Reducing Tile Complexity for Self-Assembly Through Temperature Programming

Ming-Yang Kao*

Robert Schweller[†]

Abstract

We consider the tile self-assembly model and how tile complexity can be eliminated by permitting the temperature of the self-assembly system to be adjusted throughout the assembly process. To do this, we propose novel techniques for designing tile sets that permit an arbitrary length m binary number to be encoded into a sequence of O(m) temperature changes such that the tile set uniquely assembles a supertile that precisely encodes the corresponding binary number. As an application, we show how this provides a general tile set of size O(1) that is capable of uniquely assembling essentially any $n \times n$ square, where the assembled square is determined by a temperature sequence of length $O(\log n)$ that encodes a binary description of n. This yields an important decrease in tile complexity from the required $\Omega(\frac{\log n}{\log\log n})$ for almost all n when the temperature of the system is fixed. We further show that for almost all n, no tile system can simultaneously achieve both $o(\log n)$ temperature complexity and $o(\frac{\log n}{\log \log n})$ tile complexity, showing that both versions of an optimal square building scheme have been discovered. This work suggests that temperature change can constitute a natural, dynamic method for providing input to self-assembly systems that is potentially superior to the current technique of designing large tile sets with specific inputs hardwired into the tileset.

1 Introduction

Self-assembly is the ubiquitous process by which objects autonomously assemble into complexes. This phenomenon is common in nature and yet is poorly understood from a mathematical perspective. It is believed that self-assembly technology will ultimately permit the precise fabrication of complex nanostructures. Of particular interest is DNA self-assembly. Double and triple crossover DNA molecules have been designed

that can act as four-sided building blocks for DNA self-assembly [4, 5]. Experimental work has been done to show the effectiveness of using these building blocks to assemble DNA crystals and perform DNA computation [6, 8, 11, 12]. With these building blocks (tiles) in mind, researchers have considered the power of the *tile* self-assembly model.

The tile assembly model extends the theory of Wang tilings of the plane [10] by adding a natural mechanism for growth. Informally, the model consists of a set of four sided Wang tiles whose sides are each associated with a type of glue. The bonding strength between any two glues is determined by a glue function. A special tile in the tile set is denoted as the seed tile. Assembly takes place by starting with the seed tile and attaching copies of tiles from the tile set one by one to the growing seed whenever the total strength of attraction from the glue function meets or exceeds a fixed parameter called the temperature.

In this paper we consider the power of the *multiple* temperature model proposed by Aggarwal et al. [2, 3]. The multiple temperature model generalizes the tile self-assembly model by permitting the temperature of the system to shift up and down. Aggarwal et al. showed that by raising the temperature just once during the assembly process certain shapes could be uniquely assembled using fewer distinct tiles than what is possible for a model with a fixed temperature.

We extend these results by showing how tile sets can be designed so that they assemble supertiles that encode bits of information specified by a sequence of increases and decreases in temperature. We provide a general tile set that is capable of uniquely assembling, for any arbitrary length m binary number, a corresponding supertile that encodes that number, where the encoded binary string is specified by a length O(m) sequence of temperature changes. We then extend this construction by including a constant size set of generic square building tiles that, after a final drop in temperature, read the encoded binary number and uniquely assemble the $n \times n$ square specified by the binary string. We thus provide a constant size set of tiles that are singly capable of uniquely assembling any $n \times n$ square, where

^{*}Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL 60201. Email: kao@cs.northwestern.edu.

[†]Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL 60201. Email: schwellerr@cs.northwestern.edu.

the square assembled is determined by a length $O(\log n)$ temperature sequence which encodes a description of n. This construction stands in sharp contrast to what is possible for a fixed temperature system. For almost all n, Kolmogorov complexity dictates a lower bound of $\Omega(\frac{\log n}{\log \log n})$ distinct tiles required to uniquely assembly an $n \times n$ square for almost all n [9].

While our focus is on the assembly of $n \times n$ squares, we believe the technique of temperature programming should be useful for a number of different self-assembly applications. Interesting tile self-assembly systems can usually be broken up into two parts: An input set of tiles of arbitrary size, and an execution set of tiles of constant size. For example, Rothemund et al. [9] assembled squares using a set of $O(\log n)$ input tiles that uniquely assemble a $\log n$ digit binary number, combined with a constant size set of execution tiles that read the produced binary number and uniquely assemble the corresponding size square. Similarly, tile sets designed for DNA computation require one group of input tiles of arbitrary length designed to encode a given input, and another set of constant size designed for the computation of some procedure such as exclusiveor, evaluation of 3-SAT, etc [6, 8, 11, 12]. work initializes the study of exchanging sets of tiles representing an input for a sequence of temperature

In this paper, we show how to encode the input information for the assembly of $n \times n$ squares into a sequence of $O(\log n)$ temperature changes, rather than explicitly encoding the input into the tile system. This drops the tile complexity of the system to O(1) and provides a generic tile set that can be programmed via temperature changes to assemble any $n \times n$ square. We believe this natural, dynamic method of providing input to a tile system is potentially more practical than explicitly creating a large, hardwired input set of new tiles or DNA molecules for each distinct input n. Further, we suspect that any tile set that follows the basic input, execution framework can be adjusted slightly so as to take input from a short temperature sequence rather than a set of input tiles, similar to our adaptation of square building tiles.

Paper Layout: In Section 2 we define the self-assembly model and state the main result of the paper. In Section 3 we introduce a method of encoding bits of information into self-assembled shapes by shifting temperature, which we apply to assemble arbitrary length binary strings using a general tile set of size O(1). In Section 4 we extend the construction for building binary strings to one for building arbitrary $n \times n$ squares in O(1) tiles and $O(\log n)$ temperature changes.

In Section 5 we discuss a modification for making our constructions more robust. In Section 6 we conclude with a discussion of future research directions.

2 Basics and Main Result

Definitions To describe the tile self-assembly model, we make the following definitions. A tile t in the model is a four sided Wang tile denoted by the ordered quadruple (north(t), east(t), south(t), west(t)). The entries of the quadruples are glue types taken from an alphabet Σ representing the north, east, south, and west edges of the Wang tile, respectively. A tile system is an ordered quadruple $\langle T, s, G, \tau \rangle$ where T is a set of tiles called the *tileset* of the system, τ is a positive integer called the temperature of the system, $s \in T$ is a single tile called the seed tile, and G is a function from Σ^2 to $\{0, 1, \dots, \tau\}$ called the *glue function* of the system. It is assumed that G(x,y) = G(y,x), and there exists a null in Σ such that $\forall x \in \Sigma$, G(null, x) = 0. In this paper we assume the glue function is such that G(x,y) = 0 when $x \neq y$ and denote G(x,x) by G(x)(See [2, 3] for the effect of removing this restriction). |T| is referred to as the *tile complexity* of the system.

Define a configuration to be a mapping from \mathbb{Z}^2 to $T \cup \{\text{empty}\}$, where empty is a special tile that has the null glue on each of its four edges. The shape of a configuration is defined as the set of positions (i,j) that do not map to the empty tile. For a configuration C, a tile $t \in T$ is said to be attachable at the position (i,j) if C(i,j) = empty and $G(\text{north}(t), \text{south}(C(i,j+1))) + G(\text{east}(t), \text{west}(C(i+1,j))) + G(\text{south}(t), \text{north}(C(i,j-1))) + G(\text{west}(t), \text{east}(C(i-1,j))) \geq \tau$. For configurations C and C' such that C(x,y) = empty, C'(i,j) = C(i,j) for all $(i,j) \neq (x,y)$, and C'(x,y) = t for some $t \in T$, define the act of attaching tile t to C at position (x,y) as the transformation from configuration C to C'.

Define the adjacency graph of a configuration C as follows. Let the set of vertices be the set of coordinates (i,j) such that C(i,j) is not empty. Let there be an edge between vertices (x_1,y_1) and (x_2,y_2) iff $|x_1-x_2|+|y_1-y_2|=1$. We refer to a configuration whose adjacency graph is finite and connected as a supertile. For a supertile S, denote the number of non-empty positions (tiles) in the supertile by $\operatorname{size}(S)$. We also note that each tile $t\in T$ can be thought of as denoting the unique supertile that maps position (0,0) to t and all other positions to empty. Throughout this paper we will informally refer to tiles as being supertiles.

A cut of a supertile is a cut of the adjacency graph of the supertile. In addition, for each edge e_i in a cut the edge strength s_i of e_i is the glue strength (from the glue function) of the glues on the abutting edges of the adjacent tiles corresponding to e_i . The cut strength of

a cut c is $\sum s_i$ for each edge e_i in the cut. A supertile is said to be stable at temperature τ if there exists no cut of the supertile with strength less than τ .

2.2 The Assembly Process Assembly takes place by growing a supertile starting with tile s at position (0,0). Any $t \in T$ that is attachable at some position (i,j) may attach and thus increase the size of the supertile. For a given tile system, any supertile that can be obtained by starting with the seed and attaching arbitrary attachable tiles is said to be produced. If this process comes to a point at which no tiles in T can be added, the resultant supertile is said to be terminally produced. For a given shape Υ , a tile system Γ uniquely produces shape Υ if there exists a terminal supertile S of shape Υ such that every supertile derived from the seed can be grown into S. The tile complexity of a shape Υ is the minimum tile set size required to uniquely assemble Υ .

2.3 The Multiple Temperature Model In the multiple temperature model, the integer temperature τ in the tile system description is replaced with a sequence of integers $\{\tau_i\}_{i=1}^k$ called the temperature sequence of the system. The number of temperatures k in the sequence is called the temperature complexity of the system. The size of the largest temperature in the sequence is called the temperature range of the system. In this paper, we require the temperature range to be bounded by a constant.

In a system with k temperatures, assembly takes place in k phases. In the first phase, assembly takes place as in the standard model under temperature τ_1 . Phase 1 continues until no tiles can be added. phase two, tiles can be added or removed under τ_2 . Specifically, at any point during phase 2, if there exists a cut of the resultant supertile with cut strength less than τ_2 , the portion of the supertile occurring on the side of the cut not containing the seed tile may be removed. Also, at any point in the second phase any tile in Tmay be added to the supertile if the tile is attachable at a given position under temperature τ_2 . The second phase of this assembly continues until no tiles can be added or removed. We then go to phase 3 in which tiles may be added and removed under temperature τ_3 . The process is continued up through τ_k . For any given choice of additions and removals such that each of the kphases finishes, the tile system terminally produces the corresponding shape assembled after phase k. If the kphases always finish regardless of the choice of additions and removals, and the terminally produced supertile Ris unique, the tile system uniquely assembles the shape of R.

2.4 Main Result The main result of this paper is the following theorem which shows that there exists a single tile set of constant size that can be efficiently programmed by a series of temperature changes to uniquely assembly essentially any $n \times n$ square.

THEOREM 2.1. There exists a tile set T of size O(1) such that for any $n \geq 22$ there exists a temperature sequence $\{\tau_i\}_{i=1}^k$ of length $k = O(\log n)$ such that T uniquely assembles an $n \times n$ square with temperature sequence $\{\tau_i\}_{i=1}^k$.

This theorem is proven in Section 4. We also show in Section 4 that for almost all n, a tile system that assembles an $n \times n$ square cannot simultaneously achieve $o(\frac{\log n}{\log \log n})$ tile complexity and $o(\log n)$ temperature complexity. This shows that there does not exist a smooth tradeoff between tile complexity and temperature complexity, and that our result constitutes the optimal achievable scheme for any system that hopes to drop tile complexity below the $O(\frac{\log n}{\log \log n})$ bound achieved in [1].

To design the tile set for Theorem 2.1, we first introduce in Section 3 a technique for encoding bits of information into assembled supertiles via temperature shifts, thus permitting the assembly of supertiles that encode arbitrary binary strings. We then extend this construction in Section 4 by adding a constant size set of square building tiles that read a binary string encoded into an input supertile and assemble a corresponding $n \times n$ square. We thus show that it is possible to assemble any $n \times n$ square in O(1) tile complexity and $O(\log n)$ temperature complexity. This is in contrast to the tile complexity lower bound of $\Omega(\frac{\log n}{\log \log n})$ that holds for almost all n for any system that only has a constant number of temperature shifts [9, 3].

3 Programming a Tile Set with Temperature Change

In this section we introduce the *bit-flip gadget* which permits a bit of information to be encoded into a produced supertile by shifting the temperature of the self-assembly system. We then show how these gadgets can be used to encode arbitrary length m binary strings with a fixed size tile set and O(m) temperature changes.

3.1 Bit-Flipping The basic tool used in our constructions in this paper is a set of tiles we collectively refer to as a *bit-flip gadget*. The tiles for the basic gadget are depicted in Figure 1. The idea is that the gadget uniquely assembles a shape that encodes a binary 0 for an initial temperature, then flips the bit and encodes a binary 1 after a change in temperature. At temperature

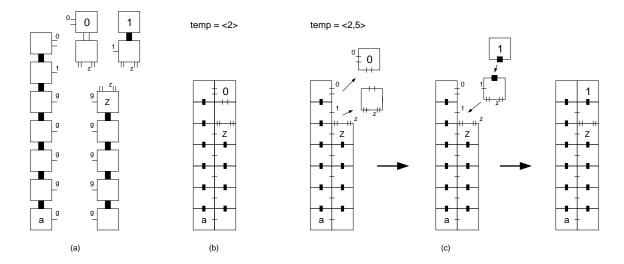


Figure 1: (a) Tiles that implement the bit flip gadget. The number of lines on the side of a tile represents the strength of the corresponding glue. The dark black line denotes a strength 5 glue. (b) At temperature 2, with tile a as the seed tile, the bit flip gadget uniquely assembles a supertile with the 0 tile in the top right corner. (c) By raising the temperature to 5, the 0 tile breaks off and is replaced by the 1 tile.

 $\tau=2$, the tiles in Figure 1 uniquely assemble a supertile containing the 0 tile in the top right corner. By raising the temperature to $\tau=5$, the two tiles in the east column that lie north of the z tile fall off and are replaced by two new tiles, the 1 tile being placed in the top right corner where the 0 tile was originally. Thus, the system uniquely assembles a supertile with tile 0 in the top right corner for temperature sequence $\tau=\langle 2\rangle$, and uniquely assembles a supertile with tile 1 in the top right corner for temperature sequence $\tau=\langle 2,5\rangle$.

In addition to permitting a single bit of information to be encoded into an assembled supertile, bit flip gadgets can be used to control the length of an assembled supertile. That is, the default 0 tile can constitute a *dead-end* in that no more tiles can attach to it, whereas the flipped 1 tile leads to the assembly of more tiles, possibly another copy of the bit flip gadget. The newly formed gadget can in turn be set to a dead-end, or flipped to continue growth. Combining these two uses for gadgets, we now show how a slightly modified version of the basic bit-flip gadget permits the assembly of arbitrary binary strings of arbitrary length.

3.2 Building Arbitrary Binary Strings with O(1) Tiles To assemble a supertile which encodes an arbitrary binary string $b_0b_1 \dots b_{m-1}$, we use a modified version of the bit flip gadget given in Figure 2. The top half of this gadget encodes either a 0 or a 1, while the bottom half encodes either an x or a y. See Figure 3 for an example of how this tile set assembles for a given

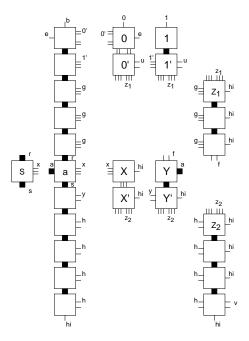


Figure 2: These tiles implement a modified bit flip gadget that constitutes a tile set of constant size that can uniquely assemble a supertile that represents any arbitrary binary string of any length m, where the string assembled is determined by a length O(m) temperature sequence. The dark black lines denote strength 9 glues. The glues 0, 1, b, u, v, and hi are not used to assemble the binary string, but are used when the tile set is extended to assemble $n \times n$ squares in Section 4.

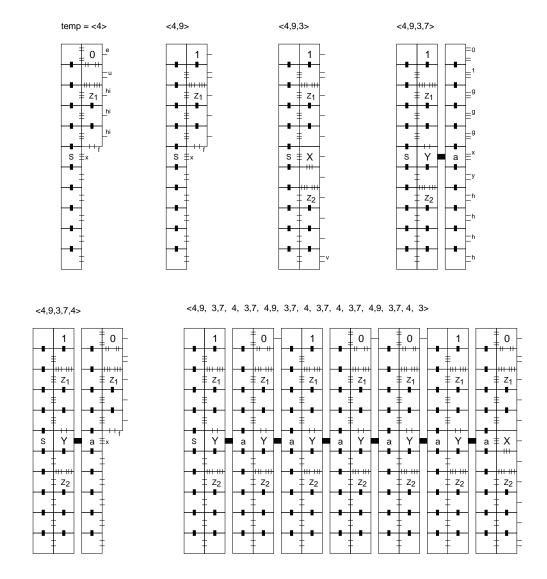


Figure 3: A sequence of temperature changes to uniquely assemble a supertile that encodes the string 1010010.

temperature sequence. The basic idea is that the top half of the gadget will encode a single bit of the given binary string. The bottom half, on the other hand, will be set to the x tile if the corresponding gadget is meant to encode the final bit of the bit string, whereas the y tile will serve the purpose of creating another copy of the gadget to encode another bit. Thus, by flipping the bottom half of the gadgets, the length of the bit string can be precisely controlled, while flipping the top half of the gadget specifies the value of each corresponding bit

THEOREM 3.1. For any given length m binary string $b = b_0b_1 \cdots b_{m-1}$, there exists a sequence of temperatures, all less than or equal to 9, of length O(m) such

that the tile set of Figure 2 uniquely assembles a supertile S that encodes b. Specifically, S is an $11 \times 2m$ rectangle such that the tile in the top row, 2i+1 in from the west, is the 0 tile if $b_i=0$ and the 1 tile if $b_i=1$.

Proof. For any arbitrary length m binary number $b = b_0b_1 \dots b_{m-1}$, consider a corresponding length 4m-1 temperature sequence $\tau^b = \langle \tau_0, \dots \tau_{4m-2} \rangle$ defined as follows.

$$\tau_{4i} = 4 \text{ for } i = 0, \dots, m - 1
\tau_{4i+1} = \begin{cases} 4 \text{ if } b_i = 0 \\ 9 \text{ if } b_i = 1 \end{cases}
\tau_{4i+2} = 3 \text{ for } i = 0, \dots, m - 1
\tau_{4i+3} = 7 \text{ for } i = 0, \dots, m - 2$$

As an example, for b = 010, we have the correspond-

ing temperature sequence $\langle 4, 4, 3, 7, 4, 9, 3, 7, 4, 4, 3 \rangle$. Conceptually, the temperature sequence is broken up into groups of four, where the sequences $\langle 4 \rangle$ and $\langle 4, 9 \rangle$ encode a 0 or a 1 respectively into the top half of the gadget, and the sequence $\langle 3, 7 \rangle$ flips the bottom half of the gadget to produce another copy of the gadget. So, at temperature 4, an 11×2 rectangle is uniquely assembled with the bottom half of the second column missing, and the two top tiles of the second column being the 0 and 0' tiles. The resultant supertile is stable at temperature 8, but tile 0 can be removed at temperature 9, which in turn leads to the removal of 0'. The 1' tile can then attach at temperature 9 north of Z_1 , followed by the 1 tile.

Whether or not the temperature is raised to 9, by lowering the temperature to 3, the lower half of the second column of the gadget is filled in with the x tile placed east of the seed. By raising the temperature to 7, the x tile is exchanged for the y tile and the first column of a second gadget is assembled, with the a tile in place of the seed tile. Further, notice that this new supertile has become stable at temperature 9, rather than 8, since if the initial gadget was set to 0, the first column of the second gadget stabilizes it with an additional strength 1 bond. By dropping the temperature to 4, and optionally raising it to 9, a 0 or a 1 respectively is encoded into the second gadget. A drop to temperature 3 fills in the rest of the gadget, and a raise to temperature 7 begins a new gadget and stabilizes the previous gadget at temperature 9. This process continues until the entire $11 \times m$ rectangle is assembled with the corresponding binary number encoded in the top row.

4 Building Arbitrary $n \times n$ Squares in O(1) Tiles

We now provide an application for the tile set of Section 3.2 for assembling an arbitrary binary number in O(1) tile complexity. We combine this tile set with a tile set for building $n \times n$ squares. The basic idea is similar to previous square building constructions [9, 1] where a constant number of square building tiles are combined with $O(\log n)$ or $O(\frac{\log n}{\log \log n})$ tiles that assemble a $\log n$ digit binary number. The square building tiles then, in essence, read the inputted binary number and assemble the square uniquely described by the number. These constructions require a large tile complexity since they must build the input binary string. The tile complexity for assembly of almost all $n \times n$ squares for a system that only changes temperature O(1) times is $\Omega(\frac{\log n}{\log \log n})$ [9, 3]. However, with $O(\log n)$ temperature shifts we can build the binary number in O(1) tiles, and thus finish the entire square in O(1) tiles as well.

Theorem 4.1. There exists a tile set T of size O(1)

such that for any $n \geq 22$ there exists a temperature sequence $\{\tau_i\}_{i=1}^k$ of length $k = O(\log n)$ such that T uniquely assembles an $n \times n$ square with temperature sequence $\{\tau_i\}_{i=1}^k$.

Proof. Consider the tiles from Figure 2 with the added tiles of Figure 4. For any $n \geq 22$, let $v = 2^{\lceil \log n \rceil} - n +$ $11+2\lceil \log n \rceil$. Note that n=22 is the smallest value such that $v < 2^{\lceil \log n \rceil}$. Now, consider the length $4\lceil \log n \rceil - 1$ temperature sequence of Theorem 3.1 for encoding the length $\lceil \log n \rceil$ binary representation of the integer v. To this sequence add a final drop in temperature to 2. Thus, the first $4\lceil \log n \rceil - 1$ temperature changes uniquely assemble an $11 \times 2\lceil \log n \rceil$ rectangle encoding the integer v. At temperature 2, the binary starter tiles can attach and begin the incrimination of a fixed length binary counter, similar to the constructions in [9]. The binary counter grows to a total length of $2^{\lceil \log n \rceil} - v =$ $n-11-\lceil \log n \rceil$. With the addition of the length 11 seed rectangle and the $2\lceil \log n \rceil$ positions filled in by the stair step tiles, a width and length of exactly n is achieved. \square

From Theorem 2.1 and the fact that any square can be assembled in $O(\frac{\log n}{\log \log n})$ tile complexity at the fixed temperature 2 [1], we get the following corollary.

COROLLARY 4.1. For any $n \ge 1$, there exists a multiple temperature tile system with tile complexity O(1) and temperature complexity $O(\log n)$ that uniquely assembles an $n \times n$ square.

Thus, we have shown that all the tile complexity for the assembly of an $n \times n$ square can be transferred into a length $O(\log n)$ temperature sequence. A natural question to ask is whether this can be reduced, or if there can be a smooth tradeoff between tile complexity and temperature complexity. The next theorem shows that there is no tradeoff.

THEOREM 4.2. For a tile set T that uniquely assembles an $n \times n$ square under temperature sequence $\{\tau_i\}_{i=1}^k$, for almost all n it cannot be the case that both $|T| = o(\frac{\log n}{\log \log n})$ and $k = o(\log n)$.

Proof. The Kolmogorov complexity of an integer N with respect to a universal Turing machine U is $K_U(N) = \min |p|$ s.t $U(p) = b_N$ where b_N is the binary representation of N. A straightforward application of the pigeonhole principle yields that $K_U(N) \geq \lceil \log N \rceil - \Delta$ for at least $1 - (\frac{1}{2})^{\Delta}$ of all N (see [7] for results on Kolmogorov complexity). Thus, for any $\epsilon > 0$, $K_U(N) \geq (1 - \epsilon) \log N = \Omega(\log N)$ for almost all N. This tells us that if we had a Turing machine that takes as input a tile system and outputs the maximum length of the shape produced by the given tile system, then

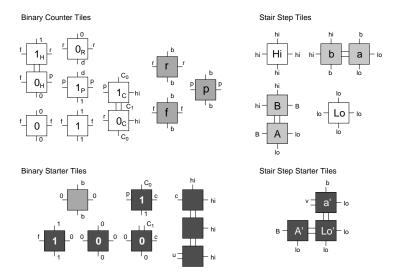


Figure 4: A tile set for reading a binary string encoded into a supertile and building a corresponding $n \times n$ square.

the total size in bits of the machine plus the size in bits of a tile system that uniquely assembles an $N \times N$ square is $\Omega(\log N)$. Such a machine exists for the multiple temperature model [2,3], implying that an encoding into bits of a tile system that uniquely assembles an $n \times n$ square must be of length $\Omega(\log n)$ for almost all n. [9] showed that a tileset and glue function can be encoded in $o(\log n)$ bits if the number of tiles in the set is $o(\frac{\log n}{\log \log n})$. Therefore, since a length k temperature sequence can be encoded in O(k) bits (assuming, as we do, a constant temperature range), a tile system with tile complexity $o(\frac{\log n}{\log \log n})$ and temperature complexity $o(\log n)$ can be completely encoded into a length $o(\log n)$ bit string, which cannot happen for almost all n.

Thus, there are two possible versions of an optimal square building assembly scheme. The first is one which obtains O(1) temperature complexity and $O(\frac{\log n}{\log \log n})$ tile complexity, which is achieved in [1], and the second is one which obtains temperature complexity $O(\log n)$ and tile complexity O(1), which is obtained by Corollary 4.1.

5 Adding Robustness

In this section we discuss how to modify the bit flip gadget construction to make it robust against certain types of potential assembly errors. In particular, the issue of concern is that the standard tile assembly model assumes that tiles attach to the growing seed supertile as singleton tiles. However, it is plausible to believe that in reality, singleton tiles could come together away from the seed to form large supertiles,

which could then cooperatively attach to the seed to create a resultant supertile that could not be created under the standard model. For example, consider the bit flip gadget tiles in Figure 1. It is plausible to believe that in implementation, the z tile and the tile to its south could come together independent of the seed tile and attach as a unit at only temperature 2, even without the placement of the 0 tile, due to the combined strength of the two strength 1 g glues. If this were to happen, the construction would not be unique as either a 0 tile or a 1 tile could then be placed in the top right corner. This non-uniqueness would prohibit the ability to program a bit of information into the supertile.

To address this concern, we modify the gadget so that the assembly is not only unique under the *standard* tile assembly model, but unique under a model in which tiles can come together and be added as supertiles as well. Consider the following assembly model introduced in [2, 3].

The Multiple Tile Model. In the multiple tile model tiles can combine into supertiles in a two-handed fashion before being added to the growing seed supertile. More specifically, a tile set T and a temperature τ have a corresponding set of addable supertiles $W(T,\tau)$. Intuitively, this set constitutes the set of supertiles that can potentially be attached to the growing seed supertile. This set is defined recursively. First, $T \subseteq W$. Second, for any two supertiles $A, B \in W$, if A and B can be abutted together to form a supertile $A \oplus B$ such that the total strength from the glue function of all abutting edges of the two supertiles meets or exceeds τ .

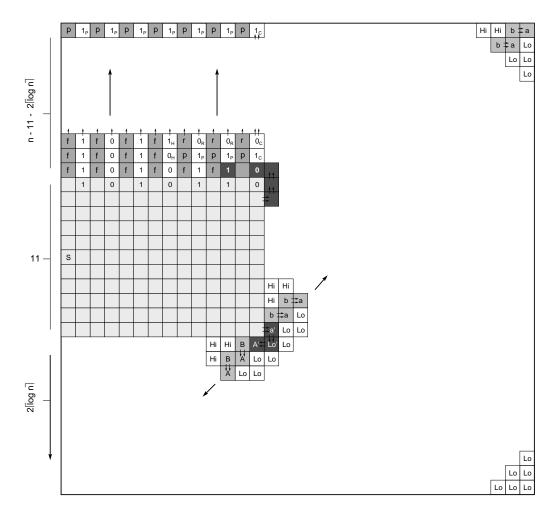


Figure 5: The assembly of a 67×67 square.

then $A \oplus B$ is also in $W(T,\tau)$. Given this set of addable supertiles, assembly takes place in the same fashion as in the standard model, except that attachments to the growing seed supertile come from the set $W(T,\tau)$, rather than just T. For a more technical definition of the multiple tile model see [2, 3].

From this definition, we see that the constructions so far in this paper are not unique under this model. However, we can make a modification to the bit flip gadget construction so that its assembly is unique. The key is to replace the chain of tiles south of the z tile with a square block of tiles. Consider the tiles for the multiple tile bit flip gadget given in Figure 6. The first property of this system is that the tiles that are placed south of the z tiles are placed cooperatively at temperature 4 with two weaker strength 3 glues. Thus, at temperature four, none of the tiles south of the z tile

can come together independent of the seed, and thus cannot be placed before the placement of the initial 0 tile.

The second important property of this set is that there are three columns of tiles south of the Z tiles. This serves the purpose of holding the Z tiles in place, as three distinct strength 3 glues are needed to stabilize Z at the higher temperature 9. Finally, note that the Z_3 and B_3 tiles are connected with strength 9 glues. All tiles in the 4×3 block of tiles including the Z row have at least 3 neighbors with the exception of the two corner tiles. These tiles thus need to be attached with strength at least 6 on one of their two edges to maintain stability at temperature 9.

By making modifications to the multiple tile bit flip gadget similar in spirit to the modifications made to the original gadget, we get corresponding constructions for $n \times n$ squares.

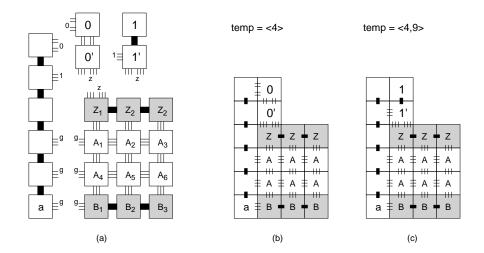


Figure 6: (a) Tiles that implement the multiple tile bit flip gadget. Dark black lines denote strength 9 glues. (b) At temperature 4 a supertile with the 0 tile at the top of the second column is assembled. (c) By raising the temperature to 9, the 0 tile breaks off and is replaced by the 1 tile.

LEMMA 5.1. Let $s_1, \ldots s_7$ be positive integers such that:

- 1. $s_1 < s_2 < s_3 < s_4 < s_5 < s_6 < s_7$
- $2. 2s_4 < s_7 < 2s_4 + s_1$
- 3. $s_7 \le s_3 + s_5$
- 4. $s_7 \leq 3s_2$
- $5. \ 2s_3 < s_6 \le s_2 + s_4$
- 6. $s_4 \leq 2s_2$.

Further, for any arbitrary length m binary number $b = b_0b_1...b_{m-1}$, define the corresponding length 4m-1 temperature sequence $\tau^b = \langle \tau_0, \ldots \tau_{4m-2} \rangle$ as follows.

$$\tau_{4i} = s_4 \text{ for } i = 0, \dots, m-1
\tau_{4i+1} = \begin{cases} s_4 \text{ if } b_i = 0 \\ s_7 \text{ if } b_i = 1 \end{cases}
\tau_{4i+2} = s_3 \text{ for } i = 0, \dots, m-1
\tau_{4i+3} = s_6 \text{ for } i = 0, \dots, m-2$$

Then, the tileset given in Figure 7 uniquely assembles a $12 \times 4m$ rectangle under the multiple tile model for temperature sequence τ^b such that the tile in the top row, 4i+1 in from the west, is labeled 0 if $b_i=0$ and 1 if $b_i=1$.

THEOREM 5.1. For any $n \ge 1$, there exists a multiple temperature tile system with tile complexity O(1) and temperature complexity $O(\log n)$ that uniquely assembles an $n \times n$ square under the multiple tile model.

Proof. Note that the integers $s_1 = 3$, $s_2 = 7$, $s_3 = 8$, $s_4 = 10$, $s_5 = 13$, $s_6 = 17$ and $s_7 = 21$ satisfy the

linear constraints in Lemma 5.1. The theorem thus follows from Lemma 5.1 and the observation that a trivial modification to the tilesets in Figures 7 and 4 permit the extension from building an arbitrary binary number to the building of an $n \times n$ square as is done in Theorem 2.1. The uniqueness of assembly under the multiple tile model for the binary counter tiles is shown in [2].

6 Future Work

We have shown that there exists a general tile set capable of building any $n \times n$ square specified by a sequence of temperature changes. More generally, is it possible to have a general shape building tile set that can be programmed to assemble any arbitrary shape via a temperature sequence that encodes a compact description of that shape? Another direction is to show that there exists a tile set that simulates an arbitrary turing machine with its input specified by a temperature sequence. A third direction is to consider how various error correcting techniques used in other work can be incorporated into temperature programmed assembly schemes. Another open question is whether or not tile complexity and temperature complexity can be reduced by increasing temperature range. question is interesting in that it seems to be the only remaining place left to hide information in a tile system. Finally, it would be interesting to implement and test the temperature programming techniques of this paper with real self-assembly systems.

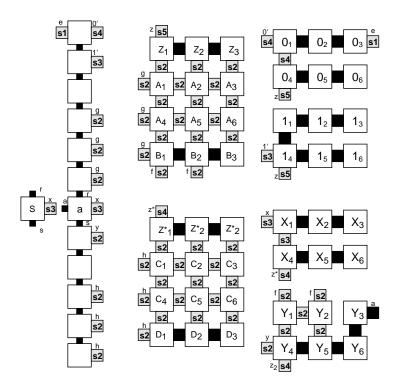


Figure 7: These tiles constitute a tile set of constant size that can uniquely assemble a supertile under the multiple tile model that represents any arbitrary binary string. The strength of each glue is given by an index s_i . Let $s_1 = 3$, $s_2 = 7$, $s_3 = 8$, $s_4 = 10$, $s_5 = 13$, $s_6 = 17$ and $s_7 = 21$ where s_7 denotes the strength of the glues denoted by dark black lines and s_6 is a value used in the temperature sequence of the tile system.

References

- [1] L. Adleman, Q. Cheng, A. Goel, and M. Huang. Running time and program size for self-assembled squares. pages 740–748, 2001.
- [2] G. Aggarwal, Q. Cheng, M. H. Goldwasser, M.-Y. Kao, P. M. de Espanes, and R. T. Schweller. Complexities for generalized models of self-assembly. SIAM Journal on Computing, 34:1493–1515, 2005.
- [3] G. Aggarwal, M. H. Goldwasser, M.-Y. Kao, and R. T. Schweller. Complexities for generalized models of self-assembly. In *Proceedings of the fifteenth annual ACM-SIAM symposium on Discrete algorithms*, pages 880–889. Society for Industrial and Applied Mathematics, 2004
- [4] T.-J. Fu and N. C. Seeman. DNA double-crossover molecules. *Biochemistry*, 32:3211–3220, 1993.
- [5] T. H. LaBean, H. Yan, J. Kopatsch, F. Liu, E. Winfree, H. J. Reif, and N. C. Seeman. The construction, analysis, ligation and self-assembly of DNA triple crossover complexes. J. Am. Chem. Soc., 122:1848–1860, 2000.
- [6] M. G. Lagoudakis and T. H. Labean. 2D DNA selfassembly for satisfiability. In Proceedings of the 5th DIMACS Workshop on DNA Based Computers, pages 459–468, June 26 1999.

- [7] M. Li and P. Vitanyi. An Introduction to Komogorov Complexity and Its Applications (Second Edition). Springer Verlag, New York, 1997.
- [8] J. Reif. Local parallel biomolecular computation. In *Proceedings of the 3rd Annual DIMACS Workshop on DNA Based Computers*, June 23-26 1997.
- [9] P. Rothemund and E. Winfree. The program-size complexity of self-assembled squares. In *Proceedings* of the 32nd Annual ACM Symposium on Theory of Computing, pages 459–468, 2000.
- [10] H. Wang. Proving theorems by pattern recognition. Bell System Technical Journal, 40:1–42, 1961.
- [11] E. Winfree, F. Liu, L. Wenzler, and N. Seeman. Design and self-assembly of two-dimensional DNA crystals. *Nature*, 394:539–544, August 1998.
- [12] E. Winfree, X. Yang, and N. C. Seeman. Universal computation via self-assembly of DNA: Some theory and experiments. In *Proceedings of the 3rd Interna*tional Meeting on DNA Based Computers, June 10-12 1996.