \xrightarrow{\sim} \partial^\alpha V$.*

Proof. By Corollary 2.4.8, the isomorphisms φ^α are uniquely defined. They restrict to unique isomorphisms $\partial^\beta(\partial^\alpha U) \xrightarrow{\sim} \partial^\beta(\partial^\alpha V)$ for all $\beta \in \{+, -\}$, which implies that the restrictions of φ^- and φ^+ to $\partial^+ U \cap \partial^- U = \partial(\partial^\alpha U)$ are equal. It follows that there is a unique extension of φ^-, φ^+ to a map $\varphi\colon \partial U \to \partial V$. Since V is also round, this map is injective, hence an isomorphism. ■

Comment 2.4.11. It follows that, if U, V are round regular molecules, there is at most *one* isomorphism $\varphi\colon \partial U \xrightarrow{\sim} \partial V$ restricting to $\varphi^\alpha\colon \partial^\alpha U \xrightarrow{\sim} \partial^\alpha V$ for all $\alpha \in \{+, -\}$, so we can write

$$U \Rightarrow V := U \Rightarrow^\varphi V,$$

and speak simply of *the rewrite of U into V.*

3. Constructions and operations

3.1. Submolecules

Submolecule relation. Every atom is a submolecule. Pasting along submolecule. Substitution based on that.

Acknowledgements

This work was supported by the ESF funded Estonian IT Academy research measure (project 2014-2020.4.05.19-0001) and by the Estonian Research Council grant PSG764.

Bibliography

[DK13] L. Dixon and A. Kissinger. Open-graphs and monoidal theories. *Mathematical Structures in Computer Science*, 23(02):308–359, 2013.

[Koc16] J. Kock. Graphs, hypergraphs, and properads. *Collectanea Mathematica*, 67(2):155–190, 2016.

Index