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Nearly Constant Tile Complexity for any Shape in Two-Handed Tile Assembly

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Abstract

Tile self-assembly is a well-studied theoretical model of geometric computation based on nanoscale DNA-based molecular systems. Here, we study the *two-handed tile self-assembly model* or *2HAM* at general temperatures, in contrast with prior study limited to small constant temperatures, leading to surprising results. We obtain constructions at larger (i.e., hotter) temperatures that disprove prior conjectures and break well-known bounds for low-temperature systems via new methods of temperature-encoded information. In particular, for all $n \in \mathbb{N}$, we assemble $n \times n$ squares using $O(2^{\log^* n})$ tile types, thus breaking the well-known information theoretic lower bound of Rothemund and Winfree. Using this construction, we then show how to use the temperature to encode general shapes and construct them at scale with $O(2^{\log^* K})$ tiles, where K denotes the Kolmogorov complexity of the target shape. Following, we refute a long-held conjecture by showing how to use temperature to construct $n \times O(1)$ rectangles using only $O(\log n / \log \log n)$ tile types. We also give two small systems to generate nanorulers of varying length based solely on varying the system temperature. These results constitute the first real demonstration of the power of high temperature systems for tile assembly in the 2HAM. This leads to several directions for future explorations which we discuss in the conclusion.

Keywords Self-assembly · Hierarchical assembly · 2HAM

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1 Introduction

In the early 1980s, Ned Seeman [19] introduced a method for creating DNA-based crystals that assemble according to base-pair interactions. Erik Winfree [23] leveraged this approach to create systems of DNA-based nanoscale *tiles* that assemble algorithmically according to programmable molecular interactions, initiating the field of *algorithmic self-assembly*. To formalize the study of these self-assembling DNA tiles, Winfree also introduced the *abstract Tile Assembly Model* or *aTAM*.

Early study of the aTAM established the model's ability to compute universally [23] and assemble desired shapes using a number of tile varieties asymptotically matching information theoretic lower bounds [1,16,23]. Since then, the sophistication of both experimental and theoretical results has grown tremendously, ranging from the 5-bit binary counters of Evans [12] and a structural complexity theory for dozens of tile assembly models [24].

Two-Handed Assembly Excluding the aTAM, perhaps the most popular tile assembly model is the *two-handed tile assembly model (2HAM)* [3], also called the *hierarchical* or *polyomino* model. The key distinction between the aTAM and the 2HAM is "seededness" or "handedness": in the (seeded, one-handed) aTAM, growth occurs via single tile addition to a growing seed assembly, whereas in the (unseeded, two-handed) 2HAM, growth occurs via unrestricted attachment of assembly pairs (or tile pairs, as a special case). The seededness of the aTAM simplifies design and analysis [5], but is difficult to enforce in experimental systems [17], motivating the study of the 2HAM.

Temperature One critical parameter in tile assembly models is *temperature*: the threshold of bonding strength needed for attachment between assemblies. A major open problem in tile assembly concerns the capabilities of systems at the lowest temperature, where one bond suffices for attachment [11,13–15]. Dynamic temperature has also been studied under the name *temperature programming* as a mechanism for guiding assembly [22].

In the aTAM, systems at higher temperatures exhibit additional dynamics [6]. These differences further incur provable reductions in the minimum number of tile types needed to build certain shapes at higher temperatures [20]. However, if scaling is permitted, then these dynamics do not confer additional capabilities [10].

This is not the case in the 2HAM: higher temperatures exhibit dynamics not found at lower temperature, regardless of scaling [8]. However, these additional dynamics have not been demonstrated to confer additional capabilities. Recently, it was proven that the unique assembly verification problem is coNP-complete in the 2HAM with arbitrary temperature [18], but is still an open problem at constant temperature. Further, it was shown that for any shape, there is a constant sized tile set that can assemble the shape at scale by setting the glues as a function of the temperature [4]. These provides further evidence that the additional dynamics allow for additional power.

Our Results Here we give several such demonstrations for benchmark problems in tile assembly, e.g. the efficient assembly of squares and thin rectangles. In some cases,

Table 1 Comparison of two of our main results with prior work

Model	Tile complexity	τ	Reference
Unique assembly of $n \times n$ squares			
aTAM	$\Theta(\frac{\log n}{\log\log n})$	$O(1)$	[1,16]
2HAM	$\Theta(\frac{\log n}{\log\log n})$	$O(1)$	[1,16]
2HAM	$O(2^{\log^* n})$	$O(n)$	Theorem 1
Unique assembly of $n \times O(1)$ thin rectangles			
aTAM	$n^{\Theta(1)}$	$O(1)$	[7]
2HAM	$O(\frac{\log n}{\log\log n})$	$O(n)$	Theorem 2

τ is the temperature of the system. Several of our results are not listed here; specifically Theorems 3, 4, and Corollary 1

these capabilities exceed those possible at low temperatures. A summary of some of our results and relation to prior work can be seen in Table 1.

Result 1: $O(2^{\log^* n})$ **Squares** Our first result achieves assembly of $n \times n$ squares using $O(2^{\log^* n})$ tile types for any n (Sect. 3).[1] Our result uses temperature $\tau = O(n)$. For any constant bounded temperature, this result beats an information theoretic lower bound of $\Omega(\frac{\log n}{\log\log n})$ tile types required for almost all integers n. By combining our square construction with the construction of [21], we get the surprising corollary that *any* connected shape S is self-assembled in $O(2^{\log^* K(S)})$ tile types, where $K(S)$ denotes the Kolmogorov complexity of S, if a scaled-up version of S is permitted. For any constant-bounded temperature system this beats the information theoretic lower bound of $\Omega(\frac{K(S)}{\log K(S)})$ tile types. Small constant factor gaps have been shown to exist between temperatures 1 and 2 within the 2HAM [3]. In the aTAM, constant factor gaps in tile complexity have been shown to exist for any pair of distinct temperatures [20]. In contrast, our result provides a provable gap in tile complexity much larger than a constant factor. Further, the previous work constructed fairly exotic shapes to achieve the desired gaps, while our result applies to both the natural, standard benchmark shape of an $n \times n$ square, as well as general shapes if scaling is permitted.

Result 2: $n \times O(1)$ **Thin Rectangles with** $O(\log(n)/\log\log(n))$ **Tiles** Our next result is the self-assembly of $n \times O(1)$ *thin*[2] rectangles using $O(\log(n)/\log\log(n))$ tile types for any positive integer n. This result overcomes not an information bound, but a "geometric bandwidth" bound: in the aTAM, $n \times O(1)$ rectangles require $n^{\Omega(1)}$ tile types to assemble [7]; a similar bound has been conjectured in the 2HAM [9]. Our result refutes this conjecture in the case of higher temperatures.

Result 3: Temperature-Controlled Shapes Finally, we present two systems with well-behaved and distinct behavior across a range of temperatures (Sect. 5). These systems assemble rectangles of dimensions $O(\log n) \times r$ for r varying across $\Theta(n)$ distinct lengths according to the $O(n)$ system temperature. Such systems thus behave as "ther-

[1] The function $\log^* n$ is the *iterated logarithm*: the number of times the logarithm must be repeatedly applied, beginning with n, until a value of less than 1 is reached.

[2] The term *thin* refers to the constant height of the rectangle.

mometers" that may be useful for measurement and calibration in high-temperature settings. These *temperature-controlled* constructions differ from previous *temperature programming* results [22], in that our temperature-controlled systems assemble a variety of shapes, each at a fixed temperature, instead of assembling a variety of shapes, each using dynamically varying temperature.

2 Definitions

Here we give a compressed presentation of the two-handed tile assembly model (2HAM) and associated definitions used throughout the paper.

Tiles 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 Π. A *strength function* $\mathrm{str} : \Pi \to \mathbb{N}$ denotes the *strength* of each glue. Two tiles that are equal up to translation have the same *type*.

Assemblies 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 coordinates of those tiles.

For a given positioned assembly Υ, the *bond graph* G_Υ is the weighted grid graph in which each tile of Υ is a vertex and the weight of an edge between tiles is the strength of the matching coincident glues or 0. A positioned assembly C is said to be τ*-stable* for positive integer τ provided the bond graph G_C has min-cut at least τ.

For a positioned assembly A and integer vector $\mathbf{v} = (v_1, v_2)$, let $A_\mathbf{v}$ denote the assembly obtained by translating each tile in A by vector $\mathbf{v}$. An *assembly* is the set of all translations $A_\mathbf{v}$ of a positioned assembly A. A *shape* is the set of all integer translations for some subset of $\mathbb{Z}^2$, and the shape of an assembly A is the shape consisting of the set of all 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.

Combinable Assemblies Informally, two assemblies are τ*-combinable* provided they may attach to form a τ-stable assembly. Formally, two assemblies A and B are τ*-combinable* into an assembly C provided there exist $A' \in A$ and $B' \in B$ such that $A' \bigcup B'$ is a τ-stable element of C.

Two-Handed Tile Assembly Model (2HAM) A *two-handed tile assembly system (2HAM system)* is an ordered pair (T, τ) where T is a set of single tile assemblies, called the *tile set*, and $\tau \in \mathbb{N}$ is the *temperature*. Assembly proceeds by repeated combination of assembly pairs to form new τ-stable assemblies, starting with single-tile assemblies. The *producible assemblies* are those constructed in this way. For a given 2HAM system $\Gamma = (T, \tau)$, the set of *producible assemblies* of Γ, denoted $\texttt{PROD}_\Gamma$, is defined recursively:

- (Base) $T \subseteq \texttt{PROD}_\Gamma$
- (Recursion) For any $A, B \in \texttt{PROD}_\Gamma$ with A and B τ-combinable into C, $C \in \texttt{PROD}_\Gamma$.

For a system $\Gamma = (T, \tau)$, we say $A \to_1^\Gamma B$ for assemblies A and B if A is τ-combinable with some producible assembly to form B, or if $A = B$. Intuitively this means that A may grow into assembly B through one or fewer combination reactions. We define the relation $\rightarrow^{\Gamma}$ to be the transitive closure of $\rightarrow_1^{\Gamma}$, i.e., $A \rightarrow^{\Gamma} B$ means that A may grow into B through a sequence of combination reactions.

A producible assembly A of a 2HAM system $\Gamma = (T, \tau)$ is *terminal* provided A is not τ-combinable with any producible assembly of Γ. A 2HAM system $\Gamma = (T, \tau)$ *uniquely assembles* a shape S provided that for all $A \in \texttt{PROD}_{\Gamma}$, there exists some $B \in \texttt{PROD}_{\Gamma}$ of shape S such that $A \rightarrow^{\Gamma} B$.

3 Squares with $O(2^{\log^* n})$ Tile Types

We prove that for any $n \in \mathbb{N}$, there exists a 2HAM tile system with $O(2^{\log^* n})$ tile types and temperature $\tau = O(n)$ that uniquely assembles an $n \times n$ square. In fact, the construction can be modified to work not only for a specific τ, but any $\tau \geq cn$ for some constant c.

Theorem 1 *For any positive integer n, there exists a 2HAM system (T, τ) with $|T| = O(2^{\log^* n})$, $\tau = O(n)$ that uniquely assembles an $n \times n$ square.*

The construction is recursive, with each level of recursion using a distinct constant-size tile set behaving identically, but independently, to corresponding tile sets at other levels. Below, the tile set is decomposed into conceptually distinct components described in separate subsections. Many of the components utilize standard techniques from prior tile assembly work; these sections give only an overview of the component, along with references to complete descriptions. The key component is a novel high-temperature unary counter utilizing both high temperature and two-handedness, described in Sect. 3.6.

3.1 Construction Sketch

We begin with a sketch of the construction, followed by details in Sects. 3.3 through 3.9. There are two primary key ideas introduced in this construction. The first key component is that the tile set is generated recursively: the size $n \times n$ square is built upon tile sets for two distinct smaller squares of size at most $\log n \times \log n$ which are generated recursively. This yields an upper bound on tile complexity described by the recurrence equation $T(n) = 2T(\log n) + O(1)$. The second key component in our construction is the application of a high-temperature unary counter. The unary counter drops a unit strength glue at each counter step, thereby ceasing to grow at a value dictated by the (high) system temperature. The components, and how they fit together, are now sketched, followed by more detailed descriptions for each component in the subsequent sections.

Figure 1a: Recursive $O(\log n) \times O(\log n)$ Squares The assembly of an $n \times n$ square is based on recursive assembly of two squares (Fig. 1a): an $x \times x$ square X and a $y \times y$ square Y, with $x, y \leq \log n$. Let $T(n)$ be an upper bound on the number of tile types used to build an $n \times n$ square; then assembling X and Y uses at most $2T(\log n)$ tile types.

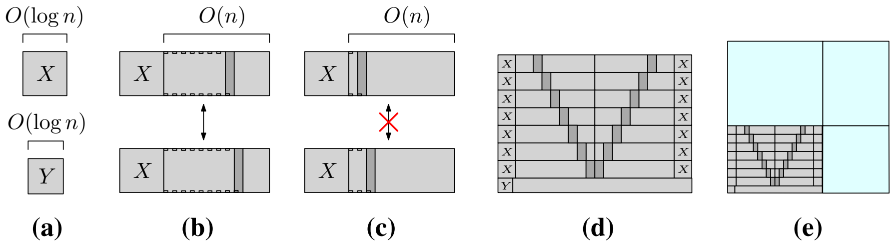

Fig. 1 A schematic of assembling $n \times n$ squares using $O(2^{\log^* n})$ tile types. **a** The starting seed squares are assembled recursively. **b** Two counter "rows" that nondeterministically assembled with matching glue arrangements that can bind together. **c** Two other counter rows with matching glue arrangements but insufficient strength (i.e., glue count). **d** Counter rows with insufficient glue counts assemble into a "reverse" counter that bonds to the east of a "normal counter". **e** The counter assembly is grown into a completed $n \times n$ square

Figure 1b:**Planks** Each $x \times x$ square X is grown into a *plank* of size roughly $x \times (2^x + x) = O(\log n) \times O(n)$ by applying a standard binary counter scheme (see [16] for an example). Planks will serve as rows in a unary counter used to assemble the $n \times n$ square. The scheme for this growth is standard: treat the east face of assembly X as a column of 0 bits denoting the initial value of a binary counter. Each successive column reads and increments the previous column's bit-wise value, stopping once the counter has reached maximum value.

We mask one modification to the counter-based plank assembly: during assembly, a *transition* column is non-deterministically selected. The exposed glues on the completed plank to the west and east of this location are *white* and *gray*, respectively. The non-deterministic selection of the transition column causes planks with every possible transition column to be assembled. Following standard previous binary counters, the number of tile types needed to implement this counting and transition scheme is $O(1)$.

Figure 1b, c: **High-Temperature Unary Counter** The assembled planks are used as rows in a unary counter (in contrast with the binary-counter approach used to assemble them). This unary counter uses high temperature to control assembly. The assembled planks from the counter-extension step are coated with tiles exposing unit-strength glues on each exposed north/south tile surface occurring *before* the planks counter transition. Thus, planks can attach if their transition occurs in a column rightward enough to cause the plank surface to expose sufficient unit-strength glues relative to τ, the system's strength.

High-strength glues at the beginning and end of the counter transition enforce that plank pairs only attach if their transition locations differ by 1. For example, the column-8-transition plank (Fig. 1b), only attaches to the top of a column-9-transition plank. Additional technical details ensure that the planks attach one at a time, from bottom to top, by way of not placing the glues on the north surface of a plank until it has attached to the growing counter.

A specified number of planks assemble into a counter, controlled by the system temperature τ, starting with the two planks that transition in the last two possible columns (exposing the largest number of glues). A special "cap" plank is the last to attach, verifying that the unary counter is completed. The detailed $O(1)$-sized tile set for this step is provided in Sect. 3.6.

Figure 1**d: Precise-Height Assembly and Reverse Counter** The assembled unary counter consists of planks with small dimension $O(\log n)$, implying that the assembly may differ from a target height by up to $\Theta(\log n)$. To reach a precise target height, a second recursively assembled square Y of dimension y is used, where y is exactly the difference between the desired height and the height of the assembled unary counter. The square Y attaches to the base of the unary counter, yielding the desired height (see Fig. 1d). The number of tile types used to assemble Y is at most $T(\log n)$ (defined earlier in this section).

The assembly of the unary counter potentially creates unused planks whose transition column is not sufficiently rightward to enable attachment to other planks. These planks are used in a second "reversed" version of the unary counter, where planks attach via glues to the right of the transition (instead of left, as in the "normal" counter). Both counter versions grow to the same height, but are assembled from planks beginning with those with the rightmost (or leftmost) transitions. The size of X is chosen so that at least half of the planks are used in the unary counter, and thus every plank is used in one or both of the two counter versions. Of note is that each plank only initially places it's unit-strength glues on it's southern face, but not it's northern face. The glues along the northern face are different for the first counter than for the reverse counter. The reverse counter is seeded with a distinct assembly, which in turn causes each attached plank in the reverse counter to attach the glues specific to the reverse counter. Thus, planks "know" which counter they are in because their attachment to the respective counter is what causes them to add the glues unique to that counter.

Both counter versions are assembled into a single assembly (see Fig. 1d) along with the square Y. The second counter version requires only $O(1)$ additional tile types.

Figure 1**e: Finishing the Square** The assembly consisting of both counter versions has a precise desired height n'. This height is chosen so that an $O(1)$-sized set of *filler* tiles can extend the dimensions of this assembly into an $n \times n$ square. This filling scheme is standard and similar to square constructions seen in prior work, e.g. [16]. A small modification is made to expose a set of glues used as invariants in the recursive square recursion (described in Sect. 3.4). This filling and formatting requires $O(1)$ tile types.

Analysis The total tile complexity for our construction based on the above steps is bounded by $T(n) = 2T(\log n) + c$ for a constant c. Solving this recurrence equations yields the final tile complexity of $O(2^{\log^* n})$.

3.2 Extension to General Shapes

Soloveichik and Winfree [21] proved that a *seed assembly* encoding a desired shape S as a binary string can be combined with an additional set of $O(1)$ tile types to assemble a scaled version of S. Theorem 1 gives a method to encode arbitrary numbers n in unary; the exposed glue invariants of the construction (see Sect. 3.4) allow compresssing such unary encodings into binary encodings of arbitrary numbers (or shapes). Thus, combining the two constructions gives the following result based on the the Kolmogorov complexity $K(S)$ of shape S:

Corollary 1 *For any shape S, there exists a tile system* (T, τ) *with* $|T| = O(2^{\log^* K(S)})$, $\tau = O(K(S))$ *that uniquely assembles a scaled version of S.*

The remainder of this section presents the detailed construction and analysis for our $n \times n$ square construction.

3.3 Preliminaries

For simplicity, we assume τ is even; replacing occurrences of $\tau/2$ with $\lfloor \tau/2 \rfloor$ and $\lceil \tau/2 \rceil$ where appropriate gives the same result for odd τ. Let $x, y = O(\log n)$ as described in Sects. 3.6 and 3.8. The complete tile set for assembling an $n \times n$ square consists of five subsets:

- T_X, assembling the $x \times x$ square X.
- T_Y, assembling the $y \times y$ square Y.
- A *plank tile set*, assembling planks from X (described in Sect. 3.5).
- A *high-temperature unary counter tile set*, assembling the unary counter from planks (described in Sect. 3.6).
- A *finishing tile set*, filling in the completed $n \times n$ square from the unary counter assembly (described in Sect. 3.7).

3.4 Exposed Glue Invariants of Assembled Squares

Given the recursive nature of our construction, we start by stating the requirements of the assembled square; specifically, of exposed glues. These exposed glue requirements may be presumed for squares X and Y. The requirements are:

1. The exposed glues are unique to the square assembled, i.e., the exposed glues on any pair of assembled squares are distinct.
2. The $4 \cdot 4 = 16$ exposed glue locations on corner tiles and tiles adjacent to corner tiles each contain a distinct glue.
3. Each remaining exposed glue location has a $\tau/2$-strength glue unique to the glue's direction (north, east, south, or west).

The eastmost glue on the north and south surfaces are referred to as p_1 and p_2, respectively.

3.5 Plank Tile Set

The plank tile set uses an $x \times x$ square assembly X (satisfying the invariants of Sect. 3.4) as a "seed" to assemble a $x \times 2^{\Theta(x)}$ assembly eastward using a standard single-tile-attachment binary counter consisting of single-tile and two-tile attachments [16]. This counter uses $x - 3$ glues of the east surface of X as an initial 0-valued column of the counter, which will grow by $2^{x-3} - 1$ additional columns before ceasing.

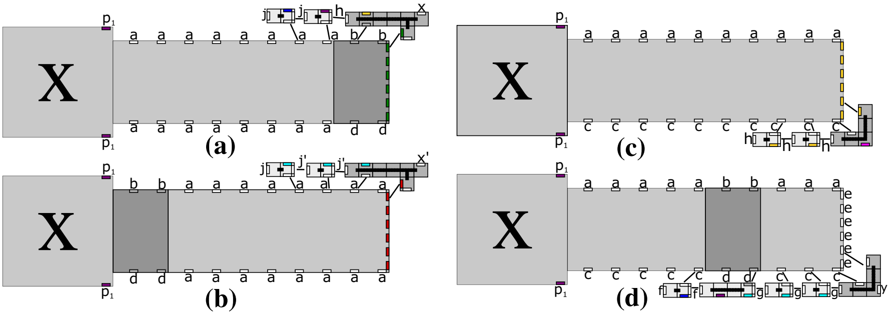

Fig. 2 Initial attachments for the high-temperature unary counter

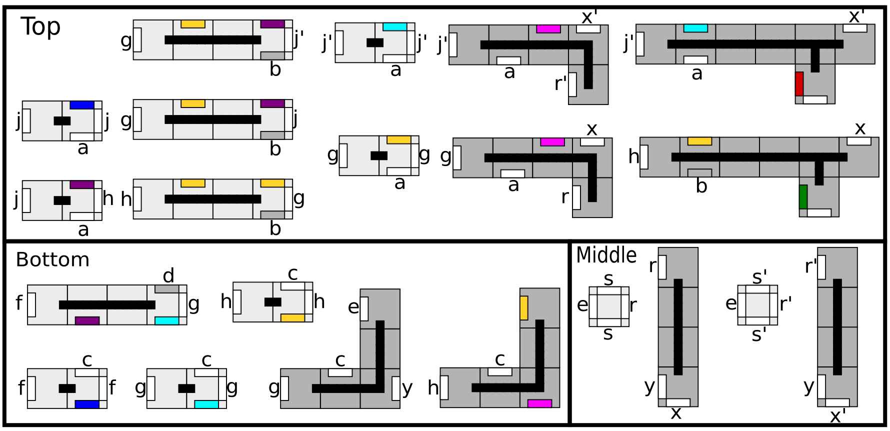

Fig. 3 The high-temperature unary counter tile set

Two of the unused glues of the east surface of X are reserved for non-counter purposes, and one more as a as well as a single glue to use as a *state bit*. The state bit's value is initalized to 1, and is through each counter column. During the assembly of each new column of the counter, 1-valued state bits are non-deterministically selected to remain 1 or transition to 0; 0-valued state bits never transition back to 1.

Each column of the counter exposes matching *white* (a, c) or *gray* (b, d) glues on the north and south ends (seen in Fig. 2a-d). White glues are exposed in all locations, except the first two columns after the state bit transition, (where gray glues are exposed instead). The resulting set of (non-deterministically) produced assemblies is a set of length $x + 2^{(x-3)}$ blocks, each with a specific transition point denoted by gray glues.

In the rare cases where the state bit transition occurs at the last possible location, first possible location, or never occurs, *green*, *red*, or *yellow* glues are exposed on the east end of the assembly, respectively (Fig. 2a–c). The 4 types of planks shown in Fig. 2a–d, are named according to their east-face glue: *green*, *yellow*, *red*, and *basic*. Let $\ell = 2^{x-3}$. Basic assemblies come in $\ell - 1$ forms, one for each number of possible white glues exposed on the north surface to the west of the transition (a glues to the west of the 2 consecutive b glues). Call the basic assembly with i pre-transition white glues B_i, for $i \in \{1, 2, \ldots, \ell - 1\}$.

3.6 High-Temperature Unary Counter Tile Set

Next, completed planks from Sect. 3.5 are assembled with a set of tile types (listed in Fig. 3) that enable them to assemble into a (high-)temperature-controlled unary counter.

The *bottom* subset of the tile set coats the south surfaces of each B_i assembly with i unit-strength *dark blue* glues, 1 p_2 glue (strength specified later), and $\ell - i$ unit-strength *light blue* glues (B_5 is shown in Fig. 2d). The *top* subset of the tile set coats the north surface of each B_i assembly with $i - 1$ unit-strength *dark blue* glues, 1 p_2 glue, and $\ell - i + 1$ yellows glues. The bottom and top subsets also coat a select subset of the the north and south surfaces of the green, red, and yellow assemblies.

Counter Growth Growth initiates from the attachment of the green and $B_{\ell-1}$ planks (Fig. 4a) using $\ell - 1$ unit strength glues, glue p_1, and glue p_2, (i.e., $g(p_1) + \ell - 1 + g(p_2) \geq \tau$). Upon combination, a cooperative attachment between the green plank and $B_{\ell-1}$ directs the attachment of top tiles to the north surface of $B_{\ell-1}$. Subsequently, basic planks $B_{\ell-2}$, $B_{\ell-3}$, etc. attach sequentially to the top of this growing counter assembly, presenting decreasing numbers ($\ell-2$, $\ell-3, \ldots$) of unit-strength dark blue glues.

Attachment of basic planks continues until assembly B_r with $g(p_1)+r+g(p_2) = \tau$ attaches. Thus choosing the strengths $g(p_1)$ and $g(p_2)$ such that $g(p_1)+r+g(p_2) = \tau$ causes the counter attachments to cease after attaching B_r, the $(\ell-r)$th basic assembly to attach (Fig. 4b). The strength of p_3 (on the yellow plank) is chosen such that $g(p_1)+g(p_3)+\ell-r = \tau$, so that the yellow plank uniquely attaches to the completed counter as a "cap" (Fig. 4c).

Reverse counter The counter seeded by the green plank serves the primary purpose of growing to within x of a desired height. In general, the assembly process excludes some basic planks, which must be incorporated as part of the final square assembly.

As a solution, the red planks are used to initiate growth of a *reverse counter*. The high-temperature unary counter tile set (Fig. 3) coats the north surface of the red plank with 1 dark blue glue, 1 p_2 glue, and $\ell - 1$ light blue glues (Fig. 2b), enabling the attachment of basic planks B_1, B_2, etc. with decreasing glue strength.

As in the original counter, the yellow plank attaches exactly when no more basic planks are able to attach via carefully chosen glue strengths. Provided the original counter includes at least half of the basic planks ($B_{\ell-1}$, $B_{\ell-2}, \ldots, B_{\ell/2}$), the entire set of basic planks have bonding positions between the two counters (see Sect. 3.8 for

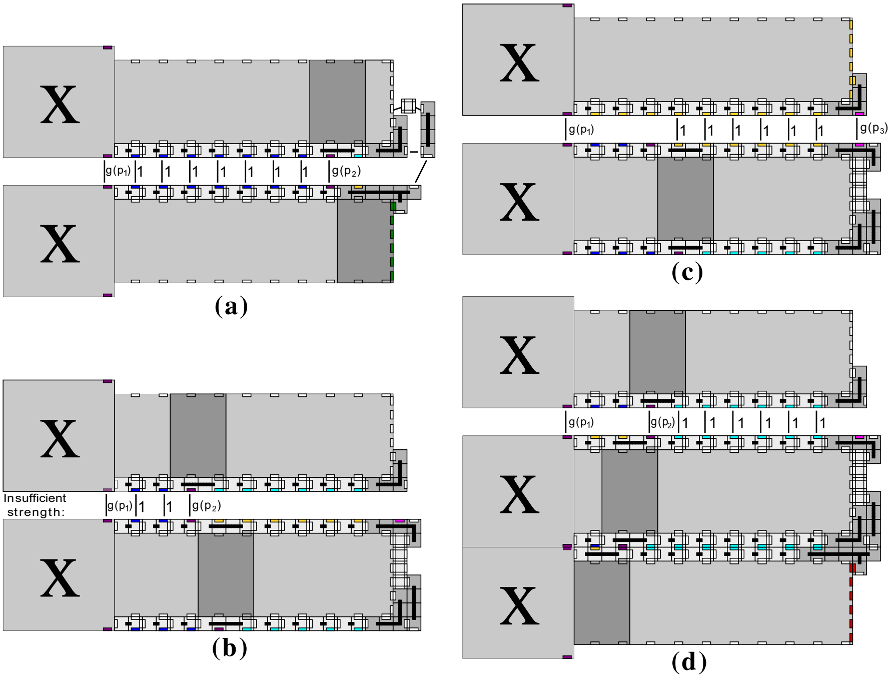

Fig. 4 **a** Seeded by the green plank, basic planks B_ℓ, $B_{\ell-1}$, etc. attach in order. Each subsequent basic plank attaches with one less strength. **b** Depending upon the strength of glue p_2 and the temperature τ, eventually no more basic planks can attach. **c** By choosing the strength of glue p_3 carefully, the yellow plank attaches exactly when no more basic planks are able to attach, thereby "capping" the finished counter. **d** To dispose of the unused basic planks, a *reversed* version of this counter is seeded by the red assembly using the same basic assemblies in reverse order (Color figure online)

details). The two completed counters attach when completed via glues on the green and red planks, yielding a finished unary counter as seen in Fig. 5.

Fixing the offset The complete (two-)counter construction grows a stack of a specified number of planks based on the chosen strengths of glues p_2 and p_3. However, each basic assembly has height $x = O(\log n)$. Thus, achieving an arbitrarily desired height requires adding $0 \le y < x$ additional length to the counter. This is done by recursive construction of a $y \times y$ assembly Y attached to the south surface of the green plank, as shown in Fig. 5.

3.7 Finishing Tile Set

The final tile set accomplishes two goals. First, "finishing" the unary counter rectangle into an $n \times n$ square. Second, "formatting" the surface glues of the final assembly to satisfy the invariants of Sect. 3.4. Given a unary counter rectangle of height n' and width m, existing tile assembly techniques can be easily applied to extend such a rectangle into a $(n' + m) \times (n' + m)$ square (the square construction in [16]). Thus, the unary counter's height is $n - m$, where $m = x + 2^{x-3}$, the width of a plank. Glue

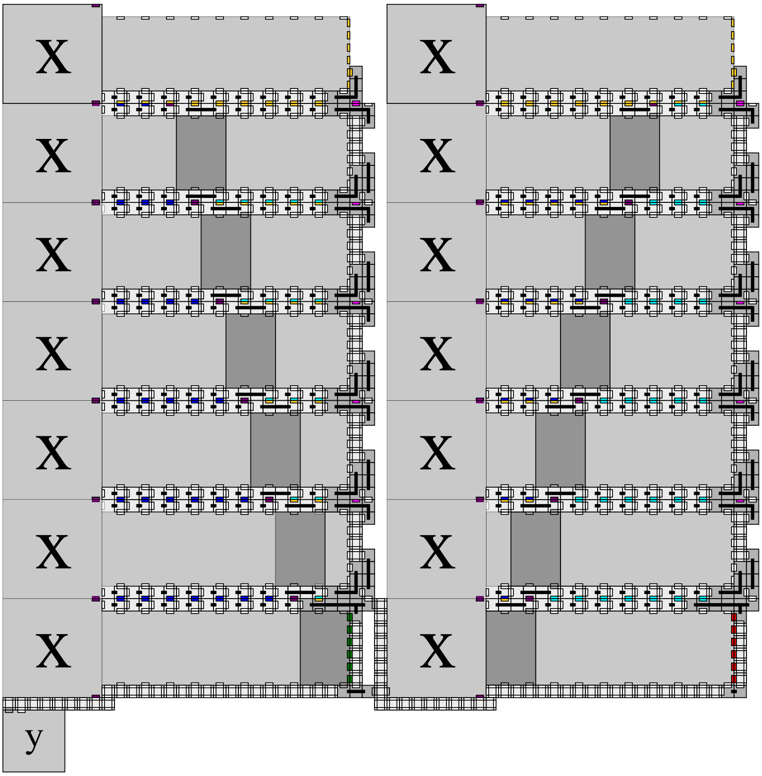

Fig. 5 The finished high-temperature unary counter attached to the reverse counter and augmented with assembly Y

formatting is easy due to the special assemblies at key locations, e.g., the square Y in the lower left corner.

3.8 Additional Details

The high-temperature unary counter must grow to height n' and width m such that $n' + m = n$. Moreover, to ensure the system has a unique terminal assembly requires that all basic planks are used in either the primary or the reverse counter, so the number of basic planks assembled cannot exceed the number needed by more than a factor of 2. So the maximum n' achievable by the counter system is a function of x, the dimension of the recursively assembled square X. The maximum height of the counter is $x \cdot 2^{x-3}$ (a maximum of 2^{x-3} basic assemblies, each of height x). The width w of the counter is $2(x + 2^{x-3}) = 2x + 2^{x-2}$, the width of two adjacent basic assemblies.

Selecting x to be the smallest even integer such that $n'+m = x2^{x-3}+2^{x-2}+2x \geq n$ ensures that the counter has sufficient capacity to grow to a height between $n' - x$ and n', yielding the exact dimensions. The counter must also use at least half of the basic assemblies to ensure a deterministic assembly. In some scenarios, due to the factor of

x in $x2^{x-3}$, the smallest value x might cause less than half of the basic blocks to be used. However, the next smallest even x *undershoots* by at most a constant multiple of 2^{x-3}. Such cases are handled by padding basic assemblies with a constant height and selecting the smaller x value.

3.9 Tile Complexity Analysis

Let $T(n)$ denote the number of distinct tile types used for a given integer n. Tile subsets T_X and T_Y each have size $T(O(\log n))$, while the other three subsets are each constant-sized. Thus $T(n) = 2T(O(\log n)) + O(1)$ and $T(1) = 1$, giving a closed form of $T(n) = O(2^{\log^* n})$.

4 Constant-Width Rectangles with $O(\log n/\log\log n)$ Tile Types

The study of precise length linear assemblies is an established benchmark problem in self-assembly for comparing the power of different models and techniques. The importance of this problem stems from both its inherent difficulty based on the limited geometric bandwidth in the thin shape, and its usefulness as a tool in the assembly of more elaborate shapes.

Tile complexity for $n \times O(1)$ rectangles in the aTAM is known to be $\Theta(n^{1/c})$, where c denotes the constant height of the rectangle [7]. The question of tile complexity for thin rectangles in the 2HAM was first asked around 2004 [7], but has remained open. It has been widely conjectured that no poly-logarithmic solution exists in the 2HAM, and substantial consideration has gone into generalizing lower bound techniques such as the *window movie lemma* [15] in order to confirm that the 2HAM cannot beat the lower bound for the aTAM. In contrast to these conjectures, we prove that by utilizing high temperature, thin rectangles of any specified length ($n \times O(1)$ lines) may be uniquely self-assembled with $O(\frac{\log n}{\log\log n})$ tile types.

While we achieve unique assembly of $n \times O(1)$ lines, this result differs from the previous result for $n \times n$ squares in that the construction does not yield a unique *assembly* (stemming from the garbage collection step of the construction). That is, our construction non-deterministically assembles a set of terminal assembles that all have the unique shape of a target $n \times O(1)$ rectangle. It is still open whether a result like ours can be obtained with a unique final assembly.

Construction sketch The construction uses a "traditional" method: small assemblies encoding consecutive counter values attach to form larger intervals of value iterations. The novelty lies in using high temperature to overcome the geometric "bandwidth" constraint: the height of the assembly is insufficient to "communicate" the value of the counter.

The construction is based on a set of $O(\log n)$-length "horizontal counter rows" that each non-deterministically encode two binary strings (a left and right string, gray and white respectively in Fig. 6a). In the (unlikely) case that the two strings are equal, the right string is incremented by 1 (via several single-tile attachments) to create a row of a "sideways" counter (Fig. 6c). The constant height of the final assembly prevents

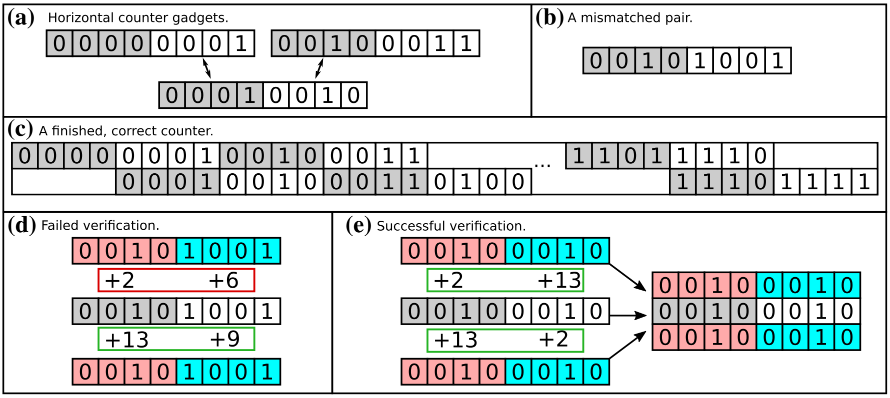

Fig. 6 A high-level schematic of assembling counter rows. **a** Left (gray) and right (white) bit strings are non-deterministically paired, including **b** mismatched pairs. **c** Correctly paired bit strings form the rows of a "horizontal counter" that grows to a precise length. **d**, **e** Incorrectly and correctly paired bit strings are identified and separated by verification assemblies

the left and right bit strings from coordinating their values by more than a constant number of bits, unavoidable assemblies of unequal bit string pairs are also assembled (Fig. 6b).

Key Idea The key idea of this constructions is to utilize high temperature to differentiate assemblies that contain equal and unequal bit string pairs. By identifying and neutralizing any unequal bit string pairs, the remaining equal counter gadgets assemble in sequence to form a precise length assembly. To identify equal bit string pairs, two "verification" assemblies potentially attach to the top and bottom of the bit string pair (Fig. 6d) via glues at each bit whose strength matches the corresponding power of two. These assemblies are both attachable exactly when the left and right bit strings are equal. This is achieved by using a strength of attachment equal to the binary value of the left counter value, plus the binary value of the complement of the right counter value, to attach the top assembly, while using the reverse for the attachment of the bottom assembly. For example, in Fig. 6d, the top assembly attaches with strength-2 from the binary value 0010 encoded in the left assembly, and strength-6 for the value 0110, which is the complement of the encoded value 1001 in the right assembly. The key insight is that the minimum strength between the top and bottom attachments under this scheme is maximized when the left and right bit-strings match, thereby allowing for a temperature value that allows both attachments only for equal bit string pairs. Assemblies without both verification assemblies attached are "disposed".

An overview of how the different parts are assembled is shown in Fig. 7. This shows where garbage is collected, how the counter pieces are put together, and then regions that must be filled to make a solid rectangle. Further details are in Sect. 4.1.

4.1 Construction Details

In [7], a lower bound of $n^{\Omega(1)}$ is given for the number of tile types needed to assemble a $n \times O(1)$ rectangle in the aTAM. In contrast to the $\Omega(\log(n)/\log\log(n))$ information

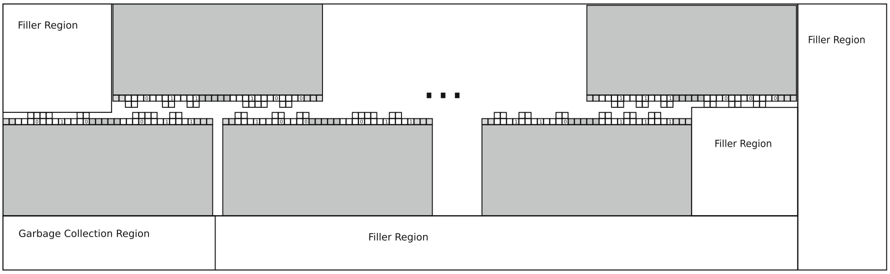

Fig. 7 The $n \times O(1)$ rectangle is grown by counter gadgets connecting in order, counting to the target length n. The key is constructing *counter blocks*: constant-height assemblies that encode a number and its increment on the southwest and southeast assembly surfaces, respectively

theoretic lower bound that applies to squares and rectangles in both the aTAM and 2HAM [16], the bound of [7] is derived from the "geometric bandwidth" restrictions of the shape's thinness. A similar bound for the 2HAM has been conjectured [7,9] but the flexibility of 2HAM assembly dynamics has made proving such a bound difficult. Here we refute the conjecture, using high temperatures to circumvent geometric bandwidth restrictions.

Theorem 2 *For any positive integer n, there exists a 2HAM system* (T, τ) *with* $|T| = O(\frac{\log n}{\log \log n})$ *and* $\tau = O(n)$ *that uniquely assembles an* $n \times O(1)$ *rectangle.*

Proof The foundation of the construction is a base-b, d-digit counter using $O(b + d)$ tile types and operating within a constant-height region by leveraging high system temperature. Forming the desired shape is finished via filler tiles and garbage collection. A high-level sketch is seen in Fig. 7.

Base b, d**-Digit Assembly** The key piece of our construction is the assembly of a $O(1)$ height counter that grows to a specific target length. To achieve this we construct counter blocks as described in Fig. 8 which, for a given b and d, assembles a height $O(1)$, width $O(bd)$ assembly consisting of d sections, with each section encoding a number from 0 to $b - 1$ through the location (in one of b positions) of a geometric bump. Together this assembly represents a given base-b, d-digit number. Further, as shown in Fig. 8e, each digit exposes the number of glues equal to the value of the given digit, and the strength of the glues for the i^{th} digit from the left is b^{i-1}. Thus, the net strength of all exposed glues is exactly the value of the number encoded by the assembly.

The next step of the process, Fig. 8d, runs a line of tiles across the assembly surface to compute whether the assembly's number is greater or equal to some given value n_0, which can be done within $O(d + b)$ tiles. By ensuring that all counter blocks start at some minimum value that we can encode in the tile set, we are able to precisely control the total length of the counter. If the assembled number is at least n_0, assembly proceeds to step (e). If not, assembly is halted at this step and the assembly will instead attach to a nearly finished rectangle assembly. To uniquely assemble our goal shape of a $n \times O(1)$ rectangle, all producible assemblies must have a forward growth path towards a terminal assembly of this shape. Thus, in this case and in a subsequent case,

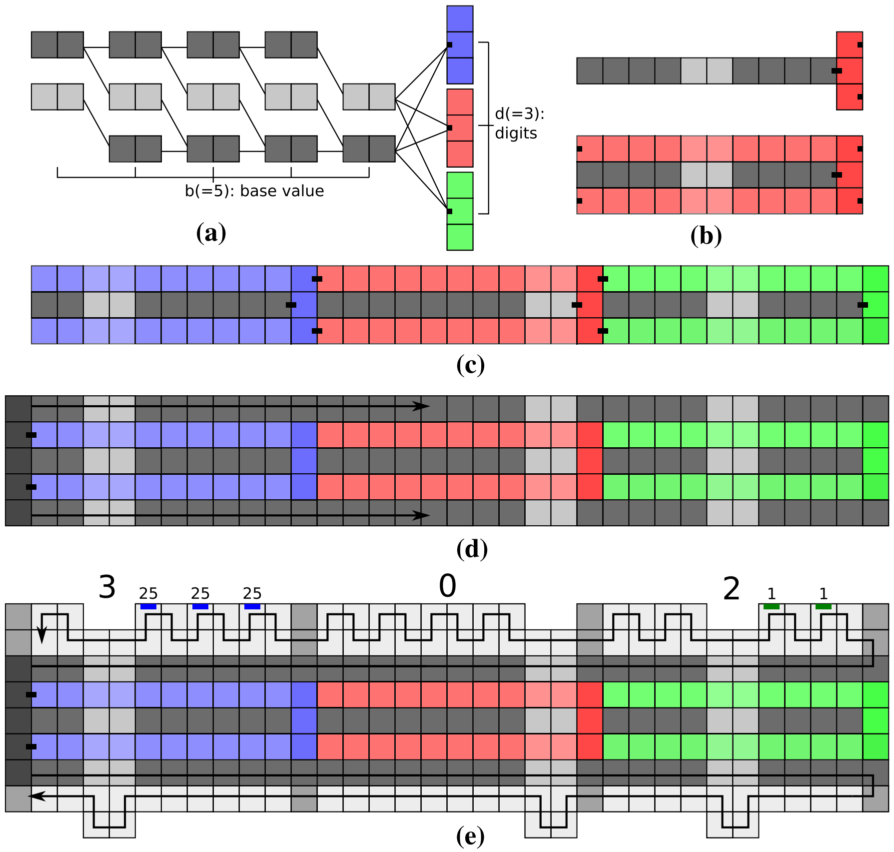

Fig. 8 The construction of a d-digit, base-b assembly, using $O(d + b)$ tile types. **a** A chain of $O(b)$ tiles assemble $2b$ long gray assemblies which nondeterministically partition the assembly into two portions separated by light gray tiles. The b possible positions of the light gray tiles represent the value of a single digit in a base b counter. **b** Each gray line assembly non-deterministically attaches to one of d distinct digit assemblies, which coat the gray assembly on each side with tiles specific to the chosen digit assembly. **c** Each of the d types of coated assemblies attach in a specific order to form a $2bd + d$ long assembly. **d** A line of tiles grows across the North and South face of the assembly to check that the non-deterministically selected number (in this case, 302 in base 5) is at least a given value n_0. **e** If the digit assembly is at least n_0 in value, a set of geometric bumps is attached that encode the value of the assembly with geometry. Further, each digit exposes a number of glues equal to the value of the digit, with each glue of strength corresponding to the digit position

we will design *garbage* assemblies such as this to have glues to attach to a special location on nearly finished correct rectangular assemblies, thereby ensuring that this *garbage* assembly still has a forward growth path to a correct final assembly.

Pairing Identical Numbers To create the counter blocks for our construction, we need a left and right number assembly to pair as increments of one another. As incrementing by one is straightforward, we simplify this goal to pair identical left and right values of two instances of the base b, d-digit assemblies from Fig. 8. The $O(1)$ height restriction of all producible assemblies makes it impossible to communicate

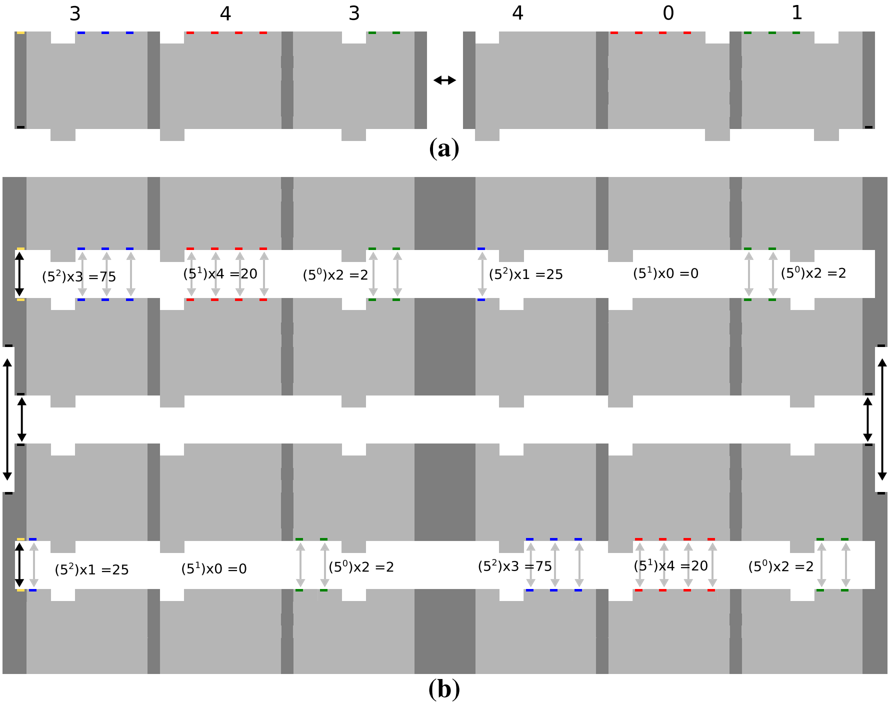

Fig. 9 **a** Two separate instances (left and right) of the d-digit, base b number assembly non-deterministically attach end to end. The sum total of exposed glue strengths for all glues is exactly $b^d - 1$ if and only if the left and right numbers match. **b** We create 4 instances of the left/right paired counter assemblies such that all 4 will combine into a single assembly if and only if the left and right numbers represented by the assemblies match. The top two assemblies can attach if the right number is less or equal to the left. The bottom two assemblies can attach if the right number is greater or equal to the left. By setting the black glues to have strength $\tau/4$, all four assemblies combine only when the left and right numbers are equal. By setting the yellow glue to have strength $\tau - b^d + 1$, this scheme can be applied for any $\tau \geq b^d - 1$

the super constant information of a left number to a right number. Therefore, we abandon trying to only pair identical numbers, but instead non-deterministically pair all possible pairs of numbers (Fig. 9a). We then select *only* the correctly paired numbers for continued growth into blocks that may be incorporated into our counter, leaving the remaining incorrectly paired blocks inert. To aid in selecting only the correctly paired assemblies for continued growth, the right versions of the paired assemblies are modified such that for a given digit value i, the digits for the left assemblies expose i glues for the given digits, and the right assemblies expose $b - i - 1$ glues (Fig. 10).

Rather than a single instance of the left-right paired counter assemblies, we construct four distinct instances of this type of assembly in a similar fashion, as shown in Fig. 9. For any given pair of left-right numbers, there exists a corresponding set of 4 such assemblies matching the pair. Our goal is to ensure that all 4 assemblies assemble if and only if the left-right pair of numbers represented by these assemblies are exact matches. To see how this works, consider the top two assemblies of Fig. 9. First, by the geometry of the shapes, we are ensured that the 4 assemblies encode the same pair

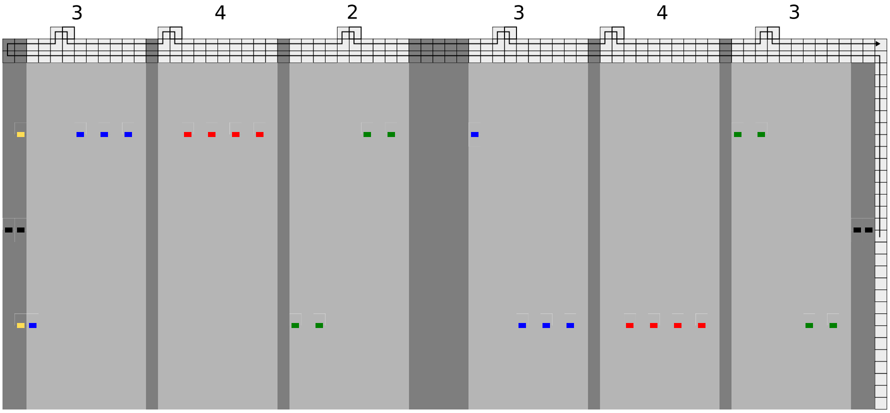

Fig. 10 The final counter assembly block is completed if and only if the left and right numbers are equal. A final collection of tiles increment the right number and place geometry that encodes the counter values

of numbers. Second, by setting the temperature to exactly $b^d - 1$, we are ensured that the right number of the pair must be less or equal to the left, as the number of glues for a given digit value x is x and $b - x$ for the left and right numbers respectively. Conversely, the bottom two gadgets combine only if the right number denotes a number that is *greater* or equal to the left. Therefore, both the top and bottom combine if and only if the left and right are exactly equal, in which case the two top and bottom assemblies may combine into one assembly. This final combination in turn causes a growth of tiles that places appropriate geometry on the surface of the assembly that denotes the left number and the increment of the right number, which is our desired counter block. The assemblies that mismatched left and right values will not become counter blocks in the counter assembly, but instead will maintain attachment sites for sticking to nearly completed rectangular assemblies.

Finishing the Rectangle Let $b = \lceil \frac{\log n}{\log \log n} \rceil$, $d = \lceil \frac{\log n}{\log \log n - \log \log \log n} \rceil$. For these parameters, note that our counter gadget is able to count up to $b^d \geq n$, and the tile complexity of the constructions is $O(b + d) = O(\frac{\log n}{\log \log n})$, and the temperature $\tau = b^d - 1 = O(n)$. Further, select n_0, the starting value of the counter, to be such that the counter grows just shy of the desired length n. The short-length will be at most the length of the counter block, which is $O(bd) = O(\log^2 n)$. With constant width (width 3 is sufficient) standard tile counter systems [7] can extend our assembly by this length within the $O(\frac{\log}{\log \log n})$ tile complexity bound. The remaining filler regions sketched in Fig. 7 can be filled in with similar techniques. Finally, a special attachment zone must be reserved to attach both types of garbage assemblies generated within the construction- ensuring that all producible assemblies have a forward growth path to a terminal rectangle of the desired dimensions. □

5 Temperature-Controlled Assembly

5.1 Temperature-Controlled rectangles

Here, we use temperature to control the assembly process of a fixed tile set. Specifically, for any $n \in \mathbb{N}$, two $O(\log n)$-sized tile sets are given that assemble $O(\log n) \times r$ rectangles, where r is in a $\Theta(n)$ range of values (that grow linearly or exponentially), depending upon the temperature. These tile sets then function as telescoping "nanorulers", where raising the temperature causes the length to reduce and vice versa. As with the previous result for thin rectangles, this construction yields multiple terminal assembles, each with the same final shape, making the system have a unique shape, but not a unique assembly.

Theorem 3 *For any positive integer n and integer r where $0 \leq r \leq n-2$, there exists a single tile set T, $|T| = O(\log n)$, such that $\Gamma = (T, \tau_r)$, where $\tau_r = n \log n + r$, uniquely assembles a $O(\log n) \times (n - r + 1)$ rectangle.*

Proof We prove this by construction. Figure 11a shows an example tile set and assembly when $1 \leq n \leq 8$, which consists of $O(\log n)$ triples. Each triple is built with τ strength glues. These triples create a binary counter, which is represented by the 1 or 0 on the center tile. Every G_i and P_i glue are of equal strength where $\text{str}(G_i) = \text{str}(P_i) = n$ for $0 \leq i \leq 2$. Since there are $\log n$ glues for each of the digits, the strength of just the special glues in a column is $n \log n$. Thus, whether the next column can attach with $\tau_r = n \log n + r$ is dependent upon the B_i glues, which encode the counting mechanism for the rectangle. Each B_i glue pair binds with strength 2^i, $\text{str}(B_i) = 2^i$. The first column has full strength and each subsequent column has one less total binding strength because of the B_i glues counting down until there are none. Let $\text{str}(S_i) = \text{str}(C_i) = \text{str}(A_i) = n \log n + n$ for $i = \{1, 2\}$.

Garbage Collection When the temperature is $\tau_r = n \log n + r$, only r columns will combine, and the other $n - r$ columns could not attach. We collect them as garbage so there is a single terminal assembly. This is be done by attaching a special column to the left of the finished assembly, attached with glue R_s that is twice the height of the rectangle. It exposes the glue R_t- providing a place for any column to attach above the

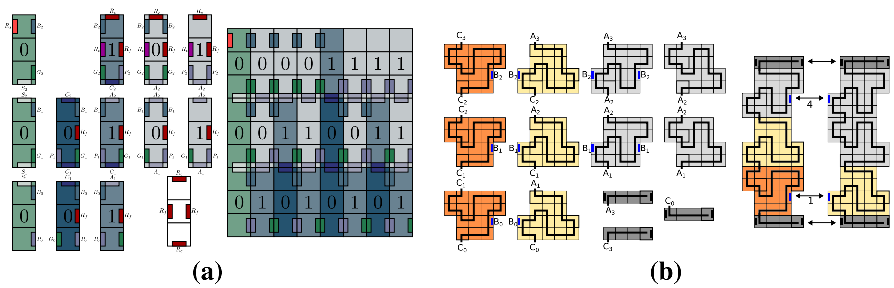

Fig. 11 **a** The tile set for a temperature controlled constant-width ruler with $1 \leq n \leq 8$ along with the maximal assembly produced. **b** A similar tile set using geometry to achieve a temperature that is linear in the length of the ruler

Fig. 12 Garbage collection can be done above the object by allowing any column to attach and filling in the empty space with cooperative binding

current rectangle. Figure 12 shows a high-level sketch. The remaining space is filled in by a single filler triple that cooperatively binds to a glue that is on the top of every column (R_c) in the original shape and the middle tile of each triple (R_f). The strength of these glues are $\mathrm{str}(R_s) = n \log n + n$, $\mathrm{str}(R_c) = n \log n$, and $\mathrm{str}(R_f) = n$. Now there is one terminal assembly of size $(6 \log n) \times (n - r + 1)$. □

Exploiting Geometry The temperature controlled rectangles require a temperature of at least $n \log n$. Here, via the use of some geometry, we are able to lower that dependency and give $\tau = 2^{k+1} + r$ where k is the number of bits needed ($\log n$), which means the temperature is linear in the size of the rectangle. Figure 11b shows the basic gadgets and how they assemble. This construction uses the same binary counting trick as the previous result. In order to ensure that both upper and lower borders must be used and at least one B_i is used (with strength 2^i), the connecting glues for the upper and lower sections have strength 2^k, and thus $\tau = 2^{k+1} + r$. Due to the geometry, each gadget has width-4, and we can take care of the garbage in a similar way as the previous result.

Theorem 4 *For any positive integer n and integer r where* $0 \le r \le n-2$*, there exists a single tile set* T, $|T| = O(\log n)$*, such that* $\Gamma = (T, \tau_r)$*, where* $\tau_r = 2^{k+1} + r$ *where* $k = \log n$*, uniquely assembles a* $O(\log n) \times 4(n-r)$ *rectangle.*

6 Future Work

Our work leads to a number of important directions for future work. A few are as follows.

– We have shown that any $n \times n$ square self-assembles in the 2HAM at temperature $\tau = O(n)$ with $O(2^{\log^* n})$ tile types. Is this the smallest achievable tile complexity? Can general n be assembled with a $O(1)$-size tile set? We have shown that with the addition of negative glues, and for special n, this is the case, but we conjecture this to be impossible in the basic model.
– Our $O(2^{\log^* n})$ tile type square construction can be viewed as a unary encoding of a target value n, and applied accordingly to problems such as building scaled-up general shapes. The unary encoding of n causes an exponential blowup in scale factors. Is it possible to utilized high-temperature systems to generate a more compact poly-logarithmic scale encoding of a target n? Achieving a more

compact encoding would allow for high-temperature techniques to be used as a more general, modular tool within lower-scale bound constructions, similar to more classic "binary counter" tile assembly subroutines.
- In the case of constant-height rectangles, we have shown assembly is possible using asymptotically as few tile types as for thicker rectangles, a provably impossible feat within the aTAM. However, it is still open whether or not any poly-logarithmic tile complexity is achievable without using a super constant temperature parameter. We conjecture the high-temperature is needed, but leave this as an open problem. Expanding on this area, a further direction is to develop trade-offs with respect to tile complexity, temperature, and rectangle height.
- Our constant-height rectangle construction achieves unique shape assembly, but non-deterministically assembles multiple distinct final assembles (of the same final shape). This type of *non-deterministic* assembly is known to allow for more efficient assembly of some classes of shapes within the abstract tile assembly model [2], but little is known how nondeterminism versus determinism affect tile type complexity within the 2HAM, and little is know in either model with regards to fundamental benchmark shapes such as rectangles. Is it possible to achieve our tile complexity, or anything close, without nondeterminism?
- We have introduced a preliminary class of temperature controlled self-assembly systems which build rectangles of dimension specified by the system temperature. This is perhaps just the beginning of a new class of tile sets that are programmable into precise and intricate shapes by way of careful temperature parameter setting. Imagine a single set of *universal* tiles for which any target shape can be constructed simply by finely tuning the temperature at which the tiles interact. Expanding on our initial results here towards this general goal is an exciting direction for future work.

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