

# COMPLEXITIES FOR GENERALIZED MODELS OF SELF-ASSEMBLY\*

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**Abstract.** In this paper, we study the complexity of self-assembly under models that are natural generalizations of the tile self-assembly model. In particular, we extend Rothemund and Winfree's study of the tile complexity of tile self-assembly [9]. They provided a lower bound of  $\Omega(\frac{\log N}{\log \log N})$  on the tile complexity of assembling an  $N \times N$  square for almost all  $N$ . Adleman et al. [1] gave a construction which achieves this bound. We consider whether the tile complexity for self-assembly can be reduced through several natural generalizations of the model. One of our results is a tile set of size  $O(\sqrt{\log N})$  which assembles an  $N \times N$  square in a model which allows flexible glue strength between non-equal glues. This result is matched for almost all  $N$  by a lower bound dictated by Kolmogorov complexity. For three other generalizations, we show that the  $\Omega(\frac{\log N}{\log \log N})$  lower bound applies to  $N \times N$  squares. At the same time, we demonstrate that there are some other shapes for which these generalizations allow reduced tile sets. Specifically, for thin rectangles with length  $N$  and width  $k$ , we provide a tighter lower bound of  $\Omega(\frac{N^{\frac{1}{k}}}{k})$  for the standard model, yet we also give a construction which achieves  $O(\frac{\log N}{\log \log N})$  complexity in a model in which the temperature of the tile system is adjusted during assembly. We also investigate the problem of verifying whether a given tile system uniquely assembles into a given shape; we show that this problem is NP-hard for three of the generalized models.

**Key words.** Kolmogorov complexity, polyominoes, self-assembly, tile complexity, tilings, Wang tiles

**AMS subject classifications.** 05B45, 05B50, 52C20, 52C45, 68Q17, 68Q25, 68Q30

**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, 12, 13]. With these building blocks (tiles) in mind, researchers have considered the power of the *tile* self-assembly model.

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\*A preliminary form of this paper appeared in *Proceedings of the 15th Annual ACM-SIAM Symposium on Discrete Algorithms*, 2004, pp. 873-882.

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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 focus on two fundamental complexities relating to this model. The first is the *tile complexity* of self-assembled shapes, defined as the minimum number of distinct Wang tiles required to assemble the shape. Rothmund and Winfree [9] introduced this concept and considered the tile complexity of self-assembled squares. The second is the complexity of verifying whether or not a system of tiles uniquely assembles into a given shape. This problem is considered by Adleman et al. [2] and shown to have a polynomial time solution for the standard tile assembly model.

We extend these studies of tile complexity and shape verification by considering the removal of various restrictions the standard model places on the assembly process. From this we obtain four natural generalizations of the tile assembly model that exhibit significant differences in tile complexity and the complexity of shape verification from that of the standard model. This suggests that some previously derived bounds on tile self-assembly are artifacts of artificial restrictions placed on the standard tile assembly model, rather than bounds on the actual process of self-assembly. Informally, the generalized models are defined as follows.

In the *flexible glue* model, the restriction imposed by Rothmund and Winfree [9] that differing glue types have bonding strength of zero is removed. In the *multiple temperature* model, the temperature of the system is permitted to change during the assembly process. In the *multiple tile* model, tiles may cooperate by assembling into supertiles before being added to the growing result. In the *unique shape* model, a system *uniquely assembles* a shape if the shape of its resultant supertiles is unique, though its produced supertile may not be unique.

In the standard tile assembly model, Kolmogorov complexity dictates a lower bound of  $\Omega(\frac{\log N}{\log \log N})$  on the tile complexity of self-assembling  $N \times N$  squares for almost all values of  $N$  [9]. Adleman et al. [1] showed how to reach this bound for all  $N$ . We show (in Theorem 6.1) that this lower bound also applies to each of the generalized models except for the flexible glue model. For this model, Kolmogorov complexity only dictates an  $\Omega(\sqrt{\log N})$  lower bound for almost all  $N$  (as shown in Theorem 6.2). We show how to achieve this bound for all  $N$  by encoding an arbitrary  $(\log N)$ -bit binary number into the glue function (Theorem 5.1).

Additionally, for some of the models we provide a lower bound of  $\Omega(\frac{N}{k})$  (see Theorem 3.1) for assembling *thin* width  $k$ , length  $N$  rectangles (a  $k \times N$  rectangle is *thin* if  $k < \frac{\log N}{\log \log N - \log \log \log N}$ ). These lower bounds show that it can require significantly larger tile sets to assemble thinner rectangles than thicker rectangles. With this in mind, we utilize the multiple temperature model to construct a thin rectangle by first constructing a thicker rectangle using a small tile set. We then raise the temperature of the system so that portions of the larger rectangle fall apart, leaving the desired rectangle (Theorem 4.1).

Given a tile system, Adleman et al. [2] give an algorithm to verify whether the tile system uniquely assembles into a given supertile. However, in the unique shape model, a tile system could uniquely assemble into a shape even if it does not produce a

TABLE 1.1

This table gives the general flavor of our results regarding upper and lower asymptotic bounds on tile complexity under the generalized models for  $k \times N$  rectangles, as well as the complexity of the UNQ-SHAPE problem, but the reader should reference precise details in the stated theorems. A rectangle is thin when  $k < \frac{\log N}{\log \log N - \log \log \log N}$  and thick otherwise. NP-X denotes the class of decision problems not in NP or co-NP unless  $P = NP$ .

Complexity of Self-Assembling $k \times N$ Rectangles, $k \leq N$ , and Shape Verification					
	Thin Rectangles		Thick Rectangles		UNQ-SHAPE
	LB	UB	LB	UB	
Standard	$\frac{N^{\frac{1}{k}}}{k}$ (Thm. 3.1)	$N^{\frac{1}{k}}$ (Thm. 3.2)	$\frac{\log N}{\log \log N}$ (see [9])	$\frac{\log N}{\log \log N}$ (see [1])	P (see [2])
Flexible Glue	$\frac{N^{\frac{1}{k}}}{k}$ (Thm. 3.1)	$N^{\frac{1}{k}}$ (Thm. 3.2)	$\sqrt{\log N}$ (Thm. 6.2)	$\sqrt{\log N}$ (Thm. 5.1)	P (see [2])
Multiple Temperature	$\frac{\log N}{\log \log N}$ (Thm. 6.1)	$\frac{\log N}{\log \log N}$ (Thm. 4.1)	$\frac{\log N}{\log \log N}$ (Thm. 6.1)	$\frac{\log N}{\log \log N}$ (see [1])	NP-X (Thm. 7.6)
Multiple Tile	$\frac{\log N}{\log \log N}$ (Thm. 6.1)	$N^{\frac{1}{k}}$ (Thm. 3.2)	$\frac{\log N}{\log \log N}$ (Thm. 6.1)	$\frac{\log N}{\log \log N}$ (see [1])	NP-X (Thm. 7.7)
Unique Shape	$\frac{N^{\frac{1}{k}}}{k}$ (Thm. 3.1)	$N^{\frac{1}{k}}$ (Thm. 3.2)	$\frac{\log N}{\log \log N}$ (Thm. 6.1)	$\frac{\log N}{\log \log N}$ (see [1])	Co-NPC (Thm. 7.1)

unique supertile. We investigate the problem of verifying whether a given tile system uniquely assembles into a given shape in the unique shape model, and show that this problem is co-NP-complete (Theorem 7.1). We also show that the problem of determining whether a tile system uniquely assembles into a given supertile is not in NP or co-NP for the multiple temperature model (Theorem 7.6) or the multiple tile model (Theorem 7.7) unless  $P = NP$ . These results are in contrast to the polynomial-time verification algorithm for the standard model [2].

**Paper Layout:** In Section 2 the standard tile model is defined as well as the generalized models. In Section 3 we introduce a construction for assembling  $k \times N$  rectangles and provide a lower bound on the tile complexity of such rectangles. In Section 4 we use this construction to show how the multiple temperature model can reduce tile complexity when  $k \ll N$ . In Section 5 we use the flexible glue model to reduce the tile-complexity of assembling  $N \times N$  squares from  $\Theta(\frac{\log N}{\log \log N})$  to  $\Theta(\sqrt{\log N})$ . In Section 6 we discuss the lower bounds for assembling shapes of extent  $N$  for the generalized models as dictated by Kolmogorov complexity. Finally, in Section 7, we show that shape verification is co-NP-complete in the unique shape model and not in NP or co-NP unless  $P = NP$  for the multiple temperature and multiple tile models.

## 2. Basics.

**2.1. The Standard Model.** For alternate descriptions of the tile assembly model, see [1, 2, 9, 11]. Briefly, a tile  $t$  in the model is a four sided Wang tile denoted by the ordered quadruple  $(\text{north}(t), \text{east}(t), \text{south}(t), \text{west}(t))$ . The entries of

the quadruples are glue types taken from an alphabet  $\Sigma$  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,  $\tau$  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  $\Sigma^2$  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  $\Sigma$  such that  $\forall x \in \Sigma, G(\mathbf{null}, x) = 0$ . In the standard tile assembly model [1, 2, 9], the glue function is such that  $G(x, y) = 0$  when  $x \neq y$ . When dealing with the standard glue model, denote  $G(x, x)$  by  $G(x)$ .

Define a *configuration* to be a mapping from  $\mathbb{Z}^2$  to  $T \cup \{\mathbf{empty}\}$ , 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  $C(i, j) = \mathbf{empty}$  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  $C(x, y) = \mathbf{empty}$ ,  $C'(i, j) = C(i, j)$  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  $\text{size}(S)$ . 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 define the *edge strength*  $s_i$  of  $e_i$  to be the glue strength (from the glue function) of the glues on the abutting edges of the adjacent tiles corresponding to  $e_i$ . Now define the *cut strength* of a cut  $c$  to be  $\sum s_i$  for each edge  $e_i$  in the cut.

In the standard model, 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  $\Upsilon$ , a tile system  $\Gamma$  *uniquely produces* shape  $\Upsilon$  if there exists a terminal supertile  $S$  of shape  $\Upsilon$  such that every supertile derived from the seed can be grown into  $S$ . The *tile complexity* of a shape  $\Upsilon$  is the minimum tile set size required to uniquely assemble  $\Upsilon$  under a given assembly model. While the definition of unique shape production provided here is the same as in [1, 2, 9], we note that it is somewhat unnatural in that it requires unique production of supertiles. In section 2.2 we introduce a model that utilizes a more natural definition of unique shape production.

## 2.2. Four Generalized Models.

**The Multiple Temperature Model.** In the *multiple temperature* model, the integer temperature  $\tau$  in the tile system description is replaced with a sequence of integers  $\{\tau_i\}_{i=1}^k$  called the *temperature sequence* of the system. A system with  $k$  temperatures in its temperature sequence is said to be a *k-temperature* system.

In a  $k$ -temperature system, assembly takes place in  $k$  phases. In the first phase, assembly takes place as in the standard model under temperature  $\tau_1$ . Phase 1 continues until no tiles can be added. In phase two, tiles can be added or removed under  $\tau_2$ . Specifically, at any point during phase 2 if there exists a cut of the resultant supertile with cut strength less than  $\tau_2$ , 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  $T$  may be added to the supertile if the tile is attachable at a given position under temperature  $\tau_2$ . 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  $\tau_3$ . The process is continued up through  $\tau_k$ . For any given choice of additions and removals such that each of the  $k$  phases finishes, the tile system *terminally* produces the corresponding shape assembled after phase  $k$ . If the  $k$  phases always finish regardless of the choice of additions and removals, and the terminally produced supertile  $R$  is unique, the tile system *uniquely assembles* the shape of  $R$  under the  $k$ -temperature model.

**The Flexible Glue Model.** In the *flexible glue* model, the restriction that  $G(x, y) = 0$  for  $x \neq y$  is removed.

**The Unique Shape Model.** In the *unique shape* model, we redefine what is meant for a system to uniquely produce a shape  $S$ . In this model, a tile system uniquely produces a shape  $S$  iff all producible supertiles can be grown into a terminal supertile with shape  $S$ . Thus, the system may produce many different terminal supertiles as long as they all have the desired shape.

**The Multiple Tile Model.** In the *multiple tile* model with parameter  $q$ , tiles can combine into supertiles of size at most  $q$  before being added to the growing seed supertile. Attaching a supertile is much like attaching a singleton tile. Intuitively, two supertiles attach to one another by abutting together and sticking if the total edge strength of the abutting edges meets or exceeds the temperature  $\tau$ . However, the formal definition of a supertile is a connected configuration of tiles on  $\mathbb{Z}^2$ . This definition makes a distinction between two supertiles that are equal up to translation. But, we actually wish to think of two such supertiles as the same supertile. We therefore use the following formal definition of supertile attachment which generalizes the notion of singleton tile attachment.

For any two supertiles  $A$  and  $B$ , define  $A \oplus B$  to be the configuration obtained by setting all empty positions  $A(i, j)$  equal to  $B(i, j)$ . Further, we say  $A \oplus B$  is *valid* if it is a supertile (i.e., it is connected), and if for all  $(i, j)$  either  $A(i, j) = \mathbf{empty}$  or  $B(i, j) = \mathbf{empty}$ . For a valid supertile  $A \oplus B$ , denote the cut defined by separating all the tile positions initially in  $A$  from all the tile positions initially in  $B$  as the *border* cut. For a supertile  $A$  and integers  $x$  and  $y$ , let  $A_{x,y}$  denote the configuration obtained by translating  $A$  by  $x$  units along the  $x$ -axis and  $y$  units along the  $y$ -axis. Finally, for a given temperature  $\tau$ , supertile  $B$  can be attached to supertile  $A$  to form supertile  $A \oplus B_{x,y}$  if  $A \oplus B_{x,y}$  is valid and the cut strength of the border of  $A \oplus B_{x,y}$  is at least  $\tau$ .

Having defined how to attach supertiles, we now define multiple tile systems. A tile system in the multiple tile model is a quintuple  $\langle T, s, G, \tau, q \rangle$ . Intuitively, in a multiple tile system any supertile of size at most  $q$  that can be obtained by combining two smaller addable supertiles is also an addable supertile. The assembly process

then permits any addable supertile to attach to the growing seed supertile if the tile can be placed so that the abutting edges of the two supertiles have a total strength that meets or exceeds the temperature  $\tau$ . For such a system define a set of *addable* supertiles  $W_T$  as follows: First,  $T \subseteq W_T$ . Second, if there exists  $A, B \in W_T$  such that  $\text{size}(A) + \text{size}(B) \leq q$ , and  $B$  can be attached to  $A$  under temperature  $\tau$  to obtain  $A \oplus B_{x,y}$ , then  $A \oplus B_{x,y}$  is also in  $W_T$ . In the multiple tile assembly model, supertiles from the set  $W_T$  may be added as well as from  $T$ . Specifically, any supertile that is in the set of addable supertiles  $W_T$  that is attachable to the seed supertile under temperature  $\tau$  can attach and increase the size of the seed supertile. For  $q = 1$ , we have  $W_T = T$ , which gives us the standard model of assembly.

**3. The Assembly of  $k \times N$  Rectangles.** In this section, we present both an upper and lower bound for assembling  $k \times N$  rectangles for arbitrary  $k$  and  $N$ . The upper bound comes from a simple construction which constitutes a  $k$ -digit, base- $N^{\frac{1}{k}}$  counter and has tile complexity  $\Theta(N^{\frac{1}{k}} + k)$ . In later sections, we use modifications of this counter to show how both the 2-temperature and flexible glue model can reduce tile complexity of certain shapes. Additionally, for the case of  $k = \log N$ , this construction constitutes a  $\log N$ -bit, base-2 counter which assembles a  $\log N \times N$  block. The tile set created by this special case is used in [3] to assemble a  $\log N \times N$  block in optimal *time complexity* (as defined in [1]) of  $\Theta(N)$ . This permits the assembly of  $N \times N$  squares in optimal tile complexity and optimal time complexity as in [1], but does so in a much simpler fashion and uses only temperature  $\tau = 2$ .

**THEOREM 3.1.** *The tile complexity of self-assembling a  $k \times N$  rectangle is  $\Omega(\frac{N^{\frac{1}{k}}}{k})$  for the standard model, the unique shape model, and the flexible glue model.*

*Proof.* Suppose there exists a tile system with fewer than  $(\frac{N}{2(k!)})^{\frac{1}{k}}$  distinct tile types, which uniquely assembles a  $k \times N$  rectangle. Then there must be fewer than  $\frac{N}{2(k!)}$  distinct  $k$  tile columns consisting of these tiles. So in a  $k \times N$  configuration, there must exist some  $k$ -tile sequence which is repeated for more than  $2(k!)$  of the columns. And under the standard, unique shape, and flexible glue models, for each of these identical columns we can assign an ordering on the  $k$  tiles that corresponds to a possible relative order in which the  $k$  tiles of the given column could be attached (in the multiple tile model, groups of tiles may be attached simultaneously, and thus this ordering is not sufficient). Since there are at most  $k!$  orderings possible, we get that at least 3 of the identical columns must also have an identical order of attachment. From this we derive a contradiction as follows. Wherever the seed tile of the construction occurs, it lies to either the west or east of two of the identically placed columns. And if the seed tile occurs to the west (respectively east) of a column, then all tiles east (respectively west) of the column are determined by (1) the tiles and their positions in the column, and (2) the relative attachment order of the tiles in the column. That is, if a rectangle has fewer than  $(\frac{N}{2(k!)})^{\frac{1}{k}} = \Omega(\frac{N^{\frac{1}{k}}}{k})$  distinct tile types, there necessarily are at least two identical columns east (respectively west) of the seed tile whose order of attachment is the same. When attaching only a single tile at a time, this guarantees the possibility of producing an infinite repeating loop of tiles. Thus, no finite shape can be uniquely produced.  $\square$

*Remark.* We also point out that the argument for Theorem 3.1 applies to any length  $N$  shape whose height at each column is bounded by a value  $k$ .

**THEOREM 3.2.** *The tile complexity of self-assembling a  $k \times N$  rectangle is  $O(N^{\frac{1}{k}} + k)$  for the standard model, the unique shape model, and the multiple tile model. We show this by first providing a construction for the standard model and*

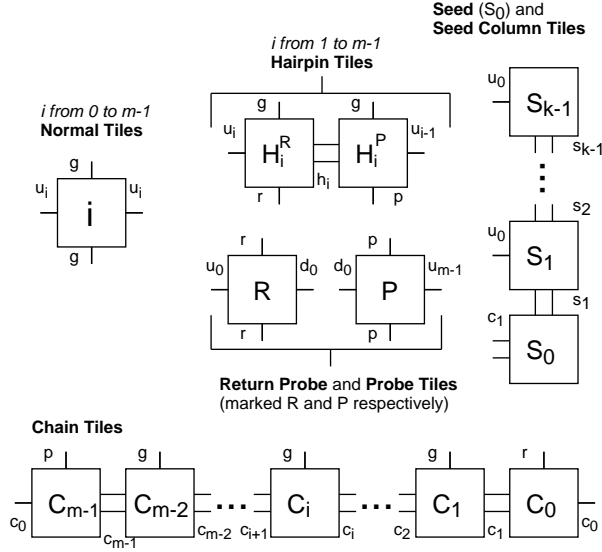


FIG. 3.1. This tile set assembles a  $k \times m^k$  rectangle in  $\Theta(k + m)$  tile complexity under the standard assembly model.

then arguing that the construction works for the unique shape model and the multiple tile model as well.

*Proof for the Standard Model.* For a given  $N$ , let  $m = \lceil N^{\frac{1}{k}} \rceil$ . To show this bound, we give a general tile set to assemble a  $k \times m^k$  rectangle in  $O(N^{\frac{1}{k}} + k)$  tiles under the standard model. We then show how to adjust the tile set so it produces a  $k \times N$  rectangle. The tile system we use constitutes a  $k$ -digit base- $m$  counter. The system has temperature  $\tau = 2$  and the tile set and glue strength function are given in Figure 3.1.

The assembly takes place as follows. The north edge of the seed tile produces a length  $k$  *seed column* from the seed column tiles. The west edge of the seed produces a length  $m$  *chain* from the chain tiles. The 0-normal tile can then fill in all the rows and columns up until column  $m - 1$ . In this column the  $H_1^P$  hairpin tile must be placed. This causes a *hairpin* growth which causes another length  $m$  chain of chain tiles to be placed in the first row. The next section of  $m$  columns are then filled with the 0-normal tile in all rows but the second, which will contain the 1-normal tile or a hairpin tile. In general, when the  $C_{m-1}$  chain tile is placed, probe tiles are added on top of each other until a row is found that does not consist of the  $(m - 1)$ -normal tile. In such a row the appropriate pair of hairpin tiles are placed and a downward growing column of return probe tiles are placed until the bottom row is encountered, at which point the  $C_0$  chain tile is placed to start the length  $m$  chain growth over again in the first row. If no such row is encountered, the assembly finishes. The idea here is that the bottom *chain* row represents the least significant digit of the counter, thus incrementing every column. After each block of  $m$  we need to find the most significant digit that requires incrementation, as well as rollover all the trailing digits displaying  $m - 1$  to 0. The hairpin tiles perform the incrementation, while the probe and return probe tiles perform the rollover.

It is easy to see that for a given  $k$  and  $m$ , this construction assembles into a  $k \times m^k$  block. In addition, we can adjust the glue types of the west edges of the seed column and seed tiles to represent any  $k$ -digit, base- $m$  number. By doing this the counter can be made to start at any number between 0 and  $m^k - 1$ . Thus, we can designate the length of the constructed shape to be any number between 1 and  $m^k$ . Therefore, to assemble a  $k \times N$  block, we use the above tile set with  $m = \lceil N^{\frac{1}{k}} \rceil$  and the west edges of the seed and seed columns tiles set to represent the number  $m^k - N$ . Thus, we can construct a  $k \times N$  block in  $4m + k = O(N^{\frac{1}{k}} + k)$  tiles.  $\square$

*Proof for the Unique Shape Model.* This follows from the construction for the standard model.  $\square$

*Proof for the Multiple Tile Model.* Now we argue that the tile set given for the standard model uniquely assembles a  $k \times N$  rectangle for the multiple tile model as well. Let  $A$  denote the uniquely produced  $k \times N$  supertile from the tile set of Figure 3.1 under the standard model. From the proof for the standard model we have that  $A$  is produced under the multiple tile model as well. We thus need to show that the multiple tile model will not produce any shape other than  $A$ . Denote any produced supertile under the standard model to be a *substructure* of  $A$ . We thus want to show that any supertile produced by a multiple tile model is a substructure of  $A$ .

To show this, consider a multiple tile system with tile set given in Figure 3.1. Consider the set  $W$  of addable supertiles and the set  $X \subset W$  of supertiles that do not contain the seed tile. For a given  $x \in X$ , denote  $x$  as a *column* if it consists of only a column of seed column tiles, a *chain* if it consists of only a chain of chain tiles, a *hairpin* if it consists of exactly two hairpin tiles, and a *singleton* if  $x \in T$ . For our argument we show the following three claims:

- Claim 1: Every supertile in the set  $X$  is either a column, chain, hairpin, or singleton.
- Claim 2: Attaching a column, chain, hairpin, or singleton to a substructure yields a new substructure.
- Claim 3: Two substructures cannot be attached to one another.

From this we have that by starting off with a single seed tile, which is a substructure, only supertiles that preserve the substructure property may be added. Thus, the multiple tile model can only produce substructures, and thus cannot produce anything the standard model cannot produce.  $\square$

*Proof of Claim 1.* Clearly all supertiles in  $X$  of size 1 can be classified as either a chain, column, hairpin, or singleton. (They are all singletons, some are chains, some are columns, none are hairpins). Inductively, suppose all supertiles in  $X$  of size less than  $k$  can be classified into the above categories. Consider an arbitrary size  $k$  supertile in  $X$ . By definition of  $W$  the supertile must be composed of two smaller supertiles. However, we cannot combine a chain with a column, nor a chain with a hairpin, nor a column with a hairpin. And clearly, if a singleton can be added to some other chain, column, hairpin, or singleton, it must yield a column, chain, or hairpin. Similarly, when two chains are combined, they yield another chain, and when two columns are combined, they yield another column. Thus, the size  $k$  supertile is either a chain, column, or hairpin.  $\square$

*Proof of Claim 2.* If a column is attachable to a substructure, it is attachable solely due to the glue strength of the south glue on the southern most tile of the column.



Instead of placing the column as a single chunk, each tile can be placed one by one under the standard model, starting with the southernmost tile. Thus, the end result is a substructure. The same type of argument applies to chains and hairpins.  $\square$

*Proof of Claim 3.* Among the tiles in an arbitrary substructure, no tile is farther north than the northern most tile in the east most column. Similarly, no tile is farther west than the west most tile in the southern most row, except for possibly a single hairpin tile. Now, since the eastern edges of all tiles in the first column and the southern edges of all tiles in the first row have bonding strength of 0, the only possible way for two substructures to bond together is for there to be an attraction between the north edge of some tile in the first column of one substructure with the south edge of a hairpin tile of the other substructure. But there is no attraction strength between the northern edges of seed column tiles and the southern edges of hairpin tiles, so this is not possible.  $\square$

**4. Reducing Tile Complexity with the 2-Temperature Model.** Now we show how a multiple temperature model can reduce tile complexity for assembling thin rectangles. For a given  $k$  and  $N$  with  $k \ll N$ , the idea is to use a modification of the construction from Section 3 to build a  $j \times N$  rectangle for optimal (bigger than  $k$ )  $j$  such that the top  $j - k$  rows are less stable than the bottom  $k$ . The temperature of the system is then raised to cause all but the bottom  $k$  rows to fall apart. We then compare the complexity of this construction with the lower bound for the standard model given in Section 3 to show that the 2-temperature model can beat a lower bound for the standard model.

*Minimizing the Complexity.* For a given  $j$  and  $N$ , assembling a  $j \times N$  rectangle using the construction of Theorem 3.2 yields an upper bound that is a function of  $j$ . If we are only interested in constructing a rectangle of length  $N$  but do not care about the width, we can choose  $j$  as a function of  $N$  such that the tile complexity is minimized. To do this we choose a value for  $j$  that balances the size of  $N^{\frac{1}{j}}$  and  $j$ . For  $j = \frac{\log N}{\log \log N - \log \log \log N} = \Theta\left(\frac{\log N}{\log \log N}\right)$ , the term  $N^{\frac{1}{j}}$  is  $\frac{\log N}{\log \log N}$ . Thus, the number of tiles used in the construction for building a  $j \times N$  block for such a  $j$  is  $j + N^{\frac{1}{j}} = \Theta\left(\frac{\log N}{\log \log N}\right)$ , which meets the lower bound dictated by Kolmogorov complexity for almost all  $N$  [9]. We use this result in the following theorem.

**THEOREM 4.1.** *Under the two-temperature model, the tile complexity of self-assembling a  $k \times N$  rectangle for an arbitrary integer  $k \geq 2$  is  $O\left(\frac{\log N}{\log \log N}\right)$ .*

*Proof.* In the case that  $k$  exceeds  $\lceil \frac{\log N}{\log \log N - \log \log \log N} \rceil$ , we can simply use a single temperature model to build the two perpendicular axes of the rectangle in optimal  $O\left(\frac{\log N}{\log \log N}\right)$  complexity. The addition of a constant number of tiles can then fill in the rest of the rectangle. Otherwise, to reach the bound we use a tile system that assembles a  $j \times N$  block for optimal value  $j = \lceil \frac{\log N}{\log \log N - \log \log \log N} \rceil$  under temperature  $\tau_1$  and breaks down to a smaller  $k \times N$  block in the second phase of the two-temperature assembly process. As in the construction from Theorem 3.2, let  $m = \lceil N^{\frac{1}{j}} \rceil$ . Consider the two-temperature tile system with  $\tau_1 = 4$  and  $\tau_2 = 6$  and the tile set and glue strength function given in Figure 3.2.

Under temperature  $\tau_1$ , this tile system assembles a  $j \times N$  block in exactly the same fashion as the single temperature system from Theorem 3.2. However, for each tile in the top  $j - k$  rows other than the seed column tiles, the north and south edges have glue strength 1. Therefore, since no glue in the system exceeds strength 4, we

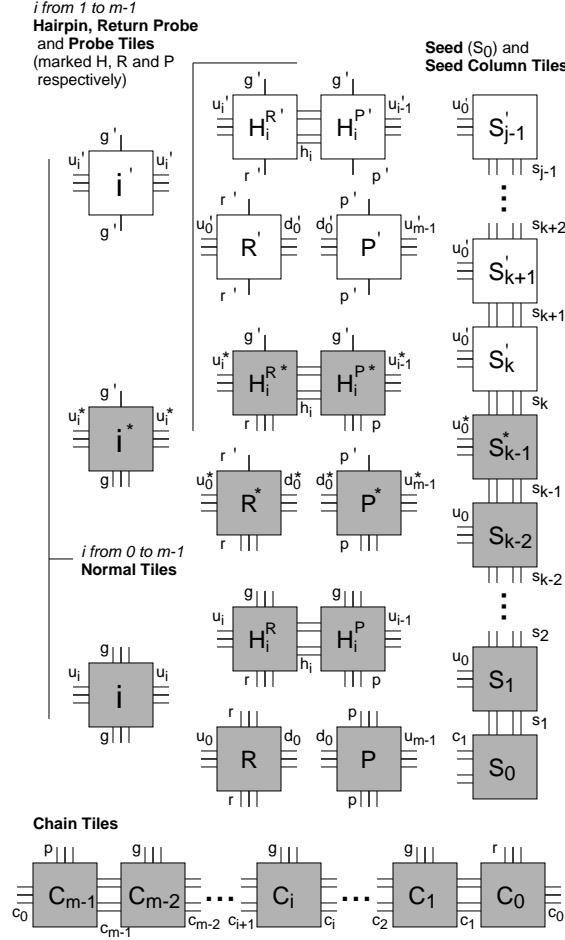


FIG. 3.2. A tile set to assemble a  $k \times N$  rectangle in  $\Theta(j + m)$  tile complexity for  $m = \lceil N^{\frac{1}{j}} \rceil$  under the 2-temperature model with  $\tau_1 = 4$  and  $\tau_2 = 6$ . At temperature  $\tau_1$  the shaded tiles fill in the bottom  $k$  rows of a  $j \times N$  rectangle while the clear tiles fill the top  $j - k$  rows. At temperature  $\tau_2$  the clear tiles fall off.

are assured that any cut consisting of one north-south edge and one east-west edge has cut strength less than  $\tau_2 = 6$ . Therefore, under the two-temperature model each tile in the top  $j - k$  rows can be removed one at a time, starting at the northwest corner of the  $j \times N$  block. We are then left with the bottom  $k$  rows. Since our design ensures that each edge in the bottom  $k$  rows has strength 3 or greater, no cut of the bottom  $k \times N$  supertile can have cut strength less than 6. Thus, no cut can break up the remaining  $k \times N$  block. And since any alternate choice of cuts would only expedite the process to this end, this construction uniquely assembles a  $k \times N$  block in  $10m + j = O(N^{\frac{1}{j}} + j) = O(\frac{\log N}{\log \log N})$  tile complexity under the two-temperature assembly model.  $\square$

For small values of  $k$ , this beats the lower bound for the standard model. Consider

	3'	3'	3'	3'	3'	3'	3'	3'	3'	3'	3'
	↑	↑	↑	↑	↑	↑	↑	↑	↑	↑	↑
	2'	2'	2'	2'	2'	H'	H'	1'	1'	1'	1'
	↑	↑	↑	↑	↑	↓	↑	↑	↑	↑	↑
	0'	0'	0'	0'	0'	R'	P'	4'	4'	4'	4'
	↑	↑	↑	↑	↑	↓	↑	↑	↑	↑	↑
	1*	H*	H*	0*	0*	0*	R*	P*	4*	4*	4*
	↑	↑	↑	↑	↑	↑	↑	↑	↑	↑	↑
	C <sub>1</sub>	C <sub>0</sub>	C <sub>4</sub>	C <sub>3</sub>	C <sub>2</sub>	C <sub>1</sub>	C <sub>0</sub>	C <sub>4</sub>	C <sub>3</sub>	C <sub>2</sub>	C <sub>1</sub>

FIG. 3.3. Here is a typical section of a self-assembled  $5 \times N$  block from the tile set in Figure 3.2 that will break down to a  $2 \times N$  block under temperature 6. Edges with strength 4 are marked by 4 adjacent arrows, while edges with strength 1 are marked with 1. All remaining edges have strength 3.

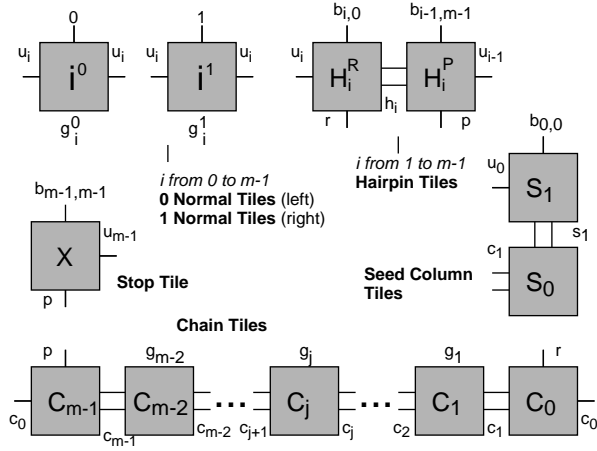


FIG. 5.1. This tile set creates a  $2 \times n$  block whose top row represents a given  $n$ -bit binary number  $b$ . Here  $b_{ij}$  is the value of the bit in position  $im + j$  in  $b$ . The glue function for glues  $g_i^1$  and  $g_j^1$  for  $i$  from 0 to  $m-1$  and  $j$  from 1 to  $m-2$  is  $G(g_i^1, g_j^1) = b_{ij}$ . All other pairs of non-equal glues have strength 0.

$k = \frac{\log N}{2 \log \log N}$ . For such  $k$  the value of  $N^{\frac{1}{k}}$  is

$$N^{\frac{2 \log \log N}{\log N}} = (\log N)^2.$$

Thus, from Theorem 3.1, the lower bound for the standard model is

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

Since this bound only gets higher for smaller values of  $k$ , the 2-temperature model yields an asymptotically smaller tile complexity for all  $k$  between 2 and  $\frac{\log N}{2 \log \log N}$ .

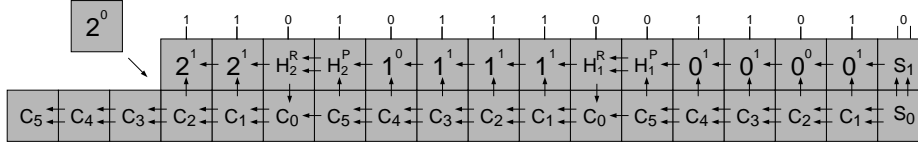


FIG. 5.2. Assembling an arbitrary  $n$ -bit binary number in  $O(\sqrt{n})$  tiles. Here we show the construction for  $n = 36$  and binary number  $b = \dots 0110101110011010$ .

**5. Assembling  $N \times N$  Squares in  $O(\sqrt{\log N})$  Tiles.** Kolmogorov complexity dictates an  $\Omega(\frac{\log N}{\log \log N})$  lower bound for almost all  $N$  on the tile complexity of self-assembling  $N \times N$  squares for the standard model in which the glue function is limited so that  $G(x, y) = 0$  for  $x \neq y$ . However, if this restriction is lifted, the bound no longer applies. In this section, we show that the tile complexity of self-assembling  $N \times N$  squares is  $\Theta(\sqrt{\log N})$  under the flexible glue model for almost all  $N$ .

**THEOREM 5.1.** *The tile complexity of self-assembling  $N \times N$  squares is  $O(\sqrt{\log N})$  under the flexible glue model.*

*Proof.* The trick as introduced in [9] is to be able to initialize a fixed length binary counter to any arbitrary  $(\log N)$ -bit binary number. This can be done trivially in  $O(\log N)$  tile complexity. By simulating base conversion, it can be done in  $O(\frac{\log N}{\log \log N})$  [1]. Here we provide a tile system that assembles a  $2 \times \log N$  block in  $O(\sqrt{\log N})$  tiles such that the top row of the block encodes a given binary number  $b$ . This is accomplished by taking advantage of the flexible glue function and encoding  $b$  into the glue function. Let  $n = \lfloor \log N \rfloor + 1$  and  $m = \lceil \sqrt{n} \rceil$ . Let  $b$  be a given  $n$ -bit binary number. Let  $b_{ij}$  be the bit in position  $im + j$  in  $b$ . We use the tile set and glue function from Figure 5.1 to construct a  $2 \times n$  block such that the top row of the block represents the number  $b$ . For convenience we denote some glues by the symbols 0 and 1.

To simplify the illustration, the tile set in Figure 5.1 assumes that  $m^2 = n$ . If this is not the case, we can do as before in Theorem 3.2 and initialize the 2-digit counter to an arbitrary value  $c$  so that a block of length exactly  $n$  is assembled. At any rate, the construction uses  $5\lceil \sqrt{n} \rceil + 1$  tiles and constructs a  $2 \times n$  block in the same fashion as the general  $k \times n$  assembly. Additionally, the glue function assures us that for the  $(i, j)$  digit of  $b$ , the corresponding position in the top row of the construction can only be tiled with either a hairpin, seed column, or normal tile with north edge glue equal to  $b_{ij}$ .

To complete the  $N \times N$  square we need to create a fixed length binary counter that is initialized to the given binary number  $b$  and grows north, incrementing row by row, until  $2^n$  is reached. The addition of a constant number of stairstep tiles can then finish off the square, as shown in [9]. The fixed length binary counter can also be implemented in a constant number of tiles as is done in [1, 9]. Alternatively, we can use the construction from Section 3 for building a  $k \times N$  block for  $k = \log N$ . This yields a binary counter consisting of eight tiles plus  $\log N$  seed column tiles. However, since we already have a “seed column” via the  $2 \times n$  seed block, we can omit the seed column tiles. Thus, the total number of tiles used for the assembly of an  $N \times N$  square is only a constant greater than the  $\Theta(\sqrt{\log N})$  tiles used to build the  $2 \times n$  seed block.

□

**6. Kolmogorov Lower Bounds.** Rothmund and Winfree [9] showed that Kolmogorov complexity dictates an  $\Omega(\frac{\log N}{\log \log N})$  lower bound on the tile complexity for self-assembling  $N \times N$  squares for almost all  $N$ . We show that their proof generalizes to the multiple temperature model, the unique shape model, and the multiple tile model. For the flexible glue model, we modify their argument to get an  $\Omega(\sqrt{\log N})$  lower bound from Kolmogorov complexity, making the construction in Theorem 5.1 tight for almost all  $N$ .

**THEOREM 6.1.** *For almost all  $N$  the tile complexity of self-assembling an  $N \times N$  square is  $\Omega(\frac{\log N}{\log \log N})$  for the multiple tile model, the multiple temperature model, and the unique shape model.*

*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 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  $\Omega(\log N)$ .

For a given assembly model, if there exists a finite size Turing machine that takes as input a tile system and outputs the maximum extent (i.e. width or length) of the shape uniquely produced by the system, then the  $\Omega(\log N)$  bound applies to the number of bits required to represent the tile system. For each of the non-flexible glue models, let  $\tau$  be the maximal temperature of the system and  $n$  the size of the tile set. Such tile sets can be represented by  $4n \log 4n + 4n \log \tau$  bits as follows. For each of the  $4n$  edges in the system assign an index to represent one of the at most  $4n$  glues of the system. Also record a mapping from each glue to an index from 0 to  $\tau$  representing the corresponding strength of the given glue. Thus, for  $\tau$  bounded by a constant, the number of bits required to represent a tile system is  $O(n \log n)$ , which implies that  $n = \Omega(\frac{\log N}{\log \log N})$  for almost all  $N$  for any system that self-assembles a shape with maximum extent  $N$  [9].

To finish this argument, we explicitly give algorithms for each model that output the maximum extent of the shape uniquely produced by a given system. For the standard model, the multiple tile model, and the unique shape model, the following algorithm can output the maximum extent of the shape produced by a given tile system:

#### Produced-Extent( $\Gamma$ )

1. Set  $D_1 = T$ . In general,  $D_i$  denotes the set of all supertiles of size  $i$  which consist of tiles in  $T$ .
2. Mark each  $t \in D_1$  as FEASIBLE.
3. Set  $i = 2$ .
4. Create  $D_i$  the set of all supertiles of size  $i$ . Mark each  $t \in D_i$  as FEASIBLE if  $t$  can be constructed from two smaller FEASIBLE supertiles from the set  $\bigcup_{r=1}^{i-1} D_r$ . If  $t$  is FEASIBLE and contains the seed tile, mark  $t$  as PRODUCED.
5. Increment  $i$  and repeat step 4 unless  $\bigcup_{r=\frac{i}{2}}^i D_r$  contains no FEASIBLE supertile.
6. Mark each PRODUCED supertile in  $\bigcup_{r=1}^i D_r$  as TERMINAL if no FEASIBLE supertile can be attached.

7. Output the maximum extent (width or length) of any smallest TERMINAL supertile in  $\bigcup_{r=1}^i D_r$ .

Under the multiple tile model, if there are no addable supertiles of size between  $\frac{i}{2}$  and  $i$ , then we know that there are no addable supertiles of size greater than  $i$ , since such a tile would need to be assembled from at least one smaller supertile of size at least  $\frac{i}{2}$ . Thus, in the case where each addable supertile is finite, this algorithm will finish and output the correct result. We also note that the algorithm outputs the extent of the smallest terminally produced supertile for the system. This tells us that the Kolmogorov bound applies to models with even more general definitions of uniqueness than what we consider. For the multiple temperature model we have the following:

### ***k*-Temperature-Produced-Extent( $\Gamma$ )**

1. Initialize the *current supertile* to be the seed tile.
2. For  $i = 1$  to  $k$  do the following: If there exists a cut  $c$  in the current supertile with  $\text{strength}(c) < \tau_i$ , remove the tiles on the side of the cut not containing the seed. If there exists some  $x \in T$  such that  $x$  is addable under  $\tau_i$ , add  $x$ . Continue adding and removing until nothing can be added or removed at temperature  $\tau_i$ .
3. Output the maximum extent of the resultant shape.

Since the definition of the  $k$ -temperature model requires that a system that uniquely produces a shape must, regardless of the sequence of additions and removals, finish each phase, we are assured that each iteration of the for loop will finish, thus giving the end result.  $\square$

**THEOREM 6.2.** *For almost all  $N$  the tile complexity of self-assembling an  $N \times N$  square is  $\Omega(\sqrt{\log N})$  under the flexible glue model.*

*Proof.* The Produced-Extent algorithm given in Theorem 6.1 for the standard assembly model works just as well for the flexible glue model. Thus, as discussed in Theorem 6.1, the number of binary digits required to represent a flexible glue tile system that self-assembles an  $N \times N$  square is bounded below by  $\Omega(\log N)$  for almost all  $N$ . We can represent a flexible glue tile system of size  $n$  tiles and temperature  $\tau$  bounded by a constant with  $f(n) = 4n \log(4n) + (4n)^2 \log \tau = O(n^2)$  bits as follows. For each tile there are four sides for which we must denote a glue. We need at most  $4n$  distinct glues, and for each glue we need to store the bonding strength with every other glue in the model. This can be stored in a  $4n \times 4n$  matrix. Now for a given  $N$ , let  $\beta(N)$  be the cardinality of the minimum tile set for assembling an  $N \times N$  square under the flexible glue model. Then, there exist constants  $C_1$  and  $C_2$  such that for almost all  $N$ ,

$$C_1 \log N \leq f(\beta(N)) \leq C_2 \beta(N)^2.$$

So  $\beta(N) = \Omega(\sqrt{\log N})$  for almost all  $N$ .  $\square$

**7. Shape Verification.** Given a shape, Adleman et al. [2] studied the problem of finding the minimum set of tiles which uniquely produces a supertile  $A$ , such that  $A$  has the given shape. To show that the decision version of the problem is in NP, they gave an algorithm to verify whether a given set of tiles uniquely produces a supertile which has the given shape. In contrast, in this section we show that for the unique shape, multiple tile, and multiple temperature models this problem is NP-hard. The problem of shape verification is defined as follows.

UNQ-SHAPE( $\Gamma, M$ ) is the problem of deciding whether the tile system  $\Gamma$  uniquely assembles into the shape  $M$ .

**7.1. Unique Shape Model.** The algorithm of [2] to verify whether a given set of tiles uniquely produces a given shape insists that the tile system should assemble into a unique terminal supertile. Under the *unique shape* model, a tile system  $\mathbb{T}$  uniquely produces a shape if all terminal supertiles of  $\mathbb{T}$  (henceforth called  $Term(\mathbb{T})$ ) have the given shape, and no larger supertiles are produced. We note that this definition automatically implies that if a tile system uniquely produces a shape, then  $Term(\mathbb{T})$  is non-empty. In this section, we show that the unique shape problem is co-NP-complete under the unique shape model, in contrast to the standard model.

**THEOREM 7.1.** *UNQ-SHAPE is co-NP-complete under the unique shape model. It remains NP-hard even when the temperature  $\tau = 2$ .*

We begin by showing that UNQ-SHAPE is in co-NP, and then show that it is NP-hard (and thus co-NP-hard).

**LEMMA 7.2.** *UNQ-SHAPE is in co-NP under the unique shape model.*

*Proof.* For this, we need to show that if an instance of UNQ-SHAPE is false, i.e. if the tile system in the instance does not assemble uniquely into the given shape, then there is a short proof of the fact. By definition, a given tile system  $\mathbb{T} = \langle T, \mathcal{S}, G, \tau \rangle$  does not uniquely assemble into the given shape  $M$  iff one of the following occurs:

1. A terminal supertile of a shape different from  $M$  can be assembled. In this case,  $Term(\mathbb{T})$  contains a supertile  $A$  with a shape different from  $M$ . Then  $A$ , along with the order in which the tiles join to assemble  $A$  would suffice as a proof. In order to check this proof, we first verify that  $A$  can indeed be assembled by adding the tiles in the order specified. Then we check that  $A$  is a terminal supertile by simply testing whether any tile is attachable at any of the empty sites adjacent to it.
2. A supertile  $C$  of size larger than the given shape can be assembled. Note that this supertile need not be terminal. We note that if any such  $C$  exists, then there exists such a  $C$  with size one larger than  $M$ . Such a  $C$ , along with the order in which tiles are added to assemble  $C$  would suffice as a proof. We verify this proof by checking that  $C$  can indeed be assembled by adding the tiles in the order specified, and that the size of the supertile is larger than the shape.

In both cases, the size of the proof is linear in the instance size, and the verification algorithm runs in time quadratic in the instance size.  $\square$

**LEMMA 7.3.** *UNQ-SHAPE is NP-hard under the unique shape model.*

*Proof.* The proof uses a construction proposed by LaBean and Lagoudakis [6] to solve SAT by exploiting the massive parallelism possible in DNA operations to emulate a non-deterministic device that solves SAT.

We reduce 3-SAT to UNQ-SHAPE using their construction. Given any instance of 3-SAT with  $m$  clauses and  $n$  different variables, we construct an instance of UNQ-SHAPE,  $(\langle T, \mathcal{S}, G, 2 \rangle, M)$  with  $|T| = O(m + n)$ , and the size of the shape  $M$  of order  $O(mn)$ . There is a one-to-one correspondence between variable assignments for the 3-SAT instance and the supertiles in  $Term(\mathbb{T})$ , i.e every possible assignment to variables is associated with a distinct terminal supertile. If the assignment satisfies the formula, the terminal supertile associated with it has the shape of an  $(n+2) \times (m+3)$  rectangle; else the shape associated with the assignment has the shape of an  $(n+2) \times (m+3)$  rectangle with its top-right corner missing. Thus, if the tile system uniquely assembles into a rectangle with its top-right corner missing, then no assignment satisfies the 3-

SAT formula; on the other hand, if the tile system does not uniquely assemble into this corner-missing rectangle, then there is at least one assignment which satisfies the 3-SAT formula. Thus, a polynomial time algorithm to decide UNQ-SHAPE will result in a polynomial time algorithm for 3-SAT.

The idea of the reduction is to have the bottom row of the rectangle encode the clauses, have the left column encode the variables, and let the second column correspond to a possible assignment of values to the variables. The rest of the assembly evaluates the formula at that assignment, and the row below the top row encodes which of the clauses get satisfied by the assignment. A tile gets added to the top-right corner iff the assignment satisfies all the clauses.

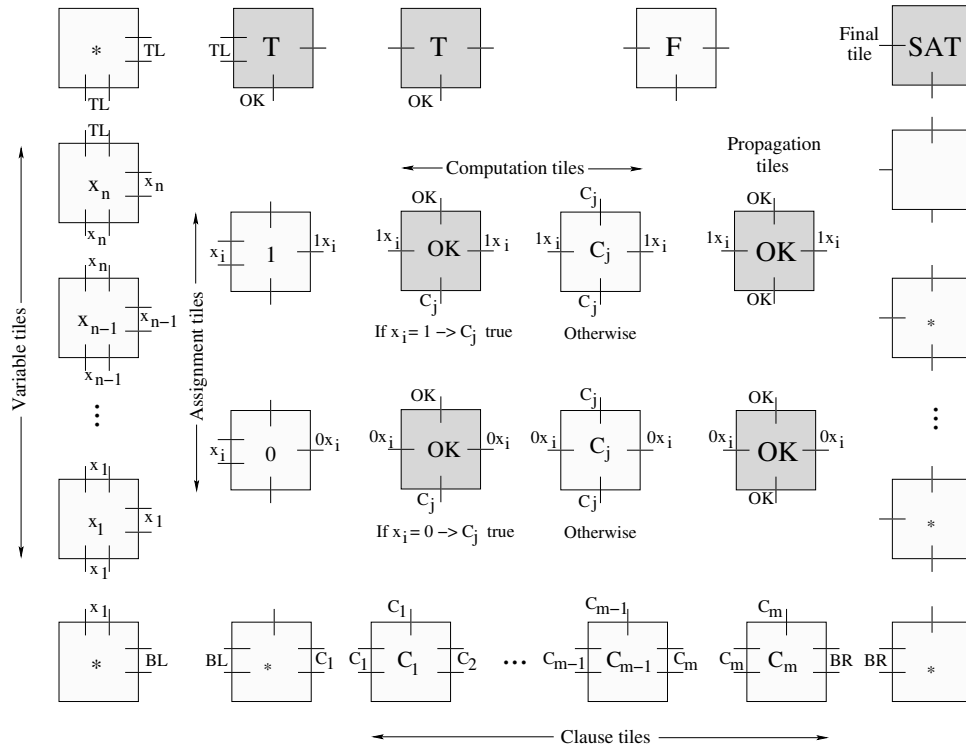


FIG. 7.1. Tile system for evaluation of a 3-SAT formula

Take any 3-SAT formula with  $n$  variables,  $x_1, x_2, \dots, x_n$ , appearing in  $m$  clauses  $C_1, C_2, \dots, C_m$ . We define a tile system as shown in Figure 7.1, where the temperature is fixed at 2. In addition to the seed tile, there are  $n$  variable tiles which attach on top of the seed tile to give the first column. The east side of these tiles provides a strength-2 glue to the assignment tiles. Besides, there are  $m$  clause tiles that attach to the east of the seed tile to form the bottom row. For any clause-variable pair,  $C_j$  and  $x_i$ , the following computation tiles are present:

1. If  $x_i$  set to 1 makes the clause  $C_j$  true, then the upper left computation tile shown in the figure is present, otherwise, the upper right one is present.
2. Similarly, if  $x_i$  set to 0 makes the clause  $C_j$  true, then the lower left computation tile in the figure is present, otherwise, the lower right one is present.

In addition, there are  $2n$  tiles to propagate  $OK$  upwards. The tile labeled  $SAT$  attaches to the top-right corner only if the formula is satisfied by the assignment in



the second column of the supertile.

Figures 7.2(a) and (b) show two of the terminal supertiles of a tile system corresponding to the formula  $(x_1 + x_2 + \overline{x_3})(x_1 + \overline{x_2} + x_3)(\overline{x_1} + x_2 + \overline{x_3})$ . Note that since the assignment  $x_1 = 0, x_2 = 1, x_3 = 1$  satisfies the formula, a tile gets attached in the top-right corner in Figure 7.2(a). Also, since the assignment  $x_1 = 0, x_2 = 1, x_3 = 0$  does not satisfy the formula, the rectangle in Figure 7.2(b) is missing a tile in the top-right corner.

*	T	T	T	T	SAT
$x_3$	1	OK	OK	OK	*
$x_2$	1	OK	C <sub>2</sub>	OK	*
$x_1$	0	C <sub>1</sub>	C <sub>2</sub>	OK	*
*	*	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	*

(a)

*	T	T	F	F	
$x_3$	0	OK	C <sub>2</sub>	OK	*
$x_2$	1	OK	C <sub>2</sub>	OK	*
$x_1$	0	C <sub>1</sub>	C <sub>2</sub>	OK	*
*	*	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	*

(b)

FIG. 7.2. Two terminal supertiles for the formula  $(x_1 + x_2 + \overline{x_3})(x_1 + \overline{x_2} + x_3)(\overline{x_1} + x_2 + \overline{x_3})$ .

□

**7.2. Multiple Tile and Multiple Temperature Models.** The algorithm of [2] to determine whether a tile system uniquely assembles a given shape does not work if the self-assembly model allows pre-assembled supertiles to be added to the growing seed supertile. The algorithm therefore does not apply to the multiple tile model. The algorithm also assumes that once a tile is placed, it can never be removed. This is not the case in the multiple temperature model. In this section we consider the complexity of the unique shape problem under the multiple tile model and the multiple temperature model. We first show that for both models the problem is NP-hard. We then generalize the proofs of this fact to show that the problem for both models is neither in NP nor co-NP unless  $P = NP$ .

**THEOREM 7.4.** *UNQ-SHAPE is NP-hard under the multiple tile model. It remains NP-hard even when the temperature  $\tau = 2$  and  $q$  is polynomial in the number of tiles in the system.*

*Proof.* The proof is a reduction from 3-SAT similar in spirit to the reduction in Theorem 7.1. For a given instance of 3-SAT with  $n$  variables and  $m$  clauses, consider a multiple tile system  $\langle T, s, G, 2, q = (n + 2)(m + 3) \rangle$  given as follows. The tile set includes the tiles given in Figure 7.3, as well as the tiles for solving 3-SAT as given in Theorem 7.1 with the following adjustment. The seed tile is no longer the seed, but just a tile in the set, and it is given a west glue  $A$  with glue strength 1. Also, the SAT tile from the construction is given a north glue  $B$  with strength 1.

This tile set assembles a single width chain of tiles that grows north for  $n + 2$  tiles and then turns east and grows for  $m + 3$  tiles. The east glue of the first tile in this chain (the seed tile) has east glue  $A$  and the last tile in the chain has south glue  $B$ . Denote the shape of this supertile as  $M$ . Now in the case that the corresponding 3-SAT formula is not satisfiable, nothing else can be attached and  $M$  is uniquely assembled. However, if there exists a satisfying assignment to the 3-SAT formula, an  $(n + 2) \times (m + 3)$  rectangle whose northeast most tile has north glue  $B$  and southwest

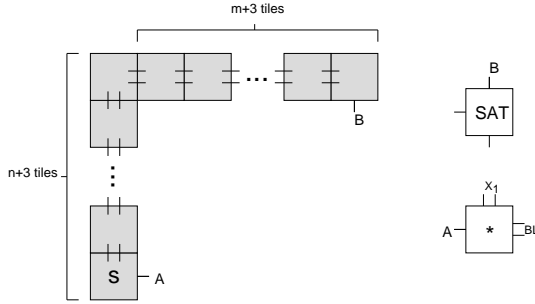


FIG. 7.3. To show that the UNQ-SHAPE problem is NP-hard for the multiple tile model we modify the tile set of Theorem 7.1. We add the tiles given above as well as change the seed tile to be  $S$ , add glue  $A$  to the west edge of the old seed tile, and add glue  $B$  to the north edge of the final SAT tile.

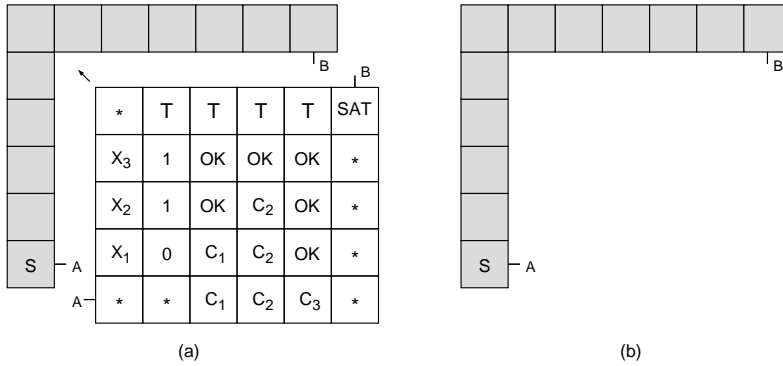


FIG. 7.4. Two terminal supertiles for the formula  $(x_1 + x_2 + \overline{x_3})(x_1 + \overline{x_2} + x_3)(\overline{x_1} + x_2 + \overline{x_3})$ . In the case that a given 3-SAT formula is not satisfiable, the tree on the right is uniquely assembled.

most tile has west glue  $A$  is in the system's addable supertile set  $W$ . Thus, a supertile of the shape of an  $(n + 3) \times (m + 4)$  rectangle can be produced. Thus, in this case  $M$  is not uniquely produced. So the output of UNQ-SHAPE when given this tile system and shape  $M$  as input is yes if and only if the corresponding 3-SAT formula is not satisfiable. Thus, UNQ-SHAPE is NP-hard under the multiple tile model.  $\square$

**THEOREM 7.5.** UNQ-SHAPE is NP-hard under the multiple temperature model. It remains NP-hard even when the temperature is raised only once.

*Proof.* We again use a reduction from 3-SAT similar in spirit to the reduction in Theorem 7.1. For a given 3-SAT formula with  $n$  variables and  $m$  clauses, consider the 2-temperature tile system with temperatures  $\tau_1 = 2, \tau_2 = 4$ , and tile set given by the construction in Theorem 7.1 with the additions and modifications given in Figure 7.5. The modifications increase the north/south glue strengths of the tiles that occur in the first column of the  $(n + 2) \times (m + 3)$  construction from strength 2 to strength 4. Additionally, four tiles are added such that the length of the first column in the construction grows to height  $n + 6$  rather than  $n + 2$ . Another modification is made to the final SAT tile such that it has a strength two glue on its north edge. This, in combination with other added tiles, allows a new chain of tiles to be added in the case that a satisfying set of variable assignments are given. The new tiles grow

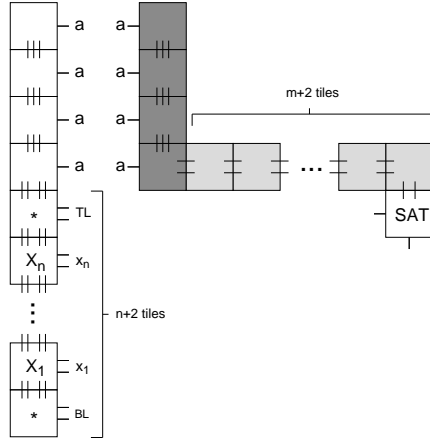


FIG. 7.5. This tile set in addition to the tile set of Theorem 7.1 under the 2-temperature model with  $\tau_1 = 2$  and  $\tau_2 = 4$  uniquely assembles a  $(n + 6) \times 1$  column if and only if the corresponding 3-SAT formula is unsatisfiable.

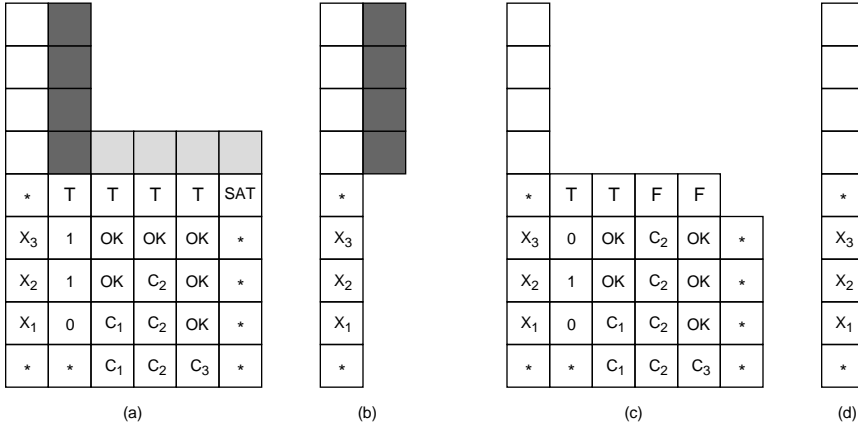


FIG. 7.6. At the initial temperature  $\tau_1 = 2$ , a supertile of shape given in (a) is formed if a satisfying assignment to the 3-SAT variables is given. Otherwise, a supertile of the shape given in (c) is constructed. At temperature  $\tau_2 = 4$ , supertiles like (a) are broken down to the supertile in (b). Supertiles of form (c) are broken down into the supertile in (d). The supertile in (d) is uniquely assembled if and only if the corresponding 3-SAT formula is unsatisfiable.

westward back to the first column of the construction. Here four tiles are placed, growing northward now, adjacent to the four *extra* tiles in the first column. These four tiles are connected to one another by strength three bonds. In addition, each has a west glue of strength one.

The idea is that now the temperature of the system is raised from two to four. At temperature four, each tile between column two and column  $m + 3$ , row 1 to  $n + 2$ , can be removed, going from bottom to top, right to left. All tiles in row  $n + 3$  from column 3 to  $m + 3$  can also be removed, leaving a height  $n + 6$  column with four extra tiles attached at the end. Nothing within this supertile can be removed, and

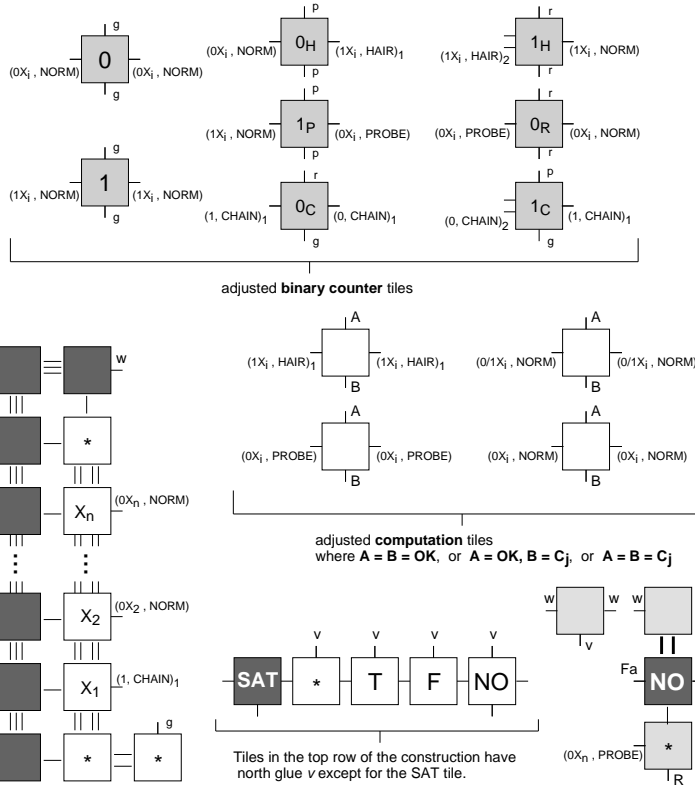


FIG. 7.7. To show that the UNQ-SHAPE problem is not in NP or co-NP unless  $P=NP$  under the multiple temperature model, we combine a binary counter with the SAT solving tiles of Section 7.1 to evaluate a given SAT formula for every possible assignment to the variables. Some tiles or glues of the construction are omitted in this figure as they are unchanged from the construction in Section 7.1.

clearly nothing can be added, so this structure is terminal. However, in the case that no satisfying arrangement exists, the four extra tiles can never get added in the first phase of the 2-temperature assembly process. So in this case the shape  $M$  equal to a  $(n + 6) \times 1$  column is uniquely assembled. Thus, when given this tile set and shape  $M$  as input, the UNQ-SHAPE problem outputs yes if and only if the corresponding 3-SAT formula is not satisfiable. So the Unique-Shape problem is NP-hard for the 2-temperature model.  $\square$

**THEOREM 7.6.** UNQ-SHAPE is not in NP or co-NP under the multiple temperature model unless  $P = NP$ . This remains true even when the temperature is raised only once.

*Proof.*

To show this we generalize the reduction from co-SAT given in Theorem 7.5. Our construction yields, depending on the input shape, a reduction from either SAT or co-SAT to the problem of deciding whether a given tile set assembles the given shape. The “not in co-NP” part of the theorem follows from the SAT reduction, and the “not in NP” part from the co-SAT reduction.

The reduction is as follows. Given a 3-SAT formula with  $n$  variables and  $m$

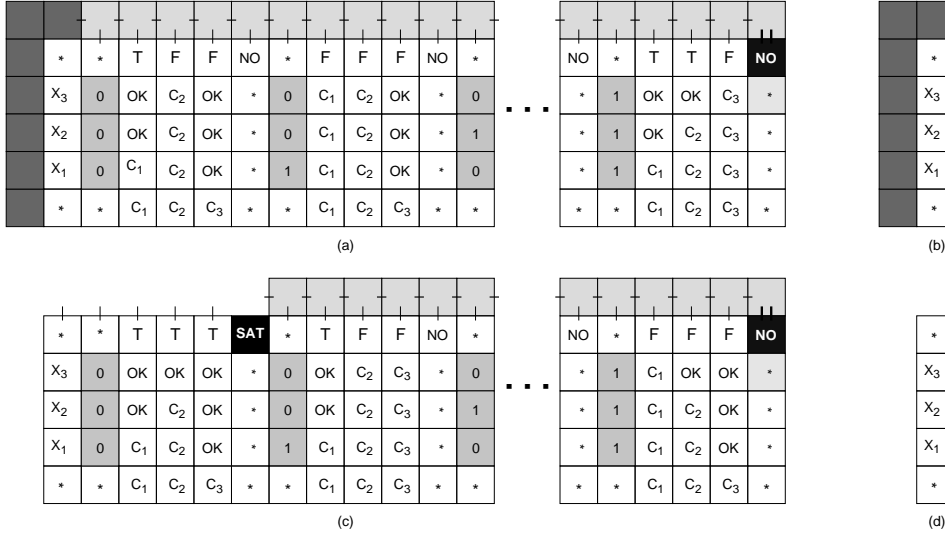


FIG. 7.8. At temperature  $\tau = 2$ , if the corresponding SAT formula has no satisfying assignment, then a growth of tiles, starting at the final NO tile is started and reaches back to the initial column of variable tiles and clamps on. In the case there are one or more satisfying assignments, the growth is stopped and a shape like (c) is formed. After raising the temperature to  $\tau = 4$ , shape (b) is uniquely produced in the first case and shape (d) in the second. Thus, the Unique-Shape problem with the tile set of Figure 7.7 yields a reduction from co-SAT with input shape (b), and a reduction from SAT with input shape (d).

clauses, we create a tile set at temperature  $\tau_1 = 2$  in the fashion of Theorem 3.2 that assembles an  $n$ -bit binary counter growing from west to east which counts from 0 to  $2^n - 1$ . In this case, however, at each incrementation of the counter the given 3-SAT formula is evaluated for the variable assignment corresponding to the current value of the binary counter. After the final iteration of the counter, a string of tiles grows back to the initial column of tiles and *latches on* by creating a second vertical column that is attached adjacently to the first. However, this growth is disrupted if any occurrence of a SAT tile is encountered. Thus, such a latch is created if and only if there is no satisfying assignment to the variables.

The temperature of the system is then raised to  $\tau_2 = 4$ . This eliminates any tile occurring east of the initial variable column. What is left is a single column supertile in the case that there exists a satisfying assignment, and a pair of adjacent columns in the case that there is no satisfying assignment. The tile set for this construction is given in Figure 7.7. Let shape  $M$  be the single column and shape  $W$  be the double column. Thus, when given this tile set and shape  $M$  as input, the UNQ-SHAPE problem outputs yes if and only if the corresponding 3-SAT formula is satisfiable. If shape  $W$  is given as input, the UNQ-SHAPE problem outputs yes if and only if the corresponding 3-SAT formula is not satisfiable. The first input exhibits the reduction from SAT, the second from co-SAT. See Figure 7.8 for an example.

□

**THEOREM 7.7.** UNQ-SHAPE is not in NP or co-NP under the multiple tile model unless  $P = NP$ . This remains true even when the temperature  $\tau = 2$ .

*Proof.* The proof is again a reduction from 3-SAT and very similar to the proof for Theorem 7.6. Consider a given instance of 3-SAT with  $n$  variables and  $m$  clauses.

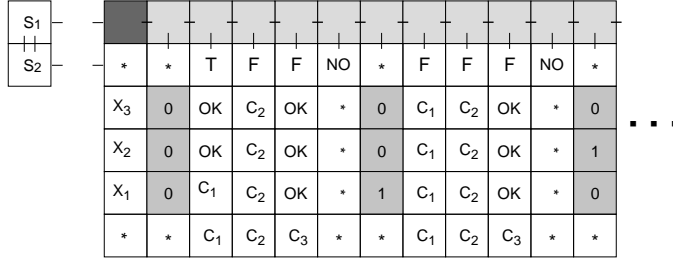


FIG. 7.9. Under the multiple tile model with  $q = 2^n(n+3)(m+2) + 2(n+3)$ , the large  $(2^n(m+2)+2) \times (n+3)$  rectangle can be attached to the two  $S$  tiles if and only if the corresponding 3-SAT formula is satisfied.

Let the size of the addable supertiles be  $q = 2^n(n+3)(m+2) + 2(n+3)$ . The tile set for the reduction is essentially that from Figure 7.7 except we remove all but one of the clamping tiles, reduce all glue strengths greater than 2 down to 2, and add tiles  $S_1$  and  $S_2$  given in Figure 7.9 with  $S_1$  being set as the seed tile.

Clearly this tile set uniquely assembles a two-tile supertile consisting only of  $S_1$  and  $S_2$  in the case that the 3-SAT formula is satisfiable. On the other hand, if there is no satisfying arrangement, the complete size  $(2^n(m+2)+2) \times (n+3)(m+2)$  rectangle from the tiles of Figure 7.7 is in the set of addable supertiles. The resultant uniquely assembled shape is then the rectangle with the tiles  $S_1$  and  $S_2$  attached to the side. Thus, the unique shape problem with the size two shape given as input gives a reduction from SAT, while the rectangle with the two  $S$  tiles attached gives a reduction from co-SAT.  $\square$

**8. Conclusions.** We have considered various natural generalizations of the self-assembly model in an attempt to reduce the tile complexity of certain shapes. In doing so, we have produced a construction for building arbitrary-sized rectangles which is particularly useful for the assembly of thin rectangles (a  $k \times N$  rectangle is thin if  $k < \frac{\log N}{\log \log N - \log \log \log N}$ ). This construction also yields a simple way to assemble thicker rectangles while achieving the same optimal tile and time complexity achieved in [1]. We use modifications of this construction to show how two of the models, the multi-temperature model and the flexible glue model, can reduce tile complexity below theoretical lower bounds for the standard model for certain shapes. In particular, the multi-temperature model assembles thin  $k \times N$  rectangles in optimal  $\Theta(\frac{\log N}{\log \log N})$ , while the flexible glue model reduces the complexity of  $\Theta(\frac{\log N}{\log \log N})$  for the assembly of  $N \times N$  squares to the tight bound of  $\Theta(\sqrt{\log N})$ . For the remaining models, we have extended Kolmogorov lower bound proofs from [9] to show that for many shapes, the new models do not improve tile complexity. We have also shown that the problem of verifying whether a given tile set assembles into a given shape is Co-NPC under the unique shape model and not in NP or co-NP unless  $P = NP$  under the multiple tile and multiple temperature models, in contrast to the polynomial time solution for the standard and flexible glue models.

There are a number of open questions remaining, some of which are as follows. First, there are some questions as to how the parameter  $q$  in the multiple tile model affects complexity. The proof of the Kolmogorov lower bound for  $N \times N$  squares does not hold if the bound of  $q$  on the size of the addable supertiles is removed. Also, to show that the UNQ-SHAPE problem under the multiple tile model is neither in

NP or co-NP we required that  $q$  be exponential in the size of the tile set. To show NP-hardness, we needed  $q$  to grow linearly in the size of the tile set. For polynomial sized  $q$ , is the problem in NP or co-NP, and for constant  $q$ , is the problem in P?

Second, can new examples be found showing that the generalized models can reduce tile complexity? For example, are there shapes for which the multiple tile or the unique shape models reduce complexity? And for the multiple temperature model, can it help to use more than two temperatures? If so, does the temperature need only be monotonically increasing or can it help to raise and lower the temperature? Also, the construction for the flexible glue model shows how to create rectangles with width at least logarithmic in their length, but does not work for thinner rectangles. However, for *medium* rectangles (width less than  $\log N$  but not thin) we can combine the flexible glue model with the 2-temperature model to attain the tight  $\Theta(\sqrt{\log N})$  tile complexity. Is it possible to assemble such a rectangle using only the flexible glue model? And finally, even in the case of the standard model, the Kolmogorov lower bounds for the assembly of  $N \times N$  squares (Theorems 6.1, 6.2) do not apply if the temperature of the system is a large exponential function of  $N$ . If this is allowed, is it possible to reduce the tile complexity of assembling  $N \times N$  squares?

**9. Acknowledgement.** We would like to thank the anonymous reviewer of this paper for the extremely detailed and helpful comments.

#### REFERENCES

- [1] L. ADLEMAN, Q. CHENG, A. GOEL, AND M. HUANG, *Running time and program size for self-assembled squares*, in Proceedings of the 33rd Annual ACM Symposium on Theory of Computing, 2001, pp. 740–748.
- [2] L. ADLEMAN, Q. CHENG, A. GOEL, M. HUANG, D. KEMPE, P. ESPANES, AND P. ROTHMUND, *Combinatorial optimization problems in self-assembly*, in Proceedings of the 34th Annual ACM Symposium on Theory of Computing, 2002, pp. 23–32.
- [3] Q. CHENG AND P. M. DE ESPANES, *Resolving two open problems in the self-assembly of squares*, Tech. Report 793, University of Southern California, June 2003.
- [4] T.-J. FU AND N. C. SEEMAN, *DNA double-crossover molecules*, *Biochemistry*, 32 (1993), pp. 3211–3220.
- [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*, *Journal of the American Chemical Society*, 122 (2000), pp. 1848–1860.
- [6] M. G. LAGOUDAKIS AND T. H. LABEAN, *2D DNA self-assembly for satisfiability*, in Proceedings of the 5th DIMACS Workshop on DNA Based Computers, June 26 1999, pp. 459–468.
- [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. ROTHMUND AND E. WINFREE, *The program-size complexity of self-assembled squares*, in Proceedings of the 32nd Annual ACM Symposium on Theory of Computing, 2000, pp. 459–468.
- [10] H. WANG, *Proving theorems by pattern recognition*, *Bell Systems Technical Journal*, 40 (1961), pp. 1–42.
- [11] E. WINFREE, *Algorithmic Self-Assembly of DNA*, PhD thesis, California Institute of Technology, Pasadena, 1998.
- [12] E. WINFREE, F. LIU, L. WENZLER, AND N. SEEMAN, *Design and self-assembly of two-dimensional DNA crystals*, *Nature*, 394 (1998), pp. 539–544.
- [13] E. WINFREE, X. YANG, AND N. C. SEEMAN, *Universal computation via self-assembly of DNA: Some theory and experiments*, in Proceedings of the 3rd International Meeting on DNA Based Computers, June 10-12 1996.