Abstract and Kinetic Tile Assembly Model

In the following section I will explain the model behind the Xgrow simulator. I will first explain the aTAM model which is the basis of kTAM, and then I will explain the improvements in kTAM.

The Abstract Tile Assembly Model (aTAM) was proposed by Erik Winfree as a practical variation on Wang tiling. Although the model generalizes to any number of dimensions, much of the research in the community so far has focused on two or three dimensions. For simplicity, we will only discuss the two-dimensional model.

A tile type $t$ is a unit square that can be translated but not rotated. Each side $u$ is covered with a "glue" of a certain "color" and "strength" specified by its type $t$. If two tiles are placed with their centers at adjacent points and if their abutting sides have glues that match in both color and strength, then they form a bond with this common strength. If the glues do not match, then no bond is formed between these tiles. Generally, glues have strength 0, 1, or 2 (although recent papers have noted that strength 2 is difficult to create in a laboratory setting).
When drawing a tile as a square, each side's glue strength is generally indicated by a dotted line (0), solid line (1), or double line (2) while "color" is indicated by an alphanumeric label.

Given a set \( T \) of tile types and a "temperature" \( \tau \in \mathbb{N} \). Intuitively, an assembly is a placement of tiles. An assembly is stable if it cannot be broken into smaller sub-assemblies without breaking total bond of strength at least \( \tau \).

A tile assembly in the aTAM always begins from a seed tile and builds outward from that. Although it is possible that tiles would bond to each other to form assemblies not including the seed tile, this is not modelled by the aTAM. Once the seed is present, the system proceeds asynchronously and nondeterministically to bond tiles to the assembly. A tile assembly system (TAS) is an ordered triple \( \mathcal{T} = (T, \sigma, \tau) \), where \( T \) is a finite set of tile types, \( \sigma \) is a seed
assembly with finite domain, and $\tau \in \mathbb{N}$ is the temperature. We write $\mathcal{A}[\mathcal{T}]$ or the set of all assemblies that can arise from $\mathcal{T}$.

$\mathcal{A}[\mathcal{T}]$, the set of terminal assemblies, represents the set of assemblies where no tile can be stably added. An assembly sequence in a TAS $\mathcal{T} = (T, \sigma, \tau)$ is an infinite sequence $\alpha = (\alpha_0, \alpha_1, \alpha_2, \ldots)$ of assemblies in which $\alpha_0 = \sigma$ and each $\alpha_{i+1}$ is obtained from $\alpha_i$ by the addition of a single tile.

The Kinetic Tile Assembly Model (kTAM) is an improvement over the aTAM, in the sense that it enables reaction rates and reversible reactions.

To model the kinetics of self-assembly, there are several simplifying assumptions made after tiles are created (Some of these assumptions can be ignored in some of the operation modes of the simulator.):

1. Tile concentrations will be held constant throughout the experiment.
2. All tile concentrations will remain the same.
3. Groups of tiles do not bond to each other, only to the aggregate including the seed tile.
4. The forward rate, or rate at which tiles add to the assembly, is constant between all the tiles. This means that, regardless of bond strength and color,
5. The reverse rate, or rate at which tiles are removed from the assembly, depends inverse exponentially on the strength of the bond.
In this model, there are two parameters that can be altered by the experimenter and one that cannot. $G_{mc} > 0$ measures the entropic cost of fixing the location of a monomer unit (and is thus dependent on monomer concentration). $G_{se} > 0$ measures the free energy cost of breaking a single-strength bond. Both are expressed in the thermal energy RT. The third parameter, the forward rate constant $k_f$, simply sets the units for the time axis. The rate of forward associations of a particular tile type at a particular site is $r_f = k_f e^{-G_{mc}}$ where $e^{-G_{mc}}$ represents the concentration of each tile. The dissociation (or backward) rate is $r_{r,b} = k_f e^{-bG_{se}}$.

Figure 2: The rates of reactions for various tile association and dissociation steps in the Kinetic Assembly Model. Note that all on-rates are identical, and that off-rates depend only upon the total strength of correct edge matches. Mismatched edges and empty neighbors are treated identically.
According to experimental work, the optimal value $G_{mc}$ and $G_{se}$ are when $G_{mc} = 2G_{se}$. The behavior of the system for different values of these parameters can be seen in the figure below:

Figure 3: Analysis of the phase diagram for 2D self-assembly.