HW3 Molecular Programming

MPRI 2.11.1

05.11.2018 - **Due on Mon. 12/11 before 12:45**

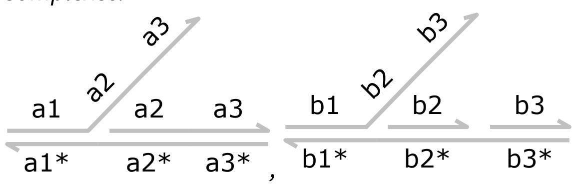
You are asked to complete the exercise marked with a [★] and to send me your solutions to:
nicolas.schabanel@ens-lyon.fr
as a PDF file named **HW3-Lastname.pdf** on **Mon. 12/11 before 12:45**.

[★] Homework: Solve exercise 1.

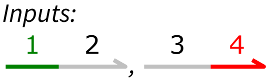
■ **Exercise 1 (DNA circuits).** In the following, long domains are represented in grey and toeholds in color.

Assume a binding rate of 0.116 and unbinding rate of 0.003 for the short domains (toeholds), compute the graph of all possible evolutions for the following mixes. Gives the main path of the evolution. What are the output(s)? Explain what each mix computes.

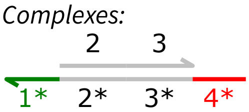
▶ ***Question 1.1)*** *Mix 1*
Complexes:



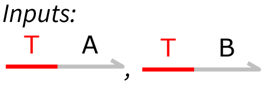
▶ ***Question 1.2)*** *Mix 2*
Inputs:



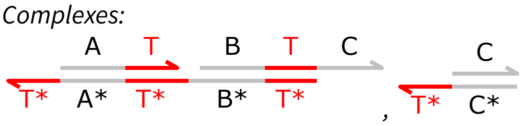
Complexes:



▶ ***Question 1.3)*** *Mix 3*
Inputs:

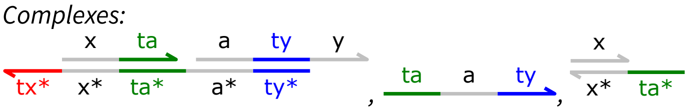


Complexes:



▶ ***Question 1.4)*** *Mix 4*
Inputs:

Complexes:



■ **Exercise 2 (Building shapes with Oritatami).** In this exercise, we will build shapes using the Oritatami co-transciptional folding model. We will show that as opposed to tile assembly systems, Oritatami systems only need a small constant upscaling to build any shape.

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 $Y =$ 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* $\mathcal{O} = (p, \heartsuit, \delta)$ is composed of:

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

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

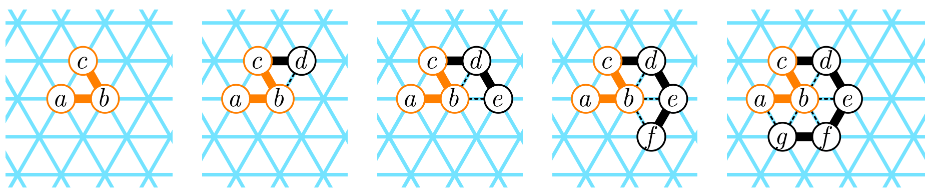
We say that two bead types a and $b \in B$ *attract* each other when $a \heartsuit b$. Furthermore, given a partial conformation c of a bead type sequence q, we say that there is a *bond* between two adjacent positions c_i and c_j of c in $\mathbb{T}$ if $q_i \heartsuit q_j$ and $|i - j| > 1$.

In this exercise, we shall only consider very simple Oritatami systems with delay time $\delta = 1$, in which the conformation grows one bead at a time, from a *seed conformation* (a few beads placed before the folding process starts, to guide the construction), and where every new bead adopts the position(s) that maximises its number of bonds with the current conformation.

Formally, given a delay-1 Oritatami system $\mathcal{O} = (p, \heartsuit, 1)$ and a *seed conformation* σ of a *seed bead type sequence* s, the conformation at time 0 is σ. The conformation at time $t + 1$ is obtained by extending the conformation at time t by placing the next bead, of type p_t, at the position(s) which maximises it number of bonds with the current conformation.

We say that the Oritatami system is *deterministic* if there is only one such position. We will only consider deterministic Oritatami systems in this exercise.

Example. The Oritatami system $\mathcal{O} = (p, \heartsuit, 1)$ with bead types $B = \{a, b, c, d, e, f, g\}$, primary structure $p = defg$, rule $\heartsuit = \{a \heartsuit g, b \heartsuit d, b \heartsuit e, b \heartsuit f, b \heartsuit g, e \heartsuit g\}$ and seed conformation $\sigma = \langle(0, 0), a; (1, 0), b; (0, -1), c\rangle$, folds as follows:



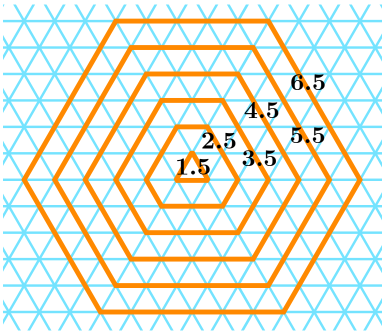
$t = 0$ $t = 1$ $t = 2$ $t = 3$ $t = 4$

The seed conformation σ is drawn in orange. The primary structure is represented by a thick black line. The bonds made are represented by dotted black lines. Note that even if g is attracted by e, it gets placed to the west of f as it makes there two bonds with a and b.

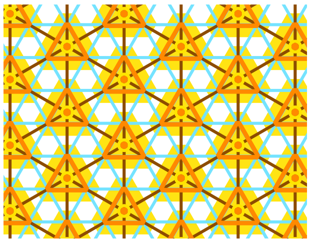
Shapes. A *shape* is a connected subset of vertices of the triangular lattice. We want to design an Oritatami system that can fold any given shape at some suitable scale.

► ***Question 2.1)*** *Exhibit a (simple) shape that cannot be folded by any given Oritatami system $\mathcal{O}$ with delay time 1. Prove it.*

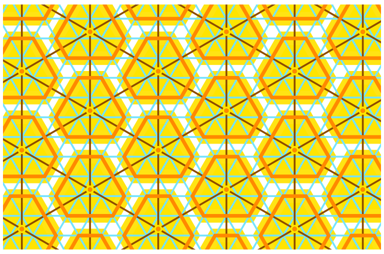
We thus need to upscale the shape if we want a general building scheme. Consider the following upscaling scheme where the vertices of the triangular lattice are replaced by nonoverlapping hexagons whose sides count respectively $n+1, n, n+1, n, n+1$, and n vertices when considered in clockwise order starting from the north side, as shown bellow:



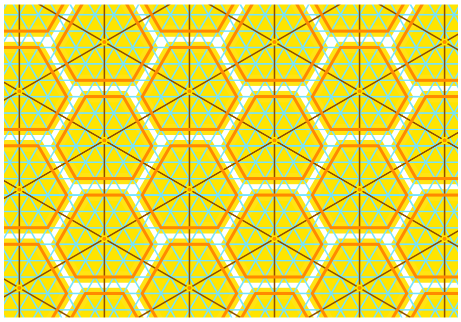
The hexagons at different scales



Scale 1.5 ($n = 1$)



Scale 2.5 ($n = 2$)



Scale 3.5 ($n = 3$)

The underlying upscaled (and rotated) triangular lattice is highlighted in brown.

We say that this correspond to scale $n+0.5$ as $n+0.5$ is the average number of vertices per side. Note that the vertices are upscaled as unit triangles when $n = 1$. Indeed, these hexagons correspond to the consecutive concentric extensions of this unit triangle. Note that any shape is rotated by 30° counterclockwise when upscaled according to this scheme, as shown in the figure 1 on page 5.

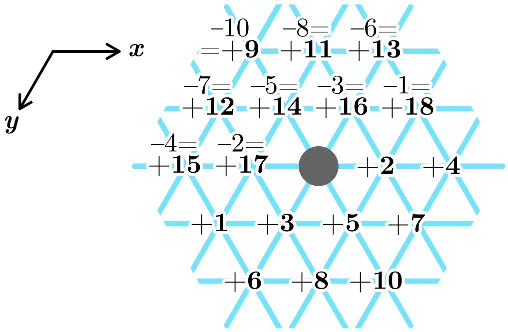
In the following, we will only consider scales $n + 0.5$ with $n \leqslant 3$.

Consider the two following paths of length 27 that cover the hexagon at scale 3.5, starting from either the smaller side (in blue), or the larger side (in black):

► ***Question 2.2)*** *Assume that all bead types of the vertices in each path are different, identified by bead types* $0, 1, \ldots, 26$*, and propose an attraction rule for each path that folds it with delay time* $\delta = 1$ *given a suitable seed conformation.* Just draw the corresponding bonds on each path.

► ***Question 2.3)*** *Describe an algorithm which, given a shape* S *of the triangular lattice as an input, outputs a path, foldable with delay time* $\delta = 1$*, which fills exactly an upscaled version of* S *at scale 3.5.*

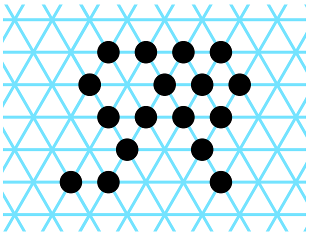
Observe that if we color every vertex (x, y) of the triangular lattice with color $(2x + 3y) \bmod 19$, then every of the 19 vertices at distance at most 2 from a given vertex receives a different color in $\{0, \ldots, 18\}$, as shown in the figure bellow displaying the color offset modulo 19 with the gray vertex.



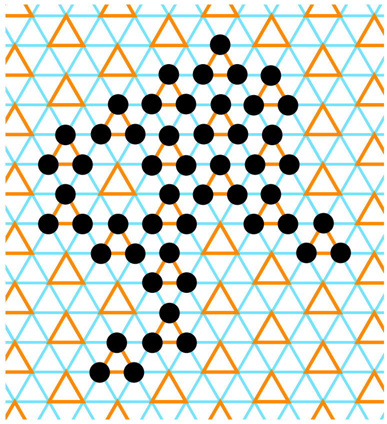
▶ ***Question 2.4)*** *Propose a set of bead types B, an attraction rule $\heartsuit$, and an algorithm which given a shape S of the triangular lattice as an input, outputs a primary structure $p \in B^*$ and a seed conformation σ such that p folds with delay time 1, exactly into an upscaled version of S at scale 3.5. What is the size of B?*

▶ ***Question 2.5)*** *Show that there is a shape at scale 1.5 which cannot be folded by any Oritatami system with delay time 1. Prove it.*

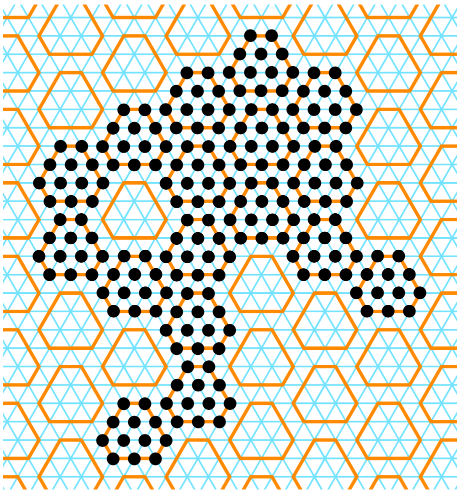
▶ ***Question 2.6)*** *What about scale 2.5?*



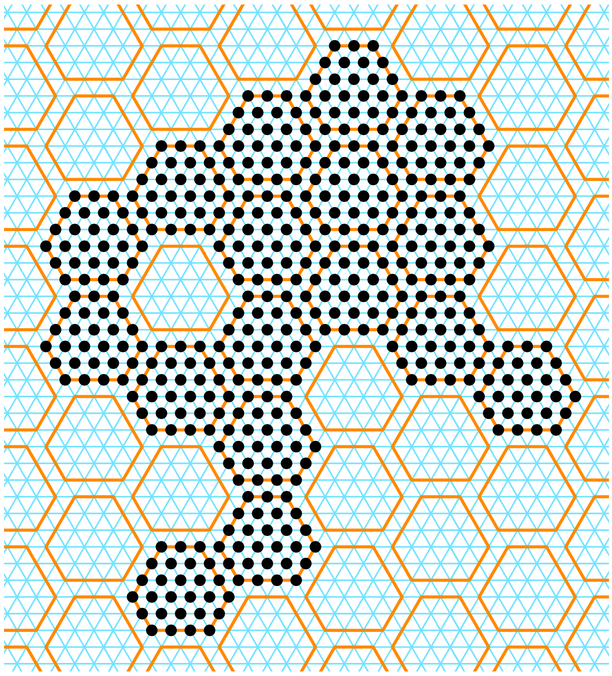
A shape S



The shape S at scale 1.5



The shape S at scale 2.5



The shape S at scale 3.5

Figure 1: Example of upscaling of a shape.