HW2 Molecular Programming

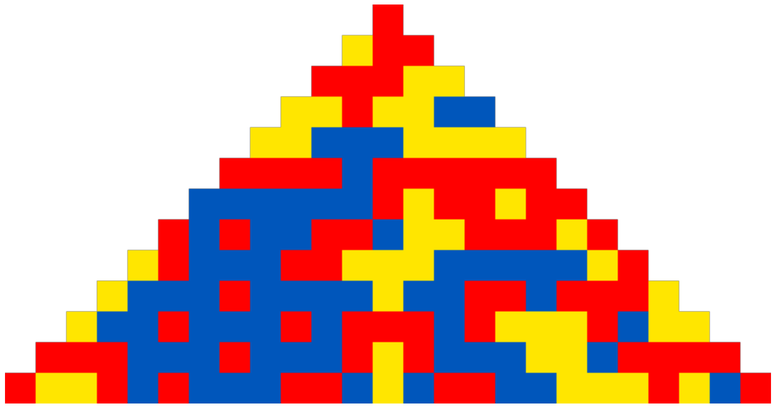
MPRI 2.11.1

29.10.2018 - **Due on Mon. 5/11 before 12:45**

You are asked to complete the exercise marked with a [★] and to send me your solutions to:
`nicolas.schabanel@cnrs.fr`
as a PDF file named `HW2-Lastname.pdf` on **Mon. 5/11 before 12:45.**

[★] Homework: Solve questions 3.1 and 3.2 of exercise 3.

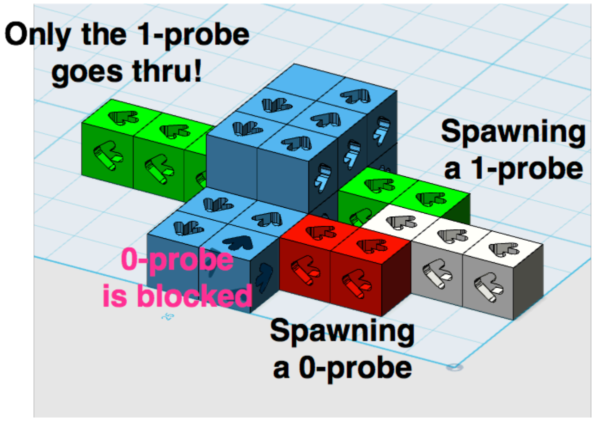
■ **Exercise 1 (Tileset for simulating cellular automata).** A cellular automaton consists of a finite set of *states* Q, a function $f : Q^3 \to Q$, called the *rule*, and an initial configuration $c^0 \in Q^*$. The configuration at time $t+1$ is obtained from the configuration at time t as follows: $c_i^{t+1} = f(c_i^t, c_{i+1}^t, c_{i+2}^t)$ for $0 \leqslant i < |c^t| - 2$. The calculation stops at the first time T such that $|c^T| < 3$ and the result of the computation is c_0^T. A classic visualization of the computation of a cellular automaton consists of a pyramid. Here is an example:



$$\text{for the rule } f(x,y,z) = \begin{cases} {\color{gold}\blacksquare} & \text{if } \{x,y,z\} = \{{\color{red}\blacksquare}\} \text{ or } \{{\color{gold}\blacksquare},{\color{blue}\blacksquare}\} \\ {\color{blue}\blacksquare} & \text{if } \{x,y,z\} = \{{\color{gold}\blacksquare}\} \text{ or } \{{\color{blue}\blacksquare},{\color{red}\blacksquare}\} \\ {\color{red}\blacksquare} & \text{if } \{x,y,z\} = \{{\color{blue}\blacksquare}\} \text{ or } \{{\color{gold}\blacksquare},{\color{red}\blacksquare}\} \text{ or } \{{\color{gold}\blacksquare},{\color{blue}\blacksquare},{\color{red}\blacksquare}\} \end{cases}$$

► ***Question 1.1)*** *Propose a finite tileset whose self-assembly simulates the computation of any Q-state cellular automata from any initial configuration and whose size is independent of the initial configuration length. Give a generic example of the execution of your assembly for generic computation steps. Express the number of variants of each tile type as a function of $|Q|$. Provide the procedure which selects the tiles used to simulate a given Q-state cellular automaton.*

■ **Exercise 2 (Probabilistic simulation Turing Machine at $T^\circ = 1$ in 2D).** Recall that in 3D, for any single-tape binary-alphabet Turing machine M, there is a tile set which simulates M using a clever trick to encode 0s and 1s. These are encoded with bridges and read using two probes where only one go through the bridge:



▶ ***Question 2.1)*** *By adjusting the concentrations (and thus the rate at which the different tiles attached), describe a tile set together with concentrations for each tile type, that simulates a given single-tape binary-alphabet Turing machine M with an arbitrary small error ε for each symbol read in 2D at temperature $T^\circ = 1$.*

■ **Exercise 3 (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 3.1)*** *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.

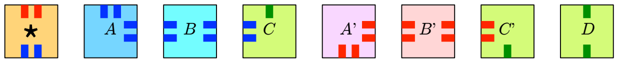
Let us now consider a (finite) tile set $\mathcal{T}$ whose final productions are 2-thick rectangles of size $2 \times \ell$ for some $\ell \geqslant 1$.

▶ ***Question 3.2)*** *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.*

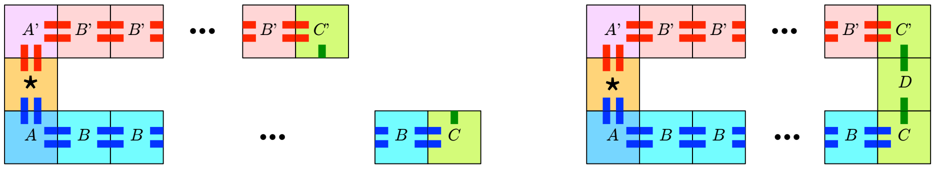
Let us now generalise and consider a (finite) tile set $\mathcal{T}$ whose final productions are q-thick rectangles of size $q \times \ell$ for some $\ell \geqslant 1$.

▶ ***Question 3.3)*** *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 3.4)*** *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?*