HW3 M2IF CR07 Molecular Programming

2023.10.10 - Due on Fri. 10.20 before 13:30

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 **HW3-Lastname.pdf** on **Fri. 10.20 before 13:30**.

■ **Exercise 1 (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 $(u, v) \in \cup_{\varepsilon=\pm1}\{(x + \varepsilon, y), (x, y + \varepsilon), (x + \varepsilon, y + \varepsilon)\}$. 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 $Y =$ 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 $p \in B^*$, a configuration c of p is a self-avoiding path in $\mathbb{T}$ where each vertex c_i is labelled by the bead type p_i.

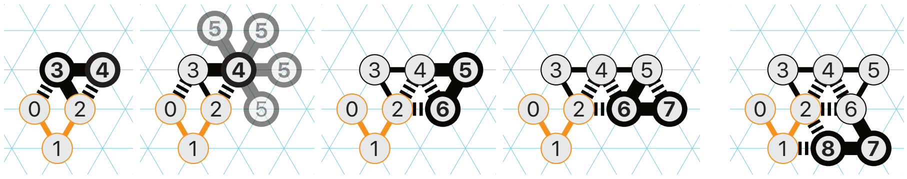
We say that two bead types a and $b \in B$ *attract* each other when $a \heartsuit b$. Furthermore, given a partial configuration c of a bead type sequence q, we say that there is a *bond* between two adjacent positions c_i and c_j of c in $\mathbb{T}$ if $q_i \heartsuit q_j$ and $|i - j| > 1$.

Notations. We denote by $c^{\rhd\delta}$ the set of all configurations extending configuration c by δ beads. We call *nascent* the δ last beads of an extension $c' \in c^{\rhd\delta}$. We denote by $h(c)$ the number of bonds made in a configuration c. We denote by $h_i(c)$ the number of bonds made with the bead indexed i in c. Given an extension $c' \in c^{\rhd\delta}$ we denote by $n(c')$ the number of bonds made by the nascent beads in c': $n(c') = h(c') - h(c)$.

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 $c^0 = \sigma$. We index negatively the beads of $\sigma = \sigma_{-|\sigma|+1} \ldots \sigma_0$ so that the non-seed beads are indexed from 1 to t in configuration c^t at time t. 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. We call *favorable extension* any such extension by δ beads which maximizes the number of bonds. We denote by $F(c) = \arg\max_{\gamma \in c^{\rhd\delta}} h(\gamma)$ the set of all favorable extensions of c by δ beads. When the maximizing position is always unique (i.e. if all favorable extension always place the next bead p^{t+1} at the same location), we say that the OS is *deterministic*. We will only consider deterministic OS in this exercise.

We say that an OS is *non-blocking* if at all step, all favorable extensions can be extended by at least one bead.

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:



$t = 1$ $\quad$ $t = 2$ $\quad$ $t = 3$ $\quad$ $t = 4$ $\quad$ $t = 5$

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 $\delta = 2$ nascent beads are represented in bold. If there are several favorable extensions, the freely moving nascent part is represented translucently. Observe two remarkable steps:

- $t = 2$ and 3: the position of 5 is not determined when 4 is placed (indeed, there are several favorable extensions placing 5 at different locations), 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.

Crucial step. Consider a deterministic OS. Let us denote by c^∞ its final configuration. We say that step t is *crucial* for the nascent bead indexed by k if all favorable extensions of c^{t-1} agree to place bead indexed by k at its final location in c^∞ whereas it was not the case for all the favorable extensions of c^{t-2}. For instance, there are exactly two crucial steps in the example above: steps 3 and 5 which are crucial for beads 5 and 7 respectively.

We now consider a non-blocking deterministic OS.

▶ **Question 1.1)** *Prove that for all configuration $c' \in c^{t \triangleright \delta}$, $n(c') \leqslant 4\delta + 1$.*
▷ *Hint. how many bonds can make a nascent bead?*

▶ **Question 1.2)** *Prove that: if for some $1 \leqslant i < \delta$, there is $c' \in F(c^{t-1})$ such that c' and c^∞ disagree on the position of the bead indexed by $t + i$ (i.e., $c'_{t+i} \neq c^\infty_{t+i}$), then there is a crucial step t' with $t < t' < t + \delta$.*

Let us denote by $N(c)$ the maximum number of bonds made by nascent beads in an extension of c: $N(c) = \max_{\gamma \in c^{\triangleright\delta}} n(\gamma) = \max_{\gamma \in c^{\triangleright\delta}} h(\gamma) - h(c)$.

▶ **Question 1.3)** *Prove that at all time t, for a non-blocking OS:*

1. $N(c^{t-1}) \leqslant N(c^t) + h_t(c^t)$
2. *furthermore, if step t is crucial, then:* $N(c^{t-1}) \leqslant N(c^t) + h_t(c^t) - 1$

We want to prove that there is no non-blocking OS that can fold a long enough straight line. By contradiction, let's consider a deterministic OS $\mathcal{O}$ with delay δ and a seed σ whose terminal configuration is a straight line of length L.

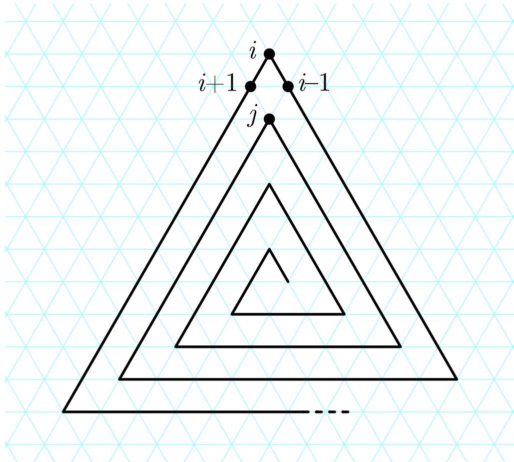
▶ **Question 1.4)** *Show that at all step t, there is always a favorable extension of c^{t-1} that does not place the last nascent bead, indexed by $t + \delta - 1$, at its final position.*

▶ **Question 1.5)** *Show that there are at least $\lfloor (L - |\sigma|)/\delta \rfloor$ crucial steps in the folding of $\mathcal{O}$.*

▶ **Question 1.6)** *Conclude that $L \leqslant |\sigma| + O(\delta^2)$.*

It follows that there is no non-blocking deterministic OS that can fold into a long enough straight line. Surprisingly enough, there is a blocking deterministic delay-6 OS that can fold into arbitrary long straight line!

[★] Exercise 2 (Oritatami — Impossible triangle path). We want to prove that no deterministic oritatami system with delay $\delta \leqslant 2$ can fold according to the infinite triangular spiral below. Recall that the transcript t of an oritatami system (t is the sequence of bead types) is *ultimately periodic*, i.e. there is an i_0 and a period T such that for all $i \geqslant 0$, $t_{i_0+i} = t_{i_0+T+i}$.

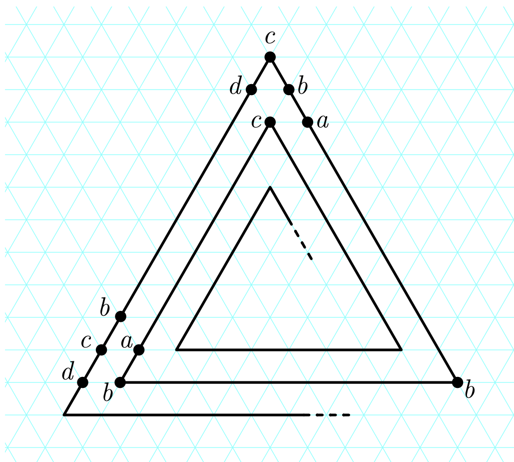


▶ Question 2.1) *Prove than no deterministic delay-1 oritatami system can fold according to this spiral.*

Let us consider now a deterministic delay-2 oritatami system that would fold according to the infinite triangular spiral.

▶ Question 2.2) *Prove that 2 bonds are required to place the bead correctly at each corner.*

▶ Question 2.3) *Show that there are 4 consecutive bead types a, b, c, d in the transcript that get placed as follows:*



▶ Question 2.4) *Show that in order to stabilize c in the lower left corner, c must bind with a.*

▶ Question 2.5) *Conclude that c cannot be placed deterministically at the top corner.*

▶ Question 2.6 (★★★)) *What about deterministic oritatami systems with larger delays?*