HW4 Molecular Programming

M2ICA CR16

2026.01.21 - Due on None

You are asked to complete the exercise marked with a [★] and to send me your solutions to:

nicolas.schabanel@ens-lyon.fr

as a PDF file named **HW4-Lastname.pdf** on **None**.

■ **Exercise 1 (The power of zigzag assembly).** In this exercise we want to assemble at temperature $T^\circ = 2$, a pyramide P_n of size $(2n+1) \times (n+1)$ with its bottom line as the seed (in darker gray) as illustrated in Fig. 1.

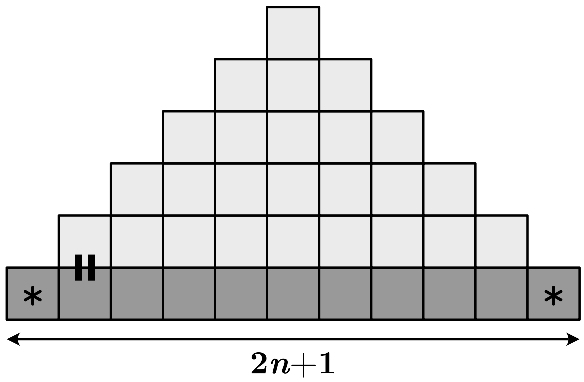


Figure 1: Question 1.1)

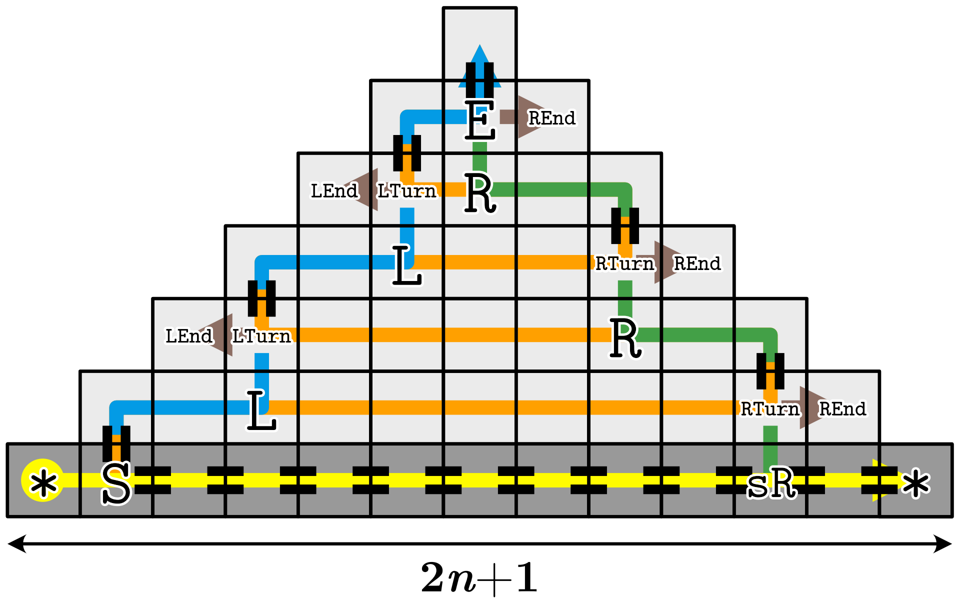
► **Question 1.1)** *Provide a fixed tile set (independent of n) that at temperature $T^\circ = 2$, assembles the pyramide P_n, for any n, from its (assumed to be already assembled) bottom row (in darker gray in Fig. 1), with the following constraints:*

- *You are only allowed one glue of strength 2 connecting each pair of rows and the first glue of strength 2 has to be in the left corner of the bottom row seed as illustrated in 1.*
- *Furthermore, you are allowed to distinguish only $o(n)$ tiles in the seed bottom row; all the other tiles must be indistinguishable.*

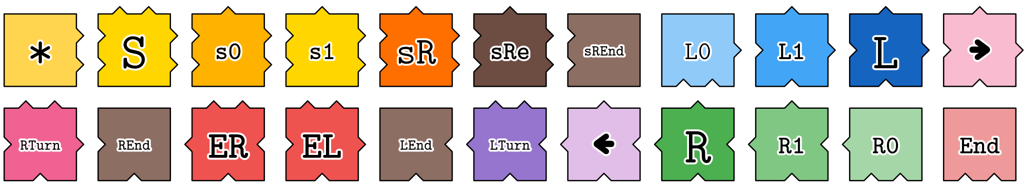
Provide the tile set as well as a generic assembly indicating the assembly order. Is it ordered? No justification asked.

▷ *Hint. Decide first where you place the glue of strength 2 between each row.*

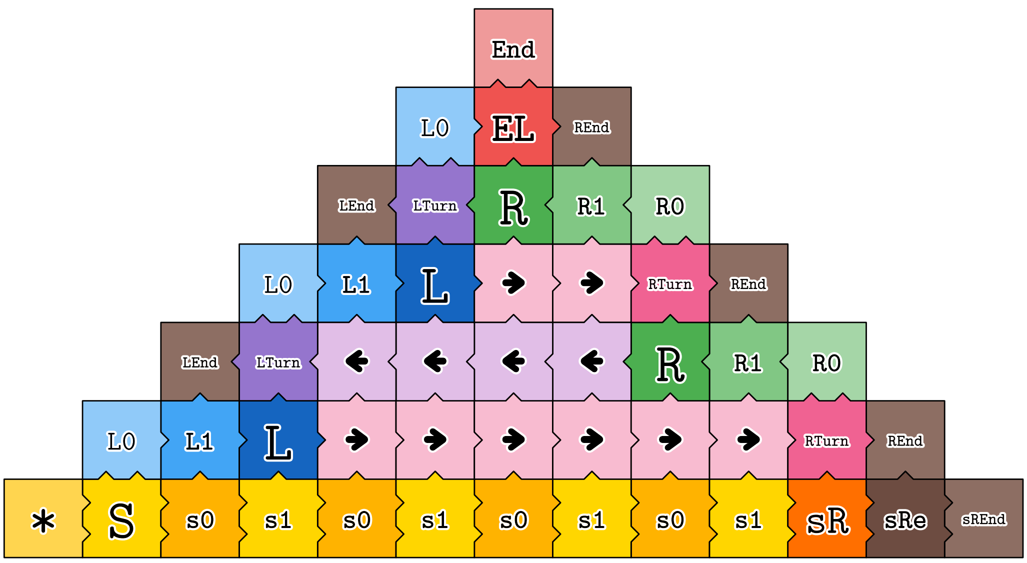
Answer. ▷ The assembly grows according to a zigzag pattern. The previous row always places a signal tile L or R two steps after it began, to indicate to the next row when to turn. This allows to turn just before the last tile of each row. Here is the order of assembly with the main signals and the positions of the glue of strength 2 between the rows:



22 tiles are enough to implement the assembly (glues are not displayed but only the tiles placed next to each other in the assembly bellow attract each other)):



Here is a generic assembly:



Note that the distinction between tiles s0 and s1 is not necessary for this question. Only 2 tiles need to be distinguished in the seed row for the assembly: S and sR. The tile set is ordered as shown above. ◁

▶ **Question 1.2)** *Provide a constant number of dedicated tiles that assemble non-deterministically the seed bottom row required for your tile set for any n, and only these bottom rows.*

Provide a generic assembly. Is it ordered? No justification asked.

▷ Hint. *The only non-determinism must be in the value of n. There must be a single assembly of the seed for every fixed value of n.*
Answer. ▷ The seed tiles (in yellow above) non-deterministically assemble from tile $\boxed{*}$, from left to right, a row for any $n \geqslant 1$:

$$\boxed{*}\boxed{\texttt{S}}\left(\boxed{\texttt{s0}}\boxed{\texttt{s1}}\right)^{n-1}\boxed{\texttt{sR}}\boxed{\texttt{sRe}}\boxed{\texttt{sREnd}}$$

which is the base of the pyramide P_n. The value of n is determined when the tile $\boxed{\texttt{sR}}$ attaches instead of tile $\boxed{\texttt{s0}}$. ◁

■ **Exercise 2 (Window Movie Lemma).** We investigate the computation power of tile assembly at temperature $T^\circ = 1$. We allow *mismatches*, i.e. a tile can be added to the current aggregate as soon as it is attached by *at least one side* to the current aggregate for which the glues match (the other sides in contact can have mismatching glues). Unless specified explicitly otherwise, all assemblies take place at $T^\circ = 1$ in this exercise.

Let us first consider a (finite) tile set $\mathcal{T}$ which only assembles unidimensional segments of size $1 \times \ell$ for some $\ell \geqslant 1$ starting from its seed tile. Let $\tau = |\mathcal{T}|$ denote the number of tile types in $\mathcal{T}$ in all of the following. Recall that the *final productions* of a tileset $\mathcal{T}$ are the shapes corresponding to every possible assembly of tiles from $\mathcal{T}$ starting from the seed tile of $\mathcal{T}$ and where no more tile can be added.

► **Question 2.1)** *Show (and explicit) that there is a constant $k(\tau)$, which depends only on τ, such that if a segment of size $1 \times \ell$ with $\ell \geqslant k(\tau)$ is a final production of $\mathcal{T}$, then there is an integer $1 \leqslant i < k(\tau)$ such that all the segments $1 \times (\ell + n \cdot i)$ are also final productions of $\mathcal{T}$ for all $n \geqslant -1$. If so, we say that the tile set $\mathcal{T}$ is pumpable.*
Answer. ▷ Any $1 \times \ell$ final production $t_1 \dots t_\ell$ of length $\ell \geqslant k(\tau) =_{\text{def}} \tau + 1$ contains a tile type t repeated twice. Let $L < R$ be the closest indices (also the smallest in case of ties) such that $t_L = t_R = t$. We have $R - L < k(\tau)$. Then, at $T^\circ = 1$, each segment $t_1 \dots t_{L-1}(t_L \dots t_R)^n t_{R+1} \dots t_\ell$ is also a final production of $\mathcal{T}$ for any $n \geqslant 0$ with length $\ell + (n-1)(R - L + 1)$. ◁

Let us now consider a (finite) tile set $\mathcal{T}$ whose final productions are 2-thick rectangles of size $2 \times \ell$ for some $\ell \geqslant 1$.

► **Question 2.2)** *Show (and explicit) that there is a constant $k_2(\tau)$, which depends only on τ, such that if a 2-thick rectangle of size $2 \times \ell$ with $\ell \geqslant k_2(\tau)$ is a final production of $\mathcal{T}$, then $\mathcal{T}$ is pumpable, i.e. that there is an integer $1 \leqslant i < k_2(\tau)$ such that all the 2-thick rectangles $2 \times (\ell + n \cdot i)$ are also final productions of $\mathcal{T}$ for all $n \geqslant -1$.*
▷ Hint. *Pay attention to the order in which the tiles are attached, make sure that the pumped structure can indeed self-assemble.*
Answer. ▷ We use the same idea, but instead on focusing on tiles, we will focus on the borders between the tiles and record on each border which glues are placed on both sides and from which direction was the tile attached: for each vertical line cutting the final production, there are two borders on top of each other; for each border, there two glues, one on each side, and three possible directions of attachment ($\rightarrow$, $\leftarrow$ and none if the glues were not used to attach the tiles on either side). Let $\gamma \leqslant 4\tau$ be the number of glues. There are thus at most: $(gamma^2 \times 3)^2 \leqslant 2304\tau^2$ different types of vertical lines. It follows that any $2 \times \ell$ final production with $\ell \geqslant k_2(\tau) := 2304\tau^2 + 1$, contains two vertical lines with identical borders (identical glues and assembly order on both sides).

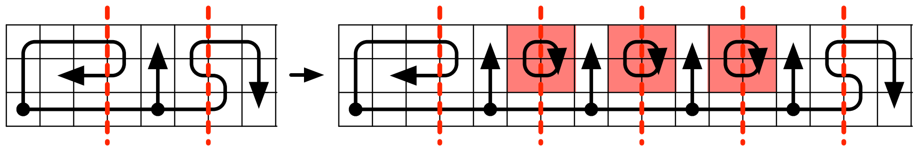
Let t_{ij}, $1 \leqslant i \leqslant 2$ and $1 \leqslant j \leqslant \ell$ be a final production with $\ell \geqslant k_2(\tau)$. Again, let $L < R$ be the closest indices (also the smallest in case of ties) such that the borders cut by the two vertical lines at L and R are identical. We have $R - L < k_2(\tau)$. Consider now the rectangles

$$\begin{matrix} t_{1,1} & \dots & t_{1,L-1} \\ t_{2,1} & \dots & t_{2,L-1} \end{matrix} \begin{pmatrix} t_{1,L} & \dots & t_{1,R} \\ t_{2,L} & \dots & t_{2,R} \end{pmatrix}^n \begin{matrix} t_{1,R+1} & \dots & t_{1,\ell} \\ t_{2,R+1} & \dots & t_{2,\ell} \end{matrix}$$

with $n \geqslant 0$. The borders (glues + assembly direction) match on each side of the pumped pattern. Thus the glues along the direction of assembly match. We just need to check that repeating the pattern does not create cycles in the assembly directions. Indeed, if there was a cycle, it would exists between two consecutive patterns (because their borders are identical, we can deleted pattern between the leftmost and rightmost part of the cycle). Now because the height of the pattern is 2 this would then imply that the cycle would disconnect the pattern in two parts that would not have been attached originally. Contradiction. It follows that every one of these rectangles can be assembled and are thus also final productions of $\mathcal{T}$ with size $2 \times (\ell + (n-1)(R-L+1))$. ◁

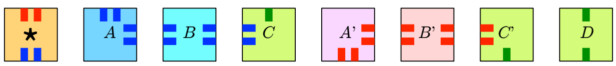
Let us now generalise and consider a (finite) tile set $\mathcal{T}$ whose final productions are q-thick rectangles of size $q \times \ell$ for some $\ell \geqslant 1$.

▶ **Question 2.3)** *Show (and explicit) that there is a constant $k_q(\tau)$, which depends only on τ, such that if a q-thick rectangle of size $q \times \ell$ with $\ell \geqslant k_q(\tau)$ is a final production of $\mathcal{T}$, then $\mathcal{T}$ is pumpable, i.e. that there is an integer $1 \leqslant i < k_q(\tau)$ such that all the q-thick rectangles $q \times (\ell + n \cdot i)$ are also final productions of $\mathcal{T}$ for all $n \geqslant -1$.*
Answer. ▷ For $q \geqslant 3$, remembering the direction in which each glue is used is not enough to avoid cycles. See for instance the example below:

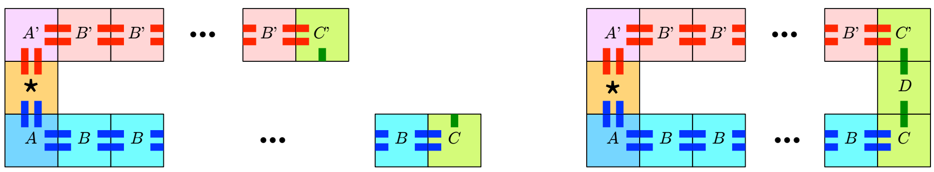


We thus record along each vertical line which tiles, where and in which order they are placed along the line. This consists in a sequence of $2q$ tiles and positions (i, s) where $1 \leqslant i \leqslant q$ and $s \in \{L, R\}$ stand for the position and side of the line resp. where the tile was placed. There are thus at most $k_q(\tau) = \tau^{2q} \cdot (2q)!$ such sequences. If $\ell > k_q(\tau)$, there must to two distinct lines with identical assembly sequence. Let us show that the segment between those two lines is indeed pumpable. [TO DO...]
◁

Consider the following tile set $\mathcal{U} = \{\bigstar, A, B, C, A', B', C', D\}$ at $T^\circ = 2$ for which $\bigstar$ is the seed tile:



The final productions of $\mathcal{U}$ at $T^\circ = 2$ consist of two arms which are either 1) of different lengths and then don't touch eachother; or 2) of equal length and then there is a tile D that makes contact between them:



▶ **Question 2.4)** *Show that no tile set can simulate intrinsically at $T^\circ = 1$, the dynamics of $\mathcal{U}$ at $T^\circ = 2$.*
▷ *Hint. As a simplification, consider that in an intrinsic simulation, all megacell corresponding to an empty position in the simulated system must never be filled by more than 30% of tiles, and all*

megacell corresponding to a non-empty position in the simulated system must be filled at 100% *by tiles. If you have time left: how would you waive these assumptions?*

Answer. ▷ Proof sketch. Consider a tile set $\mathcal{T}$ that simulates intrinsically at $T^\circ = 1$ the dynamics of $\mathcal{U}$ at some scale q. $\mathcal{T}$ grows two arms of any length. In particular, $\mathcal{T}$ has to simulate the shapes with two arms of equal length $\ell \geqslant \times k_q(|\mathcal{T}|)/q$. From the above, these two arms are thus pumpable, let's pump once the arm bellow. Then we have two contradicting situations: in the first situation $\mathcal{T}$ must fill the megacell between the two arm ends which are aligned, and in the second, it must not because they are not aligned. As the assembly takes place at $T^\circ = 1$, at least one of the two simulated arms must grow a pattern that will fill at least 50% of the megacell in both situation leading to a contradiction. ◁