Self-assembly of, and optimal encoding inside, thin rectangles at temperature-1 in 3D

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Abstract

In this paper, we study the self-assembly of rectangles in a non-cooperative, 3D version of Winfree’s abstract Tile Assembly Model. We prove four main results – the first two negative and the last two positive. First, we use Catalan numbers and a restricted version of the Window Movie Lemma (Meunier, Patitz, Summers, Theyssier, Winslow and Woods, SODA 2014) to prove two new lower bounds on the minimum number of unique tile types required for the self-assembly of rectangles. We then give a general construction for the efficient self-assembly of thin rectangles. Our construction is non-cooperative and “just-barely” 3D in the sense that it places tiles at most one step into the third dimension. Finally, we give a non-cooperative, just-barely 3D optimal encoding construction that self-assembles the bits of a given binary string along the perimeter of a thin rectangle of constant height.

1 Introduction

Intuitively, self-assembly is the process through which simple, unorganized components spontaneously combine, according to local interaction rules, to form some kind of organized final structure.

While nature exhibits numerous examples of self-assembly, researchers have been investigating the extent to which the power of nano-scale self-assembly can be harnessed for the systematic nano-fabrication of atomically-precise computational, biomedical and mechanical devices. For example, in the early 1980s, Ned Seeman [17] exhibited an experimental technique for controlling nano-scale self-assembly known as “DNA tile self-assembly”.

Erik Winfree’s abstract Tile Assembly Model (aTAM) is a simple, discrete mathematical model of DNA tile self-assembly. In the aTAM, a DNA tile is represented as an un-rotatable unit square tile. Each side of a tile may have a glue that consists of an integer strength, usually 0, 1 or 2, and an alpha-numeric label. The idea is that, if two tiles abut with matching kinds of glues, then they bind with the strength of the glue. In the aTAM, a tile set may consist of an infinite number of copies of each tile are assumed to be available during the self-assembly process in the aTAM. Self-assembly starts by designing a seed tile and placing it at the origin. Then, a tile can come in and bind to the seed-containing assembly if it binds with total strength at least a certain experimenter-chosen, integer value called the temperature that is usually 1 or 2. Self-assembly proceeds as tiles come in and bind one-at-a-time in an asynchronous and non-deterministic fashion.

Tile sets are designed to work at a certain temperature value. For instance, a tile set that self-assembles correctly at temperature-2 will probably not self-assemble correctly at temperature-1. However, if a tile set works correctly at temperature-1, then it can be easily modified to work correctly at temperature-2 (or higher). In what follows, we will refer to a “temperature-2” tile set as a tile set that self-assembles correctly only if the temperature is 2 and a “temperature-1” tile set as a tile set that self-assembles correctly if the temperature is 1.

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Temperature-2 tile sets are able to self-assemble in computationally and geometrically interesting ways, in the sense of Turing universality [19] and the efficient self-assembly of $N \times N$ squares [1,14] and algorithmically-specified shapes [15]. After all, temperature-2 tile sets give the tile set designer more control over the order in which tiles bind to the seed-containing assembly.

While it is not known whether the results cited in the previous paragraph hold for temperature-1 tile sets, the general problem of characterizing the power of non-cooperative tile self-assembly is important from both a theoretical and practical standpoint. This is because when cooperative self-assembly is implemented in the laboratory [2,11,15,16,20], erroneous non-cooperative binding events may occur, leading to the production of invalid final structures. Of course, the obvious way to minimize such erroneous non-cooperative binding events is for experimenters to always implement systems that work in non-cooperative self-assembly because temperature-1 tile sets will work at temperature-1 or temperature-2. Yet, how capable is non-cooperative self-assembly, in general, or even in certain cases? At the time of this writing, no such general characterization of the power of non-cooperative self-assembly exists, but there are numerous results that show the apparent weakness of specific classes of temperature-1 tile self-assembly [5,10,12,13].

Although these results highlight the weakness of certain types of temperature-1 tile self-assembly, if 3D (unit cube) tiles are allowed to be placed in just-barely-three-dimensional Cartesian space (where tiles may be placed in just the $z=0$ and $z=1$ planes), then temperature-1 self-assembly is nearly as powerful as its two-dimensional cooperative counterpart. For example, like 2D temperature-2 tile self-assembly, just-barely 3D temperature-1 tile self-assembly is capable of simulating Turing machines [4] and the efficient self-assembly of squares [4, 6] and algorithmically-specified shapes [7].

Furthermore, Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés [3] studied the efficient self-assembly of $k \times N$ rectangles, where $k < \frac{\log N}{\log \log N}$ at temperature-2 in 2D. They proved that the size of the smallest set of tiles that uniquely self-assemble into (i.e., the tile complexity of) a thin $k \times N$ rectangle is $O\left( N^{\frac{k}{3}} + k \right)$ and $\Omega\left( \frac{N^{\frac{k}{3}}}{k} \right)$ at temperature-2. Their lower bound actually applies to all tile sets (temperature-1, temperature-2, etc.) but their upper bound construction requires temperature-2 to work correctly. It is not clear whether their upper bound holds for temperature-1 tile self-assembly in 2D and there is no prior work related to the self-assembly of thin rectangles in just-barely 3D temperature-1 tile self-assembly. Therefore, in this paper, we study the self-assembly of thin rectangles in just-barely 3D temperature-1 tile self-assembly.

1.1 Main results of this paper

The main results of this paper are bounds on the tile complexity of, or an example of a non-trivial form of computation that can be performed inside, just-barely 3D thin rectangles at temperature-1. Intuitively, a just-barely 3D thin rectangle is like having at most two 2D thin rectangles stacked up one on top of the other. We prove four main results: the first two negative and the last two positive. Our first main result gives an asymptotic lower bound on the tile complexity of a just-barely 3D thin rectangle at temperature-1.

**Theorem 1.** The tile complexity of a just-barely 3D $k \times N$ rectangle for temperature-1 tile sets is $\Omega\left( N^{\frac{k}{3}} \right)$.

In Theorem 1 we do not require unique self-assembly of a final assembly. If we add this constraint, then we get a better lower bound:

**Theorem 2.** The tile complexity of a just-barely 3D $k \times N$ rectangle for temperature-1 tile sets that uniquely produce a final assembly is $\Omega\left( N^{\frac{k}{3}} \right)$.

Theorems 1 and 2 are more interesting when paired with our first positive result in which we give a construction for the efficient self-assembly (nearly the cube of the lower bound from Theorem 2) of a just-barely 3D thin rectangle at temperature-1.

**Theorem 3.** The tile complexity of a just-barely 3D $k \times N$ thin rectangle for temperature-1 tile sets is $O\left( N^{\frac{k}{3}} \right)$. Moreover, the tile set we built to prove this upper bound produces a unique assembly.
While Theorems 1, 2 and 3 are all bounds on the tile complexity of a just-barely 3D thin rectangle at temperature-1, our last main result is an example of a type of non-trivial computation that can be performed by self-assembly inside the bounds of a just-barely 3D thin rectangle. We define a just-barely 3D shape \( L(h, x, w, s) \) that is essentially a thin rectangle of constant height. More precisely, this shape is an approximate (thin) rectangle with height \( h \in \mathbb{Z}^+ \) and width proportional to the number \( n \) of bits in the bit string \( x \). Furthermore, this shape geometrically encodes the bits in \( x \) using one-tile-high bit bumps that protrude from the north edge of the rectangle. Each bit is encoded by a line of tiles (the “bump”) of width \( w \) in the plane \( z = 0 \) (resp., \( z = 1 \)) if the corresponding bit value is 0 (resp., 1), with an additional spacing of \( s \) empty locations on each side of the bump. Therefore, each bit occupies \( w + 2s \) positions in a horizontal line.

The following result follows from an optimal encoding construction inside a just-barely 3D thin rectangle.

**Theorem 4.** Let \( x \in \{0, 1\}^n \). There exists a temperature-1 tile set \( T_x \), such that, \( |T_x| = O\left(\frac{n}{\log n}\right) \) and \( T_x \) uniquely self-assembles into a final assembly that places tiles on, and only on, points in the shape \( L(5, x, 2, 1) \).

### 1.2 Comparison with related work

Our first two main results, Theorems 1 and 2, are most closely related to the following result.

**Theorem** (Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés in [3]). The tile complexity of a 2D \( k \times N \) rectangle (for temperature-\( \tau \) tile sets) is \( \Omega\left(\frac{N^{1/k}}{k}\right) \).

Technically, Theorems 1 and 2 are new results. However, a straightforward generalization of the previous result by Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés decreases to \( \Omega\left(\frac{N^{1/k}}{k^2}\right) \), for just-barely 3D rectangles, upon which Theorem 1 asymptotically improves, for temperature-1 tile sets. Theorem 2 is a further asymptotic improvement upon Theorem 1 for temperature-1 tile sets that are required to uniquely produce a final assembly.

Our third main result, Theorem 3, is very closely related to the following result.

**Theorem** (Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés in [3]). The tile complexity of a 2D \( k \times N \) thin rectangle (for temperature-\( \tau \) tile sets) is \( O\left(N^{\frac{1}{k} + k}\right) \).

The proof of Theorem 3 is inspired by, but substantially different from, the construction in the proof of the previous result by Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés. Our construction, like theirs, uses a counter whose base depends on the dimensions of the target rectangle but ours, unlike theirs, encodes the digits of the counter geometrically.

Finally, our fourth main result, Theorem 4, is very closely related to and asymptotically improves upon, with respect to the height of the unique final assembly in, the following result.

**Theorem** (Furcy, Micka and Summers [6]). For a bit string \( x \in \{0, 1\}^n \), there exists a temperature-1 tile set \( T_x \), such that, \( |T_x| = O\left(\frac{n}{\log n}\right) \) and \( T_x \) uniquely self-assembles into a final assembly that places tiles on, and only on, points in the shape \( L(O(\log n), x, 2, 1) \).

The difference between the previous result and Theorem 4 is that the “\( O(\log n) \)” in the former is replaced by “5” in the latter. Thus, all of our main results are closely related to and in some cases, namely Theorems 1, 2 and 4, are asymptotic improvements upon existing results.

The rest of the paper is organized as follows. In Section 2, we define notation used throughout the paper. In Section 3, we prove Theorems 1 and 2. In Section 4, we prove Theorem 3. In Section 5, we prove Theorem 4. In Section 6, we briefly discuss future work related to our results.
2 Preliminaries

In this section, we briefly sketch a 3D version of Winfree’s abstract Tile Assembly Model, give our notation for figures and gadgets and review the conditional determinism method of Lutz and Shutters[9]. Going forward, all logarithms in this paper are base-2.

2.1 3D abstract Tile Assembly Model

Fix an alphabet $\Sigma$. $\Sigma^*$ is the set of finite, $\Sigma^+$ is the set of finite, positive integers, and nonnegative integers, respectively. Let $d \in \{2, 3\}$.

A grid graph is an undirected graph $G = (V, E)$, where $V \subset \mathbb{Z}^d$, such that, for all $\{\vec{a}, \vec{b}\} \in E$, $\vec{a} - \vec{b}$ is a $d$-dimensional unit vector. The full grid graph of $V$ is the undirected graph $G^f_V = (V, E)$, such that, for all $\vec{x}, \vec{y} \in V$, $\{\vec{x}, \vec{y}\} \in E \iff ||\vec{x} - \vec{y}|| = 1$, i.e., if and only if $\vec{x}$ and $\vec{y}$ are adjacent in the $d$-dimensional integer Cartesian space.

A $d$-dimensional tile type is a tuple $t \in (\Sigma^* \times \mathbb{N})^d$, e.g., a unit square (cube), with four (six) sides, listed in some standardized order, and each side having a glue $g \in \Sigma^* \times \mathbb{N}$ consisting of a finite string label and a nonnegative integer strength. We call a $d$-dimensional tile type merely a tile type when $d$ is clear from the context.

We assume a finite set of tile types, but an infinite number of copies of each tile type, each copy referred to as a tile. A tile set is a set of tile types and is usually denoted as $T$.

A configuration is a (possibly empty) arrangement of tiles on the integer lattice $\mathbb{Z}^d$, i.e., a partial function $\alpha : \mathbb{Z}^d \rightarrow T$. Two adjacent tiles in a configuration bind, interact, or are attached, if the glues on their abutting sides are equal (in both label and strength) and have positive strength. Each configuration $\alpha$ induces a binding graph $G^b_\alpha$, a grid graph whose vertices are positions occupied by tiles, according to $\alpha$, with an edge between two vertices if the tiles at those vertices bind. For two non-overlapping configurations $\alpha$ and $\beta$, $\alpha \cup \beta$ is defined as the unique configuration $\gamma$ satisfying, for all $\vec{x} \in \text{dom } \alpha$, $\gamma(\vec{x}) = \alpha(\vec{x})$, for all $\vec{x} \in \text{dom } \beta$, $\gamma(\vec{x}) = \beta(\vec{x})$, and $\gamma(\vec{x})$ is undefined at any point $\vec{x} \in \mathbb{Z}^d \setminus (\text{dom } \alpha \cup \text{dom } \beta)$.

An assembly is a connected, non-empty configuration, i.e., a partial function $\alpha : \mathbb{Z}^d \rightarrow T$ such that $G^b_{\text{dom } \alpha}$ is connected and dom $\alpha \neq \emptyset$. Given $\tau \in \mathbb{Z}^+$, $\alpha$ is $\tau$-stable if every cut-set of $G^b_{\alpha}$ has weight at least $\tau$, where the weight of an edge is the strength of the glue it represents.[1] When $\tau$ is clear from context, we say $\alpha$ is stable. Given two assemblies $\alpha, \beta$, we say $\alpha$ is a subassembly of $\beta$, and we write $\alpha \subseteq \beta$, if dom $\alpha \subseteq$ dom $\beta$ and, for all points $\vec{p} \in$ dom $\alpha$, $\alpha(\vec{p}) = \beta(\vec{p})$.

A $d$-dimensional tile assembly system (TAS) is a triple $T = (T, \sigma, \tau)$, where $T$ is a tile set, $\sigma : \mathbb{Z}^d \rightarrow\rightarrow T$ is the finite, $\tau$-stable, seed assembly, and $\tau \in \mathbb{Z}^+$ is the temperature.

Given two $\tau$-stable assemblies $\alpha, \beta$, we write $\alpha \rightarrow\rightarrow\rightarrow _\tau \beta$ if $\alpha \subseteq \beta$ and $|\text{dom } \beta \setminus \text{dom } \alpha| = 1$. In this case we say $\alpha$ $T$-produces $\beta$ in one step. If $\alpha \rightarrow\rightarrow\rightarrow _\tau \beta$, dom $\beta \setminus$ dom $\alpha = \{ \vec{p} \}$, and $t = \beta(\vec{p})$, we write $\beta = \alpha + (\vec{p} \rightarrow t)$. The $T$-frontier of $\alpha$ is the set $\partial^T \alpha = \bigcup_{\alpha \rightarrow\rightarrow\rightarrow _\tau \beta} (\text{dom } \beta \setminus \text{dom } \alpha)$, i.e., the set of empty locations at which a tile could stably attach to $\alpha$. The $T$-frontier of $\alpha$, denoted $\partial^T \alpha$, is the subset of $\partial^T \alpha$ defined as $\{ \vec{p} \in \partial^T \alpha \mid \alpha \rightarrow\rightarrow\rightarrow _\tau \beta$ and $\beta(\vec{p}) = t \}$.

Let $A^\tau_T$ denote the set of all assemblies of tiles from $\mathbb{T}_T$, and let $A^\tau_{T,\infty}$ denote the set of finite assemblies of tiles from $\mathbb{T}$, $\{ \alpha \in A^\tau_{T,\infty} \mid \text{for all } 1 \leq i < k, \alpha_{i-1} \rightarrow\rightarrow\rightarrow _\tau \alpha_i \}$. The result of an assembly sequence $\vec{\alpha}$, denoted as res($\vec{\alpha}$), is the unique limiting assembly (for a finite sequence, this is the final assembly in the sequence).

We write $\alpha \rightarrow\rightarrow\rightarrow _\tau \beta$, and we say $\alpha$ $T$-produces $\beta$ (in 0 or more steps), if there is a $T$-assembly sequence $\alpha_0, \alpha_1, \ldots$ of length $k = |\text{dom } \beta \setminus \text{dom } \alpha| + 1$ such that (1) $\alpha = \alpha_0$, (2) dom $\beta = \bigcup_{0 \leq i < k} \text{dom } \alpha_i$, and (3) for all $0 \leq i < k$, $\alpha_i \subseteq \beta$. If $k$ is finite then it is routine to verify that $\beta = \alpha_{k-1}$.

We say $\alpha$ is $T$-producible if $\sigma \rightarrow\rightarrow\rightarrow _\tau \alpha$, and we write $A(\mathbb{T})$ to denote the set of $T$-producible assemblies.

An assembly $\alpha$ is $T$-terminal if $\alpha$ is $\tau$-stable and $\partial^T \alpha = \emptyset$. We write $A(\mathbb{T}) \subseteq A(\mathbb{T})$ to denote the set of $T$-terminal assemblies. If $|A(\mathbb{T})| = 1$ then $\mathbb{T}$ is said to be directed.

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[1] A cut-set is a subset of edges in a graph which, when removed from the graph, produces two or more disconnected subgraphs. The weight of a cut-set is the sum of the weights of all of the edges in the cut-set.
In general, a d-dimensional shape is a set \( X \subseteq \mathbb{Z}^d \). We say that a TAS \( T \) self-assembles \( X \) if, for all \( \alpha \in \mathcal{A}[:|T|], \) \( \operatorname{dom} \alpha = X \), i.e., if every terminal assembly produced by \( T \) places a tile on every point in \( X \) and does not place any tiles on points in \( \mathbb{Z}^d \setminus X \). We say that a TAS \( T \) uniquely self-assembles \( X \) if \( \mathcal{A}[:|T|] = \{ \alpha \} \) and \( \operatorname{dom} \alpha = X \).

In the spirit of [13], we define the tile complexity of a shape \( X \) at temperature \( \tau \), denoted by \( K_{\mathbb{Z}A}(X) \), as the minimum number of distinct tile types of any TAS in which it self-assembles, i.e., \( K_{\mathbb{Z}A}(X) = \min \{ n \mid T = (T, \sigma, \tau), |T| = n \text{ and } X \text{ self-assembles in } T \} \). The directed tile complexity of a shape \( X \) at temperature \( \tau \), denoted by \( K_{\mathbb{Z}A}^d(X) \), is the minimum number of distinct tile types of any TAS in which it uniquely self-assembles, i.e., \( K_{\mathbb{Z}A}^d(X) = \min \{ n \mid T = (T, \sigma, \tau), |T| = n \text{ and } X \text{ uniquely self-assembles in } T \} \).

This paper concerns the self-assembly of just-barely 3D rectangles. Let \( k, N \in \mathbb{N} \). We say that \( R^2_{k,N} \) is a 2D \( k \times N \) rectangle if \( R^2_{k,N} = \{0, 1, \ldots, N - 1\} \times \{0, 1, \ldots, k - 1\} \). We say that \( R^3_{k,N} \subseteq \mathbb{Z}^3 \) is a 3D \( k \times N \) rectangle if \( \{0, 1, \ldots, N - 1\} \times \{0, 1, \ldots, k - 1\} \times \{0\} \subseteq R^3_{k,N} \subseteq \{0, 1, \ldots, N - 1\} \times \{0, 1, \ldots, k - 1\} \times \{0, 1\} \).

If \( k < \frac{\log N}{\log \log N - \log \log \log N} \), then we say that \( R^3_{k,N} \) is thin.

### 2.2 Notation for figures and gadgets

Following standard presentation conventions for “just-barely” 3D tile self-assembly, we use big squares to represent tiles placed in the \( z = 0 \) plane and small squares to represent tiles placed in the \( z = 1 \) plane. A glue between a \( z = 0 \) tile and \( z = 1 \) tile is denoted as a small black disk. Glues between \( z = 0 \) tiles are denoted as thick lines. Glues between \( z = 1 \) tiles are denoted as thin lines.

In the context of the construction of a tile set, a gadget, referred to by a name like \textbf{Gadget}, is a group of tiles that perform a specific task as they self-assemble. All gadgets are depicted in a corresponding figure, where the input glue is explicitly specified by an arrow, output glues are inferred and glues internal to the gadget are configured to ensure unique self-assembly within the gadget. We say that a gadget is general if its input and output glues are undefined. If \textbf{Gadget} is a general gadget, then we use the notation \textbf{Gadget}(a,b) to represent the creation of the specific gadget, or simply gadget, referred to as \textbf{Gadget}, with input glue label \( a \) and output glue label \( b \) (all positive glue strengths are 1). If a gadget has two possible output glues, then we will use the notation \textbf{Gadget}(a,b,c) to denote the specific version of \textbf{Gadget}, where \( a \) is the input glue and \( b \) and \( c \) are the two possible output glues, listed in the order north, east, south and west, with all of the \( z = 0 \) output glues listed before the \( z = 1 \) output glues. If a gadget has only one output glue (and no input glue), like a gadget that contains the seed, or if a gadget has only one input glue (and no output glue), then we will use the notation \textbf{Gadget}(a). We use the notation \( \langle \cdot \rangle \) to denote some standard encoding of the concatenation of a list of symbols.

### 2.3 Conditional determinism

We use the conditional determinism method of Lutz and Shutters [14] to prove that our constructions (see Sections 4 and 5) are directed. Conditional determinism is weaker than the local determinism method of Soloveichik and Winfree [15] but strong enough to imply unique production. Although Lutz and Shutters define conditional determinism for a 2D TAS, the following holds in 3D as well.

**Theorem.** (Shutters and Lutz [14]) If \( T \) is a conditionally deterministic TAS, then \( T \) is directed.

We merely give a brief, intuitive review of conditional determinism (see [9] for a thorough discussion). Let \( T = (T, \sigma, \tau) \) be a TAS and \( \vec{a} \) be an assembly sequence of \( T \) with result \( \alpha \). Conditional determinism relies on the notion of dependence (of one position on another position in an assembly). For a position \( \vec{m} \in \operatorname{dom}(\alpha) \) and some unit vector \( \vec{u} \in \{(0, 1, 0), (1, 0, 0), (0, 1, 0), (-1, 0, 0), (0, 0, 1), (0, 0, -1)\} \), we say that \( \vec{m} + \vec{a} \) depends on \( \vec{m} \), or \( \vec{m} + \vec{u} \) is a dependent of \( \vec{m} \), if, in every assembly sequence in \( T \), a tile is placed at \( \vec{m} \) before a tile is placed at \( \vec{m} + \vec{u} \). Intuitively, \( \vec{a} \) is conditionally deterministic if the following three properties are satisfied: (1) every tile placed by \( \vec{a} \) binds with exactly temperature \( \tau \), (2) for every position \( \vec{m} \in \operatorname{dom} \alpha \), if \( \alpha(\vec{m}) \) and the union of its immediate output and dependent neighbors (adjacent positions
that depend on \( \vec{m} \) are removed from \( \alpha \) to get \( \alpha' \), then \( \alpha(\vec{m}) \) is the only tile that may bind at position \( \vec{m} \) in \( \alpha' \), and (3) \( \alpha \) is terminal. A TAS is conditionally deterministic if it exhibits a conditionally deterministic assembly sequence.

3 Lower bounds

In this section, we prove lower bounds on \( K_{SA}^3 \left( R_{k,N}^3 \right) \) (Theorem 1) and \( K_{USA}^1 \left( R_{k,N}^3 \right) \) (Theorem 2). For the sake of clarity of presentation, we prove lower bounds for \( K_{SA}^3 \left( R_{k,N}^3 \right) ) and \( K_{USA}^1 \left( R_{k,N}^3 \right) \) and note that our proof techniques generalize to 3D, giving corresponding lower bounds for \( K_{SA}^1 \left( R_{k,N}^3 \right) ) and \( K_{USA}^1 \left( R_{k,N}^3 \right) \).

Throughout this section, we will denote \( R_{k,N}^2 \) as simply \( R_{k,N} \).

3.1 A restricted Window Movie Lemma

To prove our main lower bounds, we will use a restricted version of the standard Window Movie Lemma (WML). Therefore, in this subsection, we review notation and give the statement of the restricted version of the WML.

A window \( w \) is a set of edges forming a cut-set of the full grid graph of \( \mathbb{Z}^d \). Given a window \( w \) and an assembly \( \alpha \), a window that intersects \( \alpha \) is a partitioning of \( \alpha \) into two configurations (i.e., after being split into two parts, each part may or may not be disconnected). In this case we say that the window \( w \) cuts the assembly \( \alpha \) into two configurations \( \alpha_L \) and \( \alpha_R \), where \( \alpha = \alpha_L \cup \alpha_R \). Given a window \( w \), its translation by a vector \( \vec{t} \), written \( w + \vec{t} \) is simply the translation of each one of \( w \)'s elements (edges) by \( \vec{t} \).

For a window \( w \) and an assembly sequence \( \vec{\alpha} \), we define a glue window movie \( M \) to be the order of placement, position and glue type for each glue that appears along the window \( w \) in \( \vec{\alpha} \). Given an assembly sequence \( \vec{\alpha} \) and a window \( w \), the associated glue window movie is the maximal sequence \( M_{\vec{\alpha},w} = (v_1, g_1), (v_2, g_2), \ldots \) of pairs of grid graph vertices \( v_i \) and glues \( g_i \), given by the order of appearance of the glues along window \( w \) in the assembly sequence \( \vec{\alpha} \). Furthermore, if \( k \) glues appear along \( w \) at the same instant (this happens upon placement of a tile which has multiple sides touching \( w \)) then these \( k \) glues appear contiguously and are listed in lexicographical order of the unit vectors describing their orientation in \( M_{\vec{\alpha},w} \). See Figure 1 of [12] for an example of a window, an assembly sequence and the induced glue window movie.

We will use the following restricted version of the Window Movie Lemma, where we assume \( \vec{\alpha} \) and \( \vec{\beta} \) are assembly sequences in \( \mathcal{T} = (T, \sigma, 1) \) that place tiles along simple paths \( s \) and \( s' \), respectively and \( R(M_{\vec{\alpha},w}) \) is the restricted bond-forming submovie of \( M \), which consists of only those steps of \( M \) that place glues that eventually form positive-strength bonds along \( s \).

**Lemma 1** (Restricted Window Movie Lemma). Let \( \vec{\alpha} = (\alpha_i \mid 0 \leq i < l) \) and \( \vec{\beta} = (\beta_i \mid 0 \leq i < m) \), with \( l, m \in \mathbb{Z}^+ \cup \{ \infty \} \), be assembly sequences in \( \mathcal{T} = (T, \sigma, 1) \) with results \( \alpha \) and \( \beta \), respectively, such that, \( \vec{\alpha} \) and \( \vec{\beta} \) place tiles along simple paths \( s \) and \( s' \), respectively. Let \( w \) be a window that partitions \( \alpha \) into two configurations \( \alpha_L \) and \( \alpha_R \), and \( w' = w + \vec{t} \) be a translation of \( w \) that partitions \( \beta \) into two configurations \( \beta_L \) and \( \beta_R \). Assume that \( \alpha_L \), \( \beta_L \) are the sub-configurations of \( \alpha \) and \( \beta \) containing the seed tiles of \( \alpha \) and \( \beta \), respectively. If \( R(M_{\vec{\alpha},w}) = R \left( M_{\vec{\beta},w'} - \vec{t} \right) \), then the following two assemblies are producible: (1) \( \alpha_L (\beta_R - \vec{t}) = \alpha_L \cup (\beta_R - \vec{t}) \) and (2) \( \beta_L (\alpha_R + \vec{t}) = \beta_L \cup (\alpha_R + \vec{t}) \).

The proof of Lemma 1 is identical to that of the standard WML and therefore is omitted. The proof is identical because \( \vec{\alpha} \left( \vec{\beta} \right) \) follows \( s \left( s' \right) \) and \( \tau = 1 \), so glues that do not follow \( s \left( s' \right) \) are not necessary for the self-assembly of \( \alpha \left( \beta \right) \). Note that Lemma 1 just like the standard WML, generalizes to 3D. We now turn our attention to counting the number of restricted bond-forming submovies induced by an assembly sequence that places tiles along a simple path.
3.2 Counting procedure

In this subsection, we develop a counting procedure that we will use to obtain an upper bound on the number of distinct restricted bond-forming submovies induced by an assembly sequence that places tiles along a simple path.

Let $T = (T, \sigma, 1)$ be a singly-seeded TAS. Assume that there exists $\alpha \in \mathcal{A}[T]$, such that, dom $\alpha = R_{k,N}$. Since $\tau = 1$, $G^b_{\alpha}$ contains a simple path $s$ from the location of $\sigma$ to any location in an extreme (i.e., leftmost or rightmost) column of $R_{k,N}$. Let $\tilde{\alpha}$ denote any (simple) assembly sequence that follows such a path. Since we are not currently assuming that $T$ is directed, there could be more than one $\tilde{\alpha}$ for a given $s$.

Index the columns of $R_{k,N}$ from 1 (left) to $N$ (right). Assume $c_\sigma$ is the index of the column in which the seed is contained and let $c_0$ and $c_1$ be column indices of consecutive columns of $R_{k,N}$, such that, $|c_\sigma - c_0| < |c_\sigma - c_1|$ and $s$ crosses between $c_0$ and $c_1$. Notice that $s$ crosses between columns $c_0$ and $c_1$ through $e$ crossing edges in $G^b_{\alpha}$, where $1 \leq e \leq k$ and $e$ is odd, visiting a total of $2e$ endpoints. The endpoint of a crossing edge in column $c_0$ ($c_1$) is its near (far) endpoint. A crossing edge points away from (towards) the seed if its near endpoint is visited first (second).

Observe that the first and last crossing edges visited by $s$ must point away from the seed but each crossing edge that points away from the seed (except the last crossing edge) is immediately followed by a corresponding crossing edge that points towards the seed, when skipping the part of $s$ that connects them without going through another crossing edge in between them. Assume that the rows of $R_{k,N}$ are assigned an index from 1 (top) to $k$ (bottom). Let $E \subseteq \{1, \ldots, k\}$ be such that $|E| = e$ and $f \in E$ and $l \in E$ be the row indices of the first and last crossing edges visited, respectively. We define a near (far) crossing pairing over $E$ starting at $f \in E$ (ending at $l \in E$) as a set of $p = \frac{2e}{2}$ non-overlapping pairs of elements in $E \setminus \{f\}$ $(E \setminus \{l\})$, where each pair contains (the row indices of) one crossing edge pointing away from the seed and its corresponding crossing edge pointing towards the seed. See Figure 1 for examples of the previous definitions.

For counting purposes pertaining to a forthcoming argument, we establish an injective mapping from near crossing pairings over $E$ to strings of balanced parentheses of length $e - 1$.

**Lemma 2.** There exists an injective function from the set of all near crossing pairings over $E$ starting at $f$ into the set of all strings of $2p$ balanced parentheses.

**Proof.** Given a near crossing pairing $P$ with $p$ pairs, build a string $x$ with $2p$ characters indexed from 1 to $2p$ going from left to right, as follows. For each element $\{a,b\}$ of $P$, with $a < b$ and assuming $a$ is the $i$-th lowest row index and $b$ is the $j$-th lowest row index in $E \setminus \{f\}$, place a left parenthesis at index $i$ and a right parenthesis at index $j$.

The resulting string $x$ contains exactly $p$ pairs of parentheses. Furthermore, all of the parentheses in $x$ are balanced because each opening parenthesis appears to the left of its closing parenthesis (thanks to the indexing used in the string construction algorithm just described) and, for any two pairs of parentheses in the string, it must be the case that either 1) they do not overlap (i.e., the closing parenthesis of the leftmost pair is positioned to the left of the opening parenthesis of the rightmost pair) or 2) one pair is nested inside the other (i.e., the interval defined by the indices of the nested pair is included in the interval defined by the indices of the outer pair). The other case is impossible, that is, when the two pairs $\{a,b\}$ and $\{c,d\}$ are such that $a < c < b < d$ because it would be impossible for any path crossing consecutive columns according to $P$ to be simple. Consider any simple path $\pi_{\{a,b\}}$ that links crossing edges $a$ and $b$ without going through another crossing edge in between them. Since $P$ is a near crossing pairing, $\pi_{\{a,b\}}$ is fully contained in the half-plane $H_0$ on the near side of $c_0$ toward the seed. This path partitions $H_0$ into two spaces. Since the crossing edges $c$ and $d$ belong to different components of this partition, any simple path linking these two crossing edges must cross $\pi_{\{a,b\}}$. Therefore, $s$, crossing between $c_0$ and $c_1$, could not have been simple.

Finally, note that two different near crossing pairings $P_1$ and $P_2$ over $E$ starting at $f$ will map to two different strings of balanced parentheses, so the mapping is injective. \hfill $\square$

**Corollary 1.** There exists an injective function from the set of all far crossing pairings over $E$ ending at $l$ into the set of all strings of $2p$ balanced parentheses.
The following is a systematic procedure for upper bounding the number of ways to select and order the $2e$ endpoints of the $e$ crossing edges between an arbitrary pair of consecutive columns $c_0$ and $c_1$ (see Figure 1a). Obviously, the number of ways to do this is less than or equal to $\binom{k}{e} (2e)!$. We will use crossing pairings and Catalan numbers to reduce this upper bound.

1. Choose the set $E$ of row indices of the $e$ crossing edges, out of $k$ possible edges between consecutive columns. There are $\binom{k}{e}$ ways to do this.

2. One of the crossing edges must be first, so, choose the first crossing edge $f$. There are $e$ ways to do this.

3. One of the crossing edges must be last, so, choose the last crossing edge $l$. There are $e$ ways to do this.

The three previous steps are depicted in Figure 1b. We purposely allow choosing $l = f$ because our intention is to upper bound the number of ways to select and order the endpoints of the crossing edges. Moreover, $l = f$ when $e = 1$.

Denote as $C_p$ the $p^{th}$ Catalan number (indexed starting at 0).

4. For a given pair of consecutive columns, in which $f$ is visited first, $s$ induces a near crossing pairing over $E$ starting at $f$, where the elements of each pair are row indices of near endpoints of crossing edges, including $l$, but not $f$. By Lemma 2, it suffices to count the number of ways to choose a string of $2p$ balanced parentheses. Therefore, choose a string $x_0$ of $2p$ balanced parentheses, where $x_0[i]$ corresponds to the crossing edge in $E$ with the $i$-th lowest row index, excluding $f$. There are $C_p$ ways to do this.

5. For a given pair of consecutive columns in which $l$ is visited last, $s$ induces a far crossing pairing over $E$ ending at $l$, where the elements of each pair are row indices of far endpoints of crossing edges, including $f$, but not $l$. By Corollary 1, it suffices to count the number of ways to choose a string of $2p$ balanced parentheses. Therefore, choose a string $x_1$ of $2p$ balanced parentheses, where $x_1[i]$ corresponds to the crossing edge in $E$ with the $i$-th lowest row index, excluding $l$. There are $C_p$ ways to do this.

The two previous steps are depicted in Figure 1c. At this point, we have chosen the locations and connectivity pattern of all the crossing edges. We now show that there is at most one way in which both
endpoints of every crossing edge may be visited by \( s \), subject to the constraints imposed by the previous steps.

6. Let \( I_j(r) \) be the index \( i \), such that \( x_j[i] \) corresponds to the crossing edge with row index \( r \). The following greedy algorithm attempts to build a path \( \pi \) of locations that (1) starts at the near endpoint of the first crossing edge, (2) ends at the far endpoint of the last crossing edge and (3) visits only the endpoints of the crossing edges while following the balanced parenthesis pairings of both \( x_0 \) and \( x_1 \).

Initialize \( \pi = ((c_0, f), (c_1, f)) \) to be a sequence of locations, \( j = 1 \) and \( r = f \), where \( r \) stands for “row number” and \( j \) stands for the current side, near (0) or far (1).

\[
\text{while } r \neq l \text{ do } \\
\quad \text{Let } r' \text{ be the unique row index of the crossing edge, such that, } I_j(r) \text{ and } I_j(r') \text{ are paired.} \\
\quad \text{Set } r = r'. \\
\quad \text{Append } (c_j, r) \text{ to } \pi. \\
\quad \text{Set } j = (j + 1) \mod 2. \\
\quad \text{Append } (c_j, r) \text{ to } \pi. \\
\]

First, note that no endpoint can be visited more than once, so the algorithm always terminates. Second, note that, when the algorithm terminates, either \(|\pi| = 2e\) (see Figure 1(d)), or \(|\pi| < 2e\) (see Figure 2). However, regardless of its length, \( \pi \) is the unique sequence of endpoints of crossing edges that can be visited by any simple path starting at \((c_0, f)\), ending at \((c_0, l)\) and following the balanced parenthesis pairings of both \( x_0 \) and \( x_1 \). The uniqueness of \( \pi \) follows from the uniqueness of \( r' \), given \( r \), based on the balanced parenthesis pairings of both \( x_0 \) and \( x_1 \).

\[
\begin{array}{cccccccccccc}
& & & & & & & & & & & & \\
1 & l & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & f \\
& c_1 & & & & & & & & & & & \\
& c_0 & & & & & & & & & & & \\
\end{array}
\]

Figure 2: A “bad” sample run of the counting procedure. Here, \( x_0 = (())() \) and \( x_1 = ()()() \). With \( f = 12 \), \( l = 2 \) and \( E = \{2, 4, 5, 6, 8, 10, 12\} \), there is no valid \( \pi \) (crossing edges 4 and 5 are skipped, assuming the pairs of parentheses are faithfully followed), so the algorithm terminates with \(|\pi| = 10 < 2e = 14\).

By the above counting procedure, there are at most \( \binom{k}{e} (e \cdot C_p)^2 \cdot 1 = \binom{k}{e} \left( \frac{e}{p+1} \binom{2p}{p} \right)^2 \cdot 1 \) ways to select and order the endpoints of the crossing edges between an arbitrary pair of consecutive columns \( c_0 \) and \( c_1 \) as they are visited by a simple path.

### 3.3 Lower bound for undirected self-assembly

To prove a lower bound on \( K_{3,A}^1(R_{k,N}) \), we turn our attention to upper bounding the number of restricted bond-forming submovies of the form \( \mathcal{R}(M_{\alpha,w}) \).

**Lemma 3.** If \( w \) is any window that cuts \( R_{k,N} \) into two smaller rectangles between consecutive columns, then the number of restricted bond-forming submovies of the form \( \mathcal{R}(M_{\alpha,w}) \) is less than or equal to \(|G|^k \cdot 2^{3k^2+2} \cdot k \), where \( G \) is the set of all glues of (the tile types in) \( T \).

**Proof.** Let \( e \) be an odd number such that \( 1 \leq e \leq k \) and \( \mathcal{R}(M_{\alpha,w}) = (\vec{v}_1, g_1), \ldots, (\vec{v}_{2e}, g_{2e}) \) be a restricted bond-forming submovie.

Since \( \alpha \) follows a simple path, \( g_{2i-1} = g_{2i} \) for \( i = 1, \ldots, e \). This means that we only need to assign \( e \) glues, with \(|G|\) choices for each glue. So, the number of ways to assign glues in \( \mathcal{R}(M_{\alpha,w}) \) is less than or equal to \(|G|^e\).
Since $\tilde{\alpha}$ follows a simple path, each location in $R(M_{\tilde{\alpha},v})$ corresponds to an endpoint of a crossing edge that crosses $v$. So, the number of ways to assign locations in $R(M_{\tilde{\alpha},v})$ is less than or equal to the number of ways to select and order the endpoints of $e$ crossing edges that cross $v$ via $\tilde{\alpha}$. By the above counting procedure, the number of ways to select and order the endpoints of $e$ crossing edges that cross $w$ via $\tilde{\alpha}$ is less than or equal to $\binom{k}{e} \left(\frac{1}{p+1} \left(\frac{2p}{p}\right)^2 \right)$.

Thus, if $m$ is the total number of restricted bond-forming submovies of the form $R(M_{\tilde{\alpha},w})$, then we have:

$$m \leq \sum_{1 \leq e \leq k, e \text{ odd}} \binom{k}{e} \left(\frac{1}{p+1} \left(\frac{2p}{p}\right)^2 \right) |G|^e$$

$$= \sum_{1 \leq e \leq k, e \text{ odd}} \binom{k}{e} \left(\frac{2}{e+1} \left(\frac{e-1}{(e-1)/2}\right)\right)^2 |G|^e$$

$$\leq 2^2 \sum_{1 \leq e \leq k, e \text{ odd}} \binom{k}{e} \left(\frac{e}{e+1} \left(\frac{e-1}{(e-1)/2}\right)\right)^2 |G|^e$$

$$= |G|^k \cdot 2^2 \sum_{1 \leq e \leq k, e \text{ odd}} \binom{k}{e} \left(\frac{e-1}{(e-1)/2}\right)^2$$

$$= |G|^k \cdot 2^{k+2} \sum_{0 \leq e \leq k-1, e \text{ even}} \binom{e}{e/2}^2$$

$$\leq |G|^k \cdot 2^{k+2} \sum_{0 \leq e \leq k-1, e \text{ even}} \binom{k}{e/2}^2$$

$$\leq |G|^k \cdot 2^{k+2} \cdot \sum_{0 \leq e \leq k-1, e \text{ even}} 2^e \leq |G|^k \cdot 2^{3k+2} \cdot k.$$  

$\Box$

We will use Lemma 4 to prove a 2D version of our first main lower bound, which is the following.

Lemma 4. $R_{SA}^1(R_{k,N}) = \Omega \left(N^\pm\right)$.

Note that the structure of the proof of Lemma 4 is similar to that of Theorem 3.1 of [3]. The main difference is that our proof is written in the language of the WML.

Proof. Let $\mathcal{T} = (T, \sigma, 1)$ be a singly-seeded TAS, where $G$ is the set of glues of (the tile types in) $T$ and assume that $R_{k,N}$ self-assembles in $\mathcal{T}$. It suffices to show that $|T| = \Omega \left(N^\pm\right)$. Assume that $\tilde{\alpha}$ is an assembly sequence in $\mathcal{T}$ that follows a longest simple path from $\sigma$ to some location in an extreme column in $R_{k,N}$. Let $\alpha$ be the result of $\tilde{\alpha}$. Note that $\underline{\tilde{\alpha}}$ exists because $\tau = 1$.

According to Lemma 3 if $N > 2 \cdot |G|^k \cdot 2^{3k+2} \cdot k$, then there must exist distinct windows $w_1$, $w_2$ and $w_3$ satisfying $\mathcal{R}(M_{\tilde{\alpha},w_1}) = \mathcal{R}(M_{\tilde{\alpha},w_2}) - \ell_1$ and $\mathcal{R}(M_{\tilde{\alpha},w_3}) = \mathcal{R}(M_{\tilde{\alpha},w_2}) - \ell_2$, where $\ell_1 \neq 0$, $\ell_2 \neq 0$ and $\ell_1 \neq \ell_2$. Without loss of generality, assume that $w_1$ and $w_2$ are on the same side of $\sigma$ and $w_2$ is to the east of $w_1$. Assume that $w_1$ partitions $\alpha$ into $\alpha_L$ and $\alpha_R$ and $w_2$ partitions $\beta = \alpha$ into $\beta_L$ and $\beta_R$. Then, by Lemma 4 $\beta_L(\alpha_R + \ell_1) \in A[T]$. Since $\ell_1 \neq 0$, dom $(\beta_L(\alpha_R + \ell_1)) \backslash R_{k,N} \neq \emptyset$. In other words, $\mathcal{T}$ produces some assembly that places tiles outside of $R_{k,N}$.
Therefore, it must hold that

\[ N \leq 2 \cdot |G|^k \cdot 2^{3k+2} \cdot k, \]

which implies that

\[ |G|^k \geq \frac{N}{2^{3k+3} \cdot k} \]

and thus

\[ |G| \geq \left( \frac{N}{2^{3k+3} \cdot k} \right)^{\frac{1}{k}} \geq \frac{N^{\frac{1}{k}}}{(2^{6k} \cdot 2^k)^{\frac{1}{k}}} = \frac{N^{\frac{1}{k}}}{128}. \]

Finally, note that \(|T| \geq \frac{|G|}{4}\) and it follows that \(|T| = \Omega \left( N^{\frac{1}{k}} \right) \).

\[ \square \]

Our first main result is the following.

**Theorem 1.** \( K^{1}_{SA} \left( R^{1}_{k,N} \right) = \Omega \left( N^{\frac{1}{k}} \right) \).

**Proof.** The proof of Lemma 4 generalizes to 3D. The extra “2” in the denominator of the exponent in “\( N^{\frac{1}{k}} \)” comes from the fact that every column in \( R^{1}_{k,N} \) consists of 2k positions.

In Lemma 4 we do not require unique self-assembly. If we add this constraint, then we get a better upper bound on the number of bond-forming submovies as shown in the next subsection.

### 3.4 Lower bound for directed self-assembly

We will use the following technical result, which assumes a directed TAS, to reduce the upper bound on the number of bond-forming submovies from Lemma 3.

**Lemma 5.** Assume \( T \) is directed. If \( w \) is any window that cuts \( R_{k,N} \) into two smaller rectangles between consecutive columns and \( R \left( M_{\vec{\alpha},w} \right) = (\vec{v}_1, g_1), \ldots, (\vec{v}_{2e}, g_{2e}) \) is a restricted bond-forming submovie, where \( e \) is an odd number satisfying \( 1 \leq e \leq k \), then for all restricted bond-forming submovies \( R \left( M_{\vec{\alpha}',w'} \right) = (\vec{v}'_1, g'_1), \ldots, (\vec{v}'_{2e}, g'_{2e}) \), where \( w' \) is any window that cuts \( R_{k,N} \) into two smaller rectangles between consecutive columns, if \( w' = w + \vec{t} \), for some \( \vec{t} \neq 0 \), \( \vec{v}'_i = \vec{v}_i + \vec{t} \) for \( i = 1, \ldots, 2e \) and \( g_{4i-2} = g'_{4i-2} \), for all \( i = 1, \ldots, \frac{e+1}{2} \), then \( R \left( M_{\vec{\alpha},w} \right) = R \left( M_{\vec{\alpha}',w'} \right) - \vec{t} \).

Since \( \vec{\alpha} \) follows a simple path, it must be the case that \( g_{4i-3} = g'_{4i-3} \iff g_{4i-2} = g'_{4i-2} \), for all \( i = 1, \ldots, \frac{e+1}{2} \). Thus, Lemma 5 basically says that, when counting the number of restricted bond-forming submovies of the form \( R \left( M_{\vec{\alpha},w} \right) \), where \( \vec{\alpha} \) is an assembly sequence in a directed TAS, we only need to consider roughly half of the (at most) \( k \) pairs of matching glues.

**Proof.** For the sake of obtaining a contradiction, assume that \( R \left( M_{\vec{\alpha}',w'} \right) = (\vec{v}'_1, g'_1), \ldots, (\vec{v}'_{2e}, g'_{2e}) \) is a restricted bond-forming submovie with \( w' = w + \vec{t} \), \( \vec{t} \neq 0 \), \( \vec{v}'_i = \vec{v}_i + \vec{t} \) for \( i = 1, \ldots, 2e \), \( g_{4i-2} = g'_{4i-2} \) for all \( i = 1, \ldots, \frac{e+1}{2} \), but \( g_{4i-1} \neq g'_{4i-1} \) for some \( i = 1, \ldots, \frac{e+1}{2} \). Let \( i^* \) be the smallest such value of \( i \).

Let \( \vec{\alpha}^* \) be the assembly resulting from the assembly sequence \( \vec{\alpha}' \), where \( \vec{\alpha}' \) is a sub-assembly sequence of \( \vec{\alpha} \) up to but not including the step in which a tile is placed at the location \( \vec{v}_{4i^*-1} \). Let \( \vec{\alpha}^* \) be the assembly resulting from the assembly sequence \( \vec{\beta}' \), where \( \vec{\beta}' \) is a sub-assembly sequence of \( \vec{\alpha} \) up to but not including the step in which a tile is placed at the location \( \vec{v}_{4i^*-1} \).

Recall that \( w \) is a window that partitions \( \alpha \) into two configurations \( \alpha_L^* \) and \( \alpha_R^* \), and \( w' = w + \vec{t} \) is a translation of \( w \) that partitions \( \beta \) into two configurations \( \beta_L^* \) and \( \beta_R^* \). Assume that \( \alpha_L^* \), \( \beta_L^* \) are the sub-configurations of \( \alpha \) and \( \beta \) containing the seed tiles of \( \alpha \) and \( \beta \), respectively. By the definition of \( i^* \),
we have $\mathcal{R}(M_{\overline{\bar{a}},w}) = \mathcal{R}(M_{\overline{\bar{a}},w'}) - \tilde{v}$. Therefore, Lemma 3 says that the following assembly is producible:

\[
\beta_L^*(\alpha_{\tilde{k}} + \tilde{t}) = \beta_L^* \cup (\alpha_{\tilde{k}} + \tilde{t}).
\]

The tile that $\tilde{a}$ places at $\tilde{v}_{4\tilde{i} - 1}$ can be placed at $\tilde{v}_{4\tilde{i} - 1}$ in the assembly $\beta_L^*(\alpha_{\tilde{k}} + \tilde{t})$. However, by our original assumption, $g_{4\tilde{i} - 1} \neq g_{4\tilde{i} - 1}$, so the tile that $\tilde{a}$ places at $\tilde{v}_{4\tilde{i} - 1}$ must be different than the tile that $\tilde{a}$ places at $\tilde{v}_{4\tilde{i} - 1}$. This contradicts the fact that $\overline{T}$ is directed. □

Using Lemma 6 we get the following (reduced) upper bound on the number of restricted bond-forming submovies, assuming unique self-assembly.

**Lemma 6.** If $w$ is any window that cuts $R_{k,N}$ into two smaller rectangles between consecutive columns, then the number of restricted bond-forming submovies of the form $\mathcal{R}(M_{\overline{\bar{a}},w})$ is less than or equal to $|G|^{\lceil \frac{k}{2} \rceil} \cdot 2^{3k+2} \cdot k$, where $G$ is the set of all glues of (the tile types in) $T$.

**Proof.** Let $e$ be an odd number such that $1 \leq e \leq k$. By Lemma 5 it suffices to upper bound the number of ways to assign locations $v_i$, for all $i = 1, \ldots, 2e$ and glues $g_{4i-2}$, for $i = 1, \ldots, \frac{e+1}{2}$ in a restricted bond-forming submovies of the form $\mathcal{R}(M_{\overline{\bar{a}},w}) = (\overline{\bar{v}}, g_1), \ldots, (\overline{\bar{v}}_{2e}, g_{2e})$.

The number of ways to assign glues $g_{4i-2}$, for $i = 1, \ldots, \frac{e+1}{2}$, is less than or equal to $|G|^{\lceil \frac{k}{2} \rceil}$. By the counting procedure given in Section 3.2, the number of ways to assign locations $v_i$, for all $i = 1, \ldots, 2e$, is less than or equal to $(k/e) \left( e \frac{1}{p+1} \right)^2 \cdot 1$. Thus, if $m$ is the total number of restricted bond-forming submovies of the form $\mathcal{R}(M_{\overline{\bar{a}},w})$, where all the locations have been assigned but only the glues $g_{4i-2}$, for $i = 1, \ldots, \frac{e+1}{2}$, have been assigned, then we have:

\[
m \leq \sum_{1 \leq e \leq k, e \text{ odd}} \left( \frac{k}{e} \right) \left( e \frac{1}{p+1} \right)^2 \cdot |G|^{\lceil \frac{k}{2} \rceil} \cdot 2^{3k+2} \cdot k.
\]

Thus, a 2D version of our second main lower bound is as follows.

**Lemma 7.** $K_{USA}^1(R_{k,N}) = \Omega \left( N^{\lceil \frac{k}{2} \rceil} \right)$.

**Proof.** Mimic the proof of Lemma 4 but use Lemma 6. □

Our second main result is as follows.

**Theorem 2.** $K_{USA}^1(R_{k,N}^3) = \Omega \left( N^{\lceil \frac{k}{2} \rceil} \right)$.

**Proof.** The proof of Lemma 7 generalizes to 3D. Note that the “$\lceil \frac{k}{2} \rceil$” term in Lemma 7 gets replaced by “$\lceil \frac{2k}{3} \rceil$”, which simplifies to “$k$”. The extra “2” in the numerator of $\lceil \frac{k}{2} \rceil$ comes from the fact that every column in $R_{k,N}^3$ consists of 2k positions. □

Just like the authors in [3], we also point out that the arguments for Theorems 4 and 2 apply to any shape of length $N$ with height at each column bounded by $k$.

### 4 Upper bound

In this section, we give a construction for a singly-seeded TAS in which a sufficiently large thin rectangle $R_{k,N}^3$ uniquely self-assembles. For the sake of clarity of presentation, we represent $R_{k,N}^3$ vertically. The following is our third main result.

**Theorem 3.** $K_{USA}^1(R_{k,N}^3) = O \left( N^{\lceil \frac{k}{2} \rceil} \right)$.  

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Figure 3: A full example of a $11 \times 56$ construction. The counter begins at 10-01-10 and is counting in ternary, so the initial value is $23 = 2 \cdot 3^2 + 1 \cdot 3^1 + 2 \cdot 3^0$. Note that the least significant bit for each digit, which is the lowest bit in each digit column, is actually a “left edge” indicator, where “1” means “leftmost” and “0” means “not leftmost”. In this case, we have $d = 3$, $m = 3$, $l = 3$, $s = 23$, $c = 2$, and $r = 2$. To help distinguish overlapping tiles, “write gadgets” are drawn in gray.
The basic idea of our construction for Theorem 3 is to use a counter, the base of which is a function of $k$ and $N$. Then, we initialize the counter for our construction with a certain starting value and have it increment until its maximum value, at which point it rolls over to all 0’s and the assembly goes terminal. Our construction is inspired by, but substantially different from, a similar construction by Cheng, Aggarwal, Goldwasser, Kao, Schweller and Moisset de Espanés [3] for the self-assembly of two-dimensional $k \times N$ thin rectangles at temperature-2. Like theirs, our construction uses a counter whose base depends on $k$ and $N$. But unlike theirs, we represent each digit of the counter in our construction geometrically, using a one-bit-per-bump representation in an assembly that is three tiles wide and whose height is proportional to the binary representation of the base of the counter. See Figure 3 for an example of the counter in our construction (henceforth referred to simply as the counter) at different levels of granularity. The size of the tile set produced by the construction is $O(m) = O\left( N^{\frac{k}{3}} \right)$ and correctness follows from conditional determinism. In the remainder of this section, we will discuss parameters for the counter, define the tile set for our construction and conclude with a proof of Theorem 3.

### 4.1 Parameters for the counter

Since the height (number of tile rows) of each logical row in the counter depends on $k$ and $N$, we must choose its starting value carefully. Therefore, let $d = \left\lfloor \frac{k}{3} \right\rfloor$, $m = \left\lceil \left( \frac{N}{5} \right)^{\frac{1}{2}} \right\rceil$, $l = \lceil \log m \rceil + 1$, $s = m^d - \left\lfloor \frac{N-3l-1}{3l+2} \right\rfloor$, $c = k \mod 3$, and $r = N+1 \mod 3l+2$, where $d$ is the number of digits in the counter, $m$ is the numerical base of the counter, $l$ is the number of bits needed to represent each digit in the counter’s value plus one for the “left edge”, $s$ is the numerical start of the counter, and $c$ and $r$ are the number of tile columns and tile rows, respectively, that must be filled in after and outside of the counter. Each digit of the counter requires a width of 3 tiles, which has a direct relation with the tile complexity of the construction. The values of $m$ and $s$ are chosen such that the counter stops just before reaching a height of $N$ tiles, at which point, the assembly is given a flat “roof”. We now informally justify each of the previously-defined parameters.

We define $d$ as the number of digit columns in the counter. The number of digits in the counter is limited by the width, $k$. Each digit column requires 3 tiles. We maximize the range of the counter by maximizing the number of digit columns. Given those requirements and restrictions, we end up with $d = \left\lfloor \frac{k}{3} \right\rfloor$ digit columns.

Given at least one digit column, we have the ability to count to any number of counter rows so long as we choose an appropriate base. In that sense, choosing $m$, the base of the counter, is somewhat arbitrary. So long as the maximum height of our construction, where we count $m^d$ times, is greater than $N$, and the minimum height of our construction, where we count once, is less than $N$, then there exists a corresponding value of $s$ such that the counter stops just before reaching a height of $N$. We choose $m = \left\lceil \left( \frac{N}{5} \right)^{\frac{1}{2}} \right\rceil$.

The value of $l$, which is the number of binary bits needed to encode each digit of base-$m$, plus one for the “left edge”, is easily verified by inspection.

Let $h$ be the height of the construction without any additional “roof” tiles. By inspection of the example construction in Figure 3c as well as the construction of the gadget units in subsequent sections, we see that the height of the construction without additional tiles is $3l+1$ for the Seed unit (see Section 4.2.2), plus $3l+2$ for each incrementation of the counter, adding a Counter unit (see Section 4.2.3) row each time. If we define $n$ as the number of Counter unit rows, then $h = n(3l+2) + 3l + 1$. So then the maximum height of the counter is $m^d(3l+2) + 3l + 1$.

**Lemma 8.** $N \leq m^d(3l+2) + 3l + 1$. 

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Proof. We have

\[
N = 5 \left( \frac{N}{5} \right) \left( \frac{N}{5} \right)^{\frac{1}{d}} d \\
\leq 5 \left( \frac{N}{5} \right)^{\frac{1}{d}} d \\
= 5m^d \\
\leq 3lm^d + 2m^d \\
\leq 3lm^d + 2m^d + 3l + 1 \\
= m^d(3l + 2) + 3l + 1.
\]

And the minimum height is 6\(l + 3\).

**Lemma 9.** \(6l + 3 \leq N\), for \(k \geq 3\) and sufficiently large values of \(N\).

Proof. We have

\[
6l + 3 = 6 \left\lfloor \log m \right\rfloor + 9 \\
= 6 \left\lfloor \log \left( \frac{N}{5} \right)^{\frac{1}{d}} \right\rfloor + 9 \\
\leq 6 \log \left( \frac{N}{5} \right)^{\frac{1}{d}} + 9 \\
= \frac{6}{d} \log \left( \frac{N}{5} \right) + 15 \\
\leq \frac{6}{d} \log N + 15 \\
= \frac{6}{\left\lfloor \frac{k}{3} \right\rfloor} \log N + 15 \\
\leq 6 \log N + 15 \\
= 6\log N + 15 \\
\leq N \\
\text{For } N \geq 49.
\]

By Lemma 9, one row of the counter might result in a final assembly that will not be tall enough but Lemma 8 says that having all possible rows of the counter might result in a final assembly that is too tall. Therefore, we must start the counter at an appropriate value to get the correct height of the final assembly.

The counter can start at any whole number less than \(m^d\) and ends when it reaches 0 by rolling over \(m^d - 1\). This means that the number of Counter unit rows \(n\), is \(m^d - s\), where we have defined \(s\) as the starting value of the counter. To choose the best starting value, we find the value for \(n\) that gets \(h\) close to \(N\) without exceeding \(N\). It follows from the equation \(h = n(3l + 2) + 3l + 1\), that \(n = \left\lfloor \frac{N - 3l - 1}{3l + 2} \right\rfloor\). Thus, \(s = m^d - \left\lfloor \frac{N - 3l - 1}{3l + 2} \right\rfloor\).

\[\Box\]
Recall that we must use 3d tile columns to encode the digits of the counter. Since the remaining tile columns must still be filled in to ensure a width of k, we must sometimes construct additional tile columns outside of the counter. We denote the number of additional tile columns by c and conclude that its value is $k \mod 3$.

Similarly, we must also account for the number of additional tile rows that must be filled in after the counter has finished counting. We denote the number of filler rows at the top of the construction with r, and conclude that it is the remainder of this quotient expression $N - 3l - 1 \mod 3l + 2$, which is to say that $r = N - 3l - 1\mod 3l + 2$. This modular expression simplifies to $r = N + 1 \mod 3l + 2$.

4.2 Tile set

For the purposes of this construction, we assume the function $bin(a, b)$ gives the binary representation of a that is truncated (or prepended with 0’s) to a length of b. We will use the notation $(a)_b[i]$ to denote the digit in the i-th position from the right of a in base-b. We define a gadget unit as a collection of gadgets with a singular purpose. Gadgets belonging to the same gadget unit will have their figures grouped together. The set of all gadgets created in this subsection forms the tile set $T_{k,N}$.

4.2.1 Vertical Column tiles

Since Vertical Column tiles are present in a majority of our gadget units, they will only be shown in Figure 4.

(a) Up_Column_Tile  (b) Down_Column_Tile

Figure 4: Vertical_Column tiles are used throughout the construction to adjust the height of gadget units.

4.2.2 Seed unit

We begin by encoding the initial value of the counter with the Seed unit. It has d columns, where each 3-wide column represents a digit of s in base-m. A collection of bit-bumps on the columns’ east sides encodes the digits into binary. A small “lip” is added on the west side of the Seed unit to increase the width of the assembly by c, which catches any vertical filler tiles at the end of the construction. The Guess tile on the east side of the unit initiates the first Counter unit. See Figure 5.

We define the Seed unit by creating the following gadgets:

- The first gadget depends on the value of c:
  - If $c = 0$, create Seed_Start((seed, col, d, 1)) from the general gadget in Figure 5a
  - If $c = 1$, create Seed_Start((seed, col, d, 1)) from the general gadget in Figure 5b
  - If $c = 2$, create Seed_Start((seed, col, d, 1)) from the general gadget in Figure 5c

One gadget was created in this step.

- For each $i = 1, \ldots, d$:
  - For each $j = 1, \ldots, 3l - 3$, create Up_Column((seed, col, i, j), (seed, col, i, j + 1)) from the general gadget in Figure 5a
  - Create Seed_Msb((seed, col, i, 3l - 2), (seed, bit, i, l - 1)) from the general gadget in Figure 5d if $((s)_m[i])_2[l] = 0$ or Figure 5e if $((s)_m[i])_2[l] = 1$. 

We define the Seed unit by creating the following gadgets:
For each $j = 2, \ldots, l - 1$, create $\text{Seed}_\text{Bit}((\text{seed}, \text{bit}, i, j), (\text{seed}, \text{bit}, i, j - 1))$ from the general gadget in Figure 5g if $((s)_m[i])_{2j} = 0$ or Figure 5h if $((s)_m[i])_{2j} = 1$.

In this step, $\sum_{i=1}^{d} \left( 1 + \sum_{j=1}^{l-3} 1 + \sum_{j=2}^{l-1} 1 \right) = O(dl)$ gadgets were created. This means that
dl = O(d \log m) \\
= O \left( d \log \left( \frac{N}{5} \right) \right) \\
= O \left( d \log \left( \frac{2}{\frac{N}{5}} \right) \right) \\
= O \left( d \log \left( \frac{N}{5} \right)^{\frac{1}{d}} + d \log 2 \right) \\
= O \left( d \log \left( \frac{N}{5} \right) + d \right) \\
= O \left( \log N + \left\lfloor \frac{k}{3} \right\rfloor \right) \\
= O \left( \log N \right)
gadgets were created in this step.

- Create $\text{Seed}_\text{Bit}((\text{seed}, \text{bit}, d, 1), (\text{seed}, \text{bit}, d, 0))$ from the general gadget in Figure 5h. One gadget was created in this step.

- For each $i = 1, \ldots, d - 1$:
  - Create $\text{Seed}_\text{Bit}((\text{seed}, \text{bit}, i, 1), (\text{seed}, \text{bit}, i, 0))$ from the general gadget in Figure 5g
  - Create $\text{Seed}_\text{Spacer}((\text{seed}, \text{bit}, i + 1, 0), (\text{seed}, \text{col}, i, 1))$ from the general gadget in Figure 5l

In this step, $2(d - 1) = O(k) = O(\log N)$ gadgets were created.

- Create $\text{Seed}_\text{End}((\text{seed}, \text{bit}, 1, 0), (\text{inc}, \text{read}, 1), (\text{inc}, \text{read}, 0))$ from the general gadget in Figure 5l
  One gadget was created in this step.

Since the number of tiles in each gadget in the Seed unit is $O(1)$, then based on the above computations, the number of gadgets created in this subsection is $O(\log N)$. We will show that $\log N = O \left( \frac{\log N}{\log N - \log \log N} \cdot \frac{\log N}{\log N - \log \log N} \right)$. First, by the definition of thin rectangle, we have

\[
\frac{\log N}{\log N - \log \log N} < \frac{\log N}{\log N - \log \log N} = \frac{2 \log N}{\log N}.
\]
Figure 5: The Seed gadget unit. The actual seed tile is at the far-left of any of the Seed_Start gadgets.

where the second inequality holds for $N > 2^{2^{4}}$. Then we have

$$\log N = 2^{\log \log N}$$

$$= \left( N^{\frac{\log N}{\log \log N}} \right)^{\log \log N}$$

$$= \left( N^{\log \log N} \right)^{\frac{1}{\log \log N}}$$

$$= \left( N^{\frac{1}{\log \log N}} \right)^{2}$$

$$= N^{\frac{2}{\log \log N}}$$

$$= O \left( N^{\frac{1}{\log \log N}} \right) = O \left( N^{\frac{1}{2}} \right) = O \left( N^{\frac{1}{3}} \right) = O \left( N^{\frac{1}{\lfloor 3 \rfloor}} \right).$$

Thus, the number of gadgets created in this subsection is $O \left( N^{\frac{1}{\lfloor 3 \rfloor}} \right)$.

4.2.3 Counter unit

For this construction, we require a set of $4m - 1$ Counter gadget units to encode the digits of the counter, of which $m$ units will increment a digit of the counter, $m$ units will copy a digit of the counter, $m$ units will copy the most significant digit of the counter, and $m - 1$ units will increment the most significant digit of the counter. Each row of the counter will have a total of $d$ Counter units. Each Counter unit reads over a series of bit-bumps protruding into their row from the preceding Seed unit or counter row. After a Counter unit reads its bit pattern with Guess tiles, the unit produces a new bit pattern in the row above it that encodes a copy or increment of the current digit. Of the “less significant digit” units, the one that increments $m - 1$ to 0 is unique because it initiates another increment unit, that is, a carry is passed to the digit to its left. Other increment units, as well as the copy units, will only initiate copy units (no carry is propagated to the left). The first bit read is always the “left edge” marker, which tells the unit if it represents the most
significant digit of the counter value and needs to start a new row instead of another Counter unit. The counter terminates when the most significant digit follows an increment unit and reads \(m - 1\) in its column. At that point, the counter will have rolled over \(m^d - 1\) and the Roof unit takes over. The gadgets belonging to the Counter units are shown in Figure 6.

We define the Counter units by creating the following gadgets:

- For each \(i = 0, \ldots, l - 2\) and each \(u \in \{0, 1\}^4\):
  - Create \(\text{Counter\_Read}(\langle\text{inc, read, 0u}\rangle, \langle\text{inc, read, 10u}\rangle, \langle\text{inc, read, 00u}\rangle)\) from the general gadget in Figure 6a.
  - Create \(\text{Counter\_Read}(\langle\text{inc, read, 1u}\rangle, \langle\text{inc, read, 11u}\rangle, \langle\text{inc, read, 01u}\rangle)\) from the general gadget in Figure 6b.
  - Create \(\text{Counter\_Read}(\langle\text{copy, read, 0u}\rangle, \langle\text{copy, read, 10u}\rangle, \langle\text{copy, read, 00u}\rangle)\) from the general gadget in Figure 6c.
  - Create \(\text{Counter\_Read}(\langle\text{copy, read, 1u}\rangle, \langle\text{copy, read, 11u}\rangle, \langle\text{copy, read, 01u}\rangle)\) from the general gadget in Figure 6d.

These are read gadgets for all digit positions and all bits (except the most significant bit) for both copy and increment columns. In this step, \(\sum_{i=0}^{l-2} 4 \cdot 2^i = 4 (2^{l-1} - 1) = 4 (2^{\lfloor \log_2 m \rfloor} - 1) \leq 4 (2 \cdot 2^{\log_2 m}) = O(m) = O\left( N \left( \frac{\log^2 m}{m} \right) \right)\) gadgets were created.

Recall that the least significant bit of our digit columns represents whether the digit is for the most significant digit’s place or not. It follows then, that \(\text{bin}(2m - 2, l)\) is the greatest digit of our base-\(m\) counter but with an extra 0 at the end, which is to say that it is \(m-1\) but not for the most significant digit’s place. To get \(m - 1\) for the most significant digit’s place, we simply add a 1 to that expression and get \(\text{bin}(2m - 1, l)\).

Hence, we use the range \(0\) to \(2m - 1\) to refer to all digits of base-\(m\) in all positions / places, we use the range \(0\) to \(2m - 3\) to refer to all digits of base-\(m\) except \(m - 1\) in all positions / places, we use the index \(2m - 2\) to refer to the counter value \(m - 1\) when not in the most significant digit’s place, and we use the index \(2m - 1\) to refer to the counter value \(m - 1\) when in the most significant digit’s place.

- For each \(i = 0, \ldots, 2m - 1\), create
  \[
  \text{Counter\_Read\_Msrb}(\langle\text{copy, read, bin}(i, l)\rangle, \langle\text{copy, write, bin}(i, l)\rangle, \langle\text{d\_fill}\rangle)
  \]
  from the general gadget in Figure 6a if \(\langle i \rangle_2[l] = 0\) or Figure 6d if \(\langle i \rangle_2[l] = 1\). These are all read gadgets for the most significant bit in copy columns only. In this step, \(2m = O\left( N \left( \frac{\log^2 m}{m} \right) \right)\) gadgets were created.

- For each \(i = 0, \ldots, 2m - 3\), create
  \[
  \text{Counter\_Read\_Msrb}(\langle\text{inc, read, bin}(i, l)\rangle, \langle\text{copy, write, bin}(i + 2, l)\rangle, \langle\text{d\_fill}\rangle)
  \]
  from the general gadget in Figure 6b if \(\langle i \rangle_2[l] = 0\) or Figure 6d if \(\langle i \rangle_2[l] = 1\). These are all read gadgets for the most significant bit in increment columns but only when the digit value is between 0 and \(m - 2\). In this step, \(2m - 2 = O\left( N \left( \frac{\log^2 m}{m} \right) \right)\) gadgets were created.
• Create

\[
\text{Counter\_Read\_Msb}(\langle \text{inc, read, bin}(2m - 2, i)\rangle, \\
\langle \text{inc, write\_all\_0s, 1}\rangle, \\
\langle \text{d\_fill1}\rangle)
\]

from the general gadget in Figure 6d. This is the read gadget for the most significant bit in all increment columns (except the most significant digit) but only when the digit value is \(m - 1\). One gadget was created in this step.

• For each \(i = 1, \ldots, l - 1\), create \(\text{Counter\_Write}(\langle \text{inc, write\_all\_0s, i}\rangle, \langle \text{inc, write\_all\_0s, i + 1}\rangle)\) from the general gadget in Figure 6c. These are the write gadgets for a digit value of all 0s due to incrementation of \(m - 1\). In this step, \(l - 1 = O(\log m) = O\left(\frac{\log N}{2}\right) = O(\log N) = O\left(N^{\frac{1}{\log 2}}\right)\) gadgets were created. This group of gadgets writes a series of 0 bits, because \(m - 1\) was incremented to 0.

• For each \(u \in \{0, 1\}^{l-1}:\n\)
  - Create \(\text{Counter\_Write}(\langle \text{copy, write, u0}\rangle, \langle \text{copy, write, u}\rangle)\) from the general gadget in Figure 6c
  - Create \(\text{Counter\_Write}(\langle \text{copy, write, u1}\rangle, \langle \text{msd, write, u}\rangle)\) from the general gadget in Figure 6d

  Note that “msd” stands for “most significant digit” (since the “left edge” bit is 1 in this case).

These are all gadgets to write the “left edge” marker in all copy columns. In this step, \(2 \cdot 2^{l-1} = 2 \cdot 2^{\log m} \leq 2 \cdot 2^{\log m} = O(m) = O\left(N^{\frac{1}{\log 2}}\right)\) gadgets were created.

• For each \(i = 1, \ldots, l - 2\) and each \(u \in \{0, 1\}^{i}:\n\)
  - Create \(\text{Counter\_Write}(\langle \text{copy, write, u0}\rangle, \langle \text{copy, write, u}\rangle)\) from the general gadget in Figure 6e
  - Create \(\text{Counter\_Write}(\langle \text{copy, write, u1}\rangle, \langle \text{copy, write, u}\rangle)\) from the general gadget in Figure 6f
  - Create \(\text{Counter\_Write}(\langle \text{msd, write, u0}\rangle, \langle \text{msd, write, u}\rangle)\) from the general gadget in Figure 6g
  - Create \(\text{Counter\_Write}(\langle \text{msd, write, u1}\rangle, \langle \text{msd, write, u}\rangle)\) from the general gadget in Figure 6h

These gadgets write all digits (except the “left edge” marker) in all copy columns. In this step, \(\sum_{i=1}^{l-2} 4 \cdot 2^i = 4 \cdot \left(2^{l-2} - 2\right) = 4 \cdot (2^{\log m} - 2) \leq 4 \cdot (2 \cdot 2^{\log m}) = O(m) = O\left(N^{\frac{1}{\log 2}}\right)\) gadgets were created.

• Create \(\text{Counter\_Write\_Msb}(\langle \text{inc, write, l}\rangle, \langle \text{inc, down\_0}\rangle, 1)\) from the general gadget in Figure 6i

This gadget writes 0 for the most significant bit when digit value is all 0s after incrementing \(m - 1\). One gadget was created in this step.

• Create \(\text{Counter\_Write\_Msb}(\langle \text{copy, write, 0}\rangle, \langle \text{copy, down\_0}\rangle, 1)\) from the general gadget in Figure 6j

This gadget writes 0 for the most significant bit in any copy column except the most significant digit column. One gadget was created in this step.

• Create \(\text{Counter\_Write\_Msb}(\langle \text{copy, write, 1}\rangle, \langle \text{copy, down\_0}\rangle, 1)\) from the general gadget in Figure 6k

This gadget writes 1 for the most significant bit in any copy column except the most significant digit column. One gadget was created in this step.

• Create \(\text{Counter\_Write\_Msb}(\langle \text{msd, write, 0}\rangle, \langle \text{msd, down\_0}\rangle, 1)\) from the general gadget in Figure 6l

This gadget writes 0 for the most significant bit in the most significant digit (i.e., copy) column. One gadget was created in this step.
• Create **Counter_Write_Msb**((msd, write, 1), (msd, down, 0, 1)) from the general gadget in Figure 6h. This gadget writes 1 for the most significant bit in the most significant digit (i.e., copy) column. One gadget was created in this step.

• For each $i = 1, \ldots, 3l - 2$:
  
  – Create **Down_Column**((inc, down, 0, i), (inc, down, 0, i + 1)) from the general gadget in Figure 4b.
  
  – Create **Down_Column**((copy, down, 0, i), (copy, down, 0, i + 1)) from the general gadget in Figure 4b.

These gadgets go back down to the bottom of the new counter row in all columns (except the most significant digit column) while remembering an increment or copy is taking place. In this step, $2(3l - 2) = O(l) = O(\log m) = O\left(\frac{\log N}{k}\right) = O(\log N) = O\left(N^{\frac{1}{1+\epsilon}}\right)$ gadgets were created.

• For each $i = 1, \ldots, 3l - 3$, create **Down_Column**((msd, down, 0, i), (msd, down, 0, i + 1)) from the general gadget in Figure 4b. These gadgets go back down to the bottom of the new counter row in the most significant digit column while remembering an increment or copy is taking place. In this step, $3l - 3 = O(l) = O(\log m) = O\left(\frac{\log N}{k}\right) = O(\log N) = O\left(N^{\frac{1}{1+\epsilon}}\right)$ gadgets were created.

• Create **Counter_Return_Column_Start**((inc, down, 0, 3l - 1), (inc, down, 1, 1)) from the general gadget in Figure 6h. This is the first gadget to start going down to the bottom of the previous counter row in increment columns only. One gadget was created in this step.

• Create **Counter_Return_Column_Start**((copy, down, 0, 3l - 1), (copy, down, 1, 1)) from the general gadget in Figure 6h. This is the first gadget to start going down to the bottom of the previous counter row in copy columns only. One gadget was created in this step.

• Create **Counter_Return_Column_Start**((msd, down, 0, 3l - 2), (return, start)) from the general gadget in Figure 7b. This is the first gadget to start going back to the rightmost digit of the new counter row in the most significant digit column only. One gadget was created in this step.

• For each $i = 1, \ldots, l - 1$:
  
  – Create **Counter_Return_Column**((inc, down, 1, i), (inc, down, 1, i + 1)) from the general gadget in Figure 6b.
  
  – Create **Counter_Return_Column**((copy, down, 1, i), (copy, down, 1, i + 1)) from the general gadget in Figure 6b.

These gadgets go back down to the bottom of the previous counter row in all columns (except the most significant digit column) while remembering an increment or copy is taking place. In this step, $2(l - 1) = O(l) = O(\log m) = O\left(\frac{\log N}{k}\right) = O(\log N) = O\left(N^{\frac{1}{1+\epsilon}}\right)$ gadgets were created.

• Create **Counter_Return_Column_End**((inc, down, 1, l), (inc, read, 1), (inc, read, 0)) from the general gadget in Figure 6b. This gadget gets ready to read the “left edge” marker in the next digit (to the left) in order to increment it. One gadget was created in this step.

• Create **Counter_Return_Column_End**((copy, down, 1, l), (copy, read, 1), (copy, read, 0)) from the general gadget in Figure 6b. This gadget gets ready to read the “left edge” marker in the next digit (to the left) in order to copy it. One gadget was created in this step.
Since the number of tiles in each gadget in the Counter unit is $O(1)$, then based on the above computations, the number of gadgets (and therefore the number of tile types) created in this subsection is $O\left(N^{\left\lceil \frac{1}{k} \right\rceil}\right)$.

Figure 6: The Counter gadget unit. A row of units shares half of its space with the row above and the other half of its space with the row below.

4.2.4 Return Row unit

To begin a new row of Counter units following the completion of the current row, a Return Row gadget unit must return the frontier of the assembly to the east side of the construction. After returning the frontier to the east side, it initiates an incrementing Counter unit for the least significant digit. In cases where there is only one digit column in use, a single special gadget is used instead of the multi-piece unit. See Figure 7.
We define the Return Row unit by creating the following gadgets:

- If \( d = 1 \), create \text{Return Row Single}(\langle \text{return}, \text{start} \rangle , \langle \text{inc}, \text{read}, 1 \rangle , \langle \text{d\_fill} \rangle , \langle \text{inc}, \text{read}, 0 \rangle ) \) from the general gadget in Figure 7d. One gadget was created in this step.

- Otherwise:
  - Create \text{Return Row Start}(\langle \text{return}, \text{start} \rangle , \langle \text{d\_fill} \rangle , \langle \text{return}, 1 \rangle ) \) from the general gadget in Figure 7a. One gadget was created in this step.
  - For each \( i = 1, \ldots, d - 2 \), create \text{Return Row}(\langle \text{return}, i \rangle , \langle \text{return}, i + 1 \rangle ) \) from the general gadget in Figure 7b. In this step, \( d - 2 = O(k) = O(\log N) = O\left(N^{\frac{1}{\log N}}\right) \) gadgets were created.
  - Create \text{Return Row End}(\langle \text{return}, d - 1 \rangle , \langle \text{inc}, \text{read}, 1 \rangle , \langle \text{inc}, \text{read}, 0 \rangle ) \) from the general gadget in Figure 7c. One gadget was created in this step.

Since the number of tiles in each gadget in the Return Row unit is \( O(1) \), then based on the above computations, the number of gadgets (and therefore the number of tile types) created in this subsection is \( O\left(N^{\frac{1}{\log N}}\right)\).

![Figure 7: The Return Row gadget unit.](image)

### 4.2.5 Roof unit

The Roof gadget unit consists of a vertical tile column that reaches above the tiles from the last counter row, then extends the assembly to a height of \( N \). Along the column are glues placed periodically that accept filler extensions. These extensions are designed to patch up holes that are left in the last counter row. The highest tile in the column has west-facing and east-facing glues. These glues accept shingle tiles which extend
the roof westward and eastward so that the entire construction is “covered”. (The eastward expansion is
blocked if \( r = 0 \).) Each shingle tile has a south-facing glue that binds to a filler tile, which will cover up any
remaining gaps in the \( k \times N \) shape. The Roof unit is shown in Figure 8.

We define the Roof unit by creating the following gadgets:

- Create \( \text{Up\_Column}(\langle \text{inc, read, bin}(2m - 1, l) \rangle, \langle \text{roof, col, 2} \rangle) \) from the general gadget in Figure 4a.
  One gadget was created in this step.
- Create \( \text{Up\_Column}(\langle \text{roof, col, 2} \rangle, \langle \text{roof, col, 3} \rangle) \) from the general gadget in Figure 4a. One gadget was
  created in this step.
- For each \( i = 3, \ldots, l + 2 \), create \( \text{Roof\_Chimney}(\langle \text{roof, col, } i \rangle, \langle \text{roof, col, } i + 1 \rangle, \langle \text{roof, filler, 1} \rangle) \) from
  the general gadget in Figure 8a. In this step, \( (l + 2) - 3 + 1 = O(l) = O(log m) = O\left(\frac{\log N}{k}\right) = O(log N) \) gadgets were
  created.
- For each \( i = 1, \ldots, d - 1 \), create \( \text{Roof\_Filler}(\langle \text{roof, filler, } i \rangle, \langle \text{roof, filler, } i + 1 \rangle) \) from the general
gadget in Figure 8b. In this step, \( d - 1 = O(k) = O(log N) \) gadgets were created.
- For each \( i = l + 3, \ldots, l + r + 4 \), create \( \text{Up\_Column}(\langle \text{roof, col, } i \rangle, \langle \text{roof, col, } i + 1 \rangle) \) from the general
gadget in Figure 4a. In this step, \( r + 2 = O(l) = O(log m) = O\left(\frac{\log N}{k}\right) = O(log N) \) gadgets were
  created.
- Create \( \text{Roof\_Cap}(\langle \text{roof, col, } l + r + 5 \rangle, \langle \text{roof, r\_shingle, 1} \rangle, \langle \text{roof, l\_shingle, 1} \rangle) \) from the general
gadget in Figure 8c. One gadget was created in this step.
- For each \( i = 1, \ldots, c + 2 \), create

  \[
  \text{Roof\_Left\_Shingle}(\langle \text{roof, l\_shingle, } i \rangle, \langle \text{d\_fill} \rangle, \langle \text{roof, l\_shingle, } i + 1 \rangle)
  \]

  from the general gadget in Figure 8d. In this step, \( c + 2 = O(1) \) gadgets were created.
- If \( r > 0 \), then for each \( i = 1, \ldots, 3d - 3 \), create

  \[
  \text{Roof\_Right\_Shingle}(\langle \text{roof, r\_shingle, } i \rangle, \langle \text{roof, r\_shingle, } i + 1 \rangle, \langle \text{d\_fill} \rangle)
  \]

  from the general gadget in Figure 8d. In this step, if \( r > 0 \), then \( 3d - 3 = O(d) = O(k) = O(log N) \) gadgets were created.

Since the number of tiles in each gadget in the Roof is \( O(1) \), then based on the above computations,
the number of gadgets (and therefore the number of tile types) created in this subsection is \( O(\log N) = O\left(\frac{\log N}{k}\right) \).

4.3 Proof of Theorem 3

Assume that \( \sigma \) is the seed assembly that consists of the single seed tile that was previously specified and let
\( \mathcal{T}_{k,N} = (T_{k,N}, \sigma, 1) \). We are now ready to prove Theorem 3.
Figure 8: The Roof gadget unit.
Theorem 4. For $x \in \{0, 1\}^n$, $K_{5,SA}(L(5, x, 2, 1)) = O\left(\frac{n}{\log n}\right)$.
Going forward, let $k$ be the smallest integer satisfying $2^k \geq \frac{n}{\log n}$, $m = \lceil \frac{n}{k} \rceil$, and write $x = w_0w_1\ldots w_{m-2}w_{m-1}$, where each $w_i$ is a $k$-bit substring. Note that $w_0$ is padded to the left with leading 0’s, if necessary. The basic idea of our construction for Theorem 4 is to have a modified binary counter count from 0 to $m - 1$ and extract (the bits of) each of the $m$ $k$-bit substrings of $x$ in order. We will use the notation $width(m)$ to denote the width of (i.e., the number of bits in) the modified binary counter for the construction, henceforth simply referred to as the counter. In the counter, the bits are configured horizontally, right underneath the bits of $x$. Doing so allows the height of the construction to be constant. Figure 9 shows a high-level overview of a valid optimal encoding instance, drawn to scale. The bits of the counter are written from left-to-right. Then, the bits of the counter are read from right-to-left. If the bits of the counter map to the decimal value $j < m$, then the bits of $w_j$ are extracted along the top of $L(5, x_1, 2)$ from left-to-right in a one-bit-per-bump geometric representation. After the bits of $w_j$ are extracted, the bits of the counter are re-read, but this time from left-to-right. Finally, if the current value of the counter is less than $m - 1$, then it is incremented and the bits of the counter are propagated further to the next block on the right in the assembly. Otherwise, the maximum value of the counter has been reached and the construction is terminated.

Figure 9: A high-level overview of the construction for $n = 17$, drawn to scale, showing the horizontal configuration of the bits of the counter, counting from 000 on the left to 101 on the right. In this example, $k = 3$ is the smallest integer satisfying $2^k$ greater than or equal to $\frac{17}{\log 17}$, $width(m) = 3$ and $w_0$ is padded to the left with one leading 0.

Figure 10: The full assembly for an invalid instance of the construction. Here, $n = 8$ with $x = 01001000$ and $k = 4$. Note that this example is not valid because $k = 2$ is the smallest value, such that, $2^k \geq \frac{8}{\log 8} = \frac{8}{3}$. The seed is the bottommost tile in the leftmost column and the last tile to attach is the bottommost tile in the rightmost column. See Figure 11 for an example assembly sequence.

Figure 11: The sequence of self-assembly of the first block in Figure 10. The black square in the lower left corner represents the seed tile and the gray region represents geometrically-encoded bits of the counter.

The size of the tile set produced by the construction is $O \left(2^k\right) = O \left(\frac{n}{\log n}\right)$ and correctness follows from
conditional determinism. In the remainder of this section, we will establish a relationship between \( k \) and \( width(m) \), define the tile set for our construction and conclude with a proof of Theorem 4. Figure 10 shows an example of our construction with more details.

5.1 Width of the counter

It is worthy of note that, in the valid optimal encoding instance depicted in Figure 9, we have \( width(m) = 3 \) and \( k = 3 \) and this is not a coincidence. It turns out that, in general, \( k \) and \( width(m) \) are very closely related.

**Lemma 10.** Assuming \( n, k, m \) and \( width(m) \) are defined as we did above and \( n \geq 17 \), then \( k \leq width(m) \leq k + 1 \).

**Proof.** Observe that \( 2^k < \frac{2n}{\log n} \). If this were not the case, then we would have \( 2^k \geq \frac{2n}{\log n} \). Dividing both sides by 2, we get \( 2^{k-1} \geq \frac{n}{\log n} \). Thus, \( k' = k - 1 \) would satisfy \( 2^{k'} \geq \frac{n}{\log n} \), contradicting the fact that \( k \) is the smallest integer satisfying \( 2^k \geq \frac{n}{\log n} \). Thus, for \( n \geq 17 \), we have \( \frac{1}{2} \log n < \log n - \log \log n \leq k < \log n - \log \log n + 1 < \log n \).

We will first prove that \( \frac{n}{k} \leq 2^{k+1} \). Assume that \( \frac{n}{k} > 2^{k+1} \). Then, we have \( 2^k < \frac{n}{k} < \frac{n}{2^{k+1}} \). This is a contradiction because we know that \( 2^k < \frac{2n}{\log n} \). We will now prove that \( \frac{n}{k} > 2^{k-1} \). Assume that \( \frac{n}{k} \leq 2^{k-1} \). Then, we have \( 2^k \leq \frac{2n}{k} < 2n \log n \). This is a contradiction because we know that \( 2^k < \frac{2n}{\log n} \). Thus, we have \( 2^{k-1} < \frac{n}{k} \leq 2^{k+1} \).

The width of a counter that counts from 0 to \( m - 1 \) is \( width(m) = \lceil \log m \rceil \) and we have: \( width(m) = \lceil \log \lceil \frac{n}{k} \rceil \rceil = \lceil \log \frac{n}{k} \rceil \). We conclude the proof with the following two cases:

1. First, suppose that \( 2^{k-1} < \frac{n}{k} \leq 2^k \). In this case, \( \lceil \log \frac{n}{k} \rceil = k \).
2. Second, suppose that \( 2^k < \frac{n}{k} \leq 2^{k+1} \). In this case, \( \lceil \log \frac{n}{k} \rceil = k + 1 \).

As per the upper bound of Lemma 10, we will always use \( k + 1 \) bits to represent the value of the counter that counts from 0 to \( m - 1 \). Technically, we will encode the \( k \) least significant bits geometrically whereas the most significant bit will be encoded in the glue labels of every tile type.

5.2 Tile set

The tile set \( T_x \) for our construction is defined in terms of a set of created gadgets.

5.2.1 Seed gadget

First, the Seed gadget (see Figure 12) self-assembles from the single seed tile.

![Seed gadget](image)

(a) Seed (b) The black tiles show the location of the Seed gadget in the example from Figure 10

Figure 12: The Seed gadget.
Create $\text{Seed}(\langle \text{write\_counter\_bits}, 0, 0\cdots 0 \rangle)$ from the general gadget shown in Figure 12a. The actual seed tile of the construction is the bottommost tile in Figure 12a. Every gadget in our construction will propagate the most significant bit of the counter via its input and output glues.

One $\text{Seed}$ gadget was created in this subsection and it is comprised of $O(1)$ tiles. Therefore, the number of tile types created in this subsection is $O(1)$.

### 5.2.2 Spacer gadget

In this section, we define the general $\text{Spacer}$ gadget. The purpose of the $\text{Spacer}$ gadget is to provide spacing in between other gadgets. By construction, it always propagates information from left-to-right. Since the $\text{Spacer}$ gadget is used throughout the construction, we will create instances of it in later subsections.

![Figure 13: The Spacer gadget.](image)

**Figure 13:** The $\text{Spacer}$ gadget.

### 5.2.3 Write\_Counter\_Bit gadgets

To the $\text{Seed}$ gadget, a series of $\text{Write\_Counter\_Bit}$ gadgets (see Figure 14) self-assemble the $k$ least significant bits of the counter from left-to-right, where each $\text{Write\_Counter\_Bit}$ gadget is followed by a corresponding $\text{Spacer}$ gadget (see Figure 13). The first $\text{Write\_Counter\_Bit}$ gadget takes as input the value of the counter from either the $\text{Seed}$ gadget or a previous $\text{Start\_Next\_Block}$ gadget (see Figure 21). Each $\text{Write\_Counter\_Bit}$ gadget has a height of 3 tiles, which allows each bit to be read twice without being re-written in between.

![Figure 14: The Write\_Counter\_Bit gadgets.](image)

**Figure 14:** The $\text{Write\_Counter\_Bit}$ gadgets.

We create the $\text{Write\_Counter\_Bit}$ and corresponding $\text{Spacer}$ gadgets as follows.

- For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create
  
  $\text{Write\_Counter\_Bit\_0}(\langle \text{write\_counter\_bits}, b, 0u \rangle,$
  
  $\langle \text{write\_counter\_bits\_space}, b, u \rangle )$
from the general gadget shown in Figure 14a.

- For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create

$$\text{Write\_Counter\_Bit\_I}(\langle \text{write\_counter\_bits, } b, 1u \rangle, \langle \text{write\_counter\_bits\_space, } b, u \rangle)$$

from the general gadget shown in Figure 14b.

- For each $b \in \{0, 1\}$, each $i = 1, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create

$$\text{Spacer}(\langle \text{write\_counter\_bits\_space, } b, u \rangle, \langle \text{write\_counter\_bits, } b, u \rangle)$$

from the general gadget shown in Figure 13a.

- For each $b \in \{0, 1\}$, create

$$\text{Spacer}(\langle \text{write\_counter\_bits\_space, } b, \lambda \rangle, \langle \text{start\_read\_counter\_bits\_rl, } b \rangle)$$

from the general gadget shown in Figure 13a.

The number of Write\_Counter\_Bit gadgets created in this subsection is

$$2 \left( 2 \sum_{i=0}^{k-1} 2^i \right) = O(2^k) = O\left( \frac{n}{\log n} \right).$$

The number of Spacer gadgets created in this subsection is

$$2 \left( 1 + \sum_{i=1}^{k-1} 2^i \right) = O(2^k) = O\left( \frac{n}{\log n} \right).$$

The number of tiles in the Write\_Counter\_Bit and Spacer gadgets is $O(1)$. Therefore, the number of tile types created in this subsection is $O\left( \frac{n}{\log n} \right)$.

5.2.4 Start\_Read\_Counter\_Bits\_RL and Read\_Counter\_Bit\_RL gadgets

After the bits of the counter have been written, the Start\_Read\_Counter\_Bits\_RL gadget (see Figure 15) self-assembles, initiating the process of reading the bits of the counter from right-to-left using a series of Read\_Counter\_Bit\_RL gadgets (see Figure 16).

(a) Start\_Read\_Counter\_Bits\_RL  (b) The black tiles show the locations of the Start\_Read\_Counter\_Bits\_RL gadget in the example from Figure 10

Figure 15: The Start\_Read\_Counter\_Bits\_RL gadget.

The Read\_Counter\_Bit\_RL gadget that reads bit $i$ of the counter, for $i = 0, \ldots, k - 1$, inputs a bit string of length $i$ and outputs a bit string of length $i + 1$, with the most significant bit equal to the bit that it read. Each Read\_Counter\_Bit\_RL gadget guesses the value of the next bit by attempting to self-assemble a path in both the $z = 0$ and $z = 1$ planes. However, by construction, exactly one of these paths is prevented from proceeding by a previous portion of the assembly and the correct bit is read.

We create the Start\_Read\_Counter\_Bits and Read\_Counter\_Bit\_RL gadgets as follows.
For each $b \in \{0, 1\}$, create

\[
\text{Start}_{\text{Read Counter Bits RL}}(\langle \text{start read counter bits rl}, b \rangle, \\
\langle \text{read counter bits rl}, b, 1 \rangle, \\
\langle \text{read counter bits rl}, b, 0 \rangle)
\]

from the general gadget shown in Figure 15a.

For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 2$ and each $u \in \{0, 1\}^i$, create

\[
\text{Read Counter Bit RL}_0(\langle \text{read counter bits rl}, b, 0u \rangle, \\
\langle \text{read counter bits rl}, b, 10u \rangle, \\
\langle \text{read counter bits rl}, b, 00u \rangle)
\]

from the general gadget shown in Figure 16a.

For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 2$ and each $u \in \{0, 1\}^i$, create

\[
\text{Read Counter Bit RL}_1(\langle \text{read counter bits rl}, b, 1u \rangle, \\
\langle \text{read counter bits rl}, b, 11u \rangle, \\
\langle \text{read counter bits rl}, b, 01u \rangle)
\]

from the general gadget shown in Figure 16b.

For each $b \in \{0, 1\}$ and each $u \in \{0, 1\}^{k-1}$, create

\[
\text{Read Counter Bit RL}_0(\langle \text{read counter bits rl}, b, 0u \rangle, \\
\langle \text{read counter bits rl}, b, \text{dummy} \rangle, \\
\langle \text{start extract bits}, b, 0u \rangle)
\]

from the general gadget shown in Figure 16a. We set the label of the $z = 0$ output glue label to the “dummy” glue label $\langle \text{read counter bits rl}, \text{dummy} \rangle$ (here, and in the next creation step) so we do not have to create a special gadget for this part of the construction.

For each $b \in \{0, 1\}$ and each $u \in \{0, 1\}^{k-1}$, create

\[
\text{Read Counter Bit RL}_1(\langle \text{read counter bits rl}, b, 1u \rangle, \\
\langle \text{read counter bits rl}, b, \text{dummy} \rangle, \\
\langle \text{start extract bits}, b, 1u \rangle)
\]

from the general gadget shown in Figure 16b.
Two \texttt{Start_Read.Counter.Bits.RL} gadgets were created in this subsection. The number of \texttt{Read.Counter.Bit.RL} gadgets created in this subsection is $2 \left( 2 \cdot 2^{k-1} + 2 \sum_{i=0}^{k-2} 2^i \right) = O \left( 2^k \right) = O \left( \frac{n}{\log n} \right)$. The number of tiles in the \texttt{Start_Read.Counter.Bits.RL} and \texttt{Read.Counter.Bit.RL} gadgets is $O(1)$. Therefore, the number of tile types created in this subsection is $O \left( \frac{n}{\log n} \right)$. 

5.2.5 \texttt{Start.Extract.Bits} and \texttt{Extract.Bit} gadgets

The \texttt{Start.Extract.Bits} gadget (see Figure 17) self-assembles after the final \texttt{Read.Counter.Bit.RL} gadget and maps the $k+1$ bit of the counter value to the corresponding $k$-bit substring. That is, the input to the \texttt{Start.Extract.Bits} gadget is the value of the counter as a binary string of $k+1$ bits and it outputs to the first \texttt{Extract.Bit} gadget (see Figure 18) the $k$-bit substring $w_j$, where $j$ is the value of the counter in decimal.

![Figure 17: The Start.Extract.Bits gadget.](image)

After the \texttt{Start.Extract.Bits} gadget self-assembles, a series of \texttt{Extract.Bit} gadgets self-assemble from left-to-right, where each bit in the current $k$-bit substring is extracted. Each \texttt{Extract.Bit} gadget takes as input a bit string of length $i$, for $i = 1, \ldots, k$, self-assembles the one-bit-per-bump geometric bit pattern of tiles that corresponds to its most significant bit, removes the most significant bit and then outputs the resulting bit string of length $i-1$ to the next \texttt{Extract.Bit} gadget, with two consecutive \texttt{Spacer} gadgets in between consecutive \texttt{Extract.Bit} gadgets.

![Figure 18: The Extract.Bit gadgets.](image)

We create the \texttt{Start.Extract.Bits}, \texttt{Extract.Bit} and corresponding \texttt{Spacer} gadgets as follows.

- For each $b \in \{0, 1\}$ and each $u \in \{0, 1\}^k$, if $val(bu) < m$, where $val(z)$ denotes the decimal value of the binary string $z$, then create

\[
\texttt{Start.Extract.Bits}(\langle \texttt{Start.extract.bits}, b, u \rangle, \\
\langle \texttt{extract.bits}, b, w_{val(bu)} \rangle)
\]

from the general gadget shown in Figure 17a.
For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create
\[
\text{Extract\_Bit}_0(\langle \text{extract\_bits}, b, 0u \rangle,
\langle \text{extract\_bits\_space\_1}, b, u \rangle)
\]
from the general gadget shown in Figure 18a.

For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create
\[
\text{Extract\_Bit}_1(\langle \text{extract\_bits}, b, 1u \rangle,
\langle \text{extract\_bits\_space\_1}, b, u \rangle)
\]
from the general gadget shown in Figure 18b.

For each $b \in \{0, 1\}$, each $i = 1, \ldots, k - 1$ and each $u \in \{0, 1\}^i$, create
\[
\text{Spacer}(\langle \text{extract\_bits\_space\_1}, b, u \rangle,
\langle \text{extract\_bits\_space\_2}, b, u \rangle)
\]
from the general gadget shown in Figure 13a.

The number of Start_Extract_Bits gadgets created in this subsection is less than or equal to $2 \cdot 2^k = O\left(\frac{n}{\log n}\right)$. The number of Extract_Bit gadgets created in this subsection is $2 \left(2 \sum_{i=0}^{k-1} 2^i\right) = O\left(2^k\right) = O\left(\frac{n}{\log n}\right)$. The number of Spacer gadgets created in this subsection is $2 \left(2 \sum_{i=1}^{k-1} 2^i\right) = O\left(2^k\right) = O\left(\frac{n}{\log n}\right)$. The number of tiles in the Start_Extract_Bits, Extract_Bit and Spacer gadgets is $O(1)$. Therefore, the number of tile types created in this subsection is is $O\left(\frac{n}{\log n}\right)$.

5.2.6 Start_Read.Counter.Bits.LR and Read.Counter.Bit.LR gadgets

After the final Extract_Bit gadget self-assembles, the Start_Read.Counter.Bits.LR gadget (see Figure 19) initiates the process of re-reading the bits of the counter. The width of the Start_Read.Counter.Bits.LR gadget is configured to be $4k$ (the width of a block in the construction). The bits of the counter need to be re-read because the value of the counter is, and must be, forgotten after the Start_Extract_Bits gadget maps the value of the counter to the current substring whose bits were just extracted.

A series of Read.Counter.Bit.LR gadgets (see Figure 20) self-assemble from left-to-right and re-read the bits of the counter for the second and final time. The Read.Counter.Bit.LR gadgets read the bits of the counter similarly to but in reverse order of the previously-described Read.Counter.Bit.RL gadgets.

We create the Start_Read.Counter.Bits.LR and Read.Counter.Bit.LR gadgets as follows.

- For each $b \in \{0, 1\}$, create
\[
\text{Start\_Read\_Counter\_Bits\_LR}(\langle \text{extract\_bits\_space\_1}, b, \lambda \rangle,
\langle \text{read\_counter\_bits\_lr}, b, 1 \rangle,
\langle \text{read\_counter\_bits\_lr}, b, 0 \rangle)
\]
from the general gadget shown in Figure 19a.
Figure 19: The \texttt{Start\_Read\_Counter\_Bits\_LR} gadget.

Figure 20: The \texttt{Read\_Counter\_Bit\_LR} gadgets.
• For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 2$ and each $u \in \{0, 1\}^i$, create

$$\text{Read\_Counter\_Bit\_LR}_0((\text{read\_counter\_bits\_lr}, b, u0),$$
$$\langle \text{read\_counter\_bits\_lr}, b, u01 \rangle, \langle \text{read\_counter\_bits\_lr}, b, u00 \rangle)$$

from the general gadget shown in Figure 20a.

• For each $b \in \{0, 1\}$, each $i = 0, \ldots, k - 2$ and each $u \in \{0, 1\}^i$, create

$$\text{Read\_Counter\_Bit\_LR}_1((\text{read\_counter\_bits\_lr}, b, u1),$$
$$\langle \text{read\_counter\_bits\_lr}, b, u11 \rangle, \langle \text{read\_counter\_bits\_lr}, b, u10 \rangle)$$

from the general gadget shown in Figure 20b.

• For each $b \in \{0, 1\}$, and each $u \in \{0, 1\}^{k-1}$, create

$$\text{Read\_Counter\_Bit\_LR}_0((\text{read\_counter\_bits\_lr}, b, u0),$$
$$\langle \text{read\_counter\_bits\_lr}, b, u0 \rangle, \langle \text{read\_counter\_bits\_lr, dummy} \rangle)$$

from the general gadget shown in Figure 20a. We set the label of the $z = 1$ output glue label to $\langle \text{read\_counter\_bits\_lr, dummy} \rangle$ (here, and in the next creation step) so we do not have to create a special gadget for this part of the construction.

• For each $b \in \{0, 1\}$, and each $u \in \{0, 1\}^{k-1}$, create

$$\text{Read\_Counter\_Bit\_LR}_1((\text{read\_counter\_bits\_lr}, b, u1),$$
$$\langle \text{read\_counter\_bits\_lr}, b, u1 \rangle, \langle \text{read\_counter\_bits\_lr, dummy} \rangle)$$

from the general gadget shown in Figure 20b.

Two Start\_Read\_Counter\_Bits\_LR gadgets were created in this subsection. The number of Read\_Counter\_Bit\_LR gadgets created in this subsection is $2 \left(2 \cdot 2^{k-1} + 2 \sum_{i=0}^{k-2} 2^i\right) = O \left(2^k\right) = O \left(\frac{n}{\log n}\right)$. The number of tiles in the Start\_Read\_Counter\_Bits\_LR gadget is $O(k) = O \left(\log n\right)$. The number of tiles in the Read\_Counter\_Bit\_LR gadget is $O(1)$. Therefore, the number of tile types created in this subsection is $O \left(\frac{n}{\log n}\right)$.

### 5.2.7 Start\_Next\_Block and Last\_Block gadgets

After the final Read\_Counter\_Bit\_LR gadget self-assembles, depending on whether or not the value of the counter is equal to $m - 1$, either a Last\_Block gadget (see Figure 22) or a Start\_Next\_Block gadget (see Figure 21) self-assembles.

On the one hand, if the value of the counter is less than $m - 1$, then the value of the counter is incremented and the incremented value is propagated via the Start\_Next\_Block gadget to the first Write\_Counter\_Bit gadget in the next block. On the other hand, if the value of the counter is equal to $m - 1$, then the bits of $w_{m-1}$ were just extracted and the construction terminates with the self-assembly of the Last\_Block gadget. Our construction has the property that the last tile in the Last\_Block gadget is guaranteed to be the last tile placed in any assembly sequence.

We create the Start\_Next\_Block and Last\_Block gadgets as follows.
For each $b \in \{0, 1\}$ and each $u \in \{0, 1\}^k$, if $\text{val}(bu) < m - 1$, then let $b'u'$ be the binary representation of $\text{val}(bu) + 1$, where $b' \in \{0, 1\}$ and $u' \in \{0, 1\}^k$ and create

\[
\text{Start\_Next\_Block}(\langle \text{read\_counter\_bits\_lr}, b, u \rangle, \\
\langle \text{write\_counter\_bits}, b', u' \rangle)
\]

from the general gadget shown in Figure 21a.

For each $b \in \{0, 1\}$ and each $u \in \{0, 1\}^k$, if $\text{val}(bu) = m - 1$, then create

\[
\text{Last\_Block}(\langle \text{read\_counter\_bits\_lr}, b, u \rangle)
\]

from the general gadget shown in Figure 22a.

The number of Start\_Next\_Block gadgets created in this subsection is $O(2^k) = O\left(\frac{n}{\log n}\right)$. One Last\_Block gadget was created in this subsection. The number of tiles in the Start\_Next\_Block and Last\_Block gadgets is $O(1)$. Therefore, the number of tile types created in this subsection is $O\left(\frac{n}{\log n}\right)$.

5.3 Proof of Theorem 4

Assume that $\sigma$ is the seed assembly that consists of the single seed tile that was previously specified. Let $T_x = (T_x, \sigma, 1)$. We are now ready to prove Theorem 4.

Proof. (of Theorem 4)

First, note that $|T_x| = O\left(\frac{n}{\log n}\right)$ because there are a constant number of subsections in which tile types in $T_x$ are created (Sections 5.2.1, 5.2.3, 5.2.4, 5.2.5, 5.2.6 and 5.2.7) and each subsection contributes $O\left(\frac{n}{\log n}\right)$ tile types.

Now, let $\bar{\alpha}$ be the assembly sequence in $T_x$, with result $\alpha$, such that the order in which $\bar{\alpha}$ places tiles can be inferred from Figure 10 and with the additional constraint that, when building the assembly sequence in a depth-first manner, $\bar{\alpha}$ always tries to place as many tiles as possible in the $z = 0$ before placing a tile in the $z = 1$ plane, breaking ties on which direction in which to proceed based on the ordering: north, east, south and finally west. Thus, $L(5, x, 2, 1)$ self-assembles in $T_x$. To show that $T_x$ is conditionally deterministic, and therefore directed, mimic the proof of Theorem 3.

\[\blacksquare\]
6 Future work

It is well-known that the tile complexity of a 2D \( N \times N \) square at temperature-2 is \( O \left( \frac{\log N}{\log \log \log N} \right) \). More formally, for an \( N \times N \) square \( S_N = \{0, 1, \ldots, N-1\} \times \{0, 1, \ldots, N-1\} \), \( K_{USA}^2(S_N) = O \left( \frac{\log N}{\log \log \log N} \right) \) \[1\]. However, it is conjectured \[11\] that \( K_{USA}^3(S_N) = 2N - 1 \), meaning that a 2D \( N \times N \) square does not self-assemble efficiently at temperature-1. Yet, it turns out that the tile complexity of a just-barely 3D \( N \times N \) square at temperature-1 is \( O \left( \frac{\log N}{\log \log N} \right) \). That is, \( K_{USA}^1(S_N^3) = O \left( \frac{\log N}{\log \log N} \right) \), where \( S_N^3 \) is a just-barely 3D \( N \times N \) square, satisfying \( \{0, 1, \ldots, N-1\} \times \{0, 1, \ldots, N-1\} \times \{0\} \subseteq S_N^3 \subseteq \{0, 1, \ldots, N-1\} \times \{0, 1, \ldots, N-1\} \times \{0,1\} \) \[9\].

So, a 2D \( N \times N \) square has the same asymptotic tile complexity at temperature-2 as its just-barely 3D counterpart does at temperature-1. Now consider the tile complexity of a 2D \( k \times N \) thin rectangle at temperature-2. In this case, we know that \( K_{USA}^2(R_{k,N}^2) = O \left( N^{\frac{2}{\tau}} + k \right) \) \[3\] and it is natural to speculate whether a similar upper bound holds for a just-barely 3D \( k \times N \) thin rectangle at temperature-1. In other words, is it the case that either \( K_{SA}^1(R_{k,N}^3) \) or \( K_{USA}^1(R_{k,N}^3) \) is equal to \( O \left( N^{\frac{2}{\tau}} + k \right) \)? If not, then what are tight bounds for \( K_{SA}^1(R_{k,N}^3) \) and \( K_{USA}^1(R_{k,N}^3) \)? We conjecture that \( K_{USA}^1(R_{k,N}^3) = o \left( N^{\left\lfloor \frac{2}{\tau} \right\rfloor} \right) \).

The aforementioned tile complexities, along with our conjecture, are summarized in the following table.

|                | 2D at \( \tau = 2 \) | 3D at \( \tau = 1 \) |
|----------------|-----------------------|-----------------------|
| Squares        | \( O \left( \frac{\log N}{\log \log \log N} \right) \) \[1\] | \( O \left( \frac{\log N}{\log \log \log N} \right) \) \[9\] |
| Thin rectangles | \( O \left( N^{\frac{2}{\tau}} + k \right) \) \[3\] | \( o \left( N^{\left\lfloor \frac{2}{\tau} \right\rfloor} \right) \) (conjecture) |

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