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# The self-assembly of paths and squares at temperature 1

Pierre-Étienne Meunier *

**Abstract**

We prove that the number of tile types required to build squares of size $n \times n$, in Winfree's abstract Tile Assembly Model, when restricted to using only non-cooperative tile bindings, is at least $2n - 1$, which is also the best known upper bound. Non-cooperative self-assembly, also known as "temperature 1", is where tiles bind to each other if they match on one or more sides, whereas in cooperative binding, some tiles can bind only if they match on multiple sides.

Our proof introduces a new programming technique for temperature 1, that disproves the very intuitive and commonly held belief that, in the same model, assembling *paths* between two points $A$ and $B$ cannot be done with less tile types than the Manhattan distance $\|\overrightarrow{AB}\|_1$ between them. Then, we prove a necessary condition for these "efficient paths" to be assembled, and show that this necessary condition cannot hold in completely filled squares.

This result proves the oldest conjecture in algorithmic self-assembly, published by Rothemund and Winfree in STOC 2000, in the case where growth starts from a corner of the square. As a corollary, we establish $n$ as a lower bound on the tile complexity of the general case. The problem of determining the minimal number of tile types to self-assemble a shape is known to be $\Sigma_2^p$-complete.

## 1 Introduction

Self-assembly is the process through which unorganized, simple, components automatically coalesce according to simple local rules to form some kind of target structure. It sounds simple, but the end result can be extraordinary. For example, researchers have been able to self-assemble a wide variety of structures experimentally at the nanoscale, such as regular arrays [28], fractal structures [10, 20], smiling faces [18, 26], DNA tweezers [30], logic circuits [16, 21], neural networks [17], and molecular robots [12]. These examples are fundamental because they demonstrate that self-assembly can, in principle, be used to manufacture specialized geometrical, mechanical and computational objects at the nanoscale. Potential future applications of nanoscale self-assembly include the production of smaller, more efficient microprocessors and medical technologies that are capable of diagnosing and even treating disease at the cellular level.

Controlling nanoscale self-assembly for the purposes of manufacturing atomically precise components will require a bottom-up, hands-off strategy. In other words, the self-assembling units themselves will have to be "programmed" to direct themselves to assemble efficiently and correctly. Molecular self-assembly is rapidly becoming a ubiquitous engineering paradigm, and we need to develop a theory to inform us of its algorithmic capabilities and ultimate limitations.

In 1998, Erik Winfree [27] introduced the abstract Tile Assembly Model (aTAM), a simplified discrete mathematical model of algorithmic DNA nanoscale self-assembly pioneered by Seeman [22]. The aTAM is an asynchronous nondeterministic cellular automaton that models crystal growth

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processes. Put another way, the aTAM essentially augments classical Wang tiling [25] with a mechanism for sequential growth of a tiling. This contrasts with Wang tiling in which only the existence of a valid mismatch-free tiling is considered, and *not* the order of tile placement. In the aTAM, the fundamental components are translatable but un-rotatable square or cube *tiles* whose sides are labeled with colored *glues* colors, each with an integer *strength*. Two tiles that are placed next to each other *interact* if the glue colors on their abutting sides match, and they *bind* if the strengths on their abutting sides match and sum to at least a certain (integer) *temperature*. Self-assembly starts from a *seed* tile type and proceeds nondeterministically and asynchronously as tiles bind to the seed-containing-assembly. Despite its deliberate simplification, the aTAM is a computationally expressive model. For example, by using cooperative binding (that is, by having some of the tiles bind on two or more sides), Winfree [27] proved that it is Turing universal, which implies that self-assembly can be directed by a computer program. Here, we study noncooperative binding.

Tile self-assembly in which tiles can be placed only in a *noncooperative* fashion is colloquially referred to as "temperature-1 self-assembly". Despite the esoteric name, this is a fundamental and ubiquitous form of growth: it refers to growth from *growing and branching tips* where each new tile is added if it can match on at least *one side*.

It has been known for some time that a more general form of growth where some of the tiles must match on two or more sides, i.e. *cooperative* growth, leads to highly non-trivial behavior: arbitrary Turing machine simulation [11, 19], efficient production of $n \times n$ squares and other simple shapes using $\Theta(\log n / \log \log n)$ tile types [1], efficient production of arbitrary finite connected shapes using a number of tile types that is within a log factor of the Kolmogorov complexity of the shape [24], and even intrinsic universality: the existence of a single tile set that simulates arbitrary tile assembly systems [7].

However, the capabilities of two-dimensional noncooperative self-assembly remain largely unknown: several generalizations and restrictions of this model have been studied, that conjectured in all cases that noncooperative binding could not be as powerful as cooperative binding [4, 5, 9, 13, 15, 19]. The first fully general separation results were only proven recently [14], in the context of intrinsic universality [6–8]. However, the computational capabilities, in the Turing sense, of this model, remain largely unknown.

The conjecture that we prove in this paper was first stated by Rothemund and Winfree [19][1]: the minimal number of tile types to assemble $n \times n$ squares is $2n - 1$. A restriction of this result, where it is required that all the tiles be assembled with all their neighbors, appeared in the same paper. Moreover, computing the minimal number of tile types required to *deterministically* assemble a shape from a seed of size one is known to be NP-complete [2], and $\Sigma_2^p$-complete in the non-deterministic case [3].

### 1.1 Main results

Although a number of terms have not been formally defined, we give an overview of our two main results now. See the definitions in section 2. Our ultimate goal is to prove Rothemund and Winfree's conjecture [19] that a tile assembly system assembling only squares of size $n \times n$, from a seed of size 1, has at least $2n - 1$ tile types. Our first result disproves a statement stronger than this conjecture; namely, that the tile complexity of a square is the same as the tile complexity of its diagonal. Although widely believed, this statement is false:

**Theorem 3.1.** Let $n$ be an integer. There is a tile assembly system $\mathcal{T}_n = (T_n, \sigma_n, 1)$, and two

[1] In Figure 2 of that paper

points $A, B \in \mathbb{Z}^2$, such that $\|\overrightarrow{AB}\|_1 = n$, the terminal assemblies of $\mathcal{T}_n$ are all finite, they all include a path from $A$ to $B$, and $|T_n| = 4n/5 + O(1)$.

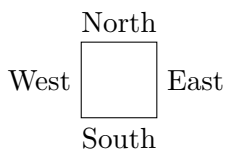
The fact that the constructions of this theorem are possible, even though they are quite elementary, is not obvious at all; indeed, the intuition from words and automata theory is that any attempt to "reuse" tile types will enable us to "pump" the path, as in the pumping lemma of finite automata [23], and thus any tile assembly system that can produce paths repeating tile types will also be able to produce ultimately periodic, infinite paths. This intuition is valid in a restricted setting where two adjacent tiles always agree on their abutting sides [9, 13].

Then, we will prove the following theorem, which gives the optimal lower bound on the tile complexity of squares, when growth starts from a corner:

**Theorem 4.2.** Let $\mathcal{T} = (T, \sigma, 1)$ be a temperature 1 tile assembly system, with $\sigma$ a single tile at $(0, 0)$, and $n$ an integer. If all terminal assemblies producible by $\mathcal{T}$ are of domain $\{0, \ldots, n-1\}^2$, then $|T| \geq 2n - 1$.

## 2 Definition and preliminaries

We begin by defining the two-dimensional abstract tile assembly model. A *tile type* is a unit square with four sides, each consisting of a glue *label* and a nonnegative integer *strength*. We call a tile's sides north, east, south, and west, respectively, according to the following picture:




We assume a finite set $T$ of tile types, but an infinite supply of copies of each type. An *assembly* is a positioning of the tiles on the discrete plane $\mathbb{Z}^2$, that is, a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$.

We say that two tiles in an assembly *interact*, or are *stably attached*, if the glue labels on their abutting side are equal, and have positive strength. An assembly $\alpha$ induces a weighted *binding graph* $G = (V, E)$, where $V = \mathrm{dom}(\alpha)$, and there is an edge $(a, b) \in E$ if and only if $a$ and $b$ interact, and this edge is weighted by the glue strength of that interaction. The assembly is said to be $\tau$-stable if any cut of $G$ has weight at least $\tau$.

A *tile assembly system* is a triple $\mathcal{T} = (T, \sigma, \tau)$, where $T$ is a finite tile set, $\sigma$ is called the *seed*, and $\tau$ is the *temperature*. Throughout this paper, we will always have $|\mathrm{dom}(\sigma)| = 1$ and $\tau = 1$. Therefore, we can make the simplifying assumption that all glues have strength one without changing the behavior of the model.

Given two assemblies $\alpha$ and $\beta$, we write $\alpha \rightarrow_1^{\mathcal{T}} \beta$ if we can get $\beta$ from $\alpha$ by the binding of a single tile, $\mathrm{dom}(\alpha) \subseteq \mathrm{dom}(\beta)$, and $|\mathrm{dom}(\beta) \setminus \mathrm{dom}(\alpha)| = 1$. We say that $\gamma$ is *producible* from $\alpha$, and write $\alpha \rightarrow^{\mathcal{T}} \gamma$ if there is a (possibly empty) sequence $\alpha = \alpha_1, \ldots, \alpha_n = \beta$ such that $\alpha_1 \rightarrow_1^{\mathcal{T}} \ldots \rightarrow_1^{\mathcal{T}} \alpha_n$.

A sequence of $k \in \mathbb{Z}^+ \cup \{\infty\}$ assemblies $\alpha_0, \alpha_1, \ldots$ over $\mathcal{A}^T$ is a $\mathcal{T}$*-assembly sequence* if, for all $1 \leq i < k$, $\alpha_{i-1} \rightarrow_1^{\mathcal{T}} \alpha_i$.

The *productions* of a tile assembly system $\mathcal{T} = (T, \sigma, \tau)$, written $\mathcal{A}[\mathcal{T}]$, is the set of all assemblies producible from $\sigma$. An assembly $\alpha$ is called *terminal* if there is no $\beta$ such that $\alpha \rightarrow_1^{\mathcal{T}} \beta$. The set of terminal assemblies is written $\mathcal{A}_\square[\mathcal{T}]$.

An important fact about temperature 1 tile assembly, that we will use heavily, is that any path of the binding graph can grow immediately from the seed, independently from anything else.

Formally, a *path* $P$ is a sequence of tile types along with positions, that is, of elements of $T \times \mathbb{Z}^2$, such that no position occurs more than once in $P$, and for all $i$, the positions of $P_i$ and $P_{i+1}$ are adjacent in the lattice grid of $\mathbb{Z}^2$.

For any path $P$ and integer $i$, we write $(x_{P_i}, y_{P_i})$ the coordinates of $P_i$'s position. Moreover, if $i < n$, we say that the *output side* of $P_i$ is the side adjacent to $P_{i+1}$, and if $i > 1$, that its *input side* is the side adjacent to $P_{i-1}$. This means that the first tile of a path does not have an input side, and the last one does not have an output side. Remark that this definition of input/output sides is only relative to a *path*, and not to the tiles themselves; indeed, the tiles, including the first and last ones, may have other glues, not used by the path.

Also, for any path $P = P_0, P_1, \ldots, P_{|P|-1}$, and any integer $i$, we call the *right-hand side* (respectively *left-hand side*) of $P_i$ the side of that is between its input and output sides, in counterclockwise (respectively clockwise) order. When there is no ambiguity, we will say "the right-hand side (respectively left-hand side)" of $P$ itself to mean "the right-hand side (respectively left-hand side) of some tile of $P$".

Finally, for $A, B \in \mathbb{Z}^2$, we use the notation $\overrightarrow{AB}$ to mean "the vector from $A$ to $B$", and the *Manhattan distance* between $A = (x_A, y_A)$ and $B = (x_B, y_B)$, written $\|\overrightarrow{AB}\|_1$, is $|x_A - x_B| + |y_A - y_B|$. We also call $O$ the *origin* on $\mathbb{Z}^2$, i.e. the point of coordinates $(0, 0)$.

### 2.1 The known upper bound

The only known way to assemble squares of size $n \times n$ at temperature 1 with $2n - 1$ tile types, is by using the "comb" design of Figure 1, already described in Rothemund and Winfree's paper [19].

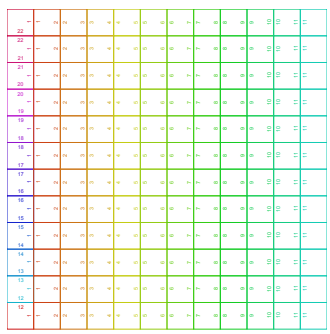


Figure 1: The comb design for size $10 \times 10$

## 3 Building efficient paths

A major obstacle in proving the claimed lower bound for squares, is that building only a square's diagonal can require less tile types than building the whole square. In this section, we show the following result:

**Theorem 3.1.** *There is a tile assembly system $\mathcal{T} = (T, \sigma, 1)$, such that for all terminal assembly $a \in \mathcal{A}_\square[\mathcal{T}]$, $a$ is finite and of width $\frac{5(|T|+2)}{4} - 23$.*

*Proof.* Since a path of height $n$ that is monotonic in the y-dimension, and has less than $n$ tile types with input side south, can be "pumped", our path will need to have "caves", or non-monotonic subpaths, and reuse them several times. Moreover, in order for all the assemblies of $\mathcal{T}$ to be finite,

the caves must be exited by a different path every time; however, since we want the caves to "save" tile types, these "exit paths" cannot all be new tile types. Therefore, one possible way to solve these constraints is to grow a regular monotonic path $P_0$ first, then build a cave $C$, and reuse a part of $P_0$ as its exit path. The next time we want to reuse $C$, we can use another part of $P_0$ as its exit path.

If the exit paths used in previous instance of a cave are all blocked in new instances, we will get only finite assemblies. Figure 2 is an example of such a path.

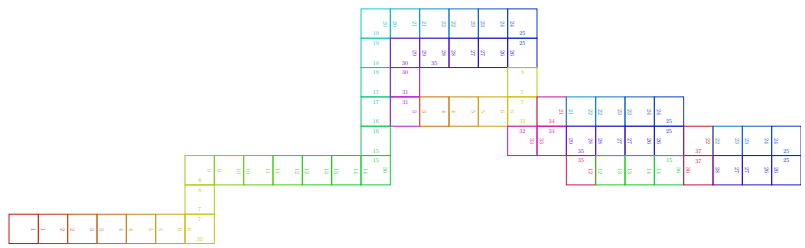


Figure 2: Reusing caves and exit paths

This figure, however, is not a terminal assembly; since our caves, and their exit paths, are used several times, the same assemblies can grow from all their repetitions. Fortunately, we can arrange the shape of our main path so that no collision ever happens between these repetitions, like on Figure 3. Now, this figure has 38 tile types, and is of width 27; it does not yet save tile types. But by inserting:

- $n$ new tile types in place of glue 6,
- $n$ new tile types in place of glue 14,
- $n$ new tile types in place of glue 24, and
- $n$ new tile types in place of glue 26

Zooming in may be needed to read these numbers on Figures 2 and 3. Printable versions are included, in Appendices A and B.

We add only $4n$ tile types, but the assembly is now $5n$ wider, and the result follows. An example of path that actually saves tile types is given on Figure 4.

□

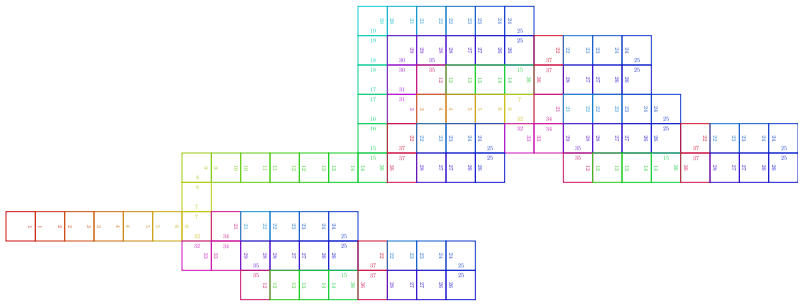


Figure 3: Early branches, not blocking the main assembly

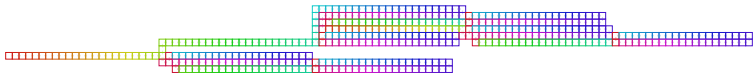


Figure 4: A path of width 112 with 106 tile types

# 4 Building filled squares requires $2n-1$ tile types

In this section, we prove that if a tileset has less than $2n-1$ tile types and all its terminal assemblies are of domain $\{0,1,\ldots,n-1\}^2$ then one of its productions is a path that does not "save" tile types. Our technique to prove this will be the following: assuming we are given such a tileset, we will first choose, using Algorithm 4.1, the assembly sequences that "lose" as much information as possible about their past, so as to "confuse" the tileset; then, if these assembly sequences can still build efficient paths, we will prove a necessary condition on these (this is Lemma 4.4), that cannot hold in completely filled squares (Theorem 4.5).

## 4.1 A path-building algorithm

We first define the algorithm we use to find assembly sequences that suit our purposes. There are two possible "priority modes" for this algorithm, namely *right-priority* and *left-priority*:

**Algorithm 4.1.** Let $\mathcal{T} = (T, \sigma, 1)$ be a tile assembly system, $\preceq$ be an ordering on $T$, and $S$ be a non-empty subset of the set of paths producible by $\mathcal{T}$. Let $P_0$ be the initial path, with just $\sigma$. For any $i \geq 0$, if several tiles can bind to $P_i$, let $P_{i+1}$ be the one such that:

1. If $P_i$ is of the same type as a previous tile $P_h$ on $P$, with $h < i$, whose output side $s$ is distinct from $P_i$'s input side, then grow $P_{h+1}$, on side $s$ of $P_i$.
2. Else, if it is possible, let $P_{i+1}$ be the tile such that:
   (a) $P_{i+1}$ binds to the first side of $P_i$ from its input side, in clockwise order if we are building a left-priority path, and in counterclockwise order if we are building a right-priority one.
   (b) There is at least one path in $S$, of which $P_0, P_1, \ldots, P_{i+1}$ is a prefix.
   (c) If there are several such choices, we choose the smallest tile with respect to $\preceq$.

3. Finally, if none of the previous cases is possible to follow (for instance, because following case 1 resulted in a collision with a previous part of the assembly), but a new branch can still grow from the existing assembly, and produce a path of $S$, then follow it. Else, the algorithm halts.

   We call the last tile that was placed before the present case the *collision tile*. In the special case that the current assembly before applying this case is already in $S$, we will adopt the convention that the *empty branch* can start.

Remark that this algorithm does not guarantee that the final path will be in $S$. If all producible paths end up being paths of $S$, it will be the case. But else, it means that we can "prevent" paths of $S$ from growing. We will use this property heavily in the rest of our proof: $S$ will be the set of all paths that reach some point in the square, and there is no way, in a filled square, to prevent a point from being covered.

## 4.2 Building filled squares from a seed in a corner

We begin by showing that a "path editing" operation is possible on the paths, built by Algorithm 4.1, that save tile types.

**Definition 4.2.** A *left-tentacular* (respectively *right-tentacular*) path is a path $P$ such that the following conditions all hold:

- at least two tiles of $P$ are of the same type. Let $i$ and $j$ be the indices of two tiles of $P$ of the same type.
- $P$ forked after a collision in case 3 of Algorithm 4.1, at some position $k > j$, and this branch started on the left-hand side (respectively right-hand side) of $P_k$.
- This same branch can also start and completely grow from tile $P_{k-j+i}$, after $P$ is itself completely grown.

Moreover, we call $\overrightarrow{P_jP_i}$ a *contraction vector* of $P$, and early branchings of $P_{k,k+1,\ldots|P|-1}$ are *tentacles*.

We say that a path is *two-way tentacular* if it is both left- and right-tentacular.

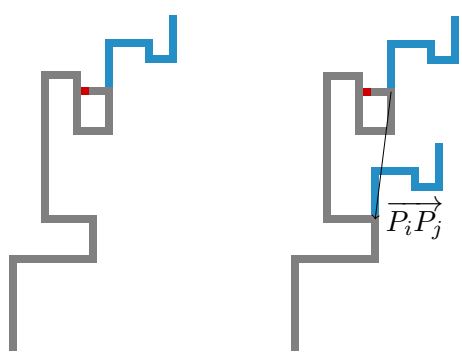



Figure 5: A right-tentacular path, with the branch in blue, and the collision tile in red. A contraction vector is drawn on the right-hand drawing.

**Definition 4.3.** Let $\mathcal{T} = (T, \sigma, 1)$ be a tile assembly system. A path $P \in \mathcal{A}[\mathcal{T}]$ is said to be *fragile* if:

- a tile type is repeated on $P$, at positions $i$ and $j$ ($i < j$), and $P_{j,j+1,\ldots,|P|-1}$, translated by $\overrightarrow{P_j P_i}$, can also start growing from $P$ immediately after $i$.
- but $P_{i,i+1,\ldots,|P|-1}$ cannot grow completely from the resulting assembly.

In the rest of the proof, we will call *breaking* $P$, the choice to start growing $P_{j,j+1,\ldots|P|-1}$, translated by $\overrightarrow{P_j P_i}$, immediately after $i$ before growing $P_{i,i+1,\ldots,|P|-1}$. Moreover, the smallest suffix of $P$ that can branched earlier than its original first point on $P$ is called the *breaking branch*.

See Figure 6 for an example of a fragile path (at this point, though, the colors of that figure are not yet defined).

**Lemma 4.4.** *Let $A = (x_A, y_A)$ be a point of $\mathbb{Z}^2$, and $\mathcal{T} = (T, \sigma, 1)$ be a tile assembly system such that the following conditions all hold:*

- $\mathrm{dom}(\sigma) = \{O\}$.
- *All assemblies can reach $A$, that is, $\forall \alpha \in \mathcal{A}_{\square}[\mathcal{T}], A \in \mathrm{dom}(\alpha)$.*
- *There is a path $P \in \mathcal{A}[\mathcal{T}]$ from $O$ to $A$, built using Algorithm 4.1 with parameter $S$ of the algorithm being the set of all producible paths of $\mathcal{T}$ from $O$ to $A$, and $P$ has strictly less than $\|\overrightarrow{OA}\|_1 - 1$ tile types.*
- *$P$ is such that for all $i$, $y_{P_i} \in \{0, \ldots, y_A\}$.*

*Then $P$ is either fragile or two-way tentacular.*

*Proof.* Let $P$ be a path from $O$ to $A$, built using Algorithm 4.1. Without loss of generality, we assume that $y_A \geq 0$ and $x_A \geq 0$ (we get other cases by rotating or flipping the argument).

We first introduce the idea of *visible glues*: we say that a glue between two tiles of $P$ is visible from the east (respectively from the south) if $P_i$ interacts with $P_{i+1}$ on its north face (respectively on its east face), and the glue between them is the rightmost (respectively lowest) one, on an infinite horizontal (respectively vertical) line between $P_i$ and $P_{i+1}$. Moreover, we adopt the convention that the rightmost tile on row $y = y_A$ has its north glue visible from the east, and its east glue visible from the south (even if this tile has 0-strength glues on these sides).

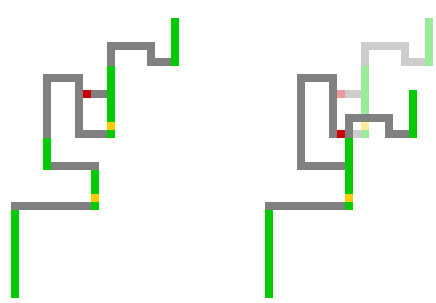


Figure 6: Tiles with glues visible from the east are in green or yellow; yellow tiles are of the same type, and red tiles are collisions. In this case, $P$ is fragile.

Let us call $P_{\mathrm{E}}$ the tiles of $P$ that have their north glue visible from the east, and $P_{\mathrm{S}}$ the tiles of $P$ that have their east glue visible from the south. First, there are at least $y_A$ tiles in $P_{\mathrm{E}}$, and $x_A$ tiles in $P_{\mathrm{S}}$. We prove this now for $P_{\mathrm{S}}$: indeed, for all $x \in \{0, \ldots, x_A - 1\}$, the visible tile of $P$ on column $x$ has output side east. To see this, suppose, for the sake of contradiction, that some tile $P_i$ is visible from the south, and has output side W. Then, draw an infinite horizontal half-line from the east side of $P_i$ to the south. Along with $P_{0,\ldots,i}$ and a horizontal infinite line at $y = 0$, it partitions the plane into two connected components, by Jordan's curve theorem (see Figure 7).

Therefore, because $P$ does not intersect itself, and for all $i$, $y_{P_i} \geq 0$, it must necessarily cross the vertical line at the east of $P_i$ again before reaching $A$. Thus, $P_i$ cannot be visible from the south, since $P$ has at least one tile below $P_i$.

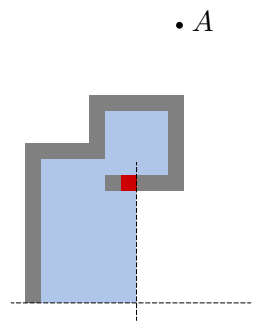



Figure 7: Jordan's curve theorem in action, with the enclosed region in blue

A similar argument, rotated by $\pi/2$, shows that $P_{\mathrm{E}}$ has at least $y_A$ tiles.

Furthermore, except possibly for the last tile of $P$, $P_{\mathrm{E}}$ and $P_{\mathrm{S}}$ are disjoint, because each tile has at most one output side: $P_{\mathrm{E}} \cap P_{\mathrm{S}} \subseteq \{P_{|P|-1}\}$, and therefore $|P_{\mathrm{E}} \cup P_{\mathrm{S}}| \geq \|\overrightarrow{OA}\|_1 - 1$.

Now, because $P$ was grown using Algorithm 4.1, if a tile type is repeated in $P_{\mathrm{E}}$, say at positions $P_i$ and $P_j$, with $i < j$, then the translation of $P_{i,i+1,\ldots,j}$ by $\overrightarrow{P_iP_j}$ started growing immediately after $P_j$, by case 1 of Algorithm 4.1, ultimately crashing into something, possibly after several repetitions (because we assumed that all productions of $\mathcal{T}$ are finite). We call this collision "collision $C_0$". Immediately after it happened, case 3 of the algorithm necessarily got used, and a new (possibly empty) branch was started from the existing assembly, and reached $A$ (because of our hypothesis that all terminal assemblies have $A$ in their domain).

Therefore, an early restart of this branch can also grow from $P_{i,i+1,\ldots,j}$. There are two cases:

1. If it can grow completely from $P$, it means that $P$ is right-tentacular, by definition of right-tentacular.

2. Else, this new branch crashes into something. We call this crash "collision $C_1$". There are two cases, according to where it crashes:

   (a) Either it crashes into a part of $P$ grown before $P_i$. In this case, first observe that the north glue of $P_i$ is still visible from the east after this operation: indeed, the north glue of $P_j$ was visible from the east before, so no $P_k$, for $k > j$, is on the right of $P_j$ on a horizontal line at $y = y_{P_j}$. And since we only translated these tiles by $\overrightarrow{P_jP_i}$, these translated tiles are not on the right of $P_i$ on a horizontal line at $y = y_{P_i}$ either (see for instance Figure 6).

   We now prove that $P$ is fragile. Indeed, grow it until index $i$. Then, grow a translation by $\overrightarrow{P_jP_i}$ of the path that grew after $P_j$, as long as it can possibly grow. We claim that

the original $P$ cannot grow anymore from this new assembly, that we call $Q$, and this is the definition of $P$ being fragile.

This is because of the definition of $P_{\mathrm{E}}$ and $P_{\mathrm{S}}$: we first argue that collision $C_1$ encloses a portion of the plane: this is indeed an application of Jordan's curve theorem, because a collision between two connected paths closes a curve in the plane. from the south in $Q$, and the side of $P_i$ exposed to the south or the east is its right-hand side (this follows from the fact that $P_i$'s output side is its north side if visible from the east, and its east side if visible from the south), the breaking branch starts from some $P_k$ (for $k > j$), on branches from its right-hand side.

Therefore, if we grow this branch early, at position $k-j+i$, and it crashes into a previous part of the assembly, then by Jordan's curve theorem, we enclose the left-hand sides of its tiles; but since this branch forks from the right-hand side of the path, the enclosed region is thus the region in which $P$ grew, because $P$ is then a "left turn" from the breaking branch $B$. Therefore, since for all $i$, $y_{P_i} \in \{0, \ldots, y_A\}$, $B$ cannot grow strictly higher than $y_A$; thus, $P$ cannot reach $A$ anymore from this assembly, which means that it cannot grow to its original endpoint, and therefore, it is fragile.

(b) Or it crashes into a part of $P$ grown after $P_i$, in which case we also choose to grow it before that part. Since $P$ is a *sequence* of points, it will not be able to grow completely after that, since a tile will already be present next to the collision tile of collision $C_1$.

Finally, the same argument on the tiles of $P_{\mathrm{W}}$ and $P_{\mathrm{N}}$ (the tiles with their north glue visible from the left, and their east glue visible from the north, respectively), proves that $P$ is also left-tentacular or fragile. Remark that $P_{\mathrm{W}} \cup P_{\mathrm{N}}$ is not necessarily disjoint from $P_{\mathrm{E}} \cup P_{\mathrm{S}}$ (in the case where $P$ has at most $2n-1$ tile types, these two sets may even be equal). □

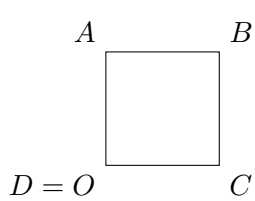
**Remark.** Consider the "tentacles" of Figure 3, restarted from the path of Figure 2: The right tentacles are after glue 32, and then glue 36, and the left one after glue 35.

We can now prove the claimed result:

**Theorem 4.5.** *Let $\mathcal{T} = (T, \sigma, 1)$ be a tile assembly system whose terminal assemblies' domains are all $\{0, \ldots, n-1\}^2$, and such that $\mathrm{dom}(\sigma) = \{(0,0)\}$. Then:*

$$|T| \geq 2n - 1$$

*Proof.* Let $A$, $B$, $C$ and $D$ be the following points of a square that $\mathcal{T}$ can assemble:




Since $\mathcal{T}$ can fill this square, it must contain in particular a path $P^0$ from $O$ to $A$, that we can build in the right-priority mode of Algorithm 4.1.

We define a sequence $(S_i)_i$ of assemblies, $S_0$ being the assembly where only $P^0$ has grown. For any $i \geq 0$, let $A_i$ be the leftmost point on the right-hand side of $S_i$, and not in $S_i$. If there are several such points, let $A_i$ be the highest one. Now, let $P^{i+1}$ be a right-priority path from $O$ to $A_i$, built using Algorithm 4.1. Moreover, let $Q^{i+1}$ be the prefix of $P^{i+1}$ that stops at the last occurrence of $P^{i+1}$'s highest point.

There are three main cases:

1. If $Q^{i+1}$ is fragile, we break it. Let $R^{i+1}$ be the assembly resulting from that operation. In the case where $Q_{i+1}$ shares parts with some other paths of $S_i$, this operation may also break these paths. Let $S_{i+1}$ be the assembly containing $R^{i+1}$ and all the parts of $S_i$ that can grow from it.

2. If $Q^{i+1}$ is right-tentacular, there are two subcases:

   (a) One of its contraction vectors $\overrightarrow{v_{i+1}}$ is to the left, i.e. $x_{\overrightarrow{v_{i+1}}} \leq 0$. In this case, we can do the same as in case 1 above. Indeed, since the last point of $Q^{i+1}$ is next to the leftmost point on the right of $S_i$, contracting it to the left will necessarily end in a collision with $S_i$, before the end of $Q^{i+1}$.
   Indeed, this is clear in the case of $Q^{i+1} = P^{i+1}$, i.e. $A_i$ is the highest point of $P^{i+1}$. Else, $P^{i+1}$ is longer than $Q^{i+1}$, and the subpath $P^{i+1} \setminus Q^{i+1}$ grows after $Q^{i+1}$, by definition of $Q^{i+1}$ as a prefix of $P^{i+1}$. Therefore, $P^{i+1} \setminus Q^{i+1}$ is on the right of $Q^{i+1}$: indeed, by Jordan's curve theorem, on the closed curve pictured on Figure 8 (the curve defined by $Q^{i+1}$, two horizontal lines, immediately above and below $Q^{i+1}$, and a vertical line on the right of the square), $P^{i+1} \setminus Q^{i+1}$ is *inside* a closed region of the plane, including a point on the right of $Q_0^{i+1}$. Therefore, $A_i$ is on the right of $Q^{i+1}$, because $Q^{i+1}$ is part of the border of this closed zone.

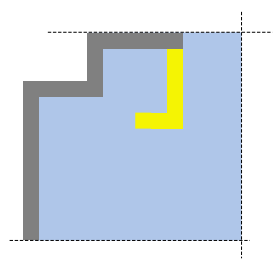


Figure 8: Jordan's curve theorem. The enclosed region is colored blue, $Q^{i+1}$ is in grey, and $P^{i+1} \setminus Q^{i+1}$ is in yellow.

   Therefore, $Q^i$ is necessarily already in $S_i$, because $A_i$ was chosen as the leftmost point on the right of $S_i$. Thus, there is an $h < i$ such that $A_h$ is the highest (and last) point of $Q^{i+1}$, and we can apply the same argument as in the case where $Q^{i+1} = P^{i+1}$, proving that $P^{i+1}$ is fragile.

   (b) Else, all its contraction vectors are strictly to the right. It is not possible that $B \in \mathrm{dom}(P^{i+1})$, for else $B$ would also be in $\mathrm{dom}(Q^{i+1})$ (indeed, by definition of $Q^{i+1}$, it includes the last occurrence of the highest point on $P^{i+1}$). and then one of the tentacles, when grown alone, would grow out of $\{0, \ldots, n-1\}^2$, contrarily to our hypothesis that all the assemblies stay within $\{0, \ldots, n-1\}^2$. Therefore, in this case, we let the tentacle grow as long as it can, until it reaches its highest point or else crashes into something.
   We continue this process with $S_{i+1}$ being the union of $S_i$, $P^{i+1}$, and the tentacles.

3. Else, by Lemma 4.4, $Q_{i+1}$ has at least $\|OA_i\|_1 - 1$ tile types. There are two subcases:

   (a) if $A_i \neq B$, we let $S_{i+1} = S_i \cup P_{i+1}$, and resume the construction.

(b) if $A_i = B$, the construction is over. Indeed, in this case $P^{i+1} = Q^{i+1}$, and $P^{i+1}$ is a path from $O$ to $B$, with at least $\|\overrightarrow{OB}\|_1 - 1 = 2n - 1$ distinct tile types.

In order to conclude the proof, we need to argue that this construction halts, even though cases 1 and 2a seem to make the assembly smaller. First, all the paths we grow in this construction are right-priority paths. Therefore, after these two cases happen, the same points $A_i$ will appear again as $A_j$, for $j > i$, but in this case, the path that we can build from $O$ to $A_j$ will necessarily be "less right-priority" than the original ones, meaning that they will turn left earlier than $P^i$. Indeed, in both case 1 and 2a, we break $P^i$, and add the resulting assembly to $S_i$.

To justify this, we examine what can possibly happen to these "broken paths" in greater detail now. When a path is broken, and we branch and grow a new one to reach $A_j$, one of two things could happen:

1. Either $P^j$ is fragile, in which case nothing can happen to earlier broken parts. The assembly sequence that we use to prove this is the following: First grow all the parts that can grow on the left of $P^j$, then the broken $P^j$. Then, grow the earlier broken parts on its right. Either these parts are on the left of $P^j$'s breaking branch, in which case they are also enclosed, or they are on its right, but in this case, even if a collision happens between the breaking branch of $P^j$, and these parts, this collision is either with the original fragile path – which still keeps it broken – or with an earlier breaking branch – which still keeps the original path enclosed, and therefore broken.

2. Else, if $P^j$ is right-tentacular, the construction will continue. If $P^j$'s tentacles crash into something, then this crash does not affect any of the arguments, since we only let them grow until their first collision.

□

**Corollary 4.6.** *Let $\mathcal{T} = (T, \sigma, 1)$ be a tile assembly system whose terminal assemblies are all of domain $\{0, \ldots, n-1\}^2$, and such that $|\mathrm{dom}(\sigma)| = 1$. Then $|T| \geq n$.*

*Proof.* Let $\Sigma$ be the position of the seed. We can use the technique of Theorem 4.2 on all the rectangles with diagonals $(\Sigma A)$, $(\Sigma B)$, $(\Sigma C)$ and $(\Sigma D)$. At least one is of width and height at least $n/2$, and verify the assumptions of Lemma 4.4, and the proof of Theorem 4.5 can be applied, either directly, or by "turning in the other direction", i.e. looking for a non-left-tentacular path. □

# 5 Future work

The next step, in proving the fully general conjecture, is to extend Lemma 4.4 to the case where the seed can be anywhere in the square. The reason why it does not apply to that case, is that a "lower restart" is not necessarily an "early restart"; indeed, let $P$ be a path from $O$ to $D$, and $Q$ be a path from $O$ to $B$. If $P_i$ and $Q_j$ are of the same type for some $i$ and $j$, then restarting $P_{i,i+1,\ldots,|P|-1}$ from $Q_j$ does not result in a competition for growth between this "lower branch" and $Q$, since the tiles of $Q$, to the north of $Q_j$, were grown before $Q_j$.

Therefore, despite Corollary 4.6, the general question remains open:

**Open Problem 1.** Is there a tile assembly system with less than $2n - 1$ tile types, that can assemble a filled square at temperature 1, starting from a single tile anywhere in the square?

Even though the recent results about its intrinsic universality [14], and the present paper, have made significant advances in that direction, the exact computational power of temperature 1 systems is still completely unknown. Moreover, the existence of single tileset simulating, at temperature 1, any other temperature 1 tile assembly system, is still open. The following open problem is particularly puzzling, especially in regard of the impressive results of [5], showing that three-dimensional temperature 1 tile assembly are capable of Turing computation:

**Open Problem 2.** Is is decidable whether two tile assembly systems have the same terminal assemblies?

Moreover, Theorem 3.1 is the first two-dimensional construction at temperature 1, with less tile types than its Manhattan diameter, in the general aTAM. On the other hand, our solution to the original conjecture relies heavily on the fact that our squares need to be completely filled. This leaves the following question open:

**Open Problem 3.** For all $n$, is there a tile assembly system $\mathcal{T}_n = (T_n, \sigma_n, 1)$, with $|\mathrm{dom}(\sigma_n)| = 1$ and $T_n < 2n - 1$, whose terminal assemblies all contain at least a square frame, that is, such that for all $\alpha \in \mathcal{A}_\square[\mathcal{T}_n]$, $(\{0, n-1\} \times \{0, \ldots, n-1\}) \cup (\{0, \ldots, n-1\} \times \{0, n-1\}) \subseteq \mathrm{dom}(\alpha)$?

The initial construction of a square with $2n - 1$ tile types, by Rothemund and Winfree, used a fairly simple design. Our result shows that this is optimal, but it does not discard the possibility of other designs:

**Open Problem 4.** Is there a way to self-assemble a square of size $n \times n$ at temperature 1 with $2n - 1$ tile types, that is not a trivial variation of Rothemund and Winfree's "comb" design (Figure 1)? How many are there?

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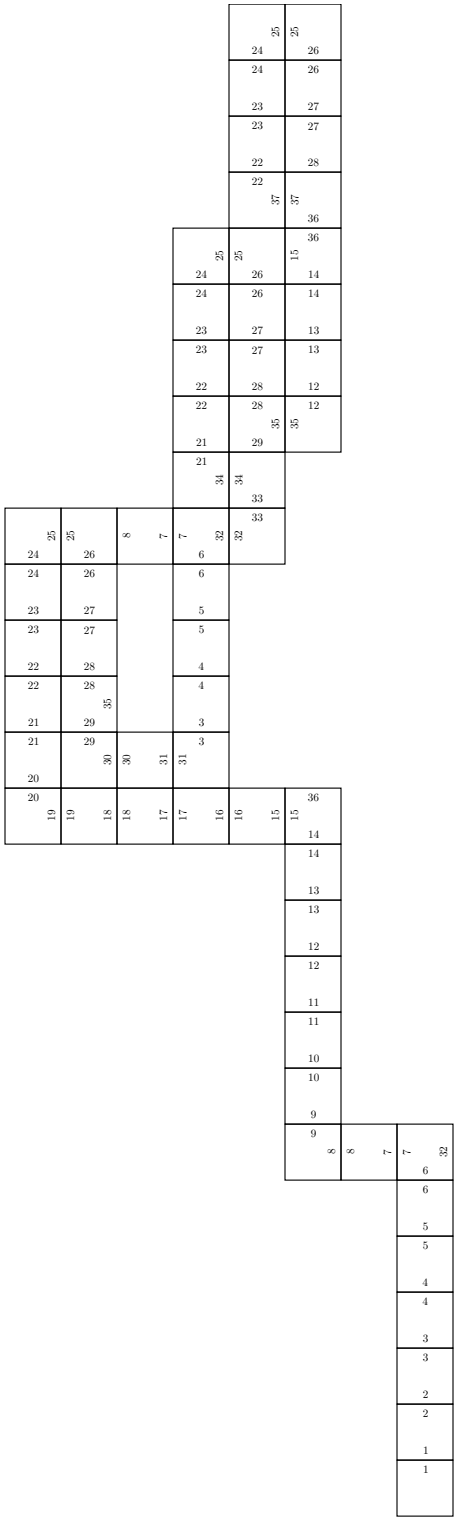
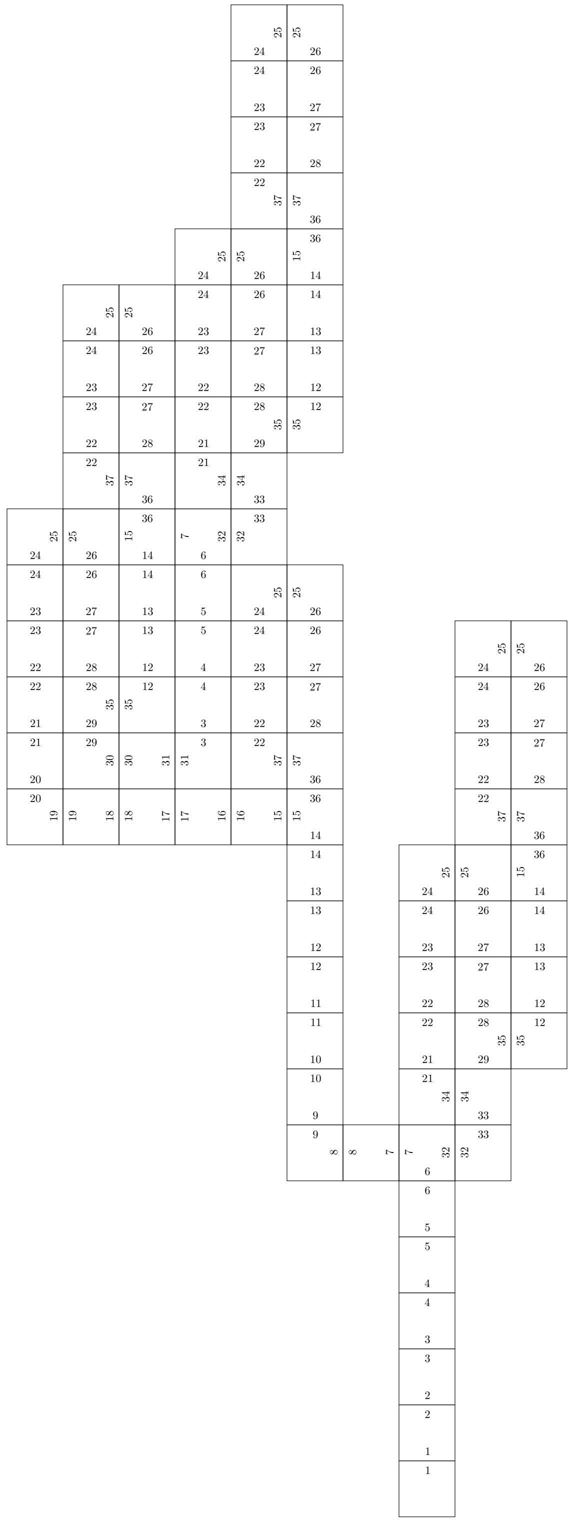
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