Membranes and Nanotubes:
Progress on Universally Programmable Intelligent Matter

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Abstract

We demonstrate how combinatory molecular computation allows parallel self-assembly of several kinds of nanomembranes and nanotubes. One such nanomembrane is a square grid constructed of cross-linked horizontal and vertical chains. We show that a relatively minor change causes it to self-assemble into a nanotube with the same cross-linked structure. A second nanomembrane is a monolayer arranged in a hexagonal grid.

1 Cross-linked Membranes

1.1 General Grid Construction

Our goal is to construct a nanomembrane structured as a cross-linked grid, as shown in Figs. 1 and 2. One row of the grid is constructed by (Eq. 73 [Mac02a]):

$$\check{\Phi}_n F Y_1 \cdots Y_n X \Longrightarrow F(Y_1 X^{(n-1)}) \cdots (Y_{n-1} X^{(1)})(Y_n X^{(0)}). \tag{1}$$

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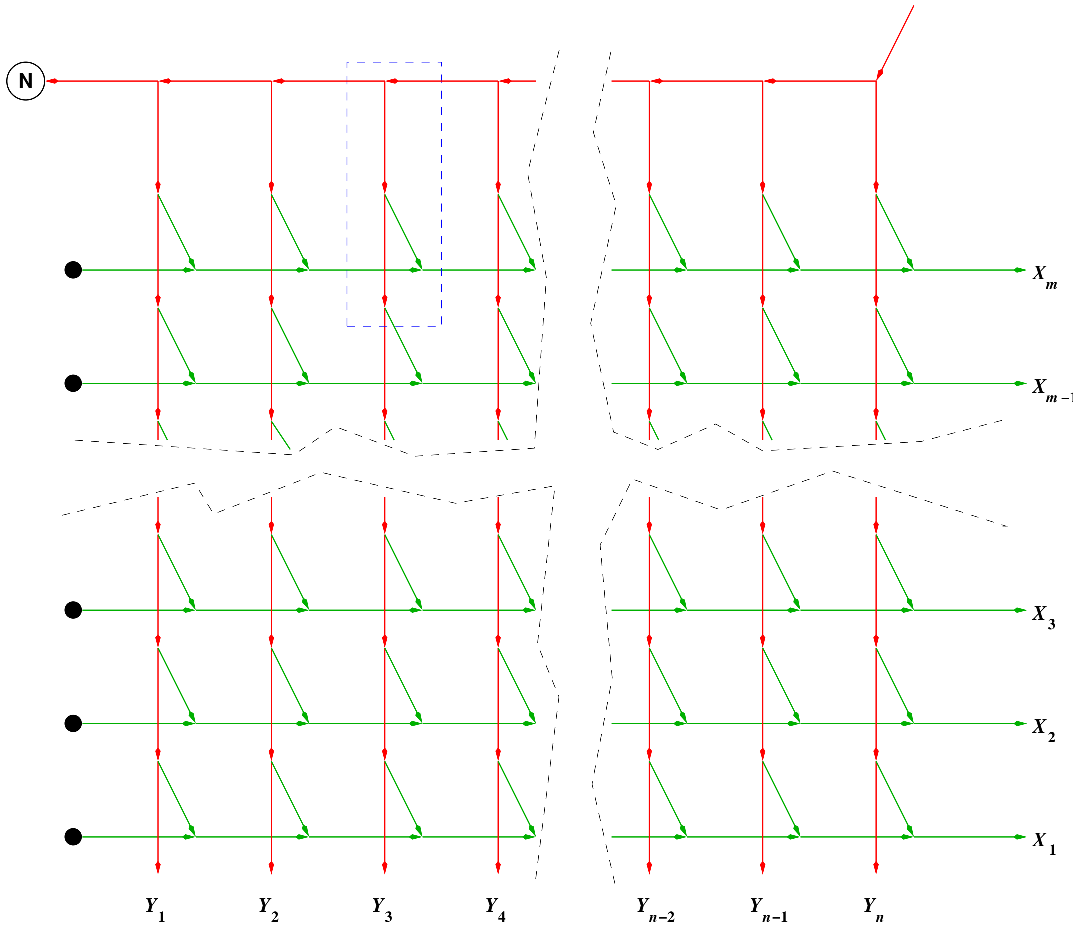

Figure 1: Nanomembrane structured as a cross-linked grid. Such a grid can be created by $\check{\Phi}^m_n \mathsf{N} Y_1 \cdots Y_n X_1 \cdots X_m$, where N is an inert combinator and $Y_1, \ldots, Y_n, X_1, \ldots, X_m$ are any complexes. The vertical red chains (the "warp") and the single horizontal red chain are composed of linked A (application) primitives. The horizontal, green chains (the "woof"), which lie below the vertical chains, are composed of linked V (sharing) primitives. The dark circles along the left border represent P primitives (result caps) that result from deleting the last sharing reference to each X_k. The red, diagonal arrow in the upper right is the *umbilical connection*, that is, the root of the combinator tree. The area in the blue dotted rectangle is expanded in more detail in Fig. 2. See Figs. 3 and 4 for visualizations of a cross-linked grid.

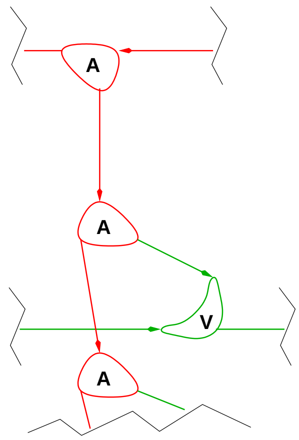

Figure 2: Detailed structure of cross-linked grid. The figure depicts an area near the top of the grid as indicated by the blue dotted rectangle in Fig. 1. Notice that the uppermost A (application) primitive is oriented differently from the other A groups.

(For the use of primes and parenthesized superscripts to indicate sharing, see **Introduction** and Sec. 17 [Mac02a].) That $\check{\Phi}_n$ constructs the indicated sharing structure follows from $\Phi_n = \mathsf{S}_n \circ \mathsf{K}$ (Eq. 72 [Mac02a]) and the following lemma.

Lemma 1 (Eq. 38 [Mac02a]) *For $n \geq 1$,*

$$\check{\mathsf{S}}_n F Y_1 \cdots Y_n X \Longrightarrow F X^{(n)}(Y_1 X^{(n-1)}) \cdots (Y_{n-1} X^{(1)})(Y_n X^{(0)}). \tag{2}$$

Proof: For the base of the induction observe that by Eq. 32 [Mac02a]:

$$\begin{aligned} \check{\mathsf{S}}_1 F Y_1 X &\Longrightarrow \check{\mathsf{S}} F Y_1 X \\ &\Longrightarrow F X^{(1)}(Y_1 X^{(0)}). \end{aligned}$$

For the induction assume $n \geq 1$ and apply Eq. 37 [Mac02a]:

$$\begin{aligned} \check{\mathsf{S}}_{n+1} F Y_1 Y_2 \cdots Y_{n+1} X &\Longrightarrow (\mathsf{B}\check{\mathsf{S}}_n \circ \check{\mathsf{S}}) F Y_1 Y_2 \cdots Y_{n+1} X \\ &\Longrightarrow \mathsf{B}\check{\mathsf{S}}_n(\check{\mathsf{S}} F) Y_1 Y_2 \cdots Y_{n+1} X \\ &\Longrightarrow \check{\mathsf{S}}_n(\check{\mathsf{S}} F Y_1) Y_2 \cdots Y_{n+1} X \\ &\Longrightarrow \check{\mathsf{S}} F Y_1 X^{(n)}(Y_2 X^{(n-1)}) \cdots (Y_n X^{(1)})(Y_{n+1} X^{(0)}) \\ &\Longrightarrow F X^{(n+1)}(Y_1 X^{(n)})(Y_2 X^{(n-1)}) \cdots (Y_n X^{(1)})(Y_{n+1} X^{(0)}). \end{aligned}$$

□

Since Φ_n is used to construct a row, it's worthwhile to look at its operation in detail:

$$\begin{aligned} \check{\Phi}_n F Y_1 \cdots Y_n X &\Longrightarrow (\mathsf{S}_n \circ \mathsf{K}) F Y_1 \cdots Y_n X \\ &\Longrightarrow \mathsf{S}_n(\mathsf{K} F) Y_1 \cdots Y_n X \\ &\Longrightarrow \mathsf{K} F X^{(n)}(Y_1 X^{(n-1)}) \cdots (Y_n X^{(0)}) \\ &\Longrightarrow F(Y_1 X^{(n-1)}) \cdots (Y_n X^{(0)}). \end{aligned} \tag{3}$$

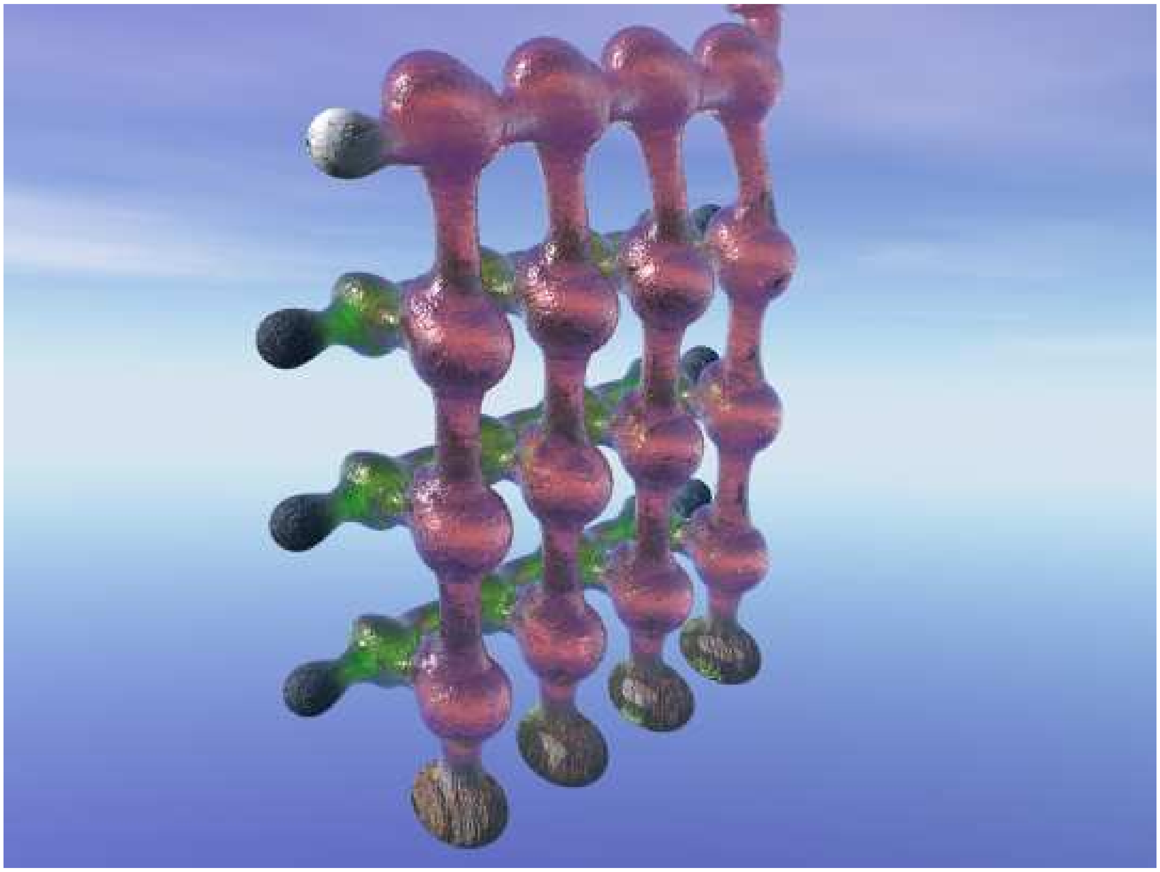

Figure 3: Visualization of front of a small cross-linked nanomembrane. Such a membrane could be created by $\mathsf{xgrid}_{3,4}\mathsf{N}YX$ with $\hat{\mathsf{W}} = \mathsf{W}$ (replicated terminal groups; see Def. 1 or 2). The view is from the front-left, so it displays the same side of the nanomembrane as Figs. 1 and 2. The vertical, red chains (warp) are composed of application (A) primitives. They are connected across the top by a horizontal chain of A primitives, starting from the umbilical connection at the upper right, and terminating in a whitish N group at the left end. The brownish groups at the lower ends of the vertical A chains are arbitrary terminal groups Y (the "loom weights," perhaps stretching the metaphor). The horizontal, green chains (woof) are composed of sharing (V) complexes. The dark groups on the nearest ends are "result caps" (P primitives). Arbitrary terminal groups X can be seen on the far ends of the horizontal chains.

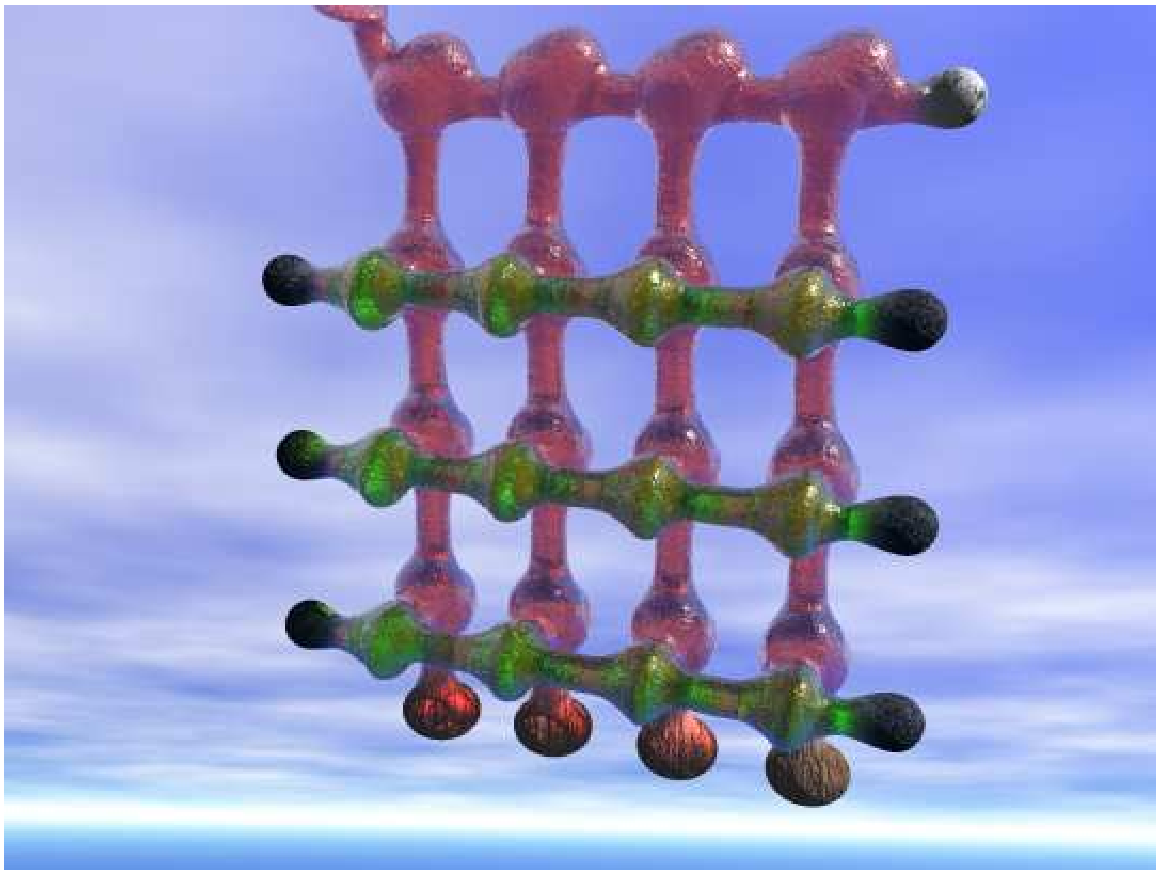

Figure 4: Visualization of rear of a small cross-linked nanomembrane. This is the same membrane as in Fig. 3, but viewed from the opposite side, to display better the horizontal chains (woof).

Notice that the K combinator in Eq. 3 discards $X^{(n)}$, the most recently made sharing reference to X:

$$\mathsf{K}FX^{(n)} \Longrightarrow F.$$

According to the rules of the deletion reaction (Sec. 6 [Mac02a]), the deleted $X^{(n)}$ complex is replaced by a "result cap" (P primitive, Sec. 11 [Mac02a]); the P primitive is shown as a black dot on the left end of each row in Fig. 1. To construct the complete grid, we iterate the row construction m times, in accord with Eq. 75 [Mac02a]:

$$(\Phi_n)^m FY_1 \cdots Y_n X_1 \cdots X_m \Longrightarrow F(Y_1 X_1 \cdots X_m) \cdots (Y_n X_1 \cdots X_m). \tag{4}$$

The following theorem shows that the correct cross-linked sharing structure (as shown in Fig. 1) is constructed.

Theorem 1 *For* $m, n \geq 1$,

$$\check{\Phi}_n^m FY_1 \cdots Y_n X_1 \cdots X_m \Longrightarrow F(Y_1 X_1^{(n-1)} \cdots X_m^{(n-1)}) \cdots (Y_n X_1^{(0)} \cdots X_m^{(0)}). \tag{5}$$

Proof: The base of the induction is established by Eq. 1. For $m \geq 1$, expand the power (Sec. 28 [Mac02a]) and use Eq. 1:

$$\begin{aligned}
&\check{\Phi}_n^{m+1} FY_1 \cdots Y_n X_1 \cdots X_m X_{m+1} \\
&\quad\Longrightarrow\ (\check{\Phi}_n^m \circ \check{\Phi}_n) FY_1 \cdots Y_n X_1 \cdots X_m X_{m+1} \\
&\quad\Longrightarrow\ \check{\Phi}_n^m (\check{\Phi}_n F) Y_1 \cdots Y_n X_1 \cdots X_m X_{m+1} \\
&\quad\Longrightarrow\ \check{\Phi}_n F(Y_1 X_1^{(n-1)} \cdots X_m^{(n-1)}) \cdots (Y_n X_1^{(0)} \cdots X_m^{(0)}) X_{m+1} \\
&\quad\Longrightarrow\ F(Y_1 X_1^{(n-1)} \cdots X_m^{(n-1)} X_{m+1}^{(n-1)}) \cdots (Y_n X_1^{(0)} \cdots X_m^{(0)} X_{m+1}^{(0)}).
\end{aligned}$$

□

1.2 Identical Terminal Groups

With the foregoing formulation, the terminal groups on the X-rows and Y-columns are all potentially different. More commonly, we would want them all the same, $X_j = X, j = 1, \ldots, m$, and $Y_k = Y, k = 1, \ldots, n$. We can use the elementary duplicators (Eqs. 40, 44 [Mac02a]) to duplicate a single X or Y. We use W if we want the terminal groups to be replicated, and $\check{\mathsf{W}}$ if we want a single copy to be shared. Letting $\hat{\mathsf{W}}$ represent either $\check{\mathsf{W}}$ or W (depending on whether sharing is wanted or not), we will show that an $m \times n$ grid with X and Y terminal groups is computed by $\mathsf{xgridp}_{m,n}$, defined as follows.

Definition 1 (xgridp)

$$\mathsf{xgridp}_{m,n} = \mathsf{B}(\mathsf{B}\hat{\mathsf{W}}^{m-1})(\mathsf{B}\hat{\mathsf{W}}^{n-1}\check{\Phi}_n^m). \tag{6}$$

We begin with the shared case, since it is more general.

Theorem 2 (xgridp**)** *For* $\hat{\mathsf{W}} = \check{\mathsf{W}}$,

$$\mathsf{xgridp}_{m,n} F Y X \Longrightarrow \check{\Phi}_n^m F Y^{(n-1)} \cdots Y^{(0)} X^{(m-1)} \cdots X^{(0)}. \tag{7}$$

Proof: Observe that

$$\begin{aligned}
\mathsf{xgridp}_{m,n} F Y X &\Longrightarrow \mathsf{B}(\mathsf{B}\check{\mathsf{W}}^{m-1})(\mathsf{B}\check{\mathsf{W}}^{n-1}\check{\Phi}_n^m) F Y X \\
&\Longrightarrow \mathsf{B}\check{\mathsf{W}}^{m-1}(\mathsf{B}\check{\mathsf{W}}^{n-1}\check{\Phi}_n^m F) Y X \\
&\Longrightarrow \mathsf{B}\check{\mathsf{W}}^{m-1}(\check{\mathsf{W}}^{n-1}(\check{\Phi}_n^m F)) Y X \\
&\Longrightarrow \check{\mathsf{W}}^{m-1}(\check{\mathsf{W}}^{n-1}(\check{\Phi}_n^m F) Y) X.
\end{aligned}$$

Here we make use of Eq. 51 [Mac02a], which shows the sharing effect of iterated $\check{\mathsf{W}}$:

$$\begin{aligned}
\check{\mathsf{W}}^{m-1}(\check{\mathsf{W}}^{n-1}(\check{\Phi}_n^m F) Y) X &\Longrightarrow \check{\mathsf{W}}^{n-1}(\check{\Phi}_n^m F) Y X^{(m-1)} \cdots X^{(0)} \\
&\Longrightarrow \check{\Phi}_n^m F Y^{(n-1)} \cdots Y^{(0)} X^{(m-1)} \cdots X^{(0)}.
\end{aligned}$$

□

Thus, $\mathsf{xgridp}_{m,n} \mathsf{N} Y X$ results in the sort of structure show in Fig. 5. Its structure is described formally by the following corollary.

Corollary 1

$$\mathsf{xgridp}_{m,n} \mathsf{N} Y X \Longrightarrow \mathsf{N}(Y^{(n-1)} X^{(m-1)(n-1)} \cdots X^{(0)(n-1)}) \cdots (Y^{(0)} X^{(m-1)(0)} \cdots X^{(0)(0)}). \tag{8}$$

The double parenthesized superscripts indicate the sharing structure. The first superscript indicates the distance from X along the vertical sharing chain (in green) on the right of Fig. 5; the second superscript indicated the distance from the right along the horizontal sharing chains (green).

Proof: Follows directly from Thms. 1 and 2. □

The case of replicated terminal groups follows from the preceding Theorem 2 by omitting the superscripts indicating sharing:

Corollary 2 *For* $\hat{\mathsf{W}} = \mathsf{W}$,

$$\mathsf{xgridp}_{m,n} F Y X \Longrightarrow \check{\Phi}_n^m F \overbrace{Y \cdots Y}^{n} \overbrace{X \cdots X}^{m}. \tag{9}$$

1.3 Size of Molecular Program Structures

We consider next the size of molecular program $\mathsf{xgridp}_{m,n}$. Referring to Def. 1 we see that several combinators ($\hat{\mathsf{W}}$, $\check{\Phi}_n$) are raised to powers. The size of these program structures is proportional to the powers, since (Sec. 28 [Mac02a]):

$$|X^N| = 9(N-1) + N|X| \text{ total primitives.}$$

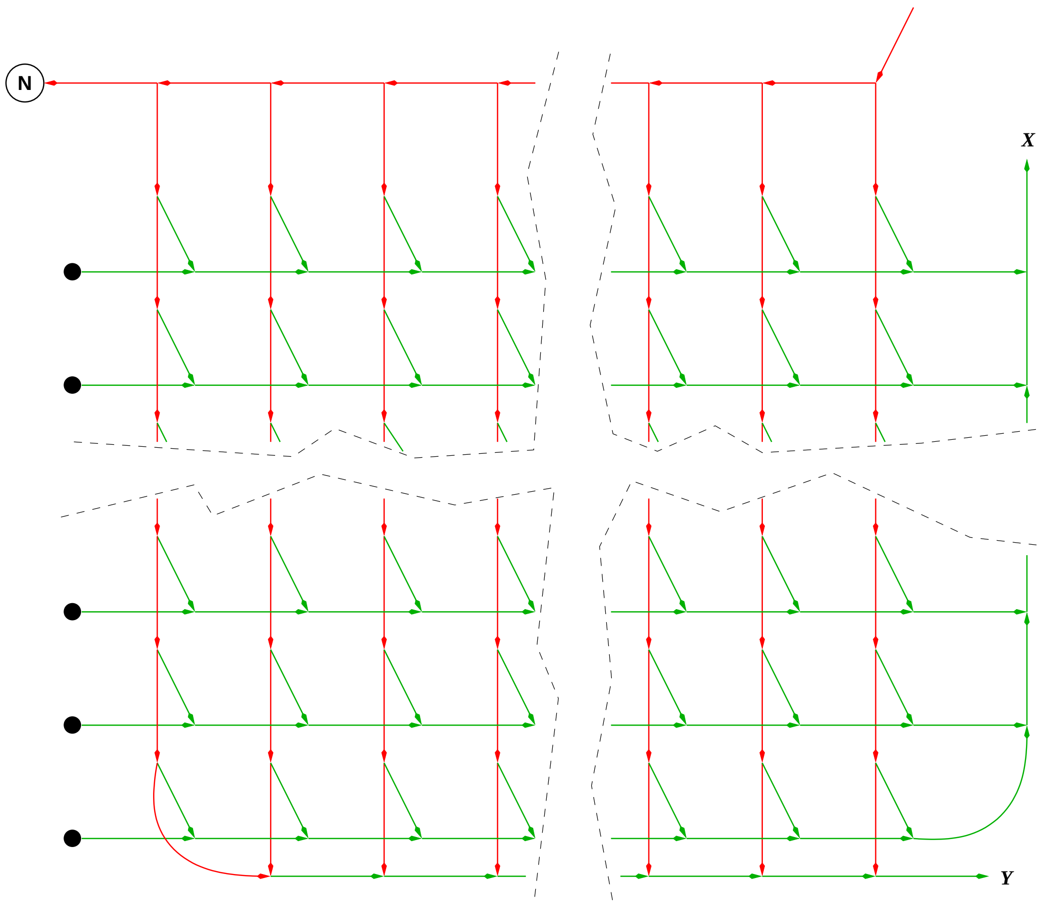

Figure 5: Nanomembrane structured as cross-linked grid with shared terminal groups. Such a structure is computed by $\mathsf{xgridp}_{m,n}\mathsf{N}YX$ or $\mathsf{xgrid}_{m,n}\mathsf{N}YX$ with $\hat{\mathsf{W}} = \check{\mathsf{W}}$. The diagram may be understood by comparison with Fig. 1. The ends of the X-rows and Y-columns are tied together by V (sharing) primitives.

(See **Introduction** [Mac02a] for a description of our notation for sizes of combinator complexes.) Furthermore (Sec. 25), $|\check{\Phi}_n| = 18n - 7$, so we can see that $|\check{\Phi}_n^m| \in \mathcal{O}(mn)$. Specifically, one can show (for $m, n \geq 1$):

$$\begin{aligned}
|\check{\Phi}_n^m| &= (5mn-2)\mathsf{S} + (4mn+m-2)\mathsf{K} + (9mn+m-5)\mathsf{A} && (10)\\
&= 18mn + 2m - 9 \text{ total primitives,} && (11)\\
|\mathsf{xgridp}_{m,n}| &= (5mn+9m+9n-18)\mathsf{S} + (4mn+9m+8n-16)\mathsf{K} + \\
&\quad (9mn+18m+17n-35)\mathsf{A} && (12)\\
&= 18mn + 36m + 34n - 57 \text{ total.} && (13)
\end{aligned}$$

This is troublesome, since it suggests that we must use a program structure of size $\mathcal{O}(mn)$ to construct a grid of size $\mathcal{O}(mn)$. However, as discussed in a previous report [Mac02b], we can avoid this problem by using iterators or "Church numerals" (Sec. 23 [Mac02a]), since $\mathsf{Z}_N X = X^N$. Then,

$$|\mathsf{Z}_N X| = 1\mathsf{A} + |\mathsf{Z}_N| + |X|; \tag{14}$$

that is, $\mathcal{O}(N + |X|)$ as opposed to $\mathcal{O}(N|X|)$. Since (Sec. 23 [Mac02a]),

$$|\mathsf{Z}_N| = (3N+1)\mathsf{S} + (2N+3)\mathsf{K} + (5N+3)\mathsf{A} = 10N + 7 \text{ total,} \tag{15}$$

this might not seem an improvement, but the advantage is apparent when we observe that $|\mathsf{Z}_m \check{\Phi}_n| \in \mathcal{O}(m+n)$; specifically,

$$|\mathsf{Z}_m \check{\Phi}_n| = (3m+5n-1)\mathsf{S} + 2(m+4n+2)\mathsf{K} + (5m+9n)\mathsf{A} = 10m + 18n + 1 \text{ total.} \tag{16}$$

As a result of the forgoing we see that it is advantageous to redefine xgridp in terms of Church numerals. Thus we modify Def. 1 to:

Definition 2 (xgrid**)**

$$\mathsf{xgrid}_{m,n} = \mathsf{B}(\mathsf{B}(\mathsf{Z}_{m-1}\hat{\mathsf{W}}))(\mathsf{B}(\mathsf{Z}_{n-1}\hat{\mathsf{W}})(\mathsf{Z}_m \check{\Phi}_n)). \tag{17}$$

By construction it immediately follows that

Corollary 3

$$\mathsf{xgrid}_{m,n} = \mathsf{xgridp}_{m,n}. \tag{18}$$

Therefore, $\mathsf{xgrid}_{m,n}\mathsf{N}YX$ will construct a grid such as shown in Fig. 5. As expected, the size is $\mathcal{O}(m+n)$:

$$\begin{aligned}
|\mathsf{xgrid}_{m,n}| &= (6m+8n+15)\mathsf{S} + (4m+6n+22)\mathsf{K} + (10m+14n+36)\mathsf{A} && (19)\\
&= 20m + 28n + 73 \text{ total.} && (20)
\end{aligned}$$

It is of course possible to factor Z_m and Z_n out of $\mathsf{xgrid}_{m,n}$ to get a program structure G independent of grid dimensions,

$$G\mathsf{Z}_m\mathsf{Z}_n = \mathsf{xgrid}_{m,n}.$$

However, there seems to be little point in this exercise, since when it comes time to construct a grid of particular dimensions, we imagine that it will be as easy to synthesize $\mathsf{xgrid}_{m,n}$ directly as to synthesize $G\mathsf{Z}_m\mathsf{Z}_n$. Both have size $\mathcal{O}(m+n)$.

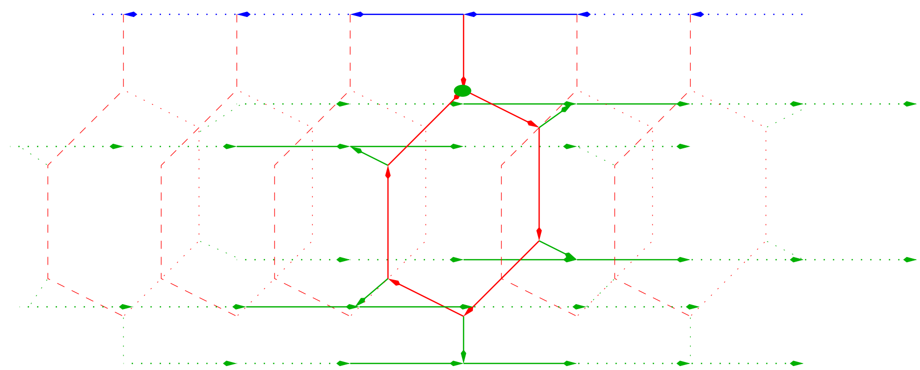

Figure 6: Basic structure of a cross-linked nanotube. Only one rib (red) is shown complete and only the middles of the staves (green), and backbone (blue). The staves are shown outside the tube (that is, it is as though the bottom of Fig. 1 has been bent forward out of the paper to form the tube), since this is the way it would most likely self-assemble. The green oval connecting the backbone to the top of the rib is the sharing (V) primitive that completes the ring. In this example the tube has circumference $m = 5$ (the number of staves) and an indeterminate length n (the number of ribs).

2 Cross-linked Tubes

The preceding construction of a cross-linked nanomembrane can be converted into a cross-linked nanotube. Consider Fig. 1; our approach will be to loop each column back to the top of itself. That is, instead of pointing to Y_k, the bottom of the column will be bent around to connect to a sharing node that points to the top of the column. The intended structure is shown in Fig. 6; Figs. 7 and 8 are visualizations of a small nanotube.

The cycle from Y_k to the top of the column may be created by Y̌, the sharing fixed-point combinator (Secs. 22 [Mac02a], 5.3 [Mac02b]), which has the following effect (see also Fig. 9 [Mac02b]):

$$\check{\mathsf{Y}} F \Longrightarrow y^{(1)} \quad \text{where } y \equiv (F\ y^{(0)}). \tag{21}$$

That is, we have a shared reference $y^{(1)}$ to an application of the function F to a shared reference $y^{(0)}$ to that same application.

From Thm. 1, we know that the kth column of the grid (Fig. 1) has the form

$$(Y_k X_1^{(n-k)} \cdots X_m^{(n-k)}).$$

The kth ring, indicated in red in Fig. 6, therefore has the form

$$y_k^{(1)} \quad \text{where } y_k \equiv (y_k^{(0)} X_1^{(n-k)} \cdots X_m^{(n-k)}). \tag{22}$$

To construct this with Y̌ we need to be able to find an F such that

$$F y = y X_1^{(n-k)} \cdots X_m^{(n-k)}. \tag{23}$$

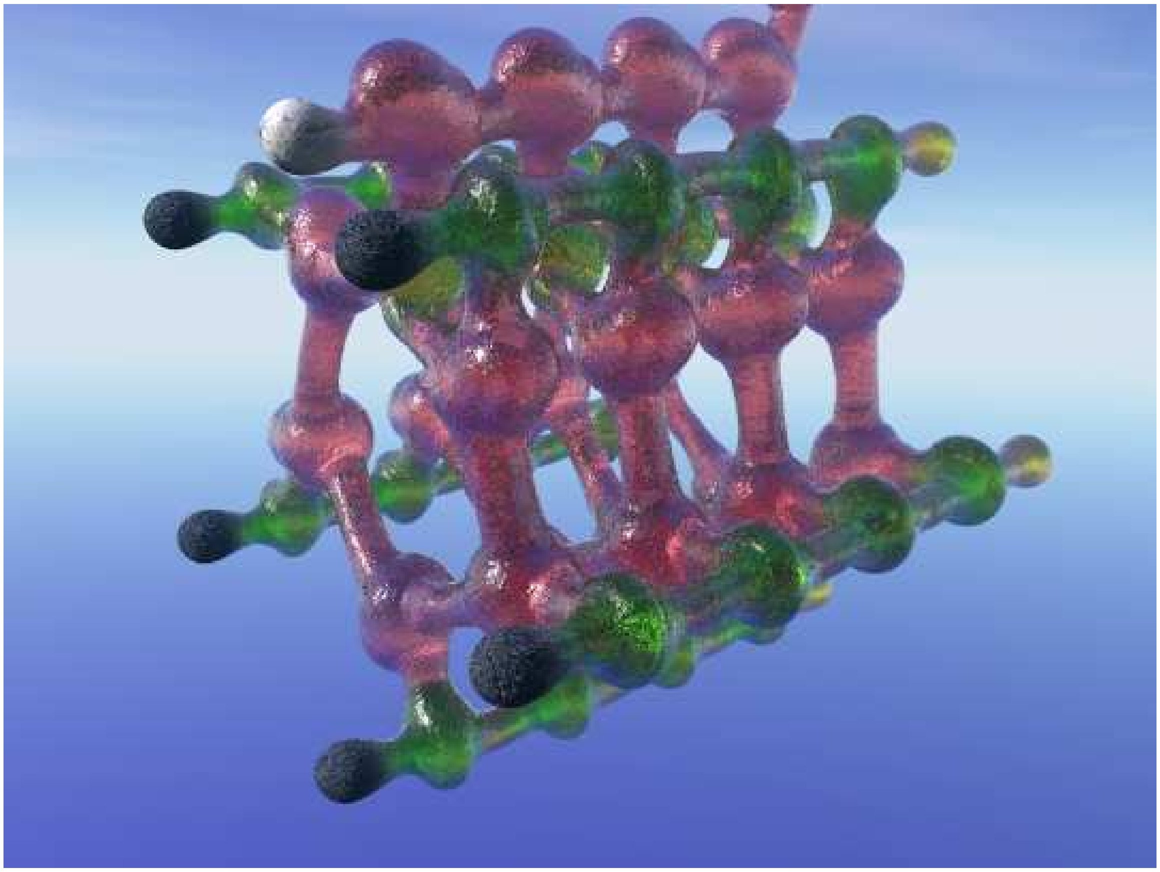

Figure 7: Visualization of small cross-linked nanotube, five staves in circumference, four ribs in length. Such a nanotube may be created by $\mathsf{xtube}_{5,4}X$ with $\hat{\mathsf{W}} = \mathsf{W}$ (replicated terminal groups; see Def. 4). The view is from the side, comparable to Fig. 6, but also shows the proximal, non-umbilical end of the tube. The N group is the whitish group at the proximal end of the backbone, which is the chain of four red A (application) groups at the top of the picture; the umbilical connection is visible at the distal end of the backbone. Each rib is a chain of five A primitives (shown in red). Along the outside of the tube are five staves, each a chain of four sharing primitives (shown in green). At the proximal end of each stave is a P primitive (result cap), shown as a small dark sphere. At the distal ends of the staves are the terminal groups X, visible as small, yellowish spheres on the two nearest staves. For a different view, see also Fig. 8.

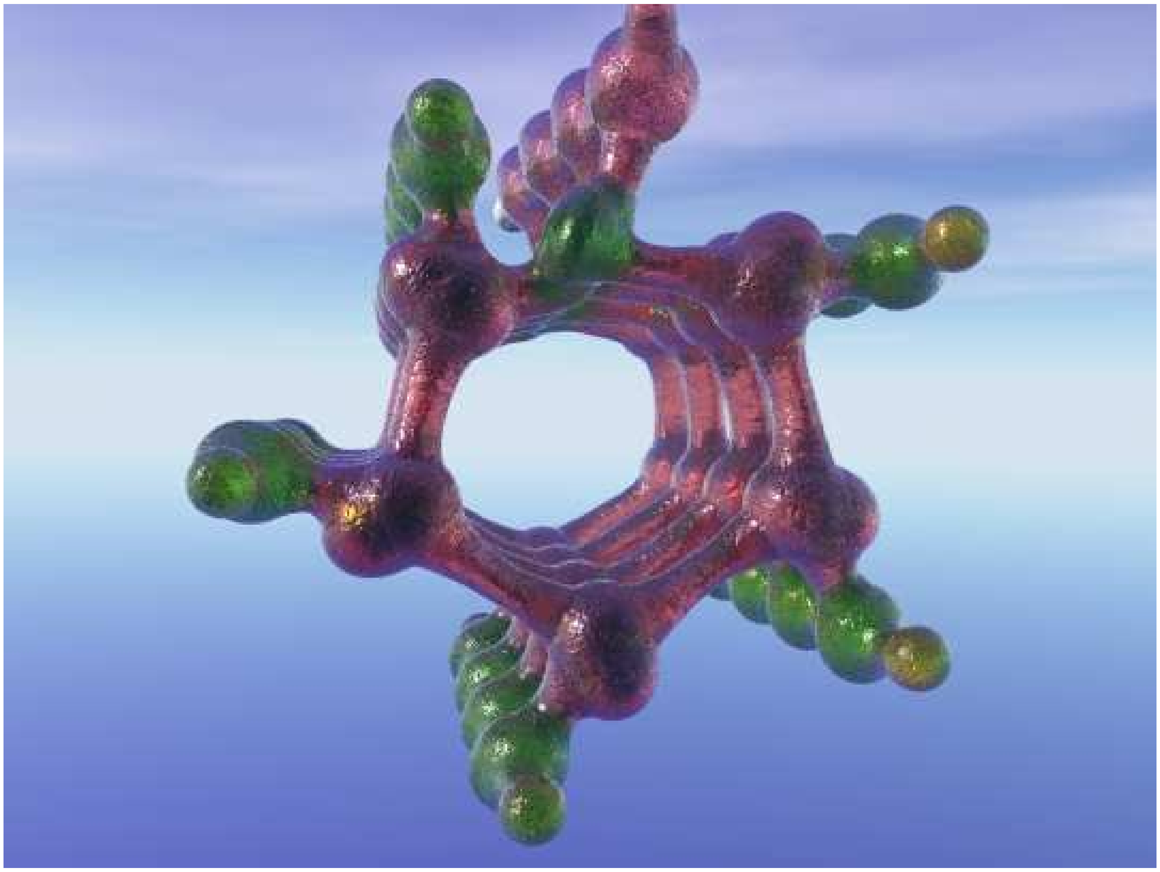

Figure 8: Visualization of small cross-linked nanotube. The view is from the umbilical end of the same nanotube shown in Fig. 7. The umbilical connection to the end of the backbone is visible at the top of the picture; the N group is barely visible at a whitish group at the distal end. The green groups immediately below the backbone are the sharing (V) primitives, which complete the pentagonal ribs and connect them to the backbone. At the proximal end of each stave is the terminal group X, shown as a small, yellowish sphere. At the distal end of each stave is a P primitive (result cap); one is slightly visible as a dark sphere at the far end of the lowest stave.

The argument y can be moved to the right by use of Eq. 109 [Mac02a]:

$$
\begin{aligned}
yX_1^{(n-k)} \cdots X_m^{(n-k)} &\Longleftarrow \mathsf{I}yX_1^{(n-k)} \cdots X_m^{(n-k)} && (24)\\
&\Longleftarrow \mathsf{C}_{[m]}\mathsf{I}X_1^{(n-k)} \cdots X_m^{(n-k)}y. && (25)
\end{aligned}
$$

Hence

$$y_k \equiv \check{\mathsf{Y}}F \quad \text{where } F = \mathsf{C}_{[m]}\mathsf{I}X_1^{(n-k)} \cdots X_m^{(n-k)}.$$

However, to apply Thm. 1 we need y_k as a function G of $X_1^{(n-k)} \cdots X_m^{(n-k)}$ so that we can write

$$y_k \equiv GX_1^{(n-k)} \cdots X_m^{(n-k)}.$$

Therefore, use Eq. 5 [Mac02a] as follows:

$$
\begin{aligned}
y_k &\equiv GX_1^{(n-k)} \cdots X_m^{(n-k)} && (26)\\
&\Longleftarrow \check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I}X_1^{(n-k)} \cdots X_m^{(n-k)}) && (27)\\
&\Longleftarrow \mathsf{B}^m\check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I})X_1^{(n-k)} \cdots X_m^{(n-k)}. && (28)
\end{aligned}
$$

Hence,

$$G = \mathsf{B}^m\check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I}). \tag{29}$$

Therefore, a nanotube m in circumference and n in length, with groups $X_1, \ldots, X_m$ on the connected (“umbilical”) end, and result caps on the distal end, can be computed by

$$\check{\Phi}_n^m\mathsf{N}\overbrace{G \cdots G}^{n}X_1 \ldots X_m.$$

We have thus proved the

Lemma 2 *Let* $G = \mathsf{B}^m\check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I})$. *Then,*

$$
\begin{aligned}
\check{\Phi}_n^m\mathsf{N}\overbrace{G \cdots G}^{n}X_1 \ldots X_m &\Longrightarrow \mathsf{N}y_1^{(1)} \cdots y_n^{(1)}\\
&\qquad \text{where } y_k \equiv (y_k^{(0)}X_1^{(n-k)} \cdots X_m^{(n-k)}).
\end{aligned}
$$

In the usual situation, all the terminal groups will be identical, $X_k = X$, so we can use $\hat{\mathsf{W}}$ (i.e., $\check{\mathsf{W}}$ or W) to simplify the definition, for example:

$$\check{\mathsf{W}}^{m-1}(\mathsf{W}^{n-1}(\check{\Phi}_n^m\mathsf{N})G)X \Longrightarrow \check{\Phi}_n^m\mathsf{N}\overbrace{G \cdots G}^{n}X^{(m-1)} \cdots X^{(0)}.$$

Thus we have

Definition 3

$$\mathsf{xtubep}_{m,n} = \hat{\mathsf{W}}^{m-1}(\mathsf{W}^{n-1}(\check{\Phi}_n^m\mathsf{N})(\mathsf{B}^m\check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I}))). \tag{30}$$

Again, because of $\check{\Phi}_n^m$ this program structure is of size $\mathcal{O}(mn)$, but we can avoid this problem by using Church numerals in a slightly more complicated definition:

Definition 4 (xtube**)**

$$\mathsf{xtube}_{m,n} = \hat{\mathsf{W}}^{m-1}(\mathsf{W}^{n-1}(\mathsf{Z}_m\check{\Phi}_n\mathsf{N})(\mathsf{B}^m\check{\mathsf{Y}}(\mathsf{C}_{[m]}\mathsf{I}))). \tag{31}$$

If the terminal groups are shared, then $\hat{\mathsf{W}} = \check{\mathsf{W}}$*; if they are replicated, then* $\hat{\mathsf{W}} = \mathsf{W}$*.*

Its size is

$$\begin{aligned} |\mathsf{xtube}_{m,n}| &= (27m + 12n - 28)\mathsf{S} + (24m + 10n - 22)\mathsf{K} + \\ &\quad (51m + 22n - 48)\mathsf{A} \qquad (32) \\ &= 102m + 44n - 96 \text{ total.} \qquad (33) \end{aligned}$$

The total includes one N and one $\check{\mathsf{Y}}$ in addition to the Ss, Ks, and As. The construction of nanotubes is described by the following theorem:

Theorem 3 (xtube**)**

$$\begin{aligned} \mathsf{xtube}_{m,n}X &\Longrightarrow \mathsf{N}y_1^{(1)} \cdots y_n^{(1)} \qquad (34) \\ &\qquad \text{where } y_k \equiv (y_k^{(0)} X^{(m-1)(n-k)} \cdots X^{(0)(n-k)}). \qquad (35) \end{aligned}$$

As before (Cor. 1), the double parenthesized superscripts represent the sharing of the terminal groups if $\hat{\mathsf{W}} = \check{\mathsf{W}}$*, otherwise, if* $\hat{\mathsf{W}} = \mathsf{W}$*, the first parenthesized number of each pair should be ignored.*

3 Hexagonal Membranes

Our goal is to define a membrane structured as a hexagonal grid such as shown in Figs. 9 and 10. To accomplish this, the following notation will be helpful:

$$\begin{aligned} y_{k,0} &= x'_{k,1}, \qquad (36) \\ y_{k,j} &= (x_{k,j}\, x'_{k,j+1}), \;\; 0 < j < n, \qquad (37) \\ y_{k,n} &= x_{k,n}, \qquad (38) \\ x_{k+1,j} &= (y_{k,j-1}\, y'_{k,j}), \;\; j = 1, \ldots, n; k \geq 1. \qquad (39) \end{aligned}$$

(The primes indicate sharing, as per **Introduction** and Sec. 17 [Mac02a].) Notice that x rows have n elements, and the y rows have $n+1$. Therefore, the grid will be built up one double-row at a time, that is, from $x_{k,j}$ to $x_{k+1,j}$. In accomplishing this, the following lemma will be useful; it will be used for constructing the V-shaped parts of the hexagons (constructed of sharing primitives, Sec. 17 [Mac02a]).

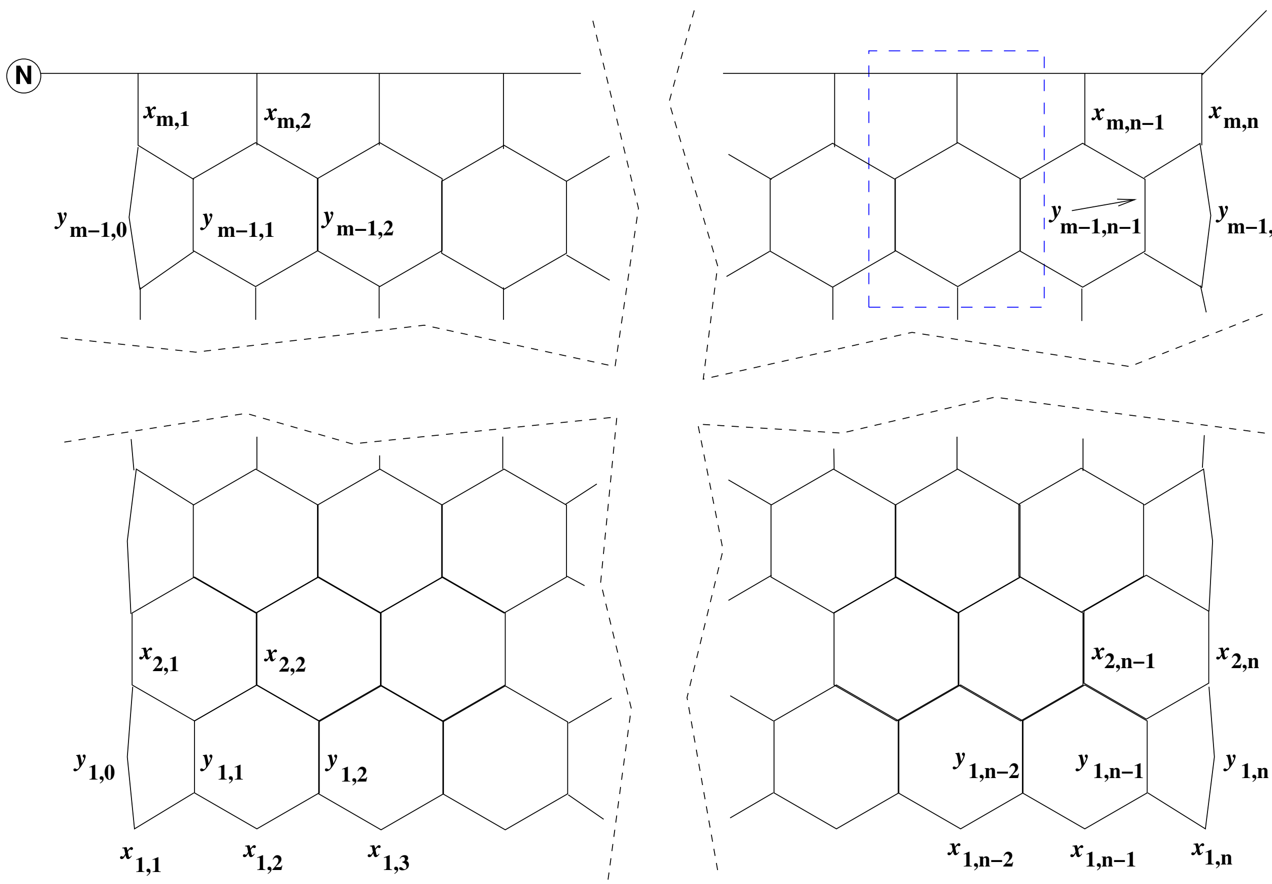

Figure 9: Nanomembrane structured as hexagonal grid. V-shaped junctures are sharing (V) primitives; inverted-V junctures are application (A) primitives. The area in the blue dotted rectangle is expanded in more detail in Fig. 10. Such a grid may be constructed by $\mathsf{hgrid}_{m,n}$ (Def. 8).

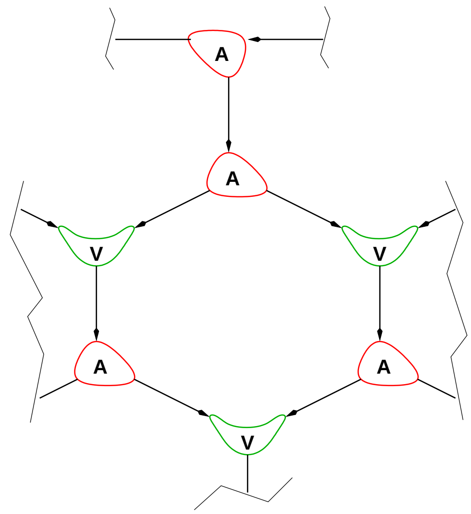

Figure 10: Detailed structure of hexagonal grid. The figure depicts an area near the top of the grid as indicated by the blue dotted rectangle in Fig. 9. A (application) primitives are shown in red; V (sharing) primitives in green. Notice that the uppermost A group is oriented differently from the other A groups.

Lemma 3 *For* $n \geq 0$,

$$\check{\mathsf{W}}_{[n]} F X_1 \cdots X_n \Longrightarrow F X_1' X_1 \cdots X_n' X_n. \tag{40}$$

Proof: This is proved inductively. By Eq. 100 [Mac02a],

$$\check{\mathsf{W}}_{[0]} F \Longrightarrow \mathsf{I} F \Longrightarrow F.$$

For $n \geq 0$ apply Eq. 102 [Mac02a]:

$$\begin{aligned}
\check{\mathsf{W}}_{[n+1]} F X_1 X_2 \cdots X_{n+1} &\Longrightarrow (\mathsf{B}\check{\mathsf{W}}_{[n]} \circ \check{\mathsf{W}}) F X_1 X_2 \cdots X_{n+1} \\
&\Longrightarrow \mathsf{B}\check{\mathsf{W}}_{[n]} (\check{\mathsf{W}} F) X_1 X_2 \cdots X_{n+1} \\
&\Longrightarrow \check{\mathsf{W}}_{[n]} (\check{\mathsf{W}} F X_1) X_2 \cdots X_{n+1} \\
&\Longrightarrow \check{\mathsf{W}} F X_1 X_2' X_2 \cdots X_{n+1}' X_{n+1} \\
&\Longrightarrow F X_1' X_1 X_2' X_2 \cdots X_{n+1}' X_{n+1}.
\end{aligned}$$

□

The following lemma will be used to construct the inverted-V parts of the hexagons (constructed of application or A primitives, Sec. 1 [Mac02a]).

Lemma 4 *For* $n \geq 0$,

$$\mathsf{B}^{[n]} F X_1 Y_1 \cdots X_n Y_n \Longrightarrow F(X_1 Y_1) \cdots (X_n Y_n). \tag{41}$$

Proof: For the base of the induction, apply Eq. 112 [Mac02a]:

$$\mathsf{B}^{[0]}F \Longrightarrow F.$$

For the induction assume $n \geq 0$ and apply Eq. 114 [Mac02a]:

$$\begin{aligned}
\mathsf{B}^{[n+1]}FX_1Y_1X_2Y_2\cdots X_{n+1}Y_{n+1} &\Longrightarrow (\mathsf{B}\circ\mathsf{BB}^{[n]})FX_1Y_1X_2Y_2\cdots X_{n+1}Y_{n+1}\\
&\Longrightarrow \mathsf{B}(\mathsf{BB}^{[n]}F)X_1Y_1X_2Y_2\cdots X_{n+1}Y_{n+1}\\
&\Longrightarrow \mathsf{BB}^{[n]}F(X_1Y_1)X_2Y_2\cdots X_{n+1}Y_{n+1}\\
&\Longrightarrow \mathsf{B}^{[n]}(F(X_1Y_1))X_2Y_2\cdots X_{n+1}Y_{n+1}\\
&\Longrightarrow F(X_1Y_1)(X_2Y_2)\cdots(X_{n+1}Y_{n+1}).
\end{aligned}$$

□

The construction of a y-row from an x-row is accomplished by the following operation:

Definition 5 (Vrow)

$$\mathsf{Vrow}_n = \check{\mathsf{W}}_{[n]}\circ\mathsf{BB}^{[n-1]}. \tag{42}$$

Theorem 4

$$\mathsf{Vrow}_nFx_{k,1}\cdots x_{k,n}\Longrightarrow Fy_{k,0}\cdots y_{k,n}.$$

Proof: By Lemma 3,

$$\check{\mathsf{W}}_{[n]}Fx_{k,1}\cdots x_{k,n}\Longrightarrow Fx'_{k,1}x_{k,1}\cdots x'_{k,n}x_{k,n}.$$

By Lemma 4,

$$\begin{aligned}
&\mathsf{BB}^{[n-1]}Fx'_{k,1}x_{k,1}x'_{k,2}x_{k,2}\cdots x'_{k,n-1}x_{k,n-1}x'_{k,n}x_{k,n}\\
&\quad\Longrightarrow \mathsf{B}^{[n-1]}(Fx'_{k,1})x_{k,1}x'_{k,2}x_{k,2}\cdots x'_{k,n-1}x_{k,n-1}x'_{k,n}x_{k,n}\\
&\quad\Longrightarrow Fx'_{k,1}(x_{k,1}x'_{k,2})\cdots(x_{k,n-1}x'_{k,n})x_{k,n}\\
&\quad= Fy_{k,0}y_{k,1}\cdots y_{k,n-1}y_{k,n}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\mathsf{Vrow}_nFx_{k,1}\cdots x_{k,n} &\Longrightarrow (\check{\mathsf{W}}_{[n]}\circ\mathsf{BB}^{[n-1]})Fx_{k,1}\cdots x_{k,n}\\
&\Longrightarrow \check{\mathsf{W}}_{[n]}(\mathsf{BB}^{[n-1]}F)x_{k,1}\cdots x_{k,n}\\
&\Longrightarrow \mathsf{BB}^{[n-1]}Fx'_{k,1}x_{k,1}\cdots x'_{k,n}x_{k,n}\\
&\Longrightarrow Fy_{k,0}\cdots y_{k,n}.
\end{aligned}$$

□

The construction of an x-row from a y-row is accomplished by the following operation:

Definition 6 (Arow)

$$\mathsf{Arow}_n = \mathsf{B}\check{\mathsf{W}}_{[n-1]} \circ \mathsf{B}^{[n]}. \tag{43}$$

Theorem 5

$$\mathsf{Arow}_n F y_{k,0} \cdots y_{k,n} \Longrightarrow F x_{k+1,1} \cdots x_{k+1,n}.$$

Proof: By Lemma 3,

$$\begin{aligned} \mathsf{B}\check{\mathsf{W}}_{[n-1]} F y_{k,0} y_{k,1} \cdots y_{k,n-1} y_{k,n} &\Longrightarrow \check{\mathsf{W}}_{[n-1]}(F y_{k,0}) y_{k,1} \cdots y_{k,n-1} y_{k,n} \\ &\Longrightarrow F y_{k,0} y'_{k,1} y_{k,1} \cdots y'_{k,n-1} y_{k,n-1} y_{k,n}. \end{aligned}$$

By Lemma 4,

$$\begin{aligned} \mathsf{B}^{[n]} F y_{k,0} y'_{k,1} y_{k,1} \cdots y'_{k,n-1} y_{k,n-1} y_{k,n} &\Longrightarrow F(y_{k,0} y'_{k,1}) \cdots (y_{k,n-1} y_{k,n}) \\ &= F x_{k+1,1} \cdots x_{k+1,n}. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathsf{Arow}_n F y_{k,0} y_{k,1} \cdots y_{k,n-1} y_{k,n} &\Longrightarrow (\mathsf{B}\check{\mathsf{W}}_{[n-1]} \circ \mathsf{B}^{[n]}) F y_{k,0} y_{k,1} \cdots y_{k,n-1} y_{k,n} \\ &\Longrightarrow \mathsf{B}\check{\mathsf{W}}_{[n-1]}(\mathsf{B}^{[n]} F) y_{k,0} y_{k,1} \cdots y_{k,n-1} y_{k,n} \\ &\Longrightarrow \mathsf{B}^{[n]} F y_{k,0} y'_{k,1} y_{k,1} \cdots y'_{k,n-1} y_{k,n-1} y_{k,n} \\ &\Longrightarrow F x_{k+1,1} \cdots x_{k+1,n}. \end{aligned}$$

□

As a consequence, the construction of a double-row is accomplished by:

Definition 7 (drow)

$$\mathsf{drow}_n = \mathsf{Vrow}_n \circ \mathsf{Arow}_n. \tag{44}$$

Theorem 6

$$\mathsf{drow}_n F x_{k,1} \cdots x_{k,n} \Longrightarrow F x_{k+1,1} \cdots x_{k+1,n}.$$

Proof:

$$\begin{aligned} \mathsf{drow}_n F x_{k,1} \cdots x_{k,n} &\Longrightarrow (\mathsf{Vrow}_n \circ \mathsf{Arow}_n) F x_{k,1} \cdots x_{k,n} \\ &\Longrightarrow \mathsf{Vrow}_n(\mathsf{Arow}_n F) x_{k,1} \cdots x_{k,n} \\ &\Longrightarrow \mathsf{Arow}_n F y_{k,0} \cdots y_{k,n} \\ &\Longrightarrow F x_{k+1,1} \cdots x_{k+1,n}. \end{aligned}$$

□

A hexagonal grid is computed by iterating drow_n.

Corollary 4

$$\mathsf{drow}_n^m F x_{k,1} \cdots x_{k,n} \Longrightarrow F x_{k+m,1} \cdots x_{k+m,n}.$$

Proof: By induction on m,

$$\begin{aligned}
(\mathsf{drow}_n)^{m+1} F x_{k,1} \cdots x_{k,n} &\Longrightarrow (\mathsf{drow}_n \circ \mathsf{drow}_n^m) F x_{k,1} \cdots x_{k,n} \\
&\Longrightarrow \mathsf{drow}_n (\mathsf{drow}_n^m F) x_{k,1} \cdots x_{k,n} \\
&\Longrightarrow \mathsf{drow}_n^m F x_{k+1,1} \cdots x_{k+1,n} \\
&\Longrightarrow F x_{k+m+1,1} \cdots x_{k+m+1,n}.
\end{aligned}$$

□

In general, the first x-row can be identical or shared copies of a single x, so $x_{1,j} = x$. Hence an $m \times n$ grid is computed by

$$\hat{\mathsf{W}}^{n-1}(\mathsf{drow}_n^m F)x \Longrightarrow \mathsf{drow}_n^m F \overbrace{xx \cdots x}^{n}$$

where $\hat{\mathsf{W}}$ is either $\check{\mathsf{W}}$ or W, depending on whether sharing of x is desired or not. Therefore we can define a generator for an $m \times n$ hexagonal grid:

Definition 8 (hgrid)

$$\mathsf{hgrid}_{m,n} = \mathsf{Z}_{n-1}\hat{\mathsf{W}}(\mathsf{Z}_m \mathsf{drow}_n \mathsf{N}). \tag{45}$$

The inert combinator (N) is used in place of the combinator F in the preceding derivations to ensure that the grid is static. To decrease the size of the complexes, we have expressed the powers by iterators: $\hat{\mathsf{W}}^{n-1} = \mathsf{Z}_{n-1}\hat{\mathsf{W}}$, $\mathsf{drow}_n^m = \mathsf{Z}_m \mathsf{drow}_n$. The sizes are as follows, for $m \geq 1, n \geq 2$:

$$\begin{aligned}
|\mathsf{Vrow}_n| &= (17n-15)\mathsf{S} + (16n-14)\mathsf{K} + (33n-30)\mathsf{A} = 66n - 59 \text{ total}, && (46) \\
|\mathsf{Arow}_n| &= (17n-10)\mathsf{S} + (16n-10)\mathsf{K} + (33n-21)\mathsf{A} = 66n - 41 \text{ total}, && (47) \\
|\mathsf{drow}_n| &= (34n-23)\mathsf{S} + (32n-22)\mathsf{K} + (66n-46)\mathsf{A} = 132n - 91 \text{ total}, && (48) \\
|\mathsf{hgrid}_{m,n}| &= (3m+37n-17)\mathsf{S} + (2m+34n-12)\mathsf{K} + (5m+71n-29)\mathsf{A} \\
&= 10m + 142n - 57 \text{ total}. && (49)
\end{aligned}$$

The latter total includes 1 for the N primitive.

As Fig. 9 shows, the vertical borders of the hexagonal grid are formed by $y_{k,0} = x'_{k,1}$ and $y_{k,n} = x^{(0)}_{k,n}$. This might be fine, but it also might stretch or bend the linking groups. Be that as it may, it presents an opportunity to show how a slightly different hexagonal grid, a "terminated grid," might be constructed (Figs. 11 and 12). In this grid, $y_{k,0}$ and $y_{k,n}$ are inert (N) complexes, and the deletion of $x'_{k,1}$ and $x^{(0)}_{k,n}$ cause them to be replaced by "result caps" (P primitives; see Secs. 3 and 6 in [Mac02b]). This structure is computed by a modified Vrow:

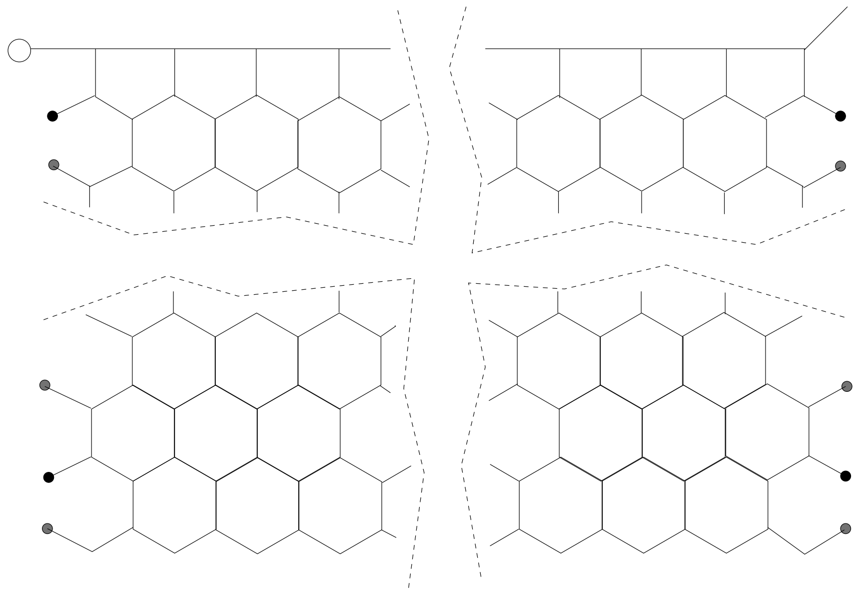

Figure 11: Nanomembrane structured as hexagonal grid with terminal groups. Such a grid may be constructed by $\mathsf{hgridt}_{m,n}$ (Def. 9). Black dots are N primitives, gray dots are P primitives. A visualization of a small grid of this kind is in Fig. 12.

Definition 9 (hgridt**)**

$$\begin{aligned}
\mathsf{Vrowt}_n &= \check{\mathsf{W}}_{[n]} \circ \mathsf{KI} \circ \mathsf{K}_{(2n-2)} \circ \mathsf{B}^{[n-1]} \circ \mathsf{C}^{[n]}\mathsf{IN} \circ \mathsf{CIN}, && (50)\\
\mathsf{drowt}_n &= \mathsf{Vrowt}_n \circ \mathsf{Arow}_n, && (51)\\
\mathsf{hgridt}_{m,n} &= \mathsf{Z}_{n-1}\hat{\mathsf{W}}(\mathsf{Z}_m \mathsf{drowt}_n \mathsf{N}). && (52)
\end{aligned}$$

The correctness of the definition of $\mathsf{hgridt}_{m,n}$ follows from the following theorem.

Theorem 7 *Let*

$$y_{k,0} = y_{k,n} = \mathsf{N}. \tag{53}$$

Then,

$$\mathsf{Vrowt}_n F x_{k,1} \cdots x_{k,n} \Longrightarrow F y_{k,0} \cdots y_{k,n}.$$

Proof: By Lemma 3,

$$\check{\mathsf{W}}_{[n]} F x_{k,1} \cdots x_{k,n} \Longrightarrow F x'_{k,1} x_{k,1} \cdots x'_{k,n} x_{k,n}.$$

By the definitions of K (Eq. 24 [Mac02a]) and I (Eq. 19 [Mac02a]),

$$\mathsf{KI} F x'_{k,1} x_{k,1} \cdots x'_{k,n} x_{k,n} \Longrightarrow F x_{k,1} \cdots x'_{k,n} x_{k,n}.$$

By Eq. 98 [Mac02a],

$$\mathsf{K}_{(2n-2)} F \underbrace{x_{k,1} \cdots x'_{k,n}}_{2n-2} x_{k,n} \Longrightarrow F x_{k,1} \cdots x'_{k,n}.$$

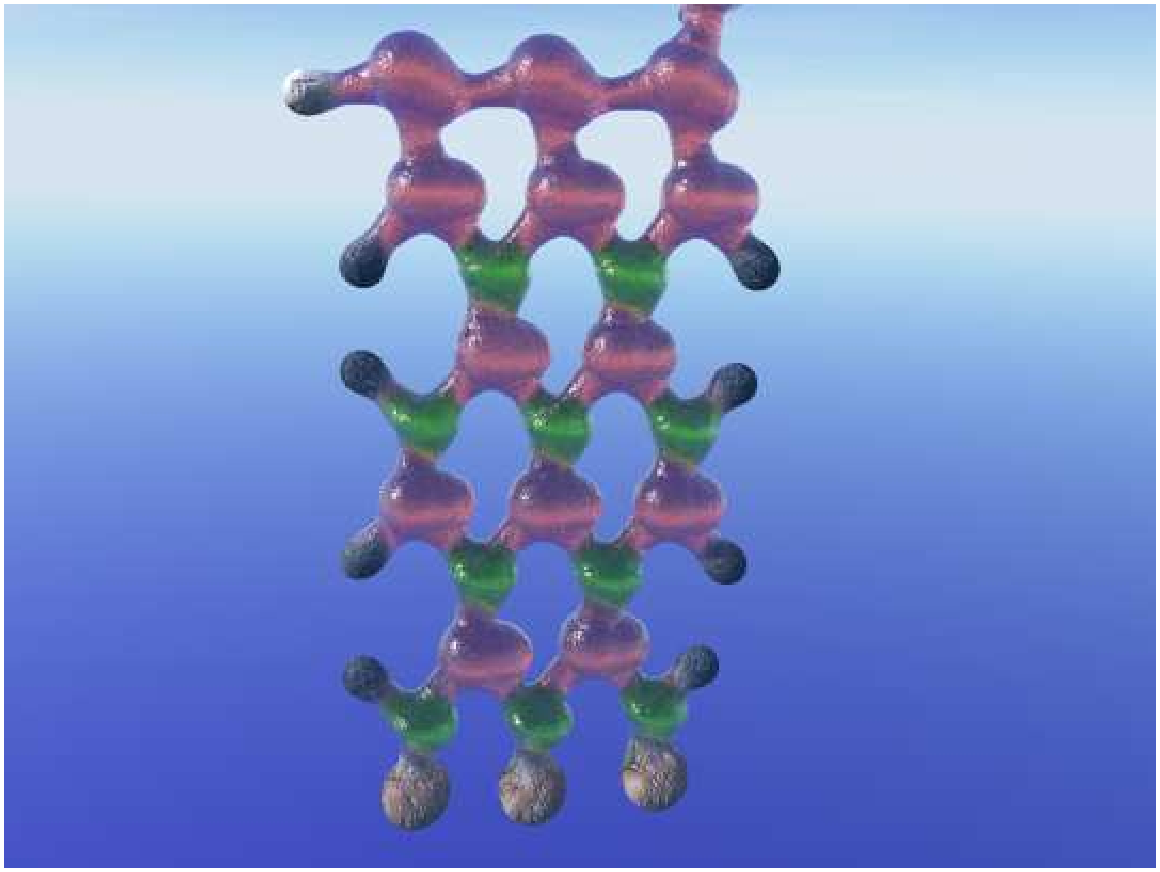

Figure 12: Visualization of small hexagonal grid produced by $\mathsf{hgridt}_{2,3}X$. The reddish structures are A (application) primitives and the greenish are V (sharing) primitives. The dark groups on the left and right are inert place-holders (P and N primitives). The light structure in the upper left is an inert (N) combinator. The three brownish structures on the bottom are copies of X, whatever it might be.

By Lemma 4,

$$\begin{aligned}\mathsf{B}^{[n-1]}Fx_{k,1}x'_{k,2}\cdots x_{k,n-1}x'_{k,n} &\Longrightarrow F(x_{k,1}x'_{k,2})\cdots(x_{k,n-1}x'_{k,n})\\ &= Fy_{k,1}\cdots y_{k,n-1}.\end{aligned}$$

By Eqs. 116 [Mac02a] and 53 (above),

$$\begin{aligned}\mathsf{C}^{[n]}\mathsf{IN}Fy_{k,1}\cdots y_{k,n-1} &\Longrightarrow \mathsf{I}Fy_{k,1}\cdots y_{k,n-1}\mathsf{N}\\ &\Longrightarrow Fy_{k,1}\cdots y_{k,n-1}y_{k,n}.\end{aligned}$$

By the definition of C (Eq. 8 [Mac02a]),

$$\begin{aligned}\mathsf{CIN}Fy_{k,1}\cdots y_{k,n-1}y_{k,n} &\Longrightarrow \mathsf{I}F\mathsf{N}y_{k,1}\cdots y_{k,n-1}y_{k,n}\\ &\Longrightarrow Fy_{k,0}y_{k,1}\cdots y_{k,n-1}y_{k,n}.\end{aligned}$$

□

Figure 12 is a depiction of the hexagonal grid constructed by $\mathsf{hgridt}_{2,3}X$; it may be understood by comparison with Figs. 10 and 11.

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[Mac02a] Bruce J. MacLennan. Molecular combinator reference manual — UPIM report 2. Technical Report CS-02-489, Dept. of Computer Science, University of Tennessee, Knoxville, 2002. Available at http://www.cs.utk.edu/~library/TechReports/ 2002/ut-cs-02-489.ps.

[Mac02b] Bruce J. MacLennan. Replication, sharing, deletion, lists, and numerals: Progress on universally programmable intelligent matter — UPIM report 3. Technical Report CS-02-493, Dept. of Computer Science, University of Tennessee, Knoxville, 2002. Available at http://www.cs.utk.edu/~library/TechReports/ 2002/ut-cs-02-493.ps.