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Self-assembly of Self-similar Structures by Active Tiles

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Self-assembly of Self-similar Structures by Active Tiles

by

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A thesis submitted in partial fulfillment of the requirements for the degree of Master of Arts
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Abstract

The natural capacity of DNA for molecular self-assembly has already been exploited to create DNA based tiles which can self-assemble into nano-scale arrays and carry out nano-scale computation. Thus far, however, all such self-assembly has been passive, in the sense that the binding capacities of a tile are never altered throughout the assembly. The idea of active tiles, tiles that can send signals to each other and activate latent binding sites, has been proposed but never incorporated into a formal model. Here, I present an extension of the existent abstract tile assembly model by defining an active tile assembly and give a detailed example of an aperiodic set of active tiles which hierarchically produces a self-similar L-shape tiling. This yields a technique utilizing active tiles for the assembly of aperiodic self-similar shapes.
1.1 Overview

DNA computing as a field owes its start to Leonard Adleman, who in 1994 proved experimentally that DNA could be used to solve computational problems[1]. Since then, different models of computing with DNA have been explored. Ned Seeman’s work in DNA nanostructures, in particular, has greatly contributed to progress in this area by providing new designs of DNA structures and new methods of working with them, as well as incorporating these into existing models (see [18, 38, 13, 32, 28, 8, 14, 29]).

The new theoretical model of computation that we present in this thesis is one whose implementation can be obtained by the two-dimensional (2D) self-assembly of DNA based tiles. We build on the foundation made by Erik Winfree with the Tile Assembly Model (TAM) as presented in his 1998 Ph.D. thesis[33], where he explores both the theoretical framework and the practical viability of such computation. On the application side, the kinetic tile assembly model (kTAM)[33] is concerned with the actual thermodynamics of the reactions involved. On the theoretical side, the abstract Tile Assembly Model (aTAM), in which DNA based tiles are used to form a 2D lattice, can simulate the dynamics of any one dimensional cellular automaton and is therefore Turing universal[33].

DNA based 2D arrays are interesting in both computing and nanotechnology. From the perspective of computing, 2D DNA based arrays allow computation to be moved to a smaller scale: problems can be encoded in the single DNA strands at the edges of the tiles (the “sticky ends”) the computation is carried out by their self-assembly. From the perspective of nanotechnology, they provide a way to obtain new materials: either directly, as the array is a physical structure in itself, or indirectly, by allowing the tiles to contain markers which could direct the assembly of some structure on top. Two-dimensional periodic tilings form crystal lattices and have been studied the
most to date (see [38]), but it is the aperiodic tilings which can carry out computation. Moreover, self-similar aperiodic motifs, if materialized, could yield quasi-crystallographic structures, which are quite rare in nature (in fact, a Nobel prize for their discovery in nature was awarded just last year to Daniel Shechtman) and in general quite difficult to design and assemble.

In what has become the standard tile assembly model (given in detail in Section 1.2), the sticky ends of the tile are formed by single stranded DNA containing a sequence of unpaired bases which can bind to a strand of complementary bases (on another tile). One important problem in the assembly process is error control: how to prevent “tiles” which have partial base matches from binding in the “wrong” place in the lattice. This is where bond stability comes into play: at high enough temperatures, weaker bonds are not stable; unfortunately, they can last long enough for the tile to form new and stable bonds in an incorrect position. One possible way to control the errors is by staging the assembly: by only allowing certain tiles in solution at a certain point, then adding other tiles in stages after a sufficient amount of time has passed for most correct bonds to form. A theoretical analysis of staged assembly is given in Demaine, et al. [5].

This thesis focuses on another possible solution, proposed in different variants in [16] and [20]. The idea is to keep certain binding sites dormant until a “signal” is received to activate them, which allows indirect control over the assembly process. A formal description of this “active assembly” method that additionally includes a possibility for sending deactivation signals is introduced in [21]. In this thesis we provide an alternate formal description to model active assembly. Although we do not allow deactivation of binding sites and make a simplifying assumption that the transmission of signals from tile to tile and binding site activation occur instantaneously, the resulting formalization allows for a more elegant and mathematically precise description of the model. We discuss possible extensions of our model in the Conclusions (for example, we show that deactivation can be easily incorporated).

The description of our formal active assembly model and its applications to the recursive assembly of self-similar structures is the main subject of this thesis. The Active Tile Assembly Model itself is introduced in Chapter 2, where we formally define active tiles and describe the hierarchical assembly in terms of a tile modification function given in Section 2.3. Then, in Chapter 3, we apply the model to an archetypal example of a self similar aperiodic tiling - the aperiodic L-shape tiling [10] - and prove that the designed tiling system recursively assembles a non-periodic L-shape
based array. We end the paper with some concluding remarks about the presented model and future avenues of research.

1.2 Background and Preliminaries

We now proceed to review in more detail some of the technical aspects of DNA based tiling and computing, including the descriptions of the abstract tile assembly model and its generalizations. We begin with some relevant segments of tiling theory.

1.2.1 Tiling

The reader is referred to [11] for a comprehensive guide to tiling. Here we review only a few key notions pertinent to this thesis. The first of these notions is that of tiling itself. A (two dimensional) tiling is a covering of $\mathbb{R}^2$ by copies of a finite set of compact sets which intersect only at their boundaries (informally, a planar arrangement of some collection of shapes with no gaps and no overlaps among them). The set of all shapes in a tiling is called the set of tiles. If tiles are decorated, that is, if the tile is marked in some way (e.g., edge colors, vertex colors, arrows), a set of matching rules governs whether or not the adjacency of two given tiles is allowed (e.g., a red edge may only be adjacent to a red edge).

Sets of square tiles of uniform size with colored edges and the requirement that the colors of abutting edges on adjacent tiles match (reflection and rotation forbidden) form a special class named after the person who first introduced them, Hao Wang. In 1975, Wang showed that one can simulate any Turing machine by a set of Wang tiles, such that the rows of the tiling simulate the tape of the machine[31]. Wang tiling forms the basis for the abstract model of DNA tiling.

To describe the particular DNA tiling presented in this paper, we must define a few more terms. A tiling is called self-similar if the tiles forming the original tiling can be composed into larger tiles that are (geometrically) similar to the original tiles in such a way that the original tiling is recovered (up to translation) if every tile in it is substituted with its larger counterpart. Self-similar tilings come in both periodic and nonperiodic varieties.

In general, a tiling of the plane is called periodic if it is invariant under some vector translation (i.e., the entire plane may be shifted in some direction and still produce the original tiling) and nonperiodic otherwise. A tile set which can only produce nonperiodic tilings is called aperiodic.
and a tiling by such a set may itself be referred to as an aperiodic tiling.

Self-similar tiling and the substitution method of tile construction is of interest because it often yields aperiodic tilings with a hierarchical structure. In fact, Goodman-Strauss[10] showed how given any substitution tiling a set of matching rules can be created to force the desired structure.

The most well-known aperiodic set constructions are modified square tiles due to Robinson[24] and the kites and darts of Penrose. Relating back to the subject of DNA based tiling, an aperiodic set of just four tiles utilizing the idea of signaling has been proposed in [20] for a set of Robinson tiles which hierarchically assemble a self-similar square pattern. In Chapter 3, we apply our model of active tile assembly to an aperiodic set of active DNA tiles that hierarchically assembles the self-similar L-shape tiling.

1.2.2 DNA Origami and Signaling

Using DNA for the purpose of self assembly is based on an inherent property of its structure: a given DNA sequence binds strongly to its perfect complement, i.e., to a sequence consisting of the bases exactly complementary to its own. Under certain conditions, partially complementary sequences may also bind but these bonds are weaker. Moreover, DNA can assume a variety of rigid forms other than the familiar linear double helix. Synthetic molecules have been designed and shown to assemble into branched species [13, 32], and more complex species that entail the lateral fusion of DNA double helices [28], such as DNA double crossover (DX) molecules [8], triple crossover (TX) molecules [14] and paranemic crossover (PX) molecules. DX and TX molecules have been used as tiles and building blocks for large nanoscale arrays [33, 34].

An important advancement in this area was DNA origami, which is essentially a method of creating arbitrary shapes from DNA by folding a single strand into the desired shape and using shorter “helper” strands to bind it rigidly together [26]. Since their appearance, DNA origami has been used as a seed for arranging DX tiles in an array [3], nanotube constructions [7] and most recently as templates for large DNA based tiles arranged in a 2D crystalline array [38] (the first such array by DNA origami tiles reported).

In a tiling which utilizes DNA structures, strands containing unmatched sequences at the tile edges act as “glues,” allowing one tile to bind to another if they contain complementary strands.\(^1\)

\(^1\)The complementary base pairs are adenine (A) and thymine (T), and guanine (G) and cytosine (C).

\(^2\)These may be referred to interchangeably in literature as “glues,” “sticky ends,” and “labels.”
A particular DNA structure that can be used as a tile, an origami cross shape, is shown in Figure 1. The size of this tile is about $100 \times 100$ nm, which allows enough space to accommodate signaling (unlike the DX and TX molecules which may and have been used for computation but are not large enough to incorporate existing signaling mechanisms).

Figure 1. A DNA origami tile.[38]

The DNA signaling mechanisms developed thus far rely on strand displacement techniques (see Fig.2) and have already been applied in a variety of ways. For example, devices whose activity is controlled by DNA strands have been produced in [37, 35]; they utilized DNA “fuel” strands, which were recently also used to construct a large number of enzyme-free logic gates [27, 22, 23]. Additionally, structures that can perform simple “walking” (based on strand displacement) on an arranged platform have been reported in [29, 36, 30]. The three most recent walking devices [12, 18, 15] showed a significant robustness, allowing the directions and the actions of the walker to be guided by a sequence of strand displacements incorporated within the walking platform.

So, a sticky end of the tile may initially be in an inactive state (Fig.2c,d), bound to a protective strand which is later stripped by a signal initiated by another tile, activating it (Fig.2e). Such signaling across and between tiles may be accomplished with a combination of the methods discussed in the previous paragraph (Fig.2). It should be noted that tile size and shape place natural restrictions on the actual amount of signal transmission and activation strands that can fit on it, but that tiles of many different shapes and sizes can in principle be created.
**Figure 2.** Signal propagation pathway: (a) seesaw gates next to an activation strand, (b) one swing of the signal along the seesaw gates, (c) transducer gates, (d) transducer cascade, energetically favorable by a gain of four base pairs at each step, (e) signal transmission to the binding site to activate it by removing a protecting strand.[19]

### 1.2.3 The Abstract Tile Assembly Model

The abstract Tile Assembly Model originally proposed by Winfree[33] is based on Wang tiles and can be described as follows. The *tile types* are unit squares with labelled edges and there are infinitely many tiles (instances) of each type. Every *edge label* has a *strength* parameter, a non-negative integer, associated with it. An *aggregate* is formed when a tile is aligned next to another tile or an existing aggregate and the sum of the strengths of the matching adjacent labels between the two structures is greater than or equal to a set “*temperature*” parameter (a non-negative integer). Neither rotation nor reflection of the tiles is allowed. A *seed tile* may be used to initiate computation, in which case it is assumed that subsequent tiles bind only to the seed tile or to the aggregate containing the seed tile. A *tile assembly system* is formed by the ordered pair \((\mathcal{T}, \tau)\) where \(\mathcal{T}\) is the set of allowed tiles and \(\tau\) is the fixed temperature parameter.

**Remark.** Note that in this description, not all edge labels of adjacent tiles have to match, just sufficiently many. This is one key difference between the aTAM and Wang tiling.

A very relevant extension and formalization of the aTAM is the two-handed assembly model
(2HAM) provided in [2] as part of what the authors call a “multiple tile model.” The 2HAM is the model that we modify and extend with signaling in the following chapter. In it, the tile types are unique squares defined as 4-tuples \((\sigma_n, \sigma_e, \sigma_s, \sigma_w)\) representing the “glues” at the north, east, south, and west edges, each glue having an associated strength in the form of a non-negative integer (cf., “edge labels” above). Tile assemblies are produced when smaller tile assemblies bind together (cf., “aggregate” above). The “two” in 2HAM refers to the number of tile assemblies which may bind at a time. A bond is formed between adjacent tiles of two assemblies if their adjacent edges have matching glue labels and has the corresponding strength. Every tile assembly is a mapping of the integer lattice into a set of tile types and the bonds between all tiles are represented by a binding graph (the vertices are the tiles and edges are the connections among them). This process and the conditions for binding are given fully in Section 2.2.

As previously mentioned, another description of signaling incorporated into the aTAM has been made in [21]. That model is also based on the 2HAM but takes an approach different from the one in this thesis to representing the active tiles and their interactions. Apart from differences in notation and representation, [21] includes an added capacity for tile glues to be deactivated and for tile assemblies to break apart, as well as an added notion of “pending actions” which allows signal transmission to be delayed by an arbitrary amount of time in order to more closely approximate the physical interactions among actual DNA tiles. Neither of these two features is incompatible with the model presented here, and we discuss the specifics of their incorporation in the concluding chapter.

### 1.2.4 Computing with Tile Assembly Models

When Winfree [33] introduced the tile assembly model, he showed that two dimensional self-assembled arrays made of DX or TX DNA tiles can simulate the dynamics of a bounded one dimensional cellular automaton and so are capable of potentially performing computations as a Universal Turing machine. Several successful experiments have confirmed the possibility of computation by array-like DNA self-assembly: binary addition (simulation of XOR) using TX molecules as tiles [17], Sierpinski triangle assembly [25, 9], and a binary counter [3] by DX molecules. Transducer simulations with programmed inputs by TX DNA molecules have also been reported [6, 4].

In each of the computational self-assembly experiments thus far, as well as in the theoretical tile assembly model, the DNA tiles are pre-designed and computation is performed by their self-
assembly into larger arrays. As mentioned before, the practical challenge posed by such passive self-assembly is the potential for errors. Since the tile sticky-ends are free to bind as long as they meet their complementary counterparts, “correct” tiles are not only competing with “incorrect” tiles (as is the case with simple multi-tile systems), but also with “partially-correct” tiles.

The formal model proposed in this paper is that of an active programmable self-assembly which is able to build up arrays hierarchically. In such a system, the signaling capabilities of the tiles allow them to assume multiple identities throughout the assembly process. Moreover, a tile is allowed to have more than one type of “glue” on any given edge and these may be initially inactive (unable to bind) until they receive an activation signal. This approach allows for step by step assembly in a potentially controlled and robust way without actually staging the process. Moreover, the work presented here suggests a potentially feasible model for the application of recursion in molecular self-assembly; and, through the use of signaling techniques, it has the potential to build self-similar structures hierarchically.
Chapter 2
Active Tile Assembly Model

In this chapter, we give the formal description of our Active Tile Assembly Model. In the first section, we define active tiles. In the second, we present binding graphs and tile assemblies. The third section introduces the tile modification function, with which we describe the dynamics of signaling within the assembly process. In the fourth and last section we use the tile modification function to construct hierarchical tile assembly sets and to define an active tile assembly system.

2.1 Basic Definitions

Definition 2.1.1. Let $\Sigma^+$ be a finite set and define the complementary set $\Sigma^- = \{-c | c \in \Sigma^+\}$. We call $\Sigma = \Sigma^+ \cup \Sigma^-$ the set of all labels.

Definition 2.1.2. The strength function is defined to be

$$s : \Sigma^+ \to \mathbb{Z}^+$$

where $\mathbb{Z}^+ = \{x \in \mathbb{Z} | x \geq 0\}$,

and for $c \in \Sigma$, $s(|c|)$ is called the strength of $c$. We use $|c|$ to denote $c$ if $c \in \Sigma^+$ and to denote $-c$ if $c \in \Sigma^-$. 

Remark. The strength of a label refers to the strength of the bond between it and its complementary label.

Definition 2.1.3. Define the set of signals:

$$\hat{\Sigma} = \left\{ c^i_j | c \in \Sigma^+; \ i, j \in \{+y, +x, -y, -x, 0\}, \ j \neq 0 \right\},$$

where $c^i_j$ for $i \neq 0$ means that $c$ can be transmitted from the direction $i$ in the direction $j$, whereas $c^i_0$ means that $c$ can be initiated in the $j$ direction and we refer to it as an initiation signal.
Remark. The directions referred to here and throughout the rest of the thesis are the axial directions of the xy-plane. This is a departure from the conventional notation of North, East, South, and West; however, we believe that this notation gives a more natural correspondence between the parts of a tile and its coordinate position in the plane and simplifies the description of signal transmission between adjacent tiles (e.g., we can say that a signal $c_j^i$ will “connect” to the signal of the form $c_k^{-j}$; here, the relation between $j$ and $-j$ is a more direct one than between, say $N$ and $S$).

**Definition 2.1.4.** A tile $t$ is a 4-tuple of tile sides, $t = (t_{+y}, t_{+x}, t_{-y}, t_{-x})$, such that each tile side $t_i$, $i \in \{+y, +x, -y, -x\}$, is an ordered pair of sets of labels:

$$t_i = (A, I) \in \mathcal{P}(\Sigma) \times \mathcal{P}(\Sigma)$$

where $\mathcal{P}(\Sigma)$ denotes the power set of $\Sigma$. We refer to $A$ as the set of active labels and to $I$ as the set of inactive labels.

**Figure 3.** a) A tile $t = (t_{+y}, t_{+x}, t_{-y}, t_{-x})$ placed on the coordinate plane. Solid lines represent active labels and dashed lines represent inactive labels. Subscripts on tile sides indicate directions normal to those tile sides. b) A tile with complementarity indicated by $+/−$. See Example 2.1.5.

**Example 2.1.5.** Refer to Figure 3 for the sample tile $t$. Let $\Sigma^+ = \{r, b, y, g\}$, corresponding to the red, blue, yellow, and green labels. Then $\Sigma^- = \{-r, -b, -y, -g\}$, so $\Sigma = \{r, b, y, g, -r, -b, -y, -g\}$,
and

\[
\begin{align*}
t_{+y} &= (\{b\}, \{r\}) \\
t_{+x} &= (\emptyset, \{-r, y, b, -g\}) \\
t_{-y} &= (\{-g\}, \emptyset) \\
t_{-x} &= (\{r\}, \emptyset)
\end{align*}
\]

are the tile sides for \( t = (t_{+y}, t_{+x}, t_{-y}, t_{-x}) \).

Definition 2.1.6. An active tile is an ordered triple \( \tau = (t, A, S) \) where \( t \) is a tile and \( A, S \subseteq \hat{\Sigma} \) such that

1. \( c_0^0 \notin A \) for any \( a \in \{+y, +x, -y, -x\} \) (the set of activation signals does not contain initiation signals),

2. if \( t_a = (A, I) \) and a) \( c \in A \), then \(-c \notin A \) and \( c, -c \notin I \); furthermore, b) if \( d \in I \), then \(-d \notin I \)

(a tile side cannot contain redundant or complementary labels).

We refer to \( A \) and \( S \) are the sets of activation signals and transmission signals respectively.

Remark. Condition 1 eliminates superfluous signaling (i.e. a tile which activates one of its own labels is equivalent to a tile with that label already active). Condition 2 comes from practical considerations of actual DNA dynamics: if a tile side contains active complementary ends, they may bind to each other instead of to complementary strands on another tile. Since a signal for a given label would also activate the complementary label, we forbid complementary labels from co-existing even in the inactive state. See Fig.2.1.7b for an example of a tile which violates these conditions.

Example 2.1.7. Refer to Figures 3 and 4a) for the sample tile with \( \Sigma = \{r, b, y, g, -r, -b, -y, -g\} \) and \( t = (t_{+y}, t_{+x}, t_{-y}, t_{-x}) \) as in Example 2.1.5. The signaling shown in Figure 4 is:

\[
A = \{r_{+y}, b_{+x}, g_{+x}, y_{+x}\}
\]

\[
S = \{b_{-y}, g_{-x}\}
\]

and the corresponding active tile is \( \tau = (t, A, S) \).

\[\Box\]
Figure 4. a) An *active tile* obtained by adding signaling to tile \( t \). See Example 2.1.7. b) Example of failed conditions (1), (2a) and (2b) in active tile Def.2.1.6.

### 2.2 Tile Assemblies and the Associated Binding Graphs

Let \( T \) be the set of all possible active tiles and consider a partial mapping:

\[
\alpha : \mathbb{Z}^2 \to T.
\]

We define the associated *binding graph* of \( \alpha \) to be a weighted graph \( G_\alpha = (V,E) \), with \( V \subset \mathbb{Z}^2 \) such that \( (i,j) \in V \) if and only if \( \alpha((i,j)) \) is defined, and \( E \subset \binom{V}{2} \) such that

\[
E = E_h \cup E_v
\]

\[
E_h = \{\{(i,j), (i + 1,j)\} | (i,j), (i + 1,j) \in V\},
\]

\[
E_v = \{\{(i,j), (i,j + 1)\} | (i,j), (i,j + 1) \in V\}.
\]

The weight function for \( G \) is defined in the following way. Let \( e = \{v,w\} = \{(i,j),(i,j+1)\} \) be a vertical edge, and let

\[
\alpha(v) = \tau_v = (t^v, A^v, S^v), \quad \alpha(w) = \tau_w = (t^w, A^w, S^w)
\]

with

\[
t^v = (t^v_{+y}, t^v_{-x}, t^v_{+y}, t^v_{-x}), \quad t^w = (t^w_{+y}, t^w_{+x}, t^w_{-y}, t^w_{-x})
\]
(where $t^v_{+y} = (A^w_{+y}, I^v_{+y})$ and similarly for the rest). We consider the intersection

$$C_e = A^v_{+y} \cap -A^w_{-y}$$

where $-A^w_{-y} = \{-c | c \in A^w_{-y}\}$. Then we define the weight of the (vertical) edge $e$ to be

$$w(e) = \begin{cases} 
\sum_{c \in C_e} s(|c|) & \text{if } C \neq \emptyset \\
0 & \text{otherwise}.
\end{cases}$$

The definition for the weight of horizontal edges is analogous.

In other words, the vertices of the binding graph are formed by points in the integer lattice which we presume are occupied by tiles. There are horizontal and vertical edges indicating horizontal and vertical adjacencies. Each edge is assigned a weight corresponding to the sum of the strengths of the complementary active labels of the adjacent tile sides.

**Remark.** We say that adjacent tiles whose adjacent sides contain complementary labels $c$ and $-c$ contain a bond of strength $s(|c|)$.

With this definition of a binding graph in hand, we proceed to make the following definitions.

**Definition 2.2.1.** Given a set of tiles $T$ and an integer $\theta \geq 0$, a *tile assembly instance* for $\theta$ is a partial mapping $\alpha : \mathbb{Z}^2 \rightarrow T$ where either

(a) $\alpha$ is defined for only a single point in $\mathbb{Z}^2$ or

(b) its associated graph $G_\alpha = (V, E)$ satisfies the following two conditions:

(i) $G$ is connected, and

(ii) the sum of the weights of the edges in any edge cut\(^1\) of $G$ is greater than or equal to $\theta$. We call $\theta$ the temperature parameter (usually $\theta = 2$).

**Remark.** Observe that condition (b), part (ii) of which is generally referred to as $\theta$-stability, forces the tile assembly instance to be composed of at least two tiles; we’ll refer to $\alpha$ in the special case of (a) as a *unit tile instance*.

\(^1\)An edge cut of a graph $G = (V, E)$ is a set of all edges with one vertex in $U$ and the other in $V \setminus U$ for some $U \subseteq V$. 

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**Definition 2.2.2.** The terms *tile assembly* and *unit tile* refer to the equivalence classes \([\alpha]\) of the respective instances under translation\(^2\):

\[ \alpha \sim \beta \text{ if and only if } \exists k, l \in \mathbb{Z} \text{ such that } \alpha(i, j) = \beta(i + k, j + l) \forall i, j \in \mathbb{Z}. \]

### 2.3 The Tile Modification Function

The Tile Modification Function \(f\) simulates signal transmission and binding site activation for each tile assembly. Let \(\alpha\) be a tile assembly instance and denote \(\alpha(z)\) by \(\alpha_z\). For \(z \in \mathbb{Z}^2\) and \(\alpha_z = \tau = (t, A, S) \in T\), let

\[
\begin{align*}
\tau_{+y} &= \alpha_{z+(0,1)} \\
\tau_{+x} &= \alpha_{z+(1,0)} \\
\tau_{-y} &= \alpha_{z+(0,-1)} \\
\tau_{-x} &= \alpha_{z+(-1,0)}
\end{align*}
\]

define the neighbors of \(\tau\) on the respective sides. If \(\tau_i\) is not defined for some \(i \in \{+y, +x, -y, -x\}\), write \(\tau_i = \varepsilon\), otherwise write \(\tau_{+y} = (t^{+y}, A^{+y}, S^{+y})\) (similarly for the other three neighbors).

Let \(N = \{(0, 1), (0, -1), (1, 0), (-1, 0)\}\). Then \(f : T^5 \rightarrow T\) is a tile modification function if

\[
f(\alpha_{z+N}) = f(\tau, \tau_{+y}, \tau_{+x}, \tau_{-y}, \tau_{-x}) = \alpha'_{z} = (t', A', S')
\]

transforms the active tile \(\tau = \alpha_z\) into another active tile \(\alpha'_{z}\) in the following way.

Let \(t = (t_{+y}, t_{+x}, t_{-y}, t_{-x})\) and \(t' = (t'_{+y}, t'_{+x}, t'_{-y}, t'_{-x})\).

1. If \(t_i = (A, I), i \in \{+y, +x, -y, -x\}\), then

\[
t'_i = (A \cup C, I \setminus (C \cup D)),
\]

where

\[
C = \left\{ c \in I \mid \exists c^{ij}_j \in A \text{ and } |c|^{ij}_0 \in S^j \text{ for some } j \in \{+y, +x, -y, -x\} \right\}
\]

\(^2\)We do not allow rotation explicitly in the model. To account for rotation, we later require that each tile set contain “rotated” copies of every tile.
\[ D = \{ c \in I \mid \exists c_j^i \in A \text{ for any } j \in \{+y, +x, -y, -x\} \} \]

(Informally, if the tile side contains an inactive label \( c \) with an activation signal for it and an adjacent tile contains a corresponding initiation signal, then the label \( c \) becomes active; inactive labels which can never be activated are removed from the tile.)

2. For \( i, j \in \{+y, +x, -y, -x\} \),

\[ A' = A \setminus A_{\text{removed}} \]

\[ A_{\text{removed}} = \left\{ c_i^j \in A \mid \tau_i \neq \varepsilon \text{ and either } \exists c_0^{-i} \in S^i \text{ or } \exists c_k^{-i} \in S^i \text{ for any } k \in \{+y, +x, -y, -x\} \right\} . \]

(Informally, when the tile receives a signal, its corresponding activation signal is used and cannot be used again, so it is removed. Activation signals that can never be activated due to being adjacent to a tile which has no possibility of sending a signal are also removed.)

3. For \( i, j \in \{+y, +x, -y, -x\} \),

\[ S' = (S \cup S_{\text{added}}) \setminus S_{\text{removed}} \]

\[ S_{\text{added}} = \left\{ c_i^j \mid \exists k \in \{+y, +x, -y, -x\} \text{ such that } c_i^j \in S \text{ and } c_k^{-i} \in S^k \right\} \]

\[ S_{\text{removed}} = \left\{ c_i^j \in S \mid \tau_i \neq \varepsilon \text{ and either } \exists c_0^{-i} \in S^i \text{ or } \exists c_k^{-i} \in S^i \text{ for any } k \in \{+y, +x, -y, -x\} \right\} \]

\[ \cup \left\{ c_i^j \in S \mid \tau_j \neq \varepsilon \text{ and } \exists c_k^{j-} \in S^j \cup A^j \text{ for any } k \in \{+y, +x, -y, -x\} \right\} \]

\[ \cup \left\{ c_0^j \in S \mid \tau_j \neq \varepsilon \right\} . \]

(Informally, when the tile receives a signal, its transmission signal is replaced with an initiation signal. Transmission signals which are not connected to matching signals in adjacent tiles, i.e., transmission signals that cannot be received or transmitted, are removed since they cannot perform any function. Initiation signals are removed since once they are adjacent to a tile they are either immediately transmitted or can never be transmitted.

We can extend \( f \) to a tile assembly instance by applying it simultaneously to every active tile in the tile assembly instance:

\[ f(\alpha) = \alpha' \text{ if and only if } \alpha_z' = f(\alpha_{z+N}) \forall z \in \mathbb{Z}^2. \]

We write \( f([\alpha]) = [\alpha'] = [f(\alpha)] \) to denote the image of the tile assembly under \( f \).
Figure 5. The tile modification function acting on a tile assembly. Two iterations of the function complete the action.

2.4 Hierarchical Tile Assembly Sets

We use the term “complete tile assembly” to refer to a tile assembly which has reached a quiescent state under iterated application of the tile modification function.

Definition 2.4.1. A complete tile assembly instance for \( \alpha \) is a tile assembly instance \( \hat{\alpha} \), such that

\[
f(\hat{\alpha}) = \hat{\alpha} \text{ and } \hat{\alpha} = f^n(\alpha) \text{ for some } n.
\]

Then, \([\hat{\alpha}]\) is the equivalence class of \( \hat{\alpha} \) under translation, so we define the complete tile assembly obtained from \([\alpha]\) as \([\hat{\alpha}]\).

A set of active tiles satisfying the following requirement is called a seed set of unit tiles, denoted \( T_0 \): for every \([\alpha] \in T_0\), if \( \alpha_z = \tau \), and \( \tau' \) is a 90° rotation of \( \tau \) (i.e., \( \tau' \) is obtained from \( \tau \) through a cyclic permutation of the direction coordinates \((+y, +x, -y, -x)\) in the tile description), then \( \exists [\beta] \in T_0 \) s.t. \( \beta_z = \tau' \) (this means that the set \( T_0 \) is closed under 90° rotations).

Fix a temperature \( \theta \). We define \( T_i \), \( i \geq 1 \), recursively as follows. \([\alpha] \in T_i\), if and only if \([\alpha] \in T_{i-1}\) or \( \alpha = \hat{\alpha}' \) where \( \alpha' \) is a tile assembly instance composed of two other tile assembly
instances, $\beta_1$ and $\beta_2$:

$$\alpha'(z) = \begin{cases} 
\beta_1(z) & \text{if } z \in \text{dom}(\beta_1) \\
\beta_2(z) & \text{if } z \in \text{dom}(\beta_2)
\end{cases}$$

and $[\beta_1], [\beta_2] \in \mathcal{T}_{i-1}$ such that the domains of $\beta_1$ and $\beta_2$ are disjoint.

We call $\mathcal{T}_n$ an active supertile set at stage $n$.

**Definition 2.4.2.** An Active Tile Assembly System (ATAS) is an ordered pair $(\mathcal{T}_0, \theta)$, where $\theta \in \mathbb{Z}^+$ is the fixed temperature parameter.
Chapter 3
L-Shape Tiling

Figure 6. Self-Similar L-Shape Tiling

In the following section we present a tile construction for a well-known aperiodic tiling of the plane, one obtained by a substitution tiling of an L-shaped tile (Fig.6). The substitution process can be obtained by repeatedly “inflating” the L-shaped tile to obtain a larger L-shape. The large L-shape is in fact produced by joining four smaller L-shaped tiles together: every subsequent tiling level is obtained from the previous one by substituting each L-shaped tile with four assembled L-shaped tiles. This is indicated in Fig.6 where each level of the substitution is outlined with a different color. The tiling of the plane generated in this process is aperiodic[10].

3.1 Active Tile Assembly System for the L-Shape Tiling

The premise in the unit tile construction is as follows. In order to obtain the smallest L-shape, we join three unit tiles together. Before moving on to the next level of the construction, one of two types of borders is built around each L-shape; then, depending on the type of border, the L-shape assumes either the center role or an outside role in the next level formed by three outside L-shapes.
and one center L-shape. To proceed to the next level, a border is built once again around each of the assembled L-shapes and the process is repeated. Three iterations of this are outlined in Fig.7.

**Figure 7.** Outline of three iterations of the L-shape unit tile construction. A yellow border represents the center role and a red one represents the outside role. Each successive level shape (left column) is composed of three red-bordered shapes (center column) and one yellow-bordered shape (right column) of the preceding level.

We claim\(^1\) that the active tile assembly system which produces the desired effect is \((\mathcal{T}_0,2)\), with \(\mathcal{T}_0\) given in Fig.8 and formally in Tables 1 and 2. The tiles in the figures and tables are presented mod rotation, so, for example, the tile G3, given by:

\[

t_{+y} = (\{1\}, \emptyset)
\]

\[

t_{+x} = (\{2\}, \emptyset)
\]

\[

t_{-y} = (\{-66\}, \emptyset)
\]

\[

t_{-x} = (\emptyset, \{-4\})
\]

\[
\mathcal{A} = \{4_{+y}^{-x}\}
\]

\[
\mathcal{S} = \{2_0^{-y}, 55_{-x}^{+y}, 55_{-y}^{-x}\}
\]

\(^1\)The formal claim is made in the last section of this chapter.
stands to also represent the tiles given by:

\[
\begin{align*}
 t_{+y} &= (\emptyset, \{-4\}) & t_{+y} &= (\{-66\}, \emptyset) & t_{+y} &= (\{2\}, \emptyset) \\
 t_{+x} &= (\{1\}, \emptyset) & t_{+x} &= (\emptyset, \{-4\}) & t_{+x} &= (\{-66\}, \emptyset) \\
 t_{-y} &= (\{2\}, \emptyset) & t_{-y} &= (\{1\}, \emptyset) & t_{-y} &= (\emptyset, \{-4\}) \\
 t_{-x} &= (\{-66\}, \emptyset) & t_{-x} &= (\{2\}, \emptyset) & t_{-x} &= (\{1\}, \emptyset) \\
 A &= \{4^+y\} & A &= \{4^+x\} & A &= \{4^-y\} \\
 S &= \{2^{-x}_0, 55^{+x}, 55^{+y}\} & S &= \{2^{+y}, 55^{+y+x}, 55^{+y}\} & S &= \{2^{+x}, 55^{-x}, 55^{-y}\}.
\end{align*}
\]

Thus, there are 28 tile classes of equivalence under rotation which encompass a total of 112 tiles required for this tiling (only 28 actual DNA tiles, however, since actual DNA tiles can rotate in the plane). As shown in Fig.8, labels 1, 2, 3, 4, and 5 are assigned a strength of 1, and labels 11, 22, 33, 44, 55, 66, 77, and 88 are assigned a strength of 2 (see Def.2.1.2). Note that these labels are to be interpreted only as strings of symbols, not numbers. The active tile assembly system for the L-shape tiling being \((T_0, 2)\) means that the sum of the strengths of all bonds which would have to be cut in order to separate a tile assembly into two parts would have to be at least 2. A consequence of this is that at the initial stage, only unit tiles with complementary labels of strength 2 can bind. This effect is shown in Fig.9, under Time 1: the four assemblies on the left are already complete assemblies (see Def.2.4.1) because there is no signaling to be transmitted; the assembly...
<table>
<thead>
<tr>
<th>Tile</th>
<th>$t_{+y}$</th>
<th>$t_{+x}$</th>
<th>$t_{-y}$</th>
<th>$t_{-x}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>(0, 0)</td>
<td>(−3, 0)</td>
<td>(−3, 0)</td>
<td>(77, 0)</td>
</tr>
<tr>
<td>X2</td>
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<td>(−77, 0)</td>
<td>(−5, 0)</td>
<td>(−2, 0)</td>
</tr>
<tr>
<td>X3</td>
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<td>(0, 0)</td>
<td>(−5, 0)</td>
<td>(88, 0)</td>
</tr>
<tr>
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<td>(5, 0)</td>
<td>(−1, 0)</td>
<td>(4, 0)</td>
</tr>
<tr>
<td>G2</td>
<td>(5, 0)</td>
<td>(−2, 0)</td>
<td>(4, 0)</td>
<td>(−2, 0)</td>
</tr>
<tr>
<td>G3</td>
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<td>(2, 0)</td>
<td>(66, 0)</td>
<td>(0, −4)</td>
</tr>
<tr>
<td>G4</td>
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<td>(−66, 0)</td>
<td>(0, −4)</td>
<td>(2, 0)</td>
</tr>
<tr>
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<td>(4, 0)</td>
<td>(1, 0)</td>
<td>(−5, −44)</td>
</tr>
<tr>
<td>F2</td>
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<td>(2, 0)</td>
<td>(0, −5, −44)</td>
<td>(0, 4)</td>
</tr>
<tr>
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<td>(0, 4)</td>
<td>(4, 0)</td>
</tr>
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<td>(55, 0)</td>
<td>(0, −4, −66)</td>
</tr>
<tr>
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<td>(4, 0)</td>
<td>(5, 0)</td>
<td>(−4, 0)</td>
</tr>
<tr>
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<td>(5, 0)</td>
<td>(−4, 0)</td>
<td>(0, −4)</td>
</tr>
<tr>
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<td>(1, 0)</td>
<td>(−2, 0)</td>
<td>(−5, 0)</td>
</tr>
<tr>
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<td>(−3, 0)</td>
<td>(−5, 0)</td>
<td>(3, 0)</td>
</tr>
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<td>(1, 0)</td>
<td>(3, 0)</td>
</tr>
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<td>(66, 0)</td>
<td>(0, 1, 2, −4)</td>
<td>(0, 0)</td>
</tr>
<tr>
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<td>(0, −5, −55)</td>
</tr>
<tr>
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<td>(−5, 0)</td>
<td>(0, −1, −2, −3)</td>
</tr>
<tr>
<td>C3</td>
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<td>(0, 0)</td>
<td>(0, −1, −2, −3)</td>
<td>(33, 0)</td>
</tr>
<tr>
<td>C4</td>
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<td>(44, 0)</td>
<td>(−4, 0)</td>
<td>(0, 0)</td>
</tr>
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<td>(1, 0)</td>
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</tr>
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<td>(2, 0)</td>
<td>(−22, 0)</td>
<td>(−5, 0)</td>
</tr>
<tr>
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<td>(−33, 0)</td>
<td>(−5, 0)</td>
<td>(3, 0)</td>
</tr>
<tr>
<td>A0</td>
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<td>(4, 0)</td>
<td>(55, 0)</td>
<td>(0, −1, −11)</td>
</tr>
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<td>(1, 0)</td>
<td>(5, 0)</td>
<td>(0, 0)</td>
</tr>
<tr>
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<td>(−2, 0)</td>
<td>(−5, 0)</td>
</tr>
<tr>
<td>A3</td>
<td>(5, 0)</td>
<td>(−3, 0)</td>
<td>(−5, 0)</td>
<td>(3, 0)</td>
</tr>
</tbody>
</table>

**Table 1** List of unit tile rotation class representatives for the L-Shape Tiling: tile sides and labels.
<table>
<thead>
<tr>
<th>Tile</th>
<th>$\mathcal{S}$</th>
<th>$\mathcal{A}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>${55_0^{-x}}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>X2</td>
<td>${55_2^+x}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>X3</td>
<td>${11_0^+y, 66_0^+y}$</td>
<td>${55_2^+y}$</td>
</tr>
<tr>
<td>G1</td>
<td>${1_0^{-x}, 4_0^-x, 5_0^-y}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>G2</td>
<td>${2_0^{-y}, 4_0^+x, 5_0^-y, 55_1^+x}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>G3</td>
<td>${2_0^-y, 55_0^+x, 55_2^-y}$</td>
<td>${4^-y}$</td>
</tr>
<tr>
<td>G4</td>
<td>${4_0^+x, 4_0^-y, 55_2^-y, 55_0^+x}$</td>
<td>${4^+x}$</td>
</tr>
<tr>
<td>F1</td>
<td>${1_0^+y, 4_0^-x, 55_2^-y}$</td>
<td>${4_0^+x, 5_0^-x, 44^+x}$</td>
</tr>
<tr>
<td>F2</td>
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<td>${4_0^-y, 5_0^+y, 44^-y}$</td>
</tr>
<tr>
<td>F3</td>
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<td>${4_0^-y, 44^-y}$</td>
</tr>
<tr>
<td>E0</td>
<td>${1_0^-y, 44^-x}$</td>
<td>${4_0^-y, 66^-y}$</td>
</tr>
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<tr>
<td>E2</td>
<td>${44^-y, 55_2^-y, 55_0^-y}$</td>
<td>${4^-y}$</td>
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<td>${5_2^+y, 55_0^+y}$</td>
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<td>C4</td>
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</tr>
<tr>
<td>B1</td>
<td>${1_2^+y, 4_2^+x}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>B2</td>
<td>${5_2^+y, 55_2^-y}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>B3</td>
<td>${1_2^+y, 2_2^+y, 3_2^+y, 5_2^+x, 55_2^-y}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>A0</td>
<td>${1_0^-y, 4_0^-x, 55_0^+x}$</td>
<td>${1_2^-y, 11_2^-y}$</td>
</tr>
<tr>
<td>A1</td>
<td>${1_2^-y, 1_2^+x, 2_2^+y, 3_2^+y, 55_2^-x}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>A2</td>
<td>${5_2^+y, 55_2^-y}$</td>
<td>$\emptyset$</td>
</tr>
<tr>
<td>A3</td>
<td>${1_2^-y, 2_2^+y, 3_2^+y, 5_2^+x, 55_2^-y}$</td>
<td>$\emptyset$</td>
</tr>
</tbody>
</table>

**Table 2** List of unit tile rotation class representatives for the L-Shape Tiling: signaling.
X2-X1 requires one application of the tile modification function, as shown, to become a complete assembly; the remaining two assemblies become complete after two applications of $f$, as shown - the first application activates the labels 2 and 4 for assemblies C0-G3 and C0-G4 respectively and removes ineffectual signal pathways; the ineffectual labels are removed by the second application of $f$. Thus, $T_1$ is the set $T_0$ plus the seven two-tile assemblies added at Time 1.

**Remark.** Note that the word “Time” here counts the assembly stages. The figures represent only the new tile assemblies added at each stage. The tile assemblies which can interact at a given stage $i$ (or “Time” $i$) are the tile assemblies in $T_i$ and are given by the set of all tiles shown in the preceding stages.

At the next stage, Time 2 (Fig.9), the only new bonds that can form are between X1 and the tile assembly X2-X3 or between X3 and the tile assembly X2-X1. The completed assembly in either case is the first L-shape: X1-X2-X3 (in the first case, it takes two iterations of $f$ and in the second just one). One can see that no other additions at this level can occur, since such would require the side by side labels on one of the two-tile assemblies to be matched with those of another two-tile assembly, which the reader may easily verify cannot happen.

In Fig.9, observe that the strength 1 labels on the outside of the X1-X2-X3 L-shape are all “negative” labels, so two “positive” labels would have to be present on the same side of a two-tile assembly in order for a bond to form. The only positive labels appropriately positioned on the existing assemblies are the +2 labels on C0-G3, but they do not match the labels on X1-X2-X3. Therefore, the only possible binding that can occur is on X3 label $-55$. We can see that this is matched by E0 and A0. This local non-determinism allows us to give L-shapes one of two different roles (center and edge, respectively) in the next assembly stage by initiating the creation of different borders around X1-X2-X3. This process is shown in Fig.10: Time 3-5 shows the only possible binding events and the resulting complete tile assemblies. Note that signals are transferred from A0 to C1 in Time 4.

**Remark.** Throughout every level of the L-shape assembly, we use the fact that the main larger shapes only have sequences of strength 1 “negative” labels along their sides, so only labels of strength 2 or corners formed by two negative labels can serve as attachment points for other tiles.

Note that in Fig.10, Time 6, both the A0-type\(^2\) assembly and the E0-type assembly may be joined.

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\(^2\)Throughout the thesis, we refer to L-shape assemblies which have a border initiated by an A0 or an E0 tile as an A0-type assembly or an E0-type assembly, respectively.
Figure 9. Time 1 shows the assemblies added to $T_1$. Time 2 shows the assemblies added to $T_2$; these are the first L-shape assemblies in the construction.

by two different assemblies, either the unit tiles B2 and G3 respectively, or the two-tile assemblies formed at Time 1, B2-C2 and G3-C0. Observe also, however, that in the former case, Time 7 would produce the latter case. Thus, Time 7 (Fig.11) will only yield new assemblies from the Time 6 assemblies created from the two-tile assemblies. Time 9 (right-most) completes the A0- and the E0-type borders.

In the E0-type assembly we see two perpendicular label 4’s (yellow) ($-$ on the E0 tile and $+$ on the G1 tile), which can be matched by the A0-type assembly, as it has a $+4$ on the A0 and a $-4$ on the D3 tile (and, again, it can be affirmed that no tile assemblies other than the ones shown can arise
up to Time 9). When these attach (see Fig.12, Time 10), a signal from G1 activates the label $-1$ (red) on C2 and C3, and a signal from D3 is sent through G1 to G3, activating the $-4$ label. Now an A0-type tile can attach to G3 and G2 at Time 11. A signal from G2 activates label $-2$ (blue) on C2 and C3, and label $-5$ on C1. The $-4$ label on G4 is activated similarly to G3. Finally, in Fig.13, the third A0-type shape can attach to G4 and F3. A signal from F3 activates label $-3$ (green) on C2 and C3, and label $-5$ on C1. Also, a signal travels from G4 to A0, then back to G4 and eventually to C1 on the top left A0-type shape, activating the $-55$ label. This completes the level 2 L-shape, which can now acquire an A0- or E0-type border in order to form the next level L-shape (level 3).

Figures 15-31 show the border-building process and the assembly of the level 3 L-shape. Fig.14 shows the borders on the level 2 shapes. Of note is the fact that the A0 border finishes at Time 36 but E0 does not finish until Time 39, thus A0-type shapes can attach to an unfinished E0-type shape. This still results in the correct assembly of the level 3 L-shape, as shown in Figures 27-31.
Figure 10. L-shape assembly, Time 3-6. The completed constructions depicted are the only constructions which can be added to $T_i$ for corresponding $i$. Beginning with this figure, only the initial and completed assemblies are shown in all figures, unless indicated otherwise; intermediate steps of the tile modification function are suppressed.
Figure 11. L-shape assembly. Time 7 (bottom left), Time 8 (top left), Time 9 (right). Again, these are the only new constructions that can be added to the active tile set.
Figure 12. Time 10-11, assembling the level 2 shape. The A0-type assembly binds via A0 and D3 to E0 and G1. The red signal from G1 is transmitted to C2 and C3, activating the corresponding labels. A signal from D3 is transmitted through G1 and activates the -4 label (yellow) in G3 which allows an A0-type assembly to bind at G3 and G2 sites. Broken transmission signals and disconnected inactive labels are cleaned up. In the figure on right, a process similar to the previous takes place, resulting in the activation of designated labels on the C1, C2, and C3 tiles in the A0-type and the G4 tile in the E0-type. Note that at this stage we also obtain incomplete L-shape constructions from completed A0-type assemblies binding to the E0-type assemblies with only a partially assembled border (for example, to the E0-type shape like in Time 7, Fig.11). These are not depicted in the following figures as they do not ultimately lead to any constructions different from the desired L-shape, although an example of the partial border mixed assemblies can be seen in Figures 27-30.
**Figure 13.** Time 12 completes the assembly of the level 2 shape from four level 1 shapes.

**Figure 14.** Level 2 L-shape assemblies with a completed A0- and E0-type border.
Figure 15. Time 13-14, initiating the A0 and E0 border formation. The only two possible binding events that can occur is the level 2 L-shape binding to an A0 or an E0. Any other events are disallowed either by geometry or by complementarity and strength: observe that all of the labels on the outside of the L-shape are “negative” strength 1. Two “positive” strength 1 labels would have to match between it and another structure in order for a bond to form. The reader may verify that none of the structures which could be produced up to this point have two positive labels in the correct configuration.
Figure 16. Time 15-16, continuing A0-E0 border formation. The assembly of the borders continues. Since B1 may already be attached to C1, both the single and the double addition structures are produced in Time 16; but the former may produce only the latter at the next step. Note also that the positive-positive corners required to fit into the negative-negative adjacencies are only ever present on single and double tiles, never on any larger structures (most tiles have only two positive labels and they use these to attach to growing assemblies, thus no positive labels remain for binding; the ones that do not follow the pattern are G2, G3, and F1, F2, and F3, but these contain positive 4 labels and there is never more than one such label on a fixed side of the assembly, so their geometry forces them to bind only with A0-type assemblies of the same level, as seen in Fig.27-31).
Figure 17. Time 17-18, the assembly continues. Note that in 17, the gold label “-44” on F1 was activated by a signal in the previous time step, which allowed a C4 tile to attach in this step.
Figure 18. Time 19-20.
Figure 19. When F1 attaches, it receives the signals 4 (yellow) and 5 (light purple) originally sent by C4 and transmitted by the E1’s.
Figure 20. Time 23-24. A similar situation arises with B2-C2 as did with B1-C1. Two assemblies are produced: one containing only B2 and one containing the B2-C2 pair; the former produces the latter at the next time step; so both evolve into the same shapes, but one does so faster.
**Figure 21.** Time 25-26. The signal originally sent by E2 is received by F2 and activates label -44 allowing C4 to attach.
Figure 22. Time 27-28.
Figure 23. Time 29-30. Notice that the second F2 receives the same signals as the second F2, activating its +4 and +5 labels and allowing E2 to attach at the next step.
**Figure 24.** Time 31-32. Just like B1-C1 and B2-C2, C3 can either be already attached to B3, or become attached immediately after.
Figure 25. Time 33-34.
Figure 26. Time 35-36. The A0-type border is completed at Time 36.
Figure 27. Time 37. Two things can occur. Either an A0-type assembly binds to a partially complete E0-type assembly as in figure on the left, or with even less of the border complete (not shown), or an A0-type assembly may gain another border tile (right).
Figure 28. Time 38. If the A0-type assembly binds, a signal from D3 is transmitted to the nearest E2, activating its -4 label and allowing it to bind to another A0-type bind if the second F2 on the E0-type border is present (left). The existing assemblies may also simply gain another border tile (right).
Figure 29. Note that the final A0-type assembly cannot attach until the border on the E0-type assembly is completed, so at this step only border additions may be gained.
Figure 30. Time 40 (top two assemblies) and 41 (bottom assembly). We see that in 41 only one new kind of assembly can be produced, because the variants of the partially assembled L-shapes converge to the same shape as more binding events occur.
Figure 31. Time 42. The first level 3 shape is assembled. Note the similarities between this and the level 2 shape. Both are given side by side in Fig.32.
3.2 The Inductive Step

In this section, we show that the smaller L-shapes self-assemble recursively into larger and larger L-shapes. First, note that the first L-shape, obtained at Time 2 (Fig.9), measures $1 \times 2$ tiles (on the short and the long sides respectively). Call this the level 1 L-shape. Given a level $n$ L-shape for $n \geq 1$, define the level $n + 1$ L-shape as the L-shape obtained by combining four bordered level $n$ L-shapes in the manner shown in Fig.32 for level 2 shapes forming the level 3 shape. Adding a border adds 1 to the dimension of the shorter side and 2 to the dimension of the longer side. The short side of level $n + 1$, $n \geq 1$ (pre-border) is just the length of the long side of level $n$ plus the border, i.e. plus 2, and the long side of level $n + 1$ is twice its short side (refer to Figure 7). So, if we denote the short side of level $n$ by $s_n$, we get:

$$s_n = 2s_{n-1} + 2, \quad \text{for } n \geq 2$$

$$= 3 \cdot 2^{n-1} - 2, \quad \text{for } n \geq 1$$

where the second equality can be easily verified using the first. As $s_1 = 1 = 3 \cdot 2^0 - 2$, if $s_n = 3 \cdot 2^{n-1} - 2, n \geq 1$,

$$s_{n+1} = 2(3 \cdot 2^{n-1} - 2) + 2 = 3 \cdot 2^n - 4 + 2 = 3 \cdot 2^n - 2$$

as required. The reader is now invited to compare level 2 and level 3 assembled L-shapes reproduced in Figure 32.

The assembly of level 1, 2, and 3 L-shapes has been shown explicitly in the previous section, if the resulting level $\geq 2$ shapes oriented as in Fig.32 are placed in the integer lattice with the bottom left corner tile (C2) on (1, 1), the resulting positioning of the tiles satisfies the format shown in Figure 33. We now show that given a level $n$ L-shape for $n \geq 2$, a level $n + 1$ L-shape will assemble.

In fact, this is not difficult to see. Suppose at some stage $N \in \mathbb{Z}$ we obtain the level $n$ L-shape assembly of the form shown in 33 and suppose furthermore that $\mathcal{T}_N$ contains the seed set of unit tiles (Fig.8) and the set of tile pairs obtained at Time=1 in Figure 9, but that the rest of the tile assemblies in $\mathcal{T}_N$ take the form of partially assembled level $\leq n - 1$ L-shapes or completely assembled level $\leq n - 1$ assemblies with partially completed borders, as was the case for $\mathcal{T}_{12}$ (Fig.13) when we obtained the level 2 L-shape, and for $\mathcal{T}_{42}$ (Fig.31) when we obtained the level 3 L-shape.
Figure 32. Level 2 and level 3 L-Shapes side by side. Note the positioning of corner markings (red labels -1, blue labels -2, green labels -3, and the purple -55 label, note that the rest of the tile edges are filled with the -5 label)
Figure 33. Level n L-Shape in $\mathbb{Z}^2$. Tiles marked with “...” represent suppressed rows and columns consisting of identical tiles. The only signaling present is on the three tiles as indicated by the red and yellow arrows (signals of the form $1^i_0$, $4^i_0$). The strength 1 labels $-1, -2, -3, -5$ are marked with red, blue, green, and light purple edges respectively. The label $-55$ at $(3 \cdot 2^{n-1} - 2, 3 \cdot 2^n - 4)$ is marked with a dark purple edge. No active or inactive labels other than the ones indicated are present.
Figure 34. Level $n$ L-Shape with A0-type border tiles.
Figure 35. Level $n$ L-Shape with E0-type border tiles.
Refer to Figures 34 and 35 for the level \( n \) L-shape assembling an A0-type border and an E0-type border respectively. It should be noted that since these two types of structure will assemble in parallel, the structure with the complete A0-type border will emerge 3 stages ahead of the complete E0-type border one, because the three corner positions of the A0-type can be filled by the paired tiles B1-C1, B2-C2, and B3-C3; this situation does not affect the final L-shape and proceeds in a manner similar to that shown in Fig.26-31 for the assembly of the level 3 shape.

Observe that the L-shape in Figure 33 consists only of “negative” labels, all but one of which are strength one. Observe also (from the set of figures describing the level 1-3 assemblies) that tiles which attach to a growing border have only negative labels on their free sides with the exception of C0 in Time 4 and 6 (Fig.10) and the tiles A0, G1, G2, F1, F2, and F3. In the former case, observe that the label on C0 is the only positive label in the entire assembly, so it could not bind with the \( n \)-level shape. In the latter case, all of these tiles carry a single label ‘4’ (yellow), which is not relevant in the \( n \)-level shape. Additionally, one can easily verify that none of the seven two-tile assemblies in Time 1(9) can bind along the \( n \)-level shape. This means that the only possible binding can occur at the \(-55\) site, matched by A0 or E0. From there, the binding sequence in Figures 34 and 35 is explained below.

In Figure 34, when A0 binds, its -1 label is activated and the -11 label is eliminated since the activation path is not connected to any corresponding transmission paths. Extraneous signaling on the tile below A0 is also eliminated. The only new binding opportunity created is in the \(-x\) direction and the only assembly containing compatible +1 and +5 label is the A1 tile, which transmits the 1 and 4 signals initiated by the A0 tile in the \(-x\) direction. The next binding opportunity is identical to the previous and so is filled by another A1 tile as the signaling gets passed along, and so on until \( x = 1 \) is reached. At this point, the corner formed by the A1 tile and the tile at \((1, 3 \cdot 2^n - 4)\) calls for a tile with two adjacent +1 sides, which is met by B1, and B1 with the necessary sides free can bind either alone or as an assembly with C1. If it binds alone, the next binding event must be the attachment of C1, which inevitably leads to a sequence of A2’s, a D1, and another sequence of A2’s until the blue edge label ‘-2’ of the assembly is reached. There B2 and C2 behave similarly to B1 and C1 above, leading to the attachment of a sequence of A3’s, a D2, and another sequence of A3’s which concludes with a B3-C3; following around the corner is a necessary sequence of A1’s and finally a D3. By this point, the extraneous signaling inside the level \( n \) shape has been removed by
the tile modification function. Once again, note that every tile attachment resulted in exclusively “negative” strength 1 labels at the edge of the assembly, except for the +4 label on A0. The -4 label, however, occurs in only one place on any A0-type assembly - on the D3 end, which makes the binding of any two A0-type assemblies geometrically impossible: the same or higher level A0-type assembly would overlap the other assembly, a lower level assembly would be too small to reach both A0 and another binding site simultaneously.

In Fig. 35, the E0 situation works similarly. When E0 attaches, it receives a -4 label activation signal, allowing E1 (and only E1) to bind. Only E1 tiles may bind until the corner is reached, at which point only F1 can attach. F1 receives the label -44 (gold) activation signal originally initiated by E0 and transmitted by the E1’s and the inactive +4 label on its +y side and -5 on its +x side is removed, since the activation pathway leading to it is cut off. The -44 label allows the C4 tile to attach, which is followed again by a sequence of E1’s terminating in F1. This time, F1 receives an activating signal for its -4 label on the −x side and its -5 label on the −y side. The E0 -4 and F1 +4 active labels are geometrically positioned in such a way as to allow only the A0 +4 and D3 -4 tiles on an assembly of the same size to attach. This can happen, at the earliest, when the E0-type border is 3 tiles short of completion (for the reasons mentioned before).

**Remark.** In fact, after the A0-type assembly has assembled, it may attach to the E0-F1 points in any incomplete E0-type assembly having these tiles, but the resulting partially assembled structure retains the capability to assemble normally and cannot assemble into any shapes other than the L-shape of its level (in particular, the -55 label cannot be activated until the full shape is assembled).

After F1, only E2 can attach, followed by a sequence of E1’s ending in F2. F2 is almost identical to F1, the only difference being that instead of an edge label 1 and a label 1 signal, F2 has an edge label 2 and a label 2 signal. It receives the -44 signal initiated by E2 and binds to a C4 tile, followed by E1’s, followed by an F2 and E2 with a sequence of E1s as before. Once the E2 that is next to F1 receives an activation signal from the D3 of an attached A0-type assembly, that E2 and F2 can bind with another A0-type assembly which will activate the second E2, which, however, cannot bind until the final F3 is in position. The first F3 sends a -55 signal to the E2, but it cannot be transmitted until the final A0-type assembly attaches, so the rest of the E0-type border is completed (eliminating unnecessary signals in the process). Notice that F1, F2, and F3 carry “special instructions.” Once an A0-type tile attaches to them, F1 initiates a “red” (label 1) signal, F2 a “blue” (label 2) and F3
a “green” (label 3) one. These get transferred along the A0-type tiles to the C2 and C3 corners, marking them with the corresponding active label. The tiles F2 and F3 also send label 5 (light purple) signals to the C1’s of the corresponding A0-type assemblies. The -55 signal from the first F3 travels to E2, then it must pass through A0 before returning to E2, then to F2 and along the border tiles until it reaches the next E2. Then its path is continued through A0 and back along the same border before it is intercepted and redirected to D3 by the F1 tile. The A0-type tile then routes the signal through its own border to C1. The tiles in the E0 and A0 borders no longer have any signaling except for the C1 tiles of the A0-type shapes which contain the signals they received from A0. The resulting outside labels are exactly as in Fig.33.

**Theorem 3.2.1.** The active tile assembly system \((T_0, 2)\) yields the recursive self-assembly of level \(n\) L-shapes for each \(n \geq 1\), which results in an aperiodic tiling of the plane.

**Proof.** The recursive process generating the L-shapes can be described as follows:

1. The level 1 L-shape assembly instances are the X1-X2-X3 structures assembled at time 2 (Fig.9).
2. Given level \(n\) L-shape assembly instances for \(n \geq 1\), assemble an A0-type or an E0-type border around each.
3. Combine three A0-type bordered level \(n\) assembly instances with an E0-type bordered level \(n\) assembly instance to form a level \(n+1\) assembly instance.

Combining the constructions of the previous section and the recursion shown in this section, we see that the only tile assemblies that can be obtained from \(T_0\) at \(\theta = 2\) are the level \(n\) L-shapes in various states of completion for all \(n \geq 1\). We note that each complete level \(n\) L-shape can be divided into three square regions, and that each of the square regions in an \(n+1\) L-shape covers more than 4 times the area covered by a square region of the level \(n\) L-shape. Thus, since these squares grow without bound, given any sized square portion of the plane, there exists some \(m\) such that the level \(m\) L-shape covers it. As \(m \to \infty\), the L-shape assembly instances provide a tiling of the plane.\(^3\)

For the proof of aperiodicity, refer to Figure 32 and Figures 34 and 35. Fix an L-shape tiling of the entire plane, \(\xi\). Notice that for a given level \(n\) L-shape, there is a unique outermost C2 marked with

\(^3\)This is, in fact, a consequence of König’s lemma.
a $-2$ label and a unique outermost C3 marked with a $-2$ label. These two unit tiles, furthermore, are separated by a line of A3’s, where the exact number of the A3’s determines the level $n$. This uniqueness is guaranteed by construction: every level $n$ L-shape is formed by an E0-type bordered level $n - 1$ L-shape in the center that is adjacent to three A0-type bordered level $n - 1$ L-shapes. Each of the A0-type shapes contains a single C2 and a single C3 as part of its border. The label counter-clockwise adjacent to the $+2\text{2}$ (dark blue) label on C2 and to the $+3\text{3}$ (dark green) label on C3 (see Fig.32) is determined by the A0-type level $n - 1$ shape’s position relative to the level $n - 1$ E0-type shape. The three possible orientations yield three possible label values (-1, -2, or -3). Consequently, the particular configuration of C2 and C3 carrying the $-2$ label is indeed unique within the level $n$ L-shape.

This unique placement of C2 and C3 followed by the fixed number of A3’s guarantees that no translation of an L-shape tiling of the plane is possible by a vector with either component less than $3 \cdot 2^{n-1} - 2$ (the length of the short side of a level $n$ L-shape) for any $n$. Otherwise, supposing this is not the case for some $n \geq 2$, consider the plane tiling $\xi$ induced by the L-shape assembly instances. Shift $\xi$ so that the bottom left corner of a level $n$ L-shape assembly is placed at the origin. Then a C2 C3 border configuration as described above for the level $n$ L-shape would have to appear more than once inside that level $n$ L-shape - and this, we have shown, cannot happen. It follows that the tiling $\xi$ is not invariant under any translation.

□
Chapter 4
Conclusions

We have formally defined a model of active tile assembly and applied it to produce a recursive self-assembly of a self-similar L-shape tiling. Several natural questions arise with respect to both.

Is the model sufficiently general? How can it be extended to tile shapes other than the square? How well does it capture the physical self-assembly process of DNA tiles? For example, the alternate attempt at an active tile model made in [21] includes the ability to deactivate what we here have called “edge labels” and allowing tiles to break away from a constructed assembly. In fact, adding a deactivation capacity to the model we have presented is not difficult. The triple \((\tau, A, S)\) could be expanded to include a set of deactivation signals and a set of deactivation pathways, becoming a 5-tuple. The tile modification function would have to be expanded to remove deactivation signals when they are used in a manner completely analogous to activation signals and to remove labels that have been deactivated. After any deactivation, it would be necessary to check whether the assembly is still \(\theta\)-stable - if not, the simulation of the remaining signal transmission would need to be continued on separate assemblies (which, if not stable themselves, would need to be broken up also). The definition of active tile sets would also have to be modified to include assemblies which are obtained in that manner.

Authors in [21] also attempt to account for variability in signal transmission rates by allowing tiles to “wait” before transmitting a signal. Our assembly model is very simplified in the sense that we assume that all signal transmissions occur simultaneously and that all signaling across a single assembly is completed before it can bind to another one. In solution, all these processes of binding and signal transmission are occurring in parallel and at variable rates; thus, a more accurate model of physical reality would allow an assembly at any point in its signal transmission cycle to bind with other assemblies, which means for any assembly \(\alpha\) we would have to add assemblies \(f^i(\alpha)\) for every \(i \geq 0\) (where \(f\) is the tile modification function) to the active supertile set of the relevant stage. An even more accurate model could account for a different rates of signal transmission by writing...
\( c_x \) instead of \( c_0 \) whenever a tile receives an activation signal from another tile; this could represent a pending signal. A tile containing such a signal could replace the \( x \) with a 0 at any iteration of the tile modification function, at which case it would act the same way as the already defined activation signals.

Another generalizing notion is that of a “flexible glue function” [2], which would assign a nonzero strength to bonds between nonmatching glues (or labels). One could directly modify the strength function and the corresponding weight function of the binding graph to accomplish this; however, in principle, this can be modelled by using a notion already provided in this paper - that of multiple active glues (or labels).

Of course, there are still more basic questions with regard to the active model: namely, just how much of an improvement is it over the standard model? In practical terms, signaling may allow more control over the assembly process while reducing the number of necessary tile types and labels. But how much can the complexity be reduced? Are there things that can be accomplished with signaling (without deactivation) which absolutely cannot be accomplished with passive tiles, regardless of the number of labels? For example, can the L-shape tiling we described be accomplished with passive tiles? What is the minimum number of tile types or labels if signaling is minimized? What is the minimum number of tile types if the number of labels is minimized? What is the absolute minimum of tile types required? Is there a tile set that will perform the assembly at temperature 1?

The attentive reader may have also noticed that the tile assemblies paired with the tile modification function as defined in Chapter 2 are essentially 2D cellular automata - this is something quite different from the simulation of a 1D cellular automaton by successive rows in a lattice. It would be interesting to analyze the possibilities of the model with regard to cellular automata, for example, to see what kinds of cellular automata can be simulated by a growing tile assembly.

These are all questions to pursue in future research. One thing that has unquestionably emerged in this thesis, however, is a special method for the construction of self-similar aperiodic tilings. We believe that the method used for the creation of the L-shape tile can be used to create a variety of aperiodic patterns, for example the square pattern in Figure 36. The principle is to use local nondeterminism to create the desired hierarchy. At each level, each instance of the shape is assigned a role in the next level by obtaining a partial border, selected at random, which grows in length with proportion to the size of the shape. This growth in length is what guarantees non-periodicity as
Figure 36. A non-periodic square tiling utilizing the border technique; here, four different border types - red, yellow, green, and blue - determine a particular square’s position in the larger shape.

Increasingly longer border lines consisting of one kind of tile types will be found further away from a given tile, disallowing translational symmetry. Essentially, the entire identity of the larger tile is contained in its outside border, so the borders mediate all binding and signaling which occurs among the shapes.

Recursive self-assembly of DNA nanostructures has not been explored in literature to date. We hope that this method together with the active tile assembly model will pave the way for much more research in this area.
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