# Self-Assembly of Any Shape with Constant Tile Types using High Temperature

## Cameron Chalk[1]

Department of Electrical and Computer Engineering, University of Texas - Austin, Austin, TX, USA
ctchalk@utexas.edu

## Austin Luchsinger[2]

Department of Computer Science, University of Texas - Rio Grande Valley, Edinburg, TX, USA
austin.luchsinger01@utrgv.edu

## Robert Schweller[3]

Department of Computer Science, University of Texas - Rio Grande Valley, Edinburg, TX, USA
robert.schweller@utrgv.edu

## Tim Wylie[4]

Department of Computer Science, University of Texas - Rio Grande Valley, Edinburg, TX, USA
timothy.wylie@utrgv.edu

#### ——— Abstract ———

Inspired by nature and motivated by a lack of top-down tools for precise nanoscale manufacture, self-assembly is a bottom-up process where simple, unorganized components autonomously combine to form larger more complex structures. Such systems hide rich algorithmic properties—notably, Turing universality—and a self-assembly system can be seen as both the object to be manufactured as well as the machine controlling the manufacturing process. Thus, a benchmark problem in self-assembly is the unique assembly of shapes: to design a set of simple agents which, based on aggregation rules and random movement, self-assemble into a particular shape and nothing else. We use a popular model of self-assembly, the 2-handed or hierarchical tile assembly model, and allow the existence of repulsive forces, which is a well-studied variant. The technique utilizes a finely-tuned temperature (the minimum required affinity required for aggregation of separate complexes).

We show that calibrating the temperature and the strength of the aggregation between the tiles, one can encode the shape to be assembled without increasing the number of distinct tile types. Precisely, we show one tile set for which the following holds: for any finite connected shape $S$, there exists a setting of binding strengths between tiles and a temperature under which the system uniquely assembles $S$ at some scale factor. Our tile system only uses one repulsive glue type and the system is growth-only (it produces no unstable assemblies). The best previous unique shape assembly results in tile assembly models use $\mathcal{O}(\frac{K(S)}{\log K(S)})$ distinct tile types, where $K(S)$ is the Kolmogorov (descriptional) complexity of the shape $S$.

## 1   Introduction

Due to the limited tool set for precise fabrication at the nanoscale, the bottom-up approach of self-assembly is an attractive area of research. Such bottom-up approaches, such as *DNA origami* [17], allow for the assembly of nanoscale materials with detailed, precisely designed shapes and patterns. Abstract self-assembly models are used to predict the behavior of systems wherein simple, separate entities form larger complex structures based on a simple rule set for movement and/or attachment using only local interactions and no global leader. Such systems include swarm robotics and molecular self-assembly, particularly self-assembling nucleic acid structures such as *DNA tiles* [9].

A common benchmark in such models, which aims at the manufacture of precise nanoscale structures, is the self-assembly of *shapes*. In our case, a shape is defined simply as a finite, connected subset of $\mathbb{Z}^2$. The model studied herein is the *two-handed tile assembly model* (also called the *hierarchical tile assembly model*) [1]. In this model, the separate entities are *tiles*, adorned with *glues*. The intuition is that tiles wander about randomly, and when tiles with matching glues meet, the tiles bind to form a larger assembly; further, such larger structures wander about and may bind to other larger assemblies or tiles.

The main measure of complexity is the number of unique types of tiles necessary and sufficient to uniquely assemble the shape, termed the *tile complexity*. The *temperature* of a system, denoted by $\tau$, is the minimum required binding strength between two entities to enforce a stable attachment; the sum of the strengths between the shared glues of two assemblies must meet or exceed the temperature. Some studies of the model include *negative-strength glues* [2, 8, 12–15, 20], which are repulsive forces which act against a particular bond between two assemblies. Studies of these repulsive forces are motivated by experimental implementation of self-assembly systems which exhibit this behavior [16].

**Our contributions.** We give one tile set with a constant number of distinct tile types which satisfies the following: given any finite connected shape $S \subset \mathbb{Z}^2$, there exists an assignment of strengths between glues (a glue function) and a temperature $\tau$ such that the system uniquely assembles $S$. The system encodes the shape in its temperature parameter $\tau$ and its glue function. Then, by utilizing the inclusion of one negative-strength glue type, the system assembles a width-$\tau$ assembly. This width-$\tau$ assembly is utilized as a seed for a tile set designed by [23] which "runs" the program encoded by the seed to assemble the shape. This work is the first to show that any shape can be built with a constant number of distinct tile types (where the glues are a function of $\tau$) at any scale without a staged model[5], i.e., it is the first to achieve this in a fully "hands-off" model which requires no experimenter intervention during the assembly process.

**Previous results.** For self-assembling a shape $S$, we list the previously known results, which do not use negative glues and use $\mathcal{O}(1)$ temperature unless otherwise specified. Let $K(S)$ be the Kolmogorov complexity[6] of $S$, and let $T(S)$ be the (smallest) runtime of a Kolmogorov-optimal program outputting $S$. A tile complexity of $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ is known, using a scale factor of $T(S)$ [23]. With negative-strength glues, a tile complexity of $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ is known, using a $\mathcal{O}(1)$ scale factor [12]. In a *staged* version of the model, where several self-assembly systems are run in parallel across a series of *bins* and then mixed together in

---

[5] In the staged self-assembly model, the results of [3] give a construction which can effectively use $\mathcal{O}(1)$ tile types to assemble the shape by increasing the number of bins and stages used.

[6] The Kolmogorov complexity of $S$ is the number of bits in the smallest program which outputs $S$ w.r.t. a universal Turing machine. For more information on Kolmogorov complexity, see [11].

*stages*, a tile complexity of $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ at scale factor $T(S)$ is known for $\mathcal{O}(1)$ bins and $\mathcal{O}(1)$ stages along with a method for (optimally) reducing the number of sufficient and necessary tile types by increasing the number of bins and stages [3].

In another staged version of the model, where tiles are partitioned into DNA and RNA types, and RNA types may be "washed away" at a given stage, a tile complexity of $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ at scale factor $\mathcal{O}(\log|S|)$ is known [7]. In a staged model where the self-assembly process is controlled by a chemical reaction network which activates and deactivates tiles' binding sites, a tile plus reaction network complexity of $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ at scale factor $\mathcal{O}(1)$ is known [19].

**Related work in high-temperature[7] self-assembly.** The first studies of utilizing temperature to encode information involved the "online", mid-assembly-process changing of temperatures [10, 24]. Our result utilizes a high temperature bonding threshold for self-assembly attachment, which we leverage to encode precise information for guiding the self-assembly process through precisely set glue strengths. A number of recent related works have also studied the effects of higher temperature self-assembly systems within various models. Within the aTAM, larger temperatures have been shown to affect the possible behavior of systems [4], and the tile complexity of self-assembled shapes [22]. Within the 2HAM, unique-assembly verification has been shown to be hard for high-temperature systems [21], while the dynamics of certain higher-temperature systems have been shown to be impossible to simulate at lower temperatures [6].

## 2    Definitions and Model

In this section we first define the two-handed tile self-assembly model with both negative and positive strength glue types. We also formulate the problem of designing a tile assembly system that constructs a constant-scaled shape given the optimal description of that shape.

**Tiles and Assemblies.** A tile is an axis-aligned unit square centered at a point in $\mathbb{Z}^2$, where each edge is labeled by a *glue* selected from a glue set $\Pi$. A *strength function* str : $\Pi \to \mathbb{Z}$ denotes the *strength* of each glue. Two tiles equal up to translation have the same *type*. A *positioned shape* is any subset of $\mathbb{Z}^2$. A *positioned assembly* is a set of tiles at unique coordinates in $\mathbb{Z}^2$, and the positioned shape of a positioned assembly $A$ is the set of those coordinates. For a given positioned assembly $\Upsilon$, define the *bond graph* $G_\Upsilon$ to be the weighted grid graph in which each element of $\Upsilon$ is a vertex and the weight of an edge between tiles is the strength of the matching coincident glues or 0.[8] A positioned assembly $C$ is $\tau$-*stable* for positive integer $\tau$ provided the bond graph $G_C$ has min-cut at least $\tau$.

For a positioned assembly $A$ and integer vector $\vec{v} = (v_1, v_2)$, let $A_{\vec{v}}$ denote the positioned assembly obtained by translating each tile in $A$ by vector $\vec{v}$. An *assembly* is a translation-free version of a positioned assembly, formally defined to be a set of all translations $A_{\vec{v}}$ of a positioned assembly $A$. An assembly is $\tau$-stable if and only if its positioned elements are $\tau$-stable. A *shape* is the set of all integer translations for some subset of $\mathbb{Z}^2$, and the shape of an assembly $A$ is defined to be the set of the positioned shapes of all positioned assemblies in $A$. The *size* of either an assembly or shape $X$, denoted as $|X|$, refers to the number of elements of any positioned element of $X$.

---

[7] We say high-temperature self-assembly for consistency with previous literature. The term high temperature may be misleading; e.g., we are not attempting to model what happens in DNA-based self-assembly systems when the literal temperature of the system is raised to high values. Intuitively, higher temperature in this model implies more fine-grained glue strengths. Another natural way to think of high temperature is to fix the temperature to one, but allow rational glue strengths.

[8] Note that only matching glues of the same type contribute a non-zero weight, whereas non-equal glues always contribute zero weight to the bond graph. Relaxing this restriction has been considered [5].

**Figure 1** The black lines between two tiles indicate unique unimportant $\tau$-strength bonds. If $\tau = 2$, $str(A) = 1$ and $str(B) = 1$, then the two assemblies in (a) are $\tau$-combinable, since $str(A) + str(B) \geq \tau$ and the positioned assemblies may be translated such that the $A$ and $B$ glues are aligned— such a combination is termed *cooperative binding*, since neither the $A$ nor $B$ glue are alone sufficient to satisfy $\tau$-combination. In (b), we consider two cases concerning the negative strength glue $X$. If $\tau = 2$, $str(C) = 2$, and $str(X) = -1$, then the assemblies in (b) are not $\tau$-combinable since $str(C) + str(X) < \tau$. If $\tau = 1$, $str(C) = 2$, $str(D) = 2$, $str(E) = 1$ and $str(X) = -1$, then the assemblies are $\tau$-combinable since $str(C) + str(X) \geq \tau$; however, the resultant assembly is unstable, since a cut along the $X$ and $E$ glue has strength $str(X) + str(E) < \tau$; this violates the valid growth-only system definition.

**Combinable Assemblies.** Two assemblies are $\tau$-*combinable* provided they may attach along a border whose strength sums to at least $\tau$. Formally, two assemblies $A$ and $B$ are $\tau$-*combinable* into an assembly $C$ provided $G_{C'}$ for any $C' \in C$ has a cut $(A', B')$ of strength at least $\tau$ for some $A' \in A$ and $B' \in B$. We call $C$ a *combination* of $A$ and $B$. Figure 1 gives examples of combinable and not combinable assemblies.

### 2.0.0.1   Two Handed Assembly Model: Growth-only Version

A *two-handed tile assembly system (2HAM system)* is an ordered pair $(T, \tau)$ where $T$ is a set of single tile assemblies, called the *tile set*, and $\tau \in \mathbb{N}$ is the *temperature*. In the *growth-only* model, assembly proceeds by repeated combination of assembly pairs to form new assemblies starting from the initial tile set. The *producible assemblies* are those constructed in this way.

▶ **Definition 1** (2HAM Producibility (growth-only)). For a given 2HAM system $\Gamma = (T, \tau)$, the set of *producible assemblies* of $\Gamma$, denoted $\texttt{PROD}_\Gamma$, is defined recursively:

- (Base) $T \subseteq \texttt{PROD}_\Gamma$
- (Combinations) For any $A, B \in \texttt{PROD}_\Gamma$ such that $A$ and $B$ are $\tau$-combinable into $C$, then $C \in \texttt{PROD}_\Gamma$.

The inclusion of negative glues, in general, allows for unstable assemblies to be producible. In previous literature, such assemblies "detach", forming two new producible assemblies. We impose the following constraint on growth-only systems which disallows production of unstable assemblies which would fall apart. Satisfying the growth-only constraint argues that the system has simpler kinetics than a non-growth-only system since the system does not rely on detachment events.

For a system $\Gamma = (T, \tau)$, we say $A \rightarrow_1^\Gamma B$ for assemblies $A$ and $B$ if $A$ is $\tau$-combinable with some producible assembly to yield $B$, or if $A = B$. Intuitively this means that $A$ may grow into assembly $B$ through one or fewer combination. We define the relation $\rightarrow^\Gamma$ to be the transitive closure of $\rightarrow_1^\Gamma$, ie., $A \rightarrow^\Gamma B$ means that $A$ may grow into $B$ through a sequence of combinations.

▶ **Definition 2** (Valid Growth-Only System). A 2HAM system $\Gamma = (T, \tau)$ is a *valid growth-only* system if for all $A \in \texttt{PROD}_\Gamma$, $A$ is $\tau$-stable.

▶ **Definition 3** (Terminal Assemblies). A *terminal* assembly of a valid growth-only 2HAM system is a producible assembly that cannot combine with any other producible assembly. Formally, an assembly $A \in \texttt{PROD}_\Gamma$ of a 2HAM system $\Gamma = (T, \tau)$ is *terminal* provided $A$ is not $\tau$-combinable with any producible assembly of $\Gamma$.

We formalize what it means for a 2HAM system to uniquely build a given assembly or a given shape.
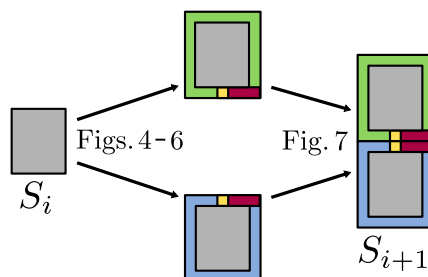
**Figure 2** A simplified overview of the growing step. $S_i$ is a width-$\Theta(i)$, height-$\Theta(2^i)$ assembly with particular exposed edge glues. $S_i$ nondeterministically assembles one of two assemblies; a *top* and *bottom*. The top and bottom share one glue of strength $2\tau - 1$ shown in yellow, and $i$ many $-1$ strength glues shown in red. Thus, the top and bottom bind with strength $2\tau - i - 1$, which is $\tau$-stable only if $i < \tau$. The resultant assembly adds two width and doubles the height of $S_i$, so its dimensions are $\Theta(i+1) \times \Theta(2^{i+1})$. Further, its exposed glues allow the process to repeat.

▶ **Definition 4** (Unique Assembly). A 2HAM system *uniquely* produces an assembly $A$ if all producible assemblies have a growth path towards the terminal assembly $A$. Formally, a 2HAM system $\Gamma = (T, \tau)$ *uniquely* produces an assembly $A$ provided that $A$ is terminal, and for all $B \in \mathtt{PROD}_\Gamma$, $B \to^\Gamma A$.

▶ **Definition 5** (Unique Shape Assembly[9]). A 2HAM system uniquely produces a shape $S$ if all producible assemblies have a growth path to a terminal assembly of shape $S$. Formally, a 2HAM system $\Gamma = (T, \tau)$ *uniquely assembles* a finite shape $S$ if for every $A \in \mathtt{PROD}_\Gamma$, there exists a terminal $A' \in \mathtt{PROD}_\Gamma$ of shape $S$ such that $A \to^\Gamma A'$.

## 3 Assembly of General Shapes with Constant Tiles

Here we give the main construction of the paper. First presented is our key contribution— assembly of a precise-width rectangle— detailed in Subsection 3.1, followed by its composition with established techniques from [23] for the main result in Subsection 3.2.

### 3.1 Key idea: precise-width rectangle using $\mathcal{O}(1)$ tile types

Here, we present a construction for building a precise-width rectangle from a constant-bounded set of tile types. Note that the convention in this paper is width × height. Formally,

▶ **Lemma 6.** *Given a temperature $\tau > 2$, there exists a negative glue, growth-only 2HAM tile system $\Gamma = \{T, \tau\}$ such that $|T| = \mathcal{O}(1)$ and $\Gamma$ uniquely produces an assembly which is a $(18 + 4\tau) \times (2^{\tau+5} - 6)$ rectangle.*

▶ **Proof 1.** We give a proof by construction. Unless explicitly stated otherwise, all glues have strength $\lceil \frac{\tau}{2} \rceil$, so at least two matching glues are required for a $\tau$-stable attachment. This is called *cooperative binding*. The construction is split into two steps: *growing* and *finishing*. Figure 2 shows a simplified overview of the growing step. The growing step of the construction concerns producing an assembly with width $7 + 2\tau$, through a process consisting of $\tau$ iterations of growth, each adding a constant-bounded width to the assembly.

---

**(a)**

**(b)**

🟨 **Figure 3** The base assembly, shown in two separate subassemblies; (a) shows the top subassembly, and (b) the bottom. The two subassemblies combine using cooperative binding at the strength-$\lceil \frac{\tau}{2} \rceil$ glues labeled $X$. The dotted line indicates distinct tile types which attach along the path with full $\tau$ strength glues. The snaking pattern ensures that each subassembly is complete before both $X$ glues are available. Once these two subassemblies bind, the resultant assembly satisfies $S_0$.

The $i + 1^{\text{th}}$ iteration of growth is initiated by a combination of two assemblies with total binding strength $2\tau - i - 1$; thus, after the $\tau^{\text{th}}$ iteration of growth, the binding strength which would initiate the next iteration of growth has total binding strength $2\tau - \tau - 1 < \tau$, and growth halts.

The finishing step involves the system's "detecting" that the growth process has completed. This is achieved using the following technique: by adding a total strength of 1 shared between two assemblies at each iteration of growth, once the assemblies have completed $\tau$ repetitions of growth, they bind with strength $\tau$. This step also gives the system its property of unique assembly of an assembly whose shape is a rectangle (and not just unique shape assembly). That is, there is exactly one terminal assembly of the system— as opposed to several terminal assemblies with the correct rectangular shape. Maintaining this property in this lemma is required to achieve the same property in Theorem 7.

### 3.1.1 Growing

The construction is described and proven correct via induction. The induction is on iterations of rectangular assemblies with well-defined exposed glues, termed $S_i$. Formally, $S_i$ refers to a $(7 + 2i) \times (2^{i+4} - 6)$ rectangular assembly with the following exposed glue labels, written as strings built by concatenating the glue labels in left-to-right/top-to-bottom order):

- North glues: $qp^i gn^{i+5}$
- East glues: $E^{2^{i+3}-5} R^2 E^{2^{i+3}-3}$
- South glues: $QP^i GN^{i+5}$
- West glues: $LW^{2^{i+3}-7} LW^4 LW^{2^{i+3}-7} L$

The goal is to show that if an assembly satisfying $S_i$ is producible, then an assembly satisfying $S_{i+1}$ is producible iff $i < \tau$. Further, only $\mathcal{O}(1)$ tile types are used in the inductive step. Then it suffices to show that $S_0$ is producible in $\mathcal{O}(1)$ tile types, implying $S_\tau$ is producible, which has width $\times$ height as in the lemma statement.

**Base case.** An assembly satisfying $S_0$ is shown to be trivially assembled by a set of $\mathcal{O}(1)$ tile types in Figure 3.

**Inductive step.** The next three paragraphs describe the inductive step. The goal is to show that if $S_i$ is producible, then a top and bottom assembly are producible which can

**Figure 4** An assembly satisfying $S_i$. The dots indicate an omitted set of repeated tiles; e.g., the dots between the tiles exposing $p$ indicate the omission of the $i$ glues with label $p$. On the right are the keystones, which attach cooperatively using $R$ glues. Only one keystone may attach, introducing nondeterminism; this is how the producibility of two assemblies, a top and bottom assembly, are implied by the production of one assembly satisfying $S_i$.

bind to produce $S_{i+1}$ iff $i < \tau$. Consider an assembly with exposed glues satisfying $S_i$. The two $R$ glues exposed allow attachment of a *keystone* assembly via cooperative binding as seen in Figure 4. There are two keystone types: *up* and *down*. Only one may attach. The $L$ glues in the middle o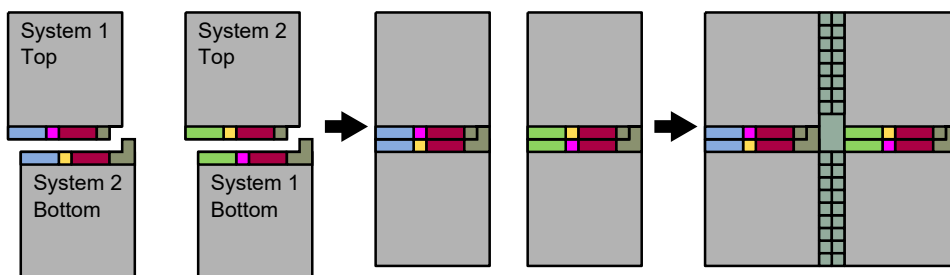f the west-side exposed glues, spaced by four $W$ glues, also allow the attachment of a supertile using cooperative binding. Once the keystone or west-side supertile has attached, a single tile type suffices to attach tiles along any long set of repeating glues on the assembly (e.g., the $E$ glues on the east side), until the glue is no longer available, as seen in Figure 5. This type of single tile type attaching along arbitrary walls is termed *propagation* of a tile.

The tiles which propagate to the corners of the west side of the assembly allow the attachment of three tiles around the corner which allow propagation of tiles along the north and south faces of the assembly. Once these tiles propagate, depending on which keystone was attached to the assembly, the attachment of a *tooth* occurs on the corresponding face (e.g., on the north face if the up keystone was attached) as shown in Figure 6. The tooth is a supertile with a specific geometry which will be motivated later on. The tooth initiates a propagation of tiles along the corresponding face. The result is the production of two assemblies, one having attached the up keystone and attached all previously discussed propagating tiles and supertiles, and one having attached the down keystone and similar tiles. We refer to the former as a *top* assembly, and the latter as a *bottom* assembly.

When a top assembly and bottom assembly attach, the result is an assembly satisfying $S_{i+1}$. A top assembly and bottom assembly are designed to attach iff $i < \tau$. When $i \geq \tau$, the binding strength between a top and bottom assembly is $\tau - 1$, and thus is insufficient. This design can be seen in Figure 7. Note that the $-1$ glues are propagated via the $N$-labeled glues from the base assembly. Since $S_i$ has $i + 5$ many $N$ glues exposed, 5 of which are

**Figure 5** Once the keystone and supertile on the left have attached, a sequence of single tile attachments may occur using cooperative binding at newly available glues. The tiles are designed such that they may attach along arbitrarily long faces, as long as the appropriate glue is exposed (e.g., a $W$ glue in the top-left tile's case).

covered by the tooth, the bottom/top assembly which assembles from $S_i$ exposes $i$ many $-1$ glues. Then the bonding strength between top and bottom assemblies is $2\tau - 1 - i$, which is less than $\tau$ iff $i \geq \tau$. The complementary geometry of the teeth ensure that a top and bottom assembly which are assembled from $S_i$ and $S_j$ respectively, with $i \neq j$, cannot align their $a$ glues and will not attach.

**Dimensions of $S_i$.** The base assembly satisfying $S_0$ is $7 \times 10$. When a top and bottom assembly attach, both have added 2 width in tiles; one tile width propagated on the west side, and one on the east. Then the width of $S_i$ is $7 + 2i$. A top and bottom assembly which have combined add 6 height in tiles on top of doubling in height: 2 via tile propagation on the top and bottom, and 4 along where the top and bottom assemblies attach. Then the height of $S_i$, $h(i)$, is defined by the recurrence $h(i) = 2h(i-1) + 6$ with $h(0) = 10$. Solving the recurrence gives a height of $2^{i+4} - 6$. Then consider a combination of a top and bottom assembly which formed from some assembly satisfying $S_{i-1}$; the resultant dimension is $(7 + 2i) \times (2^{i+4} - 6)$.

### 3.1.2   Finishing

When a top and bottom assembly combine to form an assembly satisfying $S_\tau$, the growing step shows that the process will not continue to produce $S_{\tau+1}$. However, the attachment of a supertile on the west side, a keystone, and the resultant tile propagation still occurs. The teeth attach and so do the tiles which propagate resulting from the attachment of a

**Figure 6** At the top-right and bottom-right corners, tiles attach which indicate that the left-hand side tile propagation has reached the right-hand side of the assembly. In the case of an assembly which has attached an up keystone, the tooth attaches on the top side of the assembly, and initiates a propagation of tiles along the top face. A tooth with complementary geometry will attach on the bottom side of the assembly if a down keystone attaches instead, as can be seen in Figure 7.

tooth. Then an assembly satisfying $S_\tau$ implies the production of the corresponding top and bottom assemblies. These assemblies are not rectangular. This step involves detecting that the iterative process has reached $\tau$ repetitions, and the system should finish its rectangle.

Figure 8 gives an overview of the finishing step. The technique discussed in the growing phase is employed by two disjoint tile sets, one called *system 1* and the other *system 2*. The sets of glues on the tiles in the two systems are disjoint except for two glues: the $-1$ glue, and the $+2$ glue described but not used in the growing phase. In the growing phase, recall that on the north face of a bottom assembly of system 1 which assembled from $S_i$, there are $i$ many strength 2 glues labeled $+2$ exposed which are not used (recall Figure 7). These glues are designed to match with the corresponding glues in system 2. Then the strength of binding between these shared glues is $2i - i = i$. Thus, only when $i \geq \tau$ is this binding $\tau$-stable.

**Figure 7** A bottom assembly (left) and top assembly (right). At the top of the figure are the tiles whose glues bond a bottom and top assembly; in particular, the $a$ and $-1$ glues, with $str(a) = 2\tau - 1$ and $str(-1) = -1$. A top and bottom assembly grown from an assembly $S_i$ each expose $i$ glues with strength $-1$. Then the strength of the attachment between them is $2\tau - i - 1$, and is sufficient when $i < \tau$ but insufficient when $i = \tau$. Note that $+2$ and $+2'$ glues do not match; their purpose is described later in the finishing step.

Similarly, system 1's top assembly attaches with the system 2's bottom assembly under the same constraint. These resultant assemblies expose cooperative binding locations which were not present before this attachment, allowing these two new assemblies to combine, and then fill into a rectangle using a $\mathcal{O}(1)$-sized tile set. Next, we give the dimensions of the completed rectangular assembly: system 1's top and system 2's bottom assembly, once attached, form a $(7 + 2(\tau + 1)) = (9 + 2\tau) \times (2^{(\tau+1)+4} - 6) = (2^{\tau+5} - 6)$ assembly— this can be derived from the combination of two assemblies satisfying $S_\tau$ assembling into an assembly satisfying $S_{\tau+1}$ not in exposed glues, but in size. System 1's top and system 2's bottom are combined with system 1's bottom and system 2's top into one via a width-two column, resulting in a $2(9 + 2\tau) + 2 = 18 + 4\tau \times 2^{\tau+5} - 6$ assembly. ◄

## 3.2   From rectangle to shape

To assemble the target shape, a technique is combined with Lemma 6. The technique, shown by Soloveichik and Winfree [23], first assembles a *seed block* bearing a representation (a series of exposed glues) of a Kolmogorov-optimal program which computes the spanning tree of $S$. A $\mathcal{O}(1)$-sized tile set is used to "run" the program (via Turing machine (TM) simulation) from the seed block. The seed block assembles into a $c \times c$ assembly, logically representing one coordinate of $S$. Assembly proceeds from the seed block in a subset of the four cardinal directions depending on the spanning tree computed by the program. If the spanning tree has an edge in a direction to a coordinate adjacent to the seed block, a $c \times c$ *growth block* is assembled in that direction. Each time a growth block is assembled, the program is run again to determine which adjacent coordinates (w.r.t. the growth block) are

■ **Figure 8** An overview of the finishing step. The system described in the growing step, denoted here as system 1, is repeated, denoted system 2, such that the only matching glues between the two systems are a strength-2 glue type and the one strength-($-1$) glue type. Between a system 1 top/bottom and system 2 bottom/top assembled from $S_i$, the number of shared strength-2 glues and strength-($-1$) glues is $i$, so the sum of strengths between shared glues is $2i - i = i$. This allows the top/bottom assembly of system 1 to make a $\tau$-stable attachment to the bottom/top of system 2 only after each system assembles $S_\tau$, thus detecting when the rectangle has $\Theta(\tau)$ width. Once these tops and bottoms attach, new cooperative binding locations initiate a constant-sized set of tiles to bind the two rectangles, simply to satisfy unique assembly of the rectangle.

connected by edges in the spanning tree; if so, a growth block is assembled in that direction. After assembling all growth blocks, the unique assembly is a $c \times c$ scaled version of $S$.

The seed block of [23] is assembled using $\mathcal{O}(\frac{K(S)}{\log K(S)})$ tile types. In our case, the seed block is assembled using the $\mathcal{O}(1)$-sized tile set of Lemma 6: we assemble a rectangle of width $n$ where $n$ is the length of a unary encoding of the Kolmogorov-optimal program. This seed is combined with the $\mathcal{O}(1)$-sized tile set which runs the program and assembles the shape. Figure 9 is a simplified overview of constructing a seed block compatible with a TM simulating tileset. The formal result is as follows:

▶ **Theorem 7.** *Given a shape $S$, there exists a negative glue, growth-only $2HAM$ tile system $\Gamma = \{T, \tau\}$ with $|T| = \mathcal{O}(1)$ whose unique assembly has shape $S$ at some scale factor.*

▶ **Proof 2.** The system is a union of the Lemma 6 system and a subset of the TM simulating tile set of [23]. If the entire TM simulating tile set is added to the system, depending on the seed block, some tiles may never bind to the seed block, and thus do not grow into the target shape and violate unique assembly definition. We include the subset of the TM simulating tile set which will be used by the program encoded by the seed block. Observe that the unique assembly produced by the system of Lemma 6 is not a square, nor does it have any exposed glues designed to bind with the TM simulation tile set. In order to assemble a square from the terminal assembly of Lemma 6, two such rectangular assemblies are assembled in parallel, one which is rotated 90 degrees— this "rotation" is w.r.t. the other rectangular assembly and the way the two assemblies will bind. These two assemblies combine and then "fill-in" to a square trivially using a constant-sized tile set— similar to propagation of tiles along an edge, cooperative binding can be used to add tiles between two assembled rectangles to assemble a square (technique first used in [18]). Once assembly of the square is complete, more tile propagation via another constant-sized tile set assembles a one-tile perimeter which exposes glues— described in the following paragraph— which allow the assembly to act as a seed block similar to the Soloveichik and Winfree construction [23].

Let $P$ be the (binary) program used to assemble $S$ via the construction of [23], $R$ be some mapping from binary strings to unary strings, and $R'$ be some mapping from unary strings $\{1\}^i$ with $i \in \mathbb{N}$ to unary strings $\{1\}^j$ with $j = 20 + 4m$ for $m \in \mathbb{N}$— the intuition for the mapping $R'$ is to map arbitrary unary strings to numbers which are widths of assemblies assembled by Lemma 6.
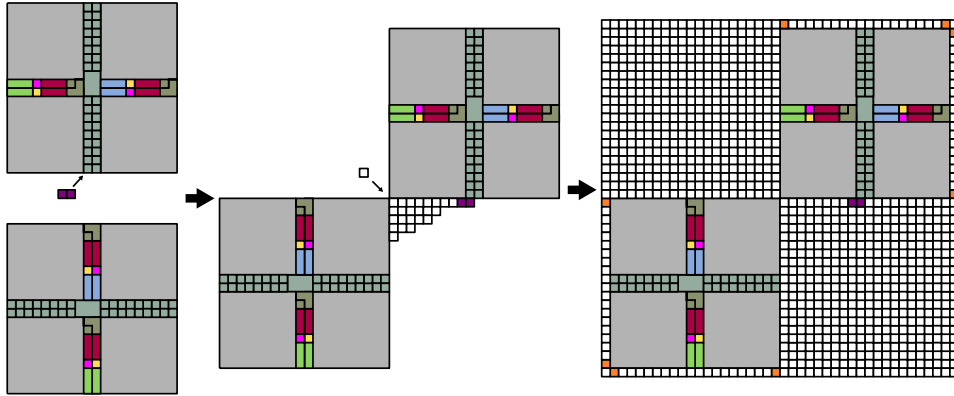
**Figure 9** The combination of two Lemma 6 constructions into a seed block. The two-tile assembly in the first subfigure initializes the attachment of the set of white tiles, which indicate a constant-sized set of *filler* tiles which are used to fill in a full square. Once the square is filled in, new cooperative binding locations are exposed where the filler tiles meet the non-filler tiles. At this location, tiles begin to propagate, adding a one-tile perimeter to the assembly. The orange tiles on the outmost perimeter of the rightmost figure demarcate the beginning and ending of glues exposing the unary program which constructs the shape $S$ via the TM simulation of [23]. The rest of the perimeter exposes glues which the TM simulation ignores. ◄

Once the square seed block is assembled and a one-tile perimeter is attached, three glue types are exposed: 1, $b$, and $\lambda$. Across the length of filler tiles (those in the square which are not from the Lemma 6 construction), $\lambda$ glues are placed; these symbols are ignored by the TM simulating tile set. The $b$ glues are placed at the beginnings and ends of the edges of the square; these indicate where to start the TM simulation. Along the edges of the rectangles from the Lemma 6 construction, glues labeled 1 are placed; these 1 glues are the relevant glues logically. The TM simulation converts these to unary strings by $R'^{-1}$, and then to $P$ by $R^{-1}$. Then the TM simulation tiles run the program $P$ which assembles the shape. ◄

## 4    Future Work

The most apparent direction for future work is to achieve the unique assembly of shapes at a $\mathcal{O}(1)$ scale factor with $\mathcal{O}(1)$ tile types. This result may be achieved through a combination of the techniques used in this work and in [12], which achieves $\mathcal{O}(1)$-scale factor with $\mathcal{O}(\frac{K(S)}{\log K(S)})$ tile types where $K(S)$ is the Kolmogorov complexity of the shape $S$. Their construction utilizes a dynamic behavior of negative glues not utilized in this work called "breaking": the combination of two assemblies may result in an unstable assembly, which then breaks into two assemblies— a formal model and some usages of breakage may be seen in [2,8,20]. Their usage of breaking involves performing a computation— via a self-assembly process which simulates a TM— which builds the shape pixel-by-pixel (using $\mathcal{O}(1)$-sized assemblies per pixel), and then breaks the TM simulating assembly into $\mathcal{O}(1)$-sized pieces, leaving the shape $S$ at a $\mathcal{O}(1)$ scale factor (along with "small garbage" of $\mathcal{O}(1)$ size). That technique may be applicable to the construction given in this work in order to break the precise-width rectangles after they are used as input for the TM which outputs $S$.

Another direction might be to achieve the unique assembly of scaled shapes with $\mathcal{O}(1)$ tile types using only positive-strength glues. We have briefly discussed previous positive-strength results which use $\Theta\left(\frac{K(S)}{\log K(S)}\right)$ tile types. Could this be lowered to $\mathcal{O}(1)$ tile types by calibrating the temperature and glue strengths, or is there some super-constant lower bound that cannot be breached?

─── **References** ───

1   Sarah Cannon, Erik D. Demaine, Martin L. Demaine, Sarah Eisenstat, Matthew J. Patitz, Robert Schweller, Scott M. Summers, and Andrew Winslow. Two hands are better than one (up to constant factors): Self-assembly in the 2ham vs. atam. In Natacha Portier and Thomas Wilke, editors, *STACS*, volume 20 of *LIPIcs*, pages 172–184. Schloss Dagstuhl - Leibniz-Zentrum fuer Informatik, 2013. Available from: `http://dblp.uni-trier.de/db/conf/stacs/stacs2013.html#CannonDDEPSSW13`.

2   Cameron Chalk, Erik D. Demiane, Martin L. Demaine, Eric Martinez, Robert Schweller, Luis Vega, and Tim Wylie. Universal shape replicators via self-assembly with attractive and repulsive forces. In *Proc. of the 28th Annual ACM-SIAM Symposium on Discrete Algorithms (SODA'17)*, 2017.

3   Cameron Chalk, Eric Martinez, Robert Schweller, Luis Vega, Andrew Winslow, and Tim Wylie. Optimal staged self-assembly of general shapes. *Algorithmica*, May 2017. Available from: `https://doi.org/10.1007/s00453-017-0318-0`.

4   H.-L. Chen, D. Doty, and S. Seki. Program size and temperature in self-assembly. *Algorithmica*, 72(3):884–899, 2015.

5   Qi Cheng, Gagan Aggarwal, Michael H. Goldwasser, Ming-Yang Kao, Robert T. Schweller, and Pablo Moisset de Espanés. Complexities for generalized models of self-assembly. *SIAM Journal on Computing*, 34:1493–1515, 2005.

6   Erik D. Demaine, Matthew J. Patitz, Trent A. Rogers, Robert T. Schweller, Scott M. Summers, and Damien Woods. The two-handed tile assembly model is not intrinsically universal. *Algorithmica*, 74(2):812–850, 2016.

7   Erik D. Demaine, Matthew J. Patitz, Robert T. Schweller, and Scott M. Summers. Self-assembly of arbitrary shapes using rnase enzymes: Meeting the kolmogorov bound with small scale factor (extended abstract). In *Proc. of the 28th International Symposium on Theoretical Aspects of Computer Science (STACS'11)*, 2011.

8   David Doty, Lila Kari, and Benoît Masson. Negative interactions in irreversible self-assembly. *Algorithmica*, 66(1):153–172, 2013.

9   Constantine Evans. *Crystals that Count! Physical Principles and Experimental Investigations of DNA Tile Self-Assembly*. PhD thesis, California Inst. of Tech., 2014.

10  Ming-Yang Kao and Robert T. Schweller. Reducing tile complexity for self-assembly through temperature programming. In *SODA 2006: Proceedings of the 17th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 571–580, 2006.

11  M. Li and P. Vitanyi. *An Introduction to Kolmogorov and Its Applications (Second Edition)*. Springer Verlag, New York, 1997.

12  Austin Luchsinger, Robert Schweller, and Tim Wylie. Self-assembly of shapes at constant scale using repulsive forces. In Matthew J. Patitz and Mike Stannett, editors, *Unconventional Computation and Natural Computation*, pages 82–97, Cham, 2017. Springer International Publishing.

13  Matthew J. Patitz, Trent A. Rogers, Robert Schweller, Scott M. Summers, and Andrew Winslow. Resiliency to multiple nucleation in temperature-1 self-assembly. In *DNA Computing and Molecular Programming*. Springer International Publishing, 2016.

14  Matthew J. Patitz, Robert T. Schweller, and Scott M. Summers. Exact shapes and turing universality at temperature 1 with a single negative glue. In *DNA Computing and Molecular Programming*, volume 6937 of *LNCS*, pages 175–189. 2011.

15  John H. Reif, Sudheer Sahu, and Peng Yin. Complexity of graph self-assembly in accretive systems and self-destructible systems. *Theoretical Comp. Sci.*, 412(17):1592–1605, 2011.

16  Paul W. K. Rothemund. Using lateral capillary forces to compute by self-assembly. *Proceedings of the National Academy of Sciences*, 97(3):984–989, 2000.

**17**    Paul W. K. Rothemund. Folding DNA to create nanoscale shapes and patterns. *Nature*, 440(7082):297–302, March 2006. Available from: `http://dx.doi.org/10.1038/nature04586`.

**18**    Paul W. K. Rothemund and Erik Winfree. The program-size complexity of self-assembled squares (extended abstract). In *Proc. of the 32nd ACM Sym. on Theory of Computing*, STOC'00, pages 459–468, 2000.

**19**    Nicholas Schiefer and Erik Winfree. *Universal Computation and Optimal Construction in the Chemical Reaction Network-Controlled Tile Assembly Model*, pages 34–54. Springer International Publishing, Cham, 2015.

**20**    Robert Schweller and Michael Sherman. Fuel efficient computation in passive self-assembly. In *SODA 2013: Proceedings of the 24th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1513–1525. SIAM, 2013.

**21**    Robert Schweller, Andrew Winslow, and Tim Wylie. Complexities for high-temperature two-handed tile self-assembly. In Robert Brijder and Lulu Qian, editors, *DNA Computing and Molecular Programming*, pages 98–109, Cham, 2017. Springer International Publishing.

**22**    Sinnosuke Seki and Yasushi Ukuno. On the behavior of tile assembly system at high temperatures. *Computability*, 2(2):107–124, 2013.

**23**    David Soloveichik and Erik Winfree. Complexity of self-assembled shapes. *SIAM Journal on Computing*, 36(6):1544–1569, 2007.

**24**    Scott M. Summers. Reducing tile complexity for the self-assembly of scaled shapes through temperature programming. *Algorithmica*, 63(1):117–136, 2012.