HW4 Molecular Programming

M2IF SCR1

12.12.2019 - **Due on *Wed 19/12* before 12:00**

You are asked to complete questions 1.1), 1.2) and 1.3) and to send me your solutions to:
`nicolas.schabanel@ens-lyon.fr`
as a PDF file named `HW4-Lastname.pdf` on ***Wed 19/12* before 12:00**.

■ **Exercise 1 (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 1.1)*** *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.

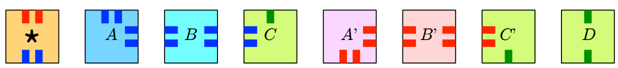
Let us now consider a (finite) tile set $\mathcal{T}$ whose final productions are 2-thick rectangles of size $2 \times \ell$ for some $\ell \geqslant 1$.

▶ ***Question 1.2)*** *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.*

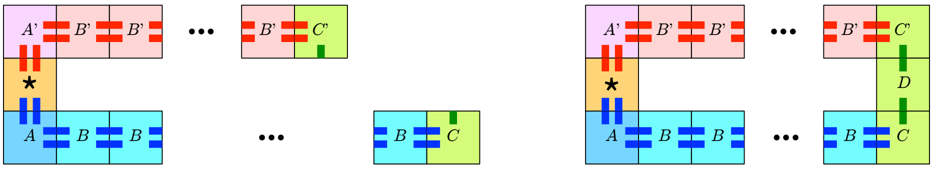
Let us now generalise and consider a (finite) tile set $\mathcal{T}$ whose final productions are q-thick rectangles of size $q \times \ell$ for some $\ell \geqslant 1$.

▶ ***Question 1.3)*** *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 $n \geqslant -1$.*

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 1.4)*** *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?*

■ **Exercise 2 (Oritatami).** Let first us recall the definition of an Oritatami system:

Triangular lattice. Consider the triangular lattice defined as $\mathbb{T} = (\mathbb{Z}^2, \sim)$, where $(x,y) \sim (u,v)$ if and only if $(u,v) \in \cup_{\varepsilon=\pm 1}\{(x+\varepsilon,y),(x,y+\varepsilon),(x+\varepsilon,y+\varepsilon)\}$. Every position (x,y) in $\mathbb{T}$ is mapped in the euclidean plane to $x \cdot X + y \cdot Y$ using the vector basis $X = (1,0) = \longrightarrow$ and $Y = \text{RotateClockwise}\,(X, 120°) = (-\frac{1}{2}, -\frac{\sqrt{3}}{2}) = \swarrow$.

Oritatami systems. Let B denote a finite set of *bead types*. Recall that an *Oritatami system* (OS) $\mathcal{O} = (p, \heartsuit, \delta)$ is composed of:

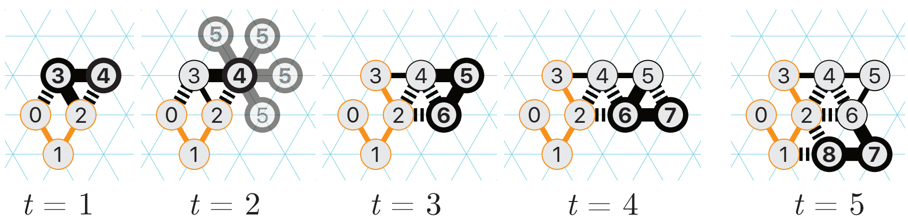
1. a bead type sequence $p \in B^*$, called the *transcript*;
2. an *attraction rule*, which is a symmetric relation $\heartsuit \subseteq B^2$;
3. a parameter δ called the *delay*.

Given a bead type sequence $q \in B^*$, a configuration c of q is a self-avoiding path in $\mathbb{T}$ where each vertex c_i is labelled by the bead type q_i.

We say that two bead types a and $b \in B$ *attract* each other when $a \heartsuit b$. Furthermore, given a partial configuration c of a bead type sequence q, we say that there is a *bond* between two adjacent positions c_i and c_j of c in $\mathbb{T}$ if $q_i \heartsuit q_j$ and $|i-j| > 1$.

Oritatami growth dynamics. given an OS $\mathcal{O} = (p, \heartsuit, \delta)$ and a *seed configuration* σ of a *seed bead type sequence* s, the configuration at time 0 is $c^0 = \sigma$. The configuration c^{t+1} at time $t+1$ is obtained by extending the configuration c^t at time t by placing the next bead, of type p_{t+1}, at the position(s) that maximize(s) the number of bonds over all the possible extensions of configuration c^t by δ beads. When the maximizing position is always unique, we say that the OS is deterministic. We shall only consider deterministic OS in this exercise.

Example. The OS $\mathcal{O} = (p, \heartsuit, \delta = 2)$ with bead types $\mathcal{B} = \{0, \ldots, 8\}$, transcript $p = \langle 3,4,5,6,7,8 \rangle$, rule $\heartsuit = \{0 \heartsuit 3, 0 \heartsuit 6, 1 \heartsuit 8, 2 \heartsuit 4, 2 \heartsuit 6, 2 \heartsuit 8, 4 \heartsuit 6, 5 \heartsuit 7\}$ and seed configuration $\sigma = \langle 0@(0,0); 1@(1,1); 2@(1,0) \rangle$, folds deterministically as follows:

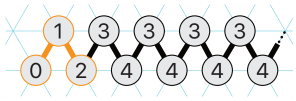


The seed configuration σ is drawn in orange. The folded transcript is represented by a black line. The bonds made are represented by dotted black lines. The $\delta = 2$ beads currently folding at time t are represented in bold. If there are several extensions that maximize the number of bonds, the freely moving part is represented translucently. Observe two remarkable steps:

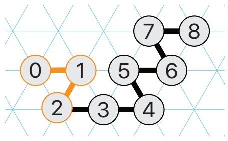
- $t = 2$ and 3: the position of 5 is not determined when 4 is placed, but will be fixed when 5 and 6 are folded together.
- $t = 4$ and 5: 7 is initially placed next to 5 when 6 and 7 are folded together but will be finally placed to the right of 8 when 7 and 8 are folded together (because two bonds can be made there instead of only one) and 7 will thus remain there.

In the following, you are asked to propose a rule and a delay that folds the transcript in the desired configuration for the given seed.

▶ ***Question 2.1)*** *Propose a delay-1 OS that, given the seed configuration $\langle 0, 1, 2\rangle$ below, folds the transcript $\langle 3, 4, 3, 4, 3, 4, \ldots\rangle$ as: (just draw the bonds, no justification asked)*

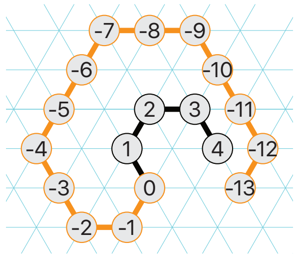


▶ ***Question 2.2)*** *Is there a delay-1 OS that, given the seed configuration $\langle 0, 1, 2\rangle$ below, folds the transcript $p = \langle 3, 4, 5, 6, 7, 8\rangle$ deterministically as below? Justify your answer.*

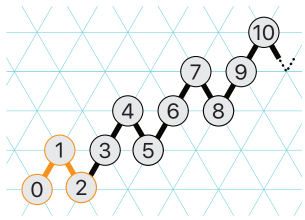


Propose a delay-2 OS that folds p as desired.

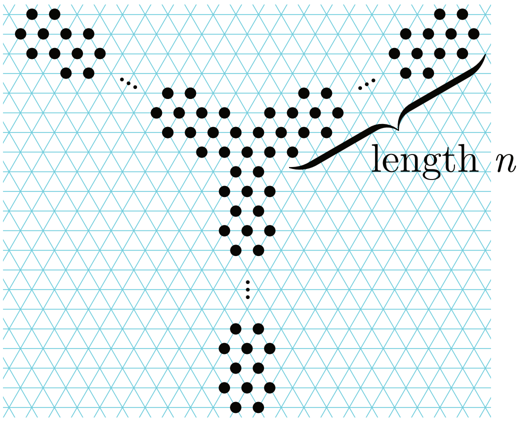
▶ ***Question 2.3)*** *Propose a delay-2 OS that, given the seed configuration $\langle -13, \ldots, -1, 0\rangle$ below, folds the transcript $p = \langle 1, 2, 3, 4\rangle$ deterministically as below. Draw and explain the key steps of the folding.*



▶ ***Question 2.4)*** *Prove that there is no delay-2 OS that, given the seed configuration $\langle 0, 1, 2\rangle$ below, folds the transcript $p = \langle 3, 4, \ldots\rangle$ deterministically along the path $(\nearrow\nearrow\searrow)^\infty$ as below.*



Conclude that there is no delay-2 deterministic OS with a fixed-size seed configuration that can cover exactly the positions of the following 3-arm star for large enough n:


length n