

# The Computation Complexity of Temperature-1 Tilings

John H. Reif<sup>1,2</sup> and Tianqi Song<sup>1</sup>

<sup>1</sup> Department of Computer Science, Duke University  
Durham, NC 27708, USA

{reif, stq}@cs.duke.edu,

<sup>2</sup> King Abdulaziz University (KAU)

**Abstract.** This paper assumes the conventional two-dimensional *aTAM* for tiling assembly due to Winfree. In this model, aTAM system has a finite set of unit size tiles with glues on their boundaries, a seed tile that is always positioned at the origin, and a glue strength function that determines the affinity of binding between adjacent tiles. It has a parameter  $\tau$  known as the *temperature* which determines the accumulative glue strength that a given tile needs to insure that it can be positioned in the assembly. An aTAM system is *deterministic* if no two assemblies each yield a different tile type in the same position, and otherwise is *nondeterministic*.

The problem of whether an aTAM tile set can be used to tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane is termed here the  $\mathbb{N}^2$  *tiling problem*. The  $\mathbb{N}^2$  tiling problem is known to be undecidable when the temperature is at least 2 even if the aTAM system is deterministic, and is also known to be undecidable when the temperature is 1 and when the aTAM system is nondeterministic. It is an open problem whether the  $\mathbb{N}^2$  tiling problem is decidable when the temperature is 1 and the system is deterministic. An aTAM system is *strongly deterministic* if it is deterministic and on any assembly sequence, it is not possible to replace a previously positioned tile in the assembly with a different tile type in the same position, without decreasing the summed glue strength with neighbors below the temperature  $\tau$ . This paper gives the first proof that there is a decision procedure for the  $\mathbb{N}^2$  tiling problem when the temperature is 1, and the system is strongly deterministic and confined in  $\mathbb{N}^2$ .

Our proof uses interesting proof techniques. We first prove that given a 2-dimensional strongly deterministic temperature-1 aTAM system  $S$  confined in  $\mathbb{N}^2$ , we can construct a 2-dimensional vector addition system with states (VASS)  $W$  such that a point on  $\mathbb{N}^2$  can be tiled by  $S$  iff it is reachable by  $W$ . Since the set of reachable points of a 2-dimensional VASS is semilinear, the set of points that can be tiled by  $S$  is also semilinear. Semilinear sets can be characterized by Presburger Arithmetic formulas, and we construct a Presburger Arithmetic formula  $P$  such that  $(x, y) \in \mathbb{N}^2$  can be tiled by  $S$  iff  $P(x, y)$  is true. Based on  $P$ , we construct another Presburger Arithmetic formula  $FC$  such that  $S$  can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane iff  $FC$  is true. The validity of Presburger Arithmetic formulas is decidable, and

then it is decidable whether  $S$  can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane. Our decision procedure has time complexity  $2^{2^{2^{2^{O(n^2)}}}}$  where  $n$  is the number of tile types in the 2-dimensional strongly deterministic temperature-1 aTAM system.

We also show that the nondeterministic temperature-1  $n \times n$  square problem is NP-complete and the strongly deterministic temperature-1  $n \times n$  square problem can be solved by a log-space bounded deterministic Turing Machine.

Keywords: Computation Complexity, Tiling, Assembly, TAM, Temperature-1, Presburger Arithmetic

# 1 Introduction

## 1.1 Domino Assembly Problems

There has long been a close association with the concept of computation and that of self-assembly. The theory of self-assembly dates to the domino assembly problem formulated in 1961 by [47], which assumed a finite set of rectilinear objects he termed dominos with colors assigned to their borders and an initial partial assembly of dominos on the plane. Wang posed the domino assembly problem: Whether the assembly can be extended by placing further of these dominos (with replication) at all positions of  $\mathbb{N}^2$ , so that all the borders of adjacent dominos have the same color. In [4] this domino assembly problem was proved to be undecidable and later the proof was simplified by [42]; both these proofs used a simulation of a universal computing model as a key element of their proof. Excellent surveys of works in domino assembly and its generalizations (e.g., to polyominoes) are given by [20], [21]. A deficiency of the formulation of the domino assembly problem was that it considered the resulting assembly, but it did not address the issue of the process of assembly, which is important to Nanoassembly.

## 1.2 DNA Nanoassembly

With the advent in the late 1990's of the experimental demonstration of molecular self-assemblies, particularly self-assembled DNA nanostructures, there was a need for more refined models for self-assembly. The DNA nanoassembly process envisioned by Seeman and Winfree begins with the self-assembly of DNA nanostructures termed DNA tiles, each consisting of a small number of DNA strands that are held together DNA hybridization. The DNA tiles have single-stranded DNA called pads that can allow the DNA tiles to bind together via DNA hybridization to form lattices of DNA tiles. Generally the temperature and geometry of the assembly are critical to this molecular assembly process.

## 1.3 The Abstract Tile Assembly Model

To provide an abstract model for such a molecular assembly process, [48, 49] introduced the aTAM. It assumes a finite number of unit size square tile types, with glues on each of their boundaries, and a glue strength function that determines the affinity of glues between adjacent tiles. It gives an explicit model for process of tile assembly: During an assembly sequence at a temperature  $\tau > 0$ , after an initial tile is placed at the origin, a tile can be placed at a position where the sum of its glue strength between adjacent tiles is at least  $\tau$ . If no two assembly processes each yield a different tile type in the same position, then the system is termed *deterministic*, and otherwise *nondeterministic*. Using a direct simulation of a universal one-dimensional cellular automata, [49] showed the undecidability of the problem of tiling assembly over all of  $\mathbb{N}^2$  when the temperature is 2. His

universal aTAM system only used a constant number of tiles and was deterministic. There have been numerous further results on the computability and complexity of assembly in the aTAM (see the surveys of [35] and its extensions and variants (e.g., [2])). Overviews of DNA self-assembly are given in [6] and [7] and comprehensive recent survey of the theory of self-assembly is given in [11].

#### 1.4 Temperature-1 Assemblies and Linear Assemblies

Tiling assemblies that have temperature-1 proceed by placing a tile that only needs to bind to one previously placed tile.

A subclass of temperature-1 tiling assemblies, here termed *linear tiling assemblies* (and also sometimes called ribbon-like assemblies), simply assemble as a (finite or infinite) one-dimensional row of tiles. Linear assemblies have some important practical applications and some interesting associated theory. The first experimentally demonstrated computation using algorithmic self-assembly of DNA tiles (see [27], [28], [50], and [31]) were linear tiling assemblies for arithmetic and logical computations (the design of many of these linear tiling assemblies for logical computations first appeared in [40]). Only later two-dimensional assemblies (of DNA Sierpinski triangles) were experimentally demonstrated by [43]. [1] showed that linear tiling assemblies are decidable. [8] and others have given tiling assemblies that assemble to given expected lengths.

In general, temperature-1 assemblies need not be linear in shape, and can form relatively complex two-dimensional tilings. Temperature-1 that are not linear assemblies also have important practical applications. For example, [29] made use of temperature-1 subassemblies (known as snake tilings) to provide error-resiliency in tiling assemblies. [30] proved lower bounds on the number of tile types needed for temperature-1 aTAM systems to form tiling assemblies of certain given shape and size.

#### 1.5 Prior Computability Results of Temperature-1 Assemblies

A number of prior results for extensions or alternative aTAMs provide Turing Universal assemblies for temperature-1 assemblies, implying the undecidability of the problem of determining if a given aTAM system allows a complete assembly over a given infinite domain:

- [9] showed this for temperature-1 two-dimensional assemblies that use probabilistic assembly processes.
- [36] showed this for temperature-1 two-dimensional assemblies with negative glue (this negative glue provides for the decrease in the strength of a tile with a previously placed tile of the assembly).
- [3] showed this for temperature-1 two-dimensional deterministic assemblies with step-wise and staged assembly. [9] also showed this for temperature-1 three-dimensional deterministic tiling assemblies.

One of the outstanding problems in the theory of tiling assembly was to determine, in the original aTAM, the decidability of the problem of temperature-1

deterministic assembly over an infinite 2D domain such as  $\mathbb{N}^2$  and to characterize the positions that the tiles types in such assemblies. [12] gave a partial, and very insightful, step toward this. In particular, they conjectured that in every temperature-1 aTAM system that produces a unique infinite assembly, there occurs a certain phenomenon they term pumpability: Every sufficiently long path of tiles in an assembly of this system contains a segment in which the same tile type repeats, and the subpath between these two occurrences can be repeated indefinitely along the same direction as the first occurrence of the segment, without colliding with a previous portion of the path. Assuming this pumpability conjecture holds, they showed that the resulting assembly is a finite union of semi-doubly periodic sets. It is not yet known if this pumpability conjecture holds, and determining the decidability and fully characterizing of the general case temperature-1 deterministic tiling assemblies remains open. Furthermore, to our knowledge there is no known decision procedure for the determination of pumpability of a tile set.

### 1.6 Our Result for Strongly Deterministic Temperature-1 Assemblies

An aTAM system is *strongly deterministic* if it is deterministic and further, on any assembly sequence, it is not possible to replace a previously positioned tile in the assembly with a different tile type in the same position, without decreasing the summed glue strength with neighbors below the temperature  $\tau$ .

In Section 3 we prove that there is a decision procedure for the  $\mathbb{N}^2$  tiling problem when the temperature is 1, and the system is strongly deterministic and confined in  $\mathbb{N}^2$ . Our proof introduces some interesting and novel (for tiling theory) proof techniques, including the use of vector addition system with states (VASS) (defined in Section 2) and Presburger Arithmetic formula (defined in Section 3.2). We first prove that given a 2-dimensional strongly deterministic temperature-1 aTAM system  $S$  confined in  $\mathbb{N}^2$ , we can construct a 2-dimensional vector addition system with states (VASS)  $W$  such that a point on  $\mathbb{N}^2$  can be tiled by  $S$  iff it is reachable by  $W$ . Since the set of reachable points of a 2-dimensional VASS is semilinear, the set of points that can be tiled by  $S$  is also semilinear. Semilinear sets can be characterized by Presburger Arithmetic formulas. Therefore, we can construct a Presburger Arithmetic formula  $P$  such that  $(x, y) \in \mathbb{N}^2$  can be tiled by  $S$  iff  $P(x, y)$  is true. Based on  $P$ , we construct another Presburger Arithmetic formula  $FC$  such that  $S$  can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane iff  $FC$  is true. The validity of Presburger Arithmetic formulas is decidable, and then it is decidable whether  $S$  can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane. Our decision procedure has time complexity  $2^{2^{2^{2^{O(n^2)}}}}$  where  $n$  is the number of tile types in the 2-dimensional strongly deterministic temperature-1 aTAM system.

### 1.7 Our Results for Temperature-1 $n \times n$ Square Tiling Assemblies

We also have some results for temperature-1 assembly of  $n \times n$  squares:

1. In Section 5 we show that the nondeterministic temperature-1  $n \times n$  square problem is NP-complete.
2. In Section 4 we show that the strongly deterministic temperature-1  $n \times n$  square problem can be solved by a log-space bounded Turing Machine.

## 2 Definitions of Tile Assembly and Vector Addition Systems

In the following, let  $\mathbb{Z}$  be the set of integers and  $\mathbb{N}$  be the non-negative integers.

### 2.1 The Abstract Tile Assembly Model

In this section, we present a terse description of abstract Tile Assembly Model (aTAM) [37]. An aTAM system ([49]) in 2-dimension is a 5-tuple:  $(\mathbb{T}, t_0, \tau, g, \Sigma)$ , where:

- $\mathbb{T}$  is a finite set termed the *set of tile types*: Each *tile type*  $t \in \mathbb{T}$  can be considered a unit length square that can not be rotated or reflected and with four glues coloring its sides; these glues are defined by a 4-tuple  $(t_N, t_E, t_S, t_W) \in \Sigma^4$  listing the glues in it's north, east, south and west directions; where  $t_N$  is the north glue,  $t_S$  is the south glue,  $t_E$  is the east glue, and  $t_W$  is the west glue.
- $t_0 \in \mathbb{T}$  is the *seed tile*: The seed tile  $t_0$  is fixed at a position (generally  $(0, 0)$ ) on integer Cartesian plane  $\mathbb{Z}^2$  at the beginning of assembly process.
- $\tau$  is a positive integer termed the *temperature*: A tile  $t$  can be incorporated into current assembly configuration at a position iff the accumulative glue strength between  $t$  and its adjacent tiles around that position is not less than  $\tau$ .
- $g : \Sigma \times \Sigma \mapsto \mathbb{N}$  is a symmetric mapping, known as the *glue strength function*, from pairs of glues to the nonnegative integers  $\mathbb{N}$  which defines the glue strength between two glue types. It is required to be symmetric: for any  $a, b \in \Sigma$ ,  $g(a, b) = g(b, a)$ .
- $\Sigma$  is the set of glue types.

Let  $\mathbb{P} \subset \mathbb{Z}^2$  be the *domain of positions* that tiles may be placed. Infinite copies of each tile type are provided during assembly process.

An assembly configuration is a partial mapping  $C$  from  $\mathbb{P}$  to  $\mathbb{T}$ . At each position  $(x, y) \in \mathbb{P}$  where  $C(x, y)$  is undefined, the configuration is said to be *empty*. For an assembly configuration  $C$ ,  $dom(C) = \{(x, y) | (x, y) \in \mathbb{P} \text{ and } C(x, y) \text{ is defined}\}$ . If  $C(x, y)$  is defined, then a tile of tile type  $C(x, y)$  is said to be *placed at position*  $(x, y)$ . The neighborhood of position  $(x, y)$  is the set  $Neighbors(x, y) = \{(x, y + 1), (x + 1, y), (x, y - 1), (x - 1, y)\}$ .

The adjacent neighbors of a tile placed in position  $(x, y) \in \mathbb{P}$  of an assembly configuration are those tiles positioned at an element of  $Neighbors(x, y)$  and can include:

- the *north neighbor* at position  $(x, y + 1) \in \mathbb{P}$ ,
- the *east neighbor* at position  $(x + 1, y) \in \mathbb{P}$ ,
- the *south neighbor* at position  $(x, y - 1) \in \mathbb{P}$ ,
- the *west neighbor* at position  $(x - 1, y) \in \mathbb{P}$ .

If the tile of tile type  $t$  at position  $(x, y) \in \mathbb{P}$  has an adjacent neighbor of tile type  $t'$ , then:

- If  $t'$  is the north neighbor at position  $(x, y + 1)$  in the north, then the glue strength between them is  $g(t_N, t'_S)$ ,
- If  $t'$  is the east neighbor at position  $(x + 1, y)$  in the east, then the glue strength between them is  $g(t_E, t'_W)$ ,
- If  $t'$  is the south neighbor at position  $(x, y - 1)$  in the south, then the glue strength between them is  $g(t_S, t'_N)$ ,
- If  $t'$  is the west neighbor at position  $(x - 1, y)$  in the west, then the glue strength between them is  $g(t_W, t'_E)$ .

For assembly configurations  $C$  and  $C'$ ,  $C \rightarrow C'$  ( $C$  produces  $C'$  in one tile assembly step  $(t, (x, y))$ ) if  $\exists t \in \mathbb{T} \exists (x, y) \in (\mathbb{P} \setminus \text{dom}(C))$  such that  $g(t_N, C(x, y + 1)_S) + g(t_S, C(x, y - 1)_N) + g(t_E, C(x + 1, y)_W) + g(t_W, C(x - 1, y)_E) \geq \tau$ ,  $C'(m, n) = C(m, n)$  for  $(m, n) \neq (x, y)$  and  $C'(x, y) = t$ . Hence an tile assembly step  $(t, (x, y))$  consisting of placing at a position  $(x, y)$  a tile type  $t \in \mathbb{T}$  where (a) position  $(x, y)$  was empty in current configuration, and (b) the accumulative glue strength between  $t$  and its (non-empty) adjacent neighboring tiles sums to at least the temperature  $\tau$ .

Given an aTAM, an assembly sequence is a sequence of assembly configurations  $C_0, C_1, \dots, C_k$  where:

- $C_0$  is the initial assembly configuration with the seed tile  $t_0$  at origin position  $(0, 0)$ , and with all other positions empty, and
- $C_i \rightarrow C_{i+1}$  for each  $i = 0, \dots, k - 1$ .

Hence each assembly configuration of the assembly sequence is produced from the previous assembly configuration: On each subsequent step  $j$  of the assembly sequence, an assembly configuration  $C_j$  is derived from the previous assembly configuration  $C_{j-1}$  by a tile assembly step  $(t, (x, y))$  consisting of placing at a position  $(x, y)$  a tile type  $t \in \mathbb{T}$  where (a) position  $(x, y)$  was empty in  $C_{j-1}$ , and (b) the accumulative glue strength between  $t$  and its (non-empty) adjacent neighboring tiles sums to at least the temperature  $\tau$ .

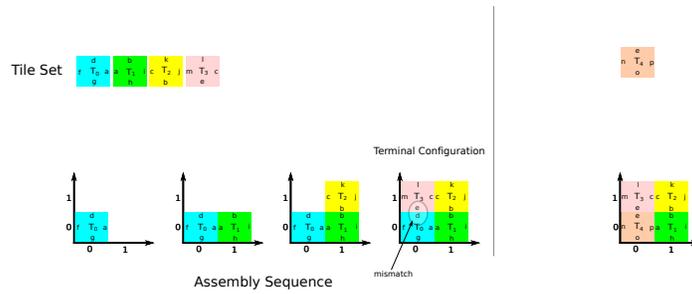
Note that for any given assembly sequence there is only at most one tile type placed at any given position  $(x, y) \in \mathbb{P}$ .

Let  $\Rightarrow$  be the transitive closure of  $\rightarrow$ . For assembly configuration  $C$  and  $C'$ ,  $C \Rightarrow C'$  (termed  $C$  produces  $C'$ ) if either  $C = C'$  or there exists assembly configuration  $C_1, C_2, \dots, C_k$  such that for each  $i = 1, \dots, k - 1$ ,  $C_i \rightarrow C_{i+1}$ , where  $C = C_1$  and  $C' = C_k$ . Given an assembly configuration  $C$ , define  $\text{terminal}(C) = \{C' \mid C \Rightarrow C' \text{ and } \neg \exists C'' \neq C' \text{ such that } C' \Rightarrow C''\}$ ; this is the set of *terminal productions* of  $C$ .

An aTAM system is *deterministic* if there is only at most one tile type placed at any given position  $(x, y) \in \mathbb{P}$  in any assembly sequence for that aTAM system. This implies that for a deterministic aTAM system and any position  $(x, y) \in \mathbb{P}$ , if an assembly sequence results in a tile type  $t$  being placed in position  $(x, y)$ , then there is no other assembly sequence resulting in a different tile type  $t' \neq t$  being placed in position  $(x, y)$ . Note however, that a given deterministic aTAM system might have multiple distinct assembly sequences, where the order in which tiles are placed might differ.

An aTAM system is *strongly deterministic* if it is deterministic and on any assembly sequence, it is not possible to remove a previously positioned tile (say of type tile  $t$  and position  $(x, y)$ ) and replace it with a different tile type  $t'$  (where  $t' \neq t$ ) at the same position  $(x, y)$ , where the summed glue strength with tiles at  $Neighbors(x, y)$  would remain not less than the temperature  $\tau$ .

Note that "strongly deterministic" does NOT necessarily mean "no mismatch" when the temperature is 1. One example is shown in Figure 1.



**Fig. 1.** There are four tile types in this temperature-1 aTAM system as shown on the left side of the line, and  $T_0$  is seed tile. The glue strength between two glues is 1 if they are the same, otherwise, it is 0. This system is strongly deterministic according to our definition: On any assembly sequence (This system has only one assembly sequence as shown.), it is not possible to remove a previously positioned tile and replace it with a different tile type at the same position, where the summed glue strength with neighbor tiles would remain not less than the temperature. However, there is a mismatch in terminal configuration between  $T_0$  and  $T_3$ . If we add another tile type  $T_4$  which has glue  $e$  on its north edge to this system, this system will not be strongly deterministic any more: On the assembly sequence, it is possible to remove the previously positioned tile of type  $T_0$  at  $(0, 0)$  and replace it with a tile of type  $T_4$ , and the summed glue strength of  $T_4$  at  $(0, 0)$  with its neighbors is not less than the temperature because of the glue match between north glue of  $T_4$  at  $(0, 0)$  and south glue of  $T_3$  at  $(0, 1)$ .

## 2.2 Vector Addition Systems and Vector Addition Systems with States

**Vector Addition Systems** A  $d$ -dimensional Vector Addition System (VAS) consists of pair  $(v_0, A)$  where  $v_0$  (called the start vector) is a vector in  $\mathbb{N}^d$  and  $A$  is a finite set of arbitrary vectors in  $\mathbb{Z}^d$ . The set of reachable vectors of a VAS  $(v_0, A)$  is the smallest set of vectors in  $\mathbb{N}^d$  containing the start vector  $v_0$  and such that if a vector  $v$  is reachable, then any (non-negative) vector  $v + a \in \mathbb{N}^d$  is reachable, for some  $a \in A$ . Note that this definition implies that if  $v$  is a reachable vector of a VAS  $(v_0, A)$ , then there exists a sequence of  $m$  (non-negative) vectors  $v_0, v_1, \dots, v_{m-1} \in \mathbb{N}^d$  where  $v_{m-1} = v$ , and  $v_k - v_{k-1}$  is an element of  $A$  for each  $k \in \{1, \dots, m-1\}$ .

**Vector Addition Systems with States:** A vector addition system with states (VASS) (see [34] and [26]) consists of a tuple  $(v_0, A, q_0, \mathbf{Q}, \Delta)$  where  $(v_0, A)$  is a VAS,  $\mathbf{Q}$  is a finite set of states,  $q_0$  is the starting state in  $\mathbf{Q}$ , and  $\Delta \subset \mathbf{Q} \times A \times \mathbf{Q}$  is a finite set of transitions. A configuration of a VASS is a pair in  $\mathbf{Q} \times \mathbb{N}^d$  consisting of a state and a nonnegative vector. The set of reachable configurations of the VASS is the smallest set of configurations containing the initial configuration  $(q_0, v_0)$  and such that if  $(q', v)$  is a reachable configuration, and  $(q', a, q) \in \Delta$  and  $v + a$  is non-negative, then  $(q, v + a)$  is a reachable configuration. Note that this definition implies that if  $(q, v)$  is reachable in the VASS, then there exists a sequence of  $m$  configurations  $(q_0, v_0), (q_1, v_1), \dots, (q_{m-1}, v_{m-1})$ , where  $(q_{m-1}, v_{m-1}) = (q, v)$ , and for each  $k \in \{1, \dots, m-1\}$ , we have:  $(q_{k-1}, v_k - v_{k-1}, q_k) \in \Delta$  where  $q_k \in \mathbf{Q}$ ,  $v_k - v_{k-1} \in A$ , and further  $v_k$  is a (non-negative) vector  $\in \mathbb{N}^d$ .

### 3 Deciding Strongly Deterministic Temperature-1 Assemblies

#### 3.1 Simulating 2D Strongly Deterministic Temperature-1 Tile Assembly via 2D Vector Addition Systems with States

##### The Simulation

Now suppose we are given an aTAM system  $(\mathbb{T}, t_0, \tau = 1, g, \Sigma)$  in  $d = 2$  dimensions (for this construction, we do not yet assume the aTAM system is strongly deterministic). Recall each tile type  $t \in \mathbb{T}$  is a 4-tuple  $(t_N, t_E, t_S, t_W) \in \Sigma^4$  listing the glues in its north, east, south and west directions. We assume the assembly sequence is confined to  $\mathbb{N}^2$ . We construct a dimension  $d = 2$  VASS  $W = (v_0, A, q_0, \mathbf{Q}, \Delta) = ((0, 0), \{(0, -1), (-1, 0), (1, 0), (0, 1)\}, t_0, \mathbb{T}, \Delta)$  that will simulate this aTAM system. This simulating VASS has the state set  $\mathbf{Q}$  = the set of tile types  $\mathbb{T}$ , the start vector  $v_0 = (0, 0)$ , the initial state  $q_0 =$  initial tile  $t_0$ , and  $A = \{(0, -1), (-1, 0), (1, 0), (0, 1)\}$ . We define  $\Delta = \{(t', (0, -1), t) | g(t_N, t'_S) \geq 1\} \cup \{(t', (-1, 0), t) | g(t_E, t'_W) \geq 1\} \cup \{(t', (0, 1), t) | g(t_S, t'_N) \geq 1\} \cup \{(t', (1, 0), t) | g(t_W, t'_E) \geq 1\}$ .

##### Proof of the Simulation

**Lemma 3.1:**  $\forall t \in \mathbb{T}, \forall x, y \in \mathbb{N}$ , if the aTAM (not assumed necessarily strongly deterministic) system has an assembly sequence that places tile type  $t$  in position  $(x, y)$ , then  $(t, (x, y))$  is a reachable configuration of  $W$ .

**Proof:** We use inductive proof. Suppose there is an assembly sequence of length  $m (m \in \mathbb{N}^+)$ :  $C_0, C_1, \dots, C_{m-1}$ , where  $C_0$  is the initial configuration and  $C_{m-1}$  is first configuration that has tile type  $t$  in position  $(x, y)$ .

Basis case: In  $C_0$ , only position  $(0, 0)$  has a tile. The tile type is  $t_0$ .  $(t_0, (0, 0))$  is a reachable configuration of  $W$ .

Inductive step: We assume that  $\forall (i, j) \in \mathbb{N}^2$  such that  $C_k$  has a tile there,  $(t_{(i,j)}, (i, j))$  is reachable by  $W$  where  $k \in \{0, 1, \dots, m-2\}$ , and  $t_{(i,j)}$  is type of the tile at  $(i, j)$ . For  $C_{k+1}$ , we only need to consider the position where  $C_k$  does not have a tile, but  $C_{k+1}$  has. Let the position be  $p = (a, b)$ , and the tile type at  $(a, b)$  be  $v$ . There should be a tile placed at a neighbor position of  $(a, b)$  in  $C_k$ , such that the glue strength between this tile and the tile of type  $v$  at  $(a, b)$  is  $\tau = 1$ . Let the neighbor position of  $(a, b)$  be  $p' = (a', b')$ , and the tile type at  $(a', b')$  be  $v'$ . According to the assumption,  $(v, (a, b))$  is reachable by  $W$ . Then  $(v', (a', b'))$  is also reachable by  $W$  because at least one of following cases occurs:

- If tile  $v$  is placed at position  $p = (a, b)$  binding in it's North with tile  $v'$  previously placed at position  $p' = (a, b+1) = (a', b')$ , then  $g(v_N, v'_S) \geq 1$  and  $p - p' = (0, -1)$ , so  $(v', p - p', v) = (v', (0, -1), v) \in \Delta$ .
- If tile  $v$  is placed at position  $p = (a, b)$  binding in it's East with tile  $v'$  previously placed at position  $p' = (a+1, b) = (a', b')$ , then  $g(v_E, v'_W) \geq 1$  and  $p - p' = (-1, 0)$ , so  $(v', p - p', v) = (v', (-1, 0), v) \in \Delta$ .
- If tile  $v$  is placed at position  $p = (a, b)$ , binding in it's South with tile  $v'$  previously placed at position  $p' = (a, b-1) = (a', b')$ , then  $g(v_S, v'_N) \geq 1$  and  $p - p' = (0, 1)$ , so  $(v', p - p', v) = (v', (0, 1), v) \in \Delta$ .
- If tile  $v$  is placed at position  $p = (a, b)$ , binding in it's West with tile  $v'$  previously placed at position  $p' = (a-1, b) = (a', b')$ , then  $g(v_W, v'_E) \geq 1$  and  $p - p' = (1, 0)$ , so  $(v', p - p', v) = (v', (1, 0), v) \in \Delta$ .

Therefore,  $\forall (x, z) \in \mathbb{N}^2$  such that  $C_{k+1}$  has a tile there,  $(t_{(x,z)}, (x, z))$  is reachable by  $W$ , where  $t_{(x,z)}$  is type of the tile at  $(x, z)$ .

In conclusion:  $\forall (c, d) \in \mathbb{N}^2$  such that  $C_{m-1}$  has a tile there,  $(t_{(c,d)}, (c, d))$  is reachable by  $W$ , where  $t_{(c,d)}$  is type of the tile at  $(c, d)$ , and then  $(t, (x, y))$  is a reachable configuration of  $W$ . **QED**

**Lemma 3.2:** Given an aTAM system with temperature  $\tau = 1$  which is strongly deterministic, let  $W$  be the VASS constructed as described above.  $\forall t \in \mathbf{Q}, \forall x, y \in \mathbb{N}$ , if  $(t, (x, y))$  is a reachable configuration of  $W$  then the aTAM has an assembly sequence that places tile type  $t$  in position  $(x, y)$ .

**Proof:** We again use inductive proof. If  $(t, (x, y))$  is a reachable configuration of  $W$ , there are a sequence of configurations  $(t_0, (x_0, y_0)), (t_1, (x_1, y_1)), \dots, (t_{m-1}, (x_{m-1}, y_{m-1}))$  where  $(x_0, y_0) = (0, 0)$ ,  $(t_{m-1}, (x_{m-1}, y_{m-1})) = (t, (x, y))$ , and  $(t_{k-1}, (x_k - x_{k-1}, y_k - y_{k-1}), t_k) \in \Delta$  for each  $k \in \{1, 2, \dots, m-1\}$ . For the basis case, it is true that the aTAM system has an assembly sequence that places tile type  $t_0$  at position  $(0, 0)$ . Inductive step: We assume that for

$i = n - 1$ , the aTAM system has an assembly sequence that places tile type  $t_{n-1}$  at position  $(x_{n-1}, y_{n-1})$  where  $n \in \{1, 2, \dots, m - 1\}$ . When  $i = n$ , because  $(t_{n-1}, (x_n - x_{n-1}, y_n - y_{n-1}), t_n) \in \Delta$ , we know that  $t_n$  can be placed at  $(x_n, y_n)$  by attaching to  $t_{n-1}$  at  $(x_{n-1}, y_{n-1})$  according to the construction of  $W$ . The only concern is that there may be already a tile at  $(x_n, y_n)$ . That tile should also be of type  $t_n$  because the system is strongly deterministic. Therefore, the aTAM system has an assembly sequence that places tile type  $t_n$  at position  $(x_n, y_n)$ .

**QED**

By the above Lemmas 3.1 and 3.2, we have:

**Theorem 3.3:** Given an aTAM system with temperature  $\tau = 1$  which is strongly deterministic and confined in  $\mathbb{N}^2$ , let  $W$  be the VASS constructed as described above.  $(t, (x, y))$  is a reachable configuration of  $W$  iff the aTAM has an assembly sequence that places tile type  $t$  in position  $(x, y)$ .

**The Set of Assembly Steps Are Semilinear** Given sets of d-vectors  $C$  and  $C' \subset \mathbb{N}^d$  ( $C$  is singleton and  $C'$  is finite), the linear set induced by  $C$  and  $C'$  is the smallest set  $S$  containing  $C$  and where if  $v \in S$ , then  $v + c' \in S$  for some  $c' \in C'$ . Note that this implies that if  $v \in S$ , then there is a sequence  $v_0, \dots, v_k$  such that  $v_0 \in C$  and  $v_i = v_{i-1} + c'$  for some  $c' \in C'$  for  $i \in \{1, \dots, k\}$ . A semilinear set is a finite union of linear sets. Semilinear Sets were first defined in [34].

Given a strongly deterministic temperature-1 aTAM system confined in  $\mathbb{N}^2$  with tile type set  $\mathbb{T}$ , we define the set  $S = \{(x, y) | x, y \in \mathbb{N}, \exists t \in \mathbb{T} \text{ such there is an assembly sequence that places a tile type } t \text{ at position } (x, y)\}$ . Also, for any tile type  $t \in \mathbb{T}$ , we define the set  $S_t = \{(x, y) | x, y \in \mathbb{N} \text{ such there is an assembly sequence that places a tile type } t \text{ at position } (x, y)\}$ .

[23] proved that the set of reachable points of any VASS of dimension 2 is effectively semilinear. [24] showed this construction could be done in doubly exponential nondeterministic time in the size of the VASS. Hence we have:

**Corollary 3.4:** For any tile type  $t \in \mathbb{T}$ , the set  $S_t$  is semilinear and the set  $S$  is semilinear.

### 3.2 Defining 2D Deterministic Temperature-1 Tile Assembly via Presburger Arithmetic

#### Presburger Arithmetic

*Presburger arithmetic* is the first order logic  $(\mathbb{Z}, <, +, =, 0, 1)$  (see [13] for a review of first order logics) with constants  $0, 1$ , the addition operation  $+$ , the order relation  $<$ , equality  $=$  as well as universal and existential quantification over the integers  $\mathbb{Z}$ . This logic was first introduced by [38]. Presburger arithmetic provides surprisingly powerful expressibility (see [10], [19], [26]) of mathematical systems that do not require multiplication.

The semilinear sets have been shown [19] to be equivalent to the sets definable by Presburger arithmetic formula, and there is an effective procedure for constructing a Presburger arithmetic formula that defines an given semilinear set.

( [25] later simplified their proof using in part some results in [18].) Combining these results with **Corollary 3.4**, we have:

**Corollary 3.5:** Given an aTAM system of temperature  $\tau = 1$  which is strongly deterministic and confined in  $\mathbb{N}^2$ , we can construct a Presburger arithmetic formula  $P(X, Y)$  such that for each position  $(x, y) \in \mathbb{N}^2$ ,  $P(x, y)$  is valid if and only if there is an assembly sequence that places a tile at position  $(x, y)$ , where  $X$  and  $Y$  are free variables of  $P$ .

### A Presburger Arithmetic Formula Characterizing Strongly Deterministic Temperature-1 $\mathbb{N}^2$ Tiling Problem

**Corollary 3.6:** Given an aTAM system of temperature  $\tau = 1$  which is strongly deterministic and confined in  $\mathbb{N}^2$ , we can construct a Presburger arithmetic formula  $\forall X, Y ((X \geq 0) \wedge (Y \geq 0)) \rightarrow P(X, Y)$  (which we call  $FC$ ), such that it is valid if and only if the given aTAM system can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane, where  $X$  and  $Y$  are free variables.

### Deciding Presburger Arithmetic

A key property of Presburger arithmetic formula, first shown by [38] (and independently discovered by [46]) is that formula validity is decidable. Much effort was devoted to decreasing the computational effort to decide the validity of Presburger formula of length  $n$ . One major class of decision methods for Presburger arithmetic is quantifier elimination (also see [14], [51], and [13] for discussions of first order theories and their decision methods, including quantifier elimination methods), first used by [38] and later improved by [10], [32], and [33] to triple exponential time. The time bounds of decision procedures for Presburger arithmetic validity can not be improved below doubly exponential time since [15] proved a double exponential nondeterministic time lower bound. [5] showed the problem of Presburger arithmetic validity to be complete for doubly exponential time alternating machines restricted to a linear number of alternations (using for their upper bounds some results of [14]). [39], [44] and [45] gave improved upper bounds for the complexity of subcases of Presburger arithmetic with bounded or restricted quantifier alternations, and [16] gave single exponential  $exp(\Omega(n))$  time lower bounds for deciding validity of Presburger arithmetic formula with a constant bound on the number of quantifier alternations. [17] has made some experiments of various methods for deciding Presburger arithmetic formula.

These decision procedures for Presburger arithmetic imply:

**Theorem 3.7:** There is a decision procedure with time complexity upper bounded by  $2^{2^{2^{2^{O(n^2)}}}}$  that determines whether a strongly deterministic temperature-1 aTAM system (confined in  $\mathbb{N}^2$ ) can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane.

### Summary of our Decision Procedure and Time Complexity Analysis

There are five steps in this decision procedure:

1. Step 1: Compute the corresponding 2-dimensional VASS  $W$  of the input  $S$  which is a 2-dimensional strongly deterministic temperature-1 aTAM system.
2. Step 2: Compute  $SL$ , the representation of the corresponding semilinear set of  $W$ .
3. Step 3: Compute  $P$ , the Presburger arithmetic formula to define  $SL$ .
4. Step 4: Construct Presburger arithmetic formula  $FC$  by  $P$  such that  $FC$  is true iff  $S$  can tile the nonnegative integer orthant  $\mathbb{N}^2$  of the cartesian plane.
5. Step 5: Decide the validity of  $FC$ .

Let the number of tile types of  $S$  be  $n$ . We assume a log-cost RAM computational model. Our time complexity is as follows:

1. Step 1 takes  $O(n^2)$  time by the simulation algorithm in 3.1. The number of the transitions of  $W$  is also  $O(n^2)$ .
2. Step 2 takes  $O(2^{2^{p(n)}})$  time by the algorithm given in [24] and  $p(n) = c * l * tr(W)$  is  $O(n^2)$ , where  $tr(W)$  is the number transitions in  $W$ ,  $l = 2$  is the length of binary encoding of the largest integer in  $W$  (We only use  $-1, 0, 1$  according to the construction of  $W$ .), and  $c$  is a constant independent of  $l$  and  $tr(W)$ . The size of  $SL$  is  $O(2^{2^{q(n)}})$  [24], where  $q(n)$  is  $O(n^2)$ .
3. Step 3 takes  $O(|SL| * 2^{r(n)})$  which is  $O(2^{(2^{q(n)} + r(n))})$  time by the construction in [25] and converting it to the formula without multiplication (The factor  $2^{r(n)}$  is from the bound of vector size in  $SL$  given in [24].), where  $|SL|$  is the size of  $SL$  and  $r(n)$  is  $O(n^2)$ . The size of  $P$  is also  $O(|SL| * 2^{r(n)})$  which is  $O(2^{(2^{q(n)} + r(n))})$ . Step 4 takes constant time and the size of  $FC$  is  $O(|P|)$  which is  $O(2^{(2^{q(n)} + r(n))})$ , where  $|P|$  is the size of  $P$ .
4. Step 5 takes  $O(2^{2^{a * |FC|}})$  which is  $O(2^{2^{d * 2^{(2^{q(n)} + r(n))}}})$  time [33] by the algorithm given in [10], where  $a, d$  are some constants and  $|FC|$  is the size of  $FC$ .

Above all, the time complexity of the decision procedure is  $O(2^{2^{d * 2^{(2^{b * n^2 + h * n^2})}}})$  where  $n$  is the number of tile types in the 2-dimensional strongly deterministic temperature-1 aTAM system, and  $d, b, h$  are constants, which is upper bounded by  $2^{2^{2^{2^{O(n^2)}}}}$ .

## 4 Strongly Deterministic Temperature-1 $n \times n$ Square Problem

In this section, we will define strongly deterministic temperature-1  $n \times n$  square problem and prove that it is in  $L$ .  $L$  is the class of decision problems that can be solved by a log-space bounded deterministic Turing Machine.

### 4.1 Strongly Deterministic Temperature-1 Tiling Reachability Problem

An aTAM system is *strongly deterministic* if it is deterministic and further, on any assembly sequence, it is not possible to replace a previously positioned tile in

the assembly with a different tile type in the same position, without decreasing the summed glue strength with neighbors below the temperature  $\tau$ .

**Strongly deterministic temperature-1 tiling reachability problem:** Given a strongly deterministic temperature-1 aTAM system  $\mathbf{S} = (\mathbb{T}, t_0, \tau = 1, g, \Sigma)$ ,  $t \in \mathbb{T}$ ,  $n \in \mathbb{N}^+$ ,  $(x, y) \in \mathbb{Z}^2$  where  $x, y \in L_n$  and  $L_n$  is defined as  $\{0, 1, 2, 3, \dots, n-1\}$ , and an initial configuration of size  $n$  at  $L_n \times \{0\}$ , decide whether there exists a linear assembly  $C_l$  from  $(0, 0)$  to  $(x, y)$  such that  $C_l(x, y) = t$  and  $C_l$  does not go beyond  $L_n \times L_n$ . A linear assembly (in section 4 and 5) is defined as a sequence of assembly steps  $(t_0, (x_0, y_0)), \dots, (t_n, (x_n, y_n))$  where if  $t_i$  is placed at  $(x_i, y_i)$ ,  $t_{i+1}$  can be placed at  $(x_{i+1}, y_{i+1})$  by attaching to  $t_i$  for any  $i \in \{1, 2, \dots, n-1\}$ , and no different tile types appear in same position.

It is well known that the composition of two functions in  $L$  is also in  $L$ . For completeness, and because we will use the same pipelining techniques in the following proofs, we give a full proof of this result.

**Proposition 4.1:** If function  $f, g \in L$ , then the composition  $g \circ f \in L$ .

**Proof:** Let  $M_f, M_g$  be the deterministic Turing machines that compute  $f$  and  $g$  in logspace respectively. We construct deterministic Turing machine  $M_{g \circ f}$  that computes  $g \circ f$ : The worktape contains 8 sections. Section 1 is for computing  $g(y)$  where  $y = f(x)$ . Section 2 is for storing the position of head on readtape. Section 3 is for storing the position of head on worktape. Section 4 is for storing the position of head on writetape. Section 5 is for storing the state of the machine. Section 6 is for storing  $i$  when the machine wants the  $i$ th bit of  $f(x)$ . Section 7 is for storing the  $i$ th bit of  $f(x)$ . Section 8 is for computing  $f(x)$ . The machine starts with working as  $M_g$  in section 1. When it needs the  $i$ th bit of  $f(x)$ , it will write corresponding information to sections 2-6, then begins to simulate  $M_f$  to compute  $f(x)$  in section 8. The machine does not write  $f(x)$  on write tape and only writes the  $i$ th bit of  $f(x)$  on section 7. When the machine gets the  $i$ th bit of  $f(x)$ , it will restore the machine according to the information in sections 2-6 and continue simulating  $M_g$  in section 1. The machine works as above until the computation is done and  $M_{g \circ f}$  computes  $g(f(x)) = (g \circ f)(x)$ .

The space complexity is determined as following: Let  $|x|$  be  $n$ , where  $|x|$  is the length of the binary encoding of  $x$ . Since  $f \in L$ ,  $|f(x)|$  should be  $poly(n)$ , where  $poly(n)$  is polynomial of  $n$ . Therefore, Section 1 is  $O(\log |f(x)|)$  which is  $O(\log n)$  size. Section 2 is  $O(\log |x|)$  which is  $O(\log n)$  size. Section 3 is  $O(\log |section\ 1|)$  which is  $O(\log \log n)$  size.  $g \in L$ , then  $|g(f(x))|$  should be  $poly(|f(x)|)$  which is  $poly(n)$ . Therefore, Section 4 is  $O(\log |g(f(x))|)$  which is  $O(\log n)$  size. Section 5 is  $O(1)$  size. Section 6 is  $O(\log |f(x)|)$  which is  $O(\log n)$  size. Section 7 is  $O(1)$  size. Section 8 is  $O(\log |x|)$  which is  $O(\log n)$  size. Therefore, the space complexity is  $O(\log n)$ . Above all,  $g \circ f \in L$ . **QED.**

**Theorem 4.2:** The strongly deterministic temperature-1 tiling reachability problem is in  $L$ .

**Proof:** To prove that strongly deterministic temperature-1 tiling reachability problem is in  $L$ , we just need to show that it is logspace reducible to  $USTCON$  because it has been proved that  $USTCON \in L$  by [41].

Let  $A$  be an instance of strongly deterministic temperature-1 tiling reachability problem. Description of  $A$ : Strongly deterministic temperature-1 aTAM system  $\mathbf{S} = (\mathbb{T}, t_0, \tau = 1, g, \Sigma)$ ,  $t \in \mathbb{T}$ ,  $n \in \mathbb{N}^+$ ,  $(x, y) \in \mathbb{Z}^2$  where  $x, y \in L_n$  and  $L_n = \{0, 1, 2, 3, \dots, n-1\}$ , and an initial configuration of size  $n$  at  $L_n \times \{0\}$ . We transform  $A$  to an instance of *USTCON*  $A'$ . Construct an undirected graph  $G = (V, E)$  according to  $A$ . For any triple  $(t, \beta, \gamma) \in \mathbb{T} \times L_n \times L_n$ , put a vertex  $v(t, \alpha, \beta)$  in  $V$ . For any two different vertices  $v(t_1, \beta_1, \gamma_1)$  and  $v(t_2, \beta_2, \gamma_2)$ , there is an edge between them if the contiguous glue strength is positive when we put  $t_1$  at  $(\beta_1, \gamma_1)$  and  $t_2$  at  $(\beta_2, \gamma_2)$ . For any vertex  $v(t, \alpha, \beta) \in V$ , delete it and its related edges if  $t \neq C_0(\alpha, \beta)$  where  $C_0$  is the initial configuration of the aTAM system  $\mathbf{S}$  of  $A$ . Description of  $A'$ : An undirected graph  $G = (V, E)$ , two vertices  $v(t_0, 0, 0)$  and  $v(t, x, y)$ . We prove that this transformation is a reduction next.

If the answer to  $A$  is yes, then there exists a linear assembly  $C_l$  from  $(0, 0)$  to  $(x, y)$  such that  $C_l(x, y) = t$  and  $C_l$  does not go beyond  $L_n \times L_n$ . Let the path of  $C_l$  be  $(x_0, y_0), (x_1, y_1), \dots, (x_k, y_k)$  where  $(x_0, y_0) = (0, 0)$  and  $(x_k, y_k) = (x, y)$ . Let the tiles on the path be  $t_0, t_1, \dots, t_k$  where  $t_0$  is the seed tile and  $t_k = t$ . According to the construction mechanism of graph  $G$  in  $A'$ , there should be an edge between  $v(t_i, x_i, y_i)$  and  $v(t_{i+1}, x_{i+1}, y_{i+1})$  for any  $i \in \{0, 1, \dots, k-1\}$ . Therefore, there is a path from  $v(t_0, 0, 0)$  to  $v(t, x, y)$  in  $G$  and the answer to  $A'$  is yes.

If the answer to  $A'$  is yes, then there is a path from  $v(t_0, 0, 0)$  to  $v(t, x, y)$  in  $G$ . Let the path be  $v(t'_0, x'_0, y'_0), v(t'_1, x'_1, y'_1), \dots, v(t'_r, x'_r, y'_r)$  where  $v(t'_0, x'_0, y'_0) = v(t_0, 0, 0)$  and  $v(t'_r, x'_r, y'_r) = v(t, x, y)$ . We construct a linear assembly  $C'_l$  under aTAM system  $\mathbf{S}$  of  $A$ . The path of  $C'_l$  is  $(x'_0, y'_0), (x'_1, y'_1), \dots, (x'_r, y'_r)$ . The tiles along the path are  $t'_0, t'_1, \dots, t'_r$ . According to the construction mechanism of graph  $G$  in  $A'$ ,  $C'_l$  is a legal linear assembly and then the answer to  $A$  is yes (The only concern may be that different tile types appear in the same position along the path. This situation is not possible because the aTAM system is strongly deterministic.). By now, we have proven that the transformation is a reduction.

Next we prove that the reduction can be done by a deterministic Turing machine  $M$  using logspace:  $M$  only needs  $O(\log(n) + \log(|\mathbb{T}|))$  which is  $O(\log(|A|))$  space in its worktape to enumerate all  $(p, p')$  to check whether there should be an edge between them, where  $|A|$  is the length of binary encoding of  $A$  and  $p, p' \in \mathbb{T} \times L_n \times L_n$ .

In conclusion, strongly deterministic temperature-1 tiling reachability problem is in  $L$ . **QED**.

## 4.2 Strongly Deterministic Temperature-1 $n \times n$ Square Problem

**Strongly deterministic temperature-1  $n \times n$  square problem:** Given a strongly deterministic temperature-1 aTAM system  $\mathbf{S} = (\mathbb{T}, t_0, \tau = 1, g, \Sigma)$ ,  $n \in \mathbb{N}^+$ , and an initial configuration of size  $n$  at  $L_n \times \{0\}$ , decide whether shape of the unique terminal configuration is  $n \times n$  square at  $L_n \times L_n$ .

**Lemma 4.3:** Given a strongly deterministic temperature-1 aTAM system  $\mathbf{S} = (\mathbb{T}, t_0, \tau = 1, g, \Sigma)$ ,  $n \in \mathbb{N}^+$ , and an initial configuration of size  $n$  at  $L_n \times \{0\}$ , the shape of the unique terminal configuration is  $n \times n$  square at  $L_n \times L_n$  iff

$\forall(x, y) \in L_n \times L_n, \exists t_{(x,y)} \in \mathbb{T}$  such that, there exists a linear assembly  $C_{l_{(x,y)}}$  from  $(0, 0)$  to  $(x, y)$  such that  $C_{l_{(x,y)}}(x, y) = t$  and  $C_{l_{(x,y)}}$  does not go beyond  $L_n \times L_n$ , and  $\forall(x, y)$  beyond  $L_n \times L_n$ , they are not reachable from  $(0, 0)$ .

**Proof:**  $\Rightarrow$ :  $\forall(x, y) \in L_n \times L_n$ , we should be able to find a linear assembly inside  $L_n \times L_n$  that reaches  $(x, y)$  by  $C_T(x, y)$  where  $C_T$  is the terminal configuration.  $\forall(x, y)$  beyond  $L_n \times L_n$ , they are not reachable from  $(0, 0)$ .

$\Leftarrow$ : The shape of the terminal configuration should be  $n \times n$  square at  $L_n \times L_n$  because  $\forall(x, y) \in \mathbb{Z}^2$ ,  $(x, y)$  is reachable from  $(0, 0)$  iff  $(x, y) \in L_n \times L_n$ , and no contradiction among linear assemblies under strongly deterministic temperature-1 aTAM system. **QED.**

**Theorem 4.4:** The strongly deterministic temperature-1  $n \times n$  square problem is in  $L$ .

**Proof:** Construct a deterministic Turing machine  $M$  to compute strongly deterministic temperature-1  $n \times n$  square problem.  $M$  works as following: It tests the reachability from  $(0, 0)$  to each position in or contiguous to  $L_n \times L_n$ . If a position is reachable iff it is in  $L_n \times L_n$ ,  $M$  gives "yes" answer, otherwise,  $M$  gives "no" answer.

Correctness: Proof of lemma 4.3.

Space complexity:  $M$  needs  $O(\log(n))$  space to enumerate all the positions and  $O(\log(|I|))$  space to resolve a reachability problem where  $|I|$  is the length of binary encoding of an instance of strongly deterministic temperature-1  $n \times n$  square problem. Therefore, space complexity is  $O(\log(|I|))$ .

In conclusion, strongly deterministic temperature-1  $n \times n$  square problem is in  $L$ . **QED.**

## 5 Nondeterministic Temperature-1 $n \times n$ Square Problem

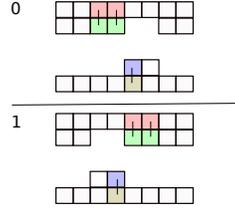
In this section, we will show that the nondeterministic temperature-1  $n \times n$  square problem is  $NP - complete$ .

**Nondeterministic temperature-1  $n \times n$  square problem:** Given an aTAM system  $\mathbf{S} = (\mathbb{T}, \tau = 1, g, \Sigma)$ , a positive integer  $n$  and an initial configuration of size  $n$  at  $\{0, 1, 2, \dots, n-1\} \times \{0\}$ , decide whether there is a terminal configuration that is an  $n \times n$  square without mismatches at  $L_n \times L_n$ . The initial configuration of size  $n$  is to make sure that this problem is in  $NP$  [22].

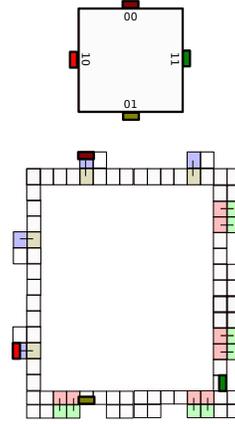
**Theorem 5.1:** Nondeterministic temperature-1  $n \times n$  square problem is  $NP - complete$ .

**Proof:** To check whether a given configuration is legal, we just need to check three things: (1) Whether it is terminal. (2) Whether it is a  $n \times n$  square at  $L_n \times L_n$ . (3) Whether all tiles are reachable from the initial configuration. Time complexity of three tasks should be  $poly(|D|)$  where  $|D|$  is the encoding length of the problem. Therefore, nondeterministic temperature-1  $n \times n$  square problem is in  $NP$ .

Reduce a known  $NP - complete$  problem, Bounded Tiling [22], to nondeterministic temperature-1  $n \times n$  square problem. Let  $I$  be an instance of



**Fig. 2.** The *micro* tile set is designed such that the only way that red tiles are incorporated into the configuration is via green tiles, and the only way that grey tiles are incorporated into the configuration is via blue tiles as shown. If there is a mismatch between two  $(8 * \log|\Sigma_I|) \times (8 * \log|\Sigma_I|)$  approximate squares, either green tile or blue tile will be squeezed out, and then there is no way for a red tile or grey tile to be incorporated into the configuration. It causes gaps that are not fixable by tiles from  $\cup_{t \in \mathbb{T}_1} F_t$ .



**Fig. 3.** Example of simulating a tile of temperature-2 system by a set of *micro* tiles.

Bounded Tiling:  $\mathbf{S}_I = (\mathbb{T}_1, \tau = 2, g_I, \Sigma_I)$ , positive integer  $n_I$ , initial configuration  $C_I: \{0, 1, 2, \dots, n_I - 1\} \mapsto T_I$ . Convert  $I$  to an instance of nondeterministic temperature-1  $n \times n$  square problem  $I'$ :  $\mathbf{S}_{I'} = (\mathbb{T}_1, \tau = 1, g_{I'}, \Sigma_{I'})$ , positive integer  $n_{I'}$ , initial configuration  $C_{I'}: \{0, 1, 2, \dots, n_{I'} - 1\} \mapsto T_{I'}$ .  $I'$  is constructed as:  $\forall t \in \mathbb{T}_1$ , we design a set of *micro* tiles  $T_t$  which assembles into an approximate  $(8 * \log|\Sigma_I|) \times (8 * \log|\Sigma_I|)$  square (each binary bit of encoding of a glue type is represented by length 8), where  $|\Sigma_I|$  is the number of glue types of  $I$ . We use geometry tricks for all four pads of a tile in  $\mathbb{T}_1$ . Details are shown Figure 2 and Figure 3.  $\forall t \in \mathbb{T}_1$ , we design a set of *micro* tiles  $F_t$  which fills the approximate square into a square. The glues for connection between approximate squares locate at the first tile of the notch or protrusion for the first binary bit of encoding of a glue type in  $\Sigma_I$ . We let:  $\mathbb{T}_{I'} = \cup_{t \in \mathbb{T}_1} (T_t \cup F_t)$ .  $g_{I'}$  specifies the strength for glue reactions inside each approximate square, between  $T_t$  and  $F_t$  where  $t \in \mathbb{T}_1$ , and between two approximate squares.  $\Sigma_{I'}$  includes all the glues.

$n_{I'} = 1 + n_I * (8 * \log|\Sigma_I|)$ .  $C_{I'}$  is constructed as: Use corresponding approximate squares to simulate  $C_I$ , then get the most southern row and fill the notches by proper tiles from  $\cup_{t \in \mathbb{T}_I} F_t$  to get a linear structure of size  $n_{I'}$ .

Correctness: (1) If the answer to  $I$  is yes: An approximate  $n_{I'} \times n_{I'}$  square can be assembled by  $\mathbf{S}_{I'}$  via simply simulating  $\mathbf{S}_I$ , and then an  $n_{I'} \times n_{I'}$  square can be assembled via filling the gaps by tiles in  $\cup_{t \in \mathbb{T}_I} F_t$ . Therefore, the answer to  $I'$  is yes. (2) If the answer to  $I'$  is yes:  $\mathbf{S}_{I'}$  simulates  $\mathbf{S}_I$  correctly, otherwise, there will be mismatches, or gaps that are not fixable by tiles from  $\cup_{t \in \mathbb{T}_I} F_t$  according to the trick explained in Figure 2. Eliminate tiles from  $\cup_{t \in \mathbb{T}_I} F_t$  in the  $n_{I'} \times n_{I'}$  square, then we get an approximate  $n_I \times n_I$  square which is assembled by  $n_I^2$  approximate  $(8 * \log|\Sigma_I|) \times (8 * \log|\Sigma_I|)$  squares. Replace every  $(8 * \log|\Sigma_I|) \times (8 * \log|\Sigma_I|)$  approximate square by its corresponding tile in  $\mathbb{T}_I$ , then we get a legal terminal configuration of  $\mathbf{S}_I$  which is an  $n_I \times n_I$  square. Therefore, the answer to  $I$  is yes.

Reduction complexity: Time complexity of constructing  $\mathbb{T}_{I'}$  is  $O(|\mathbb{T}_I| * (\log|\Sigma_I|)^2)$ ; time complexity of constructing  $\Sigma_{I'}$  is  $O(|\mathbb{T}_I| * (\log|\Sigma_I|)^2)$ ; time complexity of constructing  $g_{I'}$  is  $O(|\mathbb{T}_I|^2 * (\log|\Sigma_I|)^4)$ ; time complexity of constructing  $C_{I'}$  is  $O(n_I * (\log|\Sigma_I|)^2)$ . Therefore, the reduction complexity is  $poly(|I|)$  where  $|I|$  is the encoding length of  $I$ .

In conclusion, nondeterministic temperature-1  $n \times n$  square problem is *NP-complete*. **QED**.

## 6 Conclusions

We showed that the nondeterministic temperature-1  $n \times n$  square problem is NP-complete and the strongly deterministic temperature-1  $n \times n$  square problem can be solved by a log-space bounded Turing Machine. Our main result is that we

proved that there is a decision procedure with time complexity  $2^{2^{2^{2^{O(n^2)}}}}$  for the strongly deterministic tiling problem when the temperature is 1, where  $n$  is the number of tile types, and the system is confined in  $\mathbb{N}^2$ . The proofs made use of some interesting and novel (for tiling theory) proof techniques, including the use of vector addition system with states (VASS) and Presburger arithmetic formula. It remains an open problem whether the  $\mathbb{N}^2$  tiling problem is decidable when the temperature is 1 and the system is deterministic.

## Acknowledgments

Acknowledge Reem Mokhtar, Sudhanshu Garg, Hieu Bui and DNA19 referees for their valuable suggestions. This work was supported by NSF Grants CCF-1217457, CCF-1141847, and CCF-1320360.

## References

1. L. Adleman, J. Kari, L. Kari, and D. Reishus. On the decidability of self-assembly of infinite ribbons. In *Proceedings of IEEE Symposium on Foundations of Computer Science (FOCS 2002)*, pages 530–537, 2002.

2. G. Aggarwal, Q. Cheng, M. Goldwasser, M. Kao, P. de Espanes, and R. Schweller. Complexities for generalized models of self-assembly. *SIAM Journal on Computing*, 34(6):1493–1515, 2005.
3. Bahar Behsaz, Ján Maňuch, and Ladislav Stacho. Turing universality of step-wise and stage assembly at temperature 1. *LNCS*, 7433:1–11, 2012.
4. R. Berger. The undecidability of the domino problem. *Memoirs of the American Mathematical Society*, 66, 1966.
5. L. Berman. The complexity of logical theories. *Theoretical Computer Science*, 11:71–77, 1980.
6. Hieu Bui, Harish Chandran, Sudhanshu Garg, Nikhil Gopalkrishnan, Reem Mokhtar, Tianqi Song, and John H Reif. *DNA Computing, Chapter in Computing Handbook*, volume I: Computer Science and Software Engineering, Section 3: Architecture and Organization. Edited by Teofilo F. Gonzalez, Taylor & Francis Group, 2013.
7. Harish Chandran, Nikhil Gopalkrishnan, Sudhanshu Garg, and John Reif. *Biomolecular Computing Systems - From Logic Systems to Smart Sensors and Actuators, Invited Chapter 11, Molecular and Biomolecular Information Processing*. Wiley-VCH, Weinheim, Germany, July 2012.
8. Harish Chandran, Nikhil Gopalkrishnan, and John Reif. The tile complexity of linear assemblies. In *Proceedings of the 36th International Colloquium on Automata, Languages and Programming*, volume ICALP ‘09, pages 235–253 (Accepted to SIAM Journal of Computation (SICOMP), 2012), Berlin, Heidelberg, 2009. Springer-Verlag.
9. M. Cook, Y. Fu, and R. Schweller. Temperature 1 self-assembly: Deterministic assembly in 3d and probabilistic assembly in 2d. In *Proceedings of the 22nd Annual ACM-SIAM Symposium on Discrete Algorithms (SODA 2011)*, pages 570–589. ACM and SIAM, 2011.
10. D. C. Cooper. Theorem proving in arithmetic without multiplication. In B. Meltzer and D. Michie, editors, *Machine Intelligence*, pages 91–100. Edinburgh University Press, 1972.
11. David Doty. Theory of algorithmic self-assembly. *Communications of the ACM (CACM)*, 55(12):78–88, 2012.
12. David Doty, Matthew J. Patitz, and Scott M. Summers. Limitations of self-assembly at temperature 1. *Theoretical Computer Science*, 412(1-2):145–158, January 2011.
13. Herbert Enderton. *A mathematical introduction to logic*. ISBN 978-0-12-238452-3. Academic Press, Boston, MA, 2nd edition, 2001.
14. Jeanne Ferrante and Charles W. Rackoff. *The Computational Complexity of Logical Theories*. Number 718 in Lecture Notes in Mathematics. Springer-Verlag, 1979.
15. M. J. Fischer and Michael O. Rabin. Super-exponential complexity of presburger arithmetic. In *Proceedings of the SIAM-AMS Symposium in Applied Mathematics*, volume 7, pages 27–41, 1974.
16. Martin Fürer. The complexity of presburger arithmetic with bounded quantifier alternation depth. *Theoretical Computer Science*, 18(1):105–111, April 1982.
17. Ganesh V. Ganesh, S. Berezin, and D.L. Dill. Deciding presburger arithmetic by model checking and comparisons with other methods. In *Proceedings of 3rd Formal Methods of Computer-Aided Design*, Lecture Notes In Computer Science, November 2002.
18. Seymour Ginsburg and Edwin H. Spanier. Bounded algol-like languages. *Transactions of the American Mathematical Society*, 113:333–368, 1964.

19. Seymour Ginsburg and Edwin H. Spanier. Semigroups, presburger formulas, and languages. *Pacific Journal of Mathematics*, 16:285–296, 1966.
20. S. Golomb. *Polyominoes*. Princeton University Press, Princeton, 1994.
21. G.C. Shephard Grunbaum, B. *Tilings and Patterns*. W. H. Freeman and Company, New York, 1987.
22. Harry Lewis and Christos Papadimitriou. *Elements of the Theory of Computation*. Prentice Hall, 1981.
23. J.E. Hopcroft and J.J. Pansiot. On the reachability problem for 5- dimensional vector addition systems. *Theor. Comput. Sci.*, 8:135–159, 1979.
24. Rodney R. Howell, Louis E. Rosier, Dung T. Huynh, and Hsu-Chun Yen. Some complexity bounds for problems concerning finite and 2-dimensional vector addition systems with states. *Theoretical Computer Science*, 46:107–140, 1986.
25. Marcus Kracht. A new proof of a theorem by ginsburg and spanier. UCLA, December 2002.
26. Marcus Kracht. *The Mathematics of Language*, chapter Presburger, pages 147–160. de Gruyter, Jan 2003.
27. Thomas H. LaBean, Erik Winfree, and John H. Reif. Experimental progress in computation by self-assembly of dna tilings. In Erik Winfree and D.K. Gifford, editors, *Proceeding of DNA Based Computers V*, volume 54 of *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, pages 123–140, Cambridge, MA (published in 2000, Providence, RI), June 1999. American Mathematical Society.
28. Thomas H. LaBean, Hao Yan, Jens Kopatsch, Furong Liu, Erik Winfree, John H. Reif, and Nadrian C. Seeman. The construction, analysis, ligation and self-assembly of dna triple crossover complexes. *Journal of the American Chemical Society(JACS)*, 122(1848–1860), 2000.
29. X. Ma, J. Huang, and F. Lombardi. Error tolerant dna self-assembly using  $(2k - 1) \times (2k - 1)$  snake tile sets. *IEEE Trans Nanobioscience*, 7(1):56–64, Mar 2008.
30. Jan Manuch, Ladislav Stacho, and Christine Stoll. Two lower bounds for self-assemblies at temperature 1. *Journal of Computational Biology*, 17(6):841–852, 2010.
31. Chengde Mao, Thomas H. LaBean, John H. Reif, and Nadrian C. Seeman. Logical computation using algorithmic self-assembly of dna triple-crossover molecules. *Nature*, 407(6803):493–496, 2000.
32. Derek C. Oppen. Elementary bounds for presburger arithmetic. In *Fifth Annual ACM Symposium on Theory of Computing*, pages 34–37, Austin, Tex., 1973. Assoc. Comput. Mach.
33. Derek C. Oppen. A  $2^{2^{2^{p^n}}}$  upper bound on the complexity of presburger arithmetic. *J. Comput. Syst. Sci.*, 16(3):323–332, doi:10.1016/0022-0000(78)90021-1 1978.
34. R. J. Parikh. Language-generating devices. Technical report, Massachusetts Institute of Technology, January 1961.
35. Matthew J. Patitz and Scott M. Summers. Self-assembly of infinite structures: A survey. *Theoretical Computer Science*, 412(1-2):159–165, January 2011.
36. M.J. Patitz, R.T. Schweller, and S.M. Summers. Exact shapes and turing universality at temperature 1 with a single negative glue. In L. Cardelli and W. Shih, editors, *DNA 17*, volume 6937 of *LNCS*, pages 175–189, Heidelberg, 2011. Springer.
37. Paul W. K. Rothemund and Erik Winfree. The program-size complexity of self-assembled squares(extended abstract). *Proceedings of the Thirty-Second Annual ACM Symposium on Theory of Computing*, pages 459–468, 2000.
38. Mojżesz Presburger. Über die vollständigkeit eines gewissen systems der arithmetik ganzer zahlen, in welchem die addition als einzige operation hervortritt. *Comptes*

- Rendus du I congrès de Mathématiciens des Pays Slaves, Warszawa*, 1(92–101), 1929.
39. C. R. Reddy and D. W. Loveland. Presburger arithmetic with bounded quantifier alternation. In *ACM Symposium on Theory of Computing*, pages 320–325, 1978.
  40. John H. Reif. *Proc. DNA-Based Computers, II*, volume 48 of *Series in Discrete Mathematics and Theoretical Computer Science*, chapter Local Parallel Biomolecular Computation, pages 217–254. DIMACS, University of Pennsylvania, 1997.
  41. O. Reingold. Undirected st-connectivity in log-space. *STOC*, pages 376–385, 2005.
  42. R.M. Robinson. Undecidability and nonperiodicity for tilings of the plane. *Inventiones Math.*, 12:177–209, 1971.
  43. P.W.K. Rothmund, N. Papadakis, and E. Winfree. Algorithmic self-assembly of dna sierpinski triangles. *PLoS Biol.*, 2(12):424 doi:10.1371/journal.pbio.0020424, 2004.
  44. Bruno Scarpellini. Complexity of subcases of presburger arithmetic. *Trans. Amer. Math. Soc.*, 284:203–218, 1984.
  45. Uwe Schöning. Complexity of presburger arithmetic with fixed quantifier dimension. *Theory of Computing Systems*, 30(4):423–428, July 1997.
  46. T. Skolem. Skrifter utgitt av det norske videnskaps-akademi i oslo, i. matematisk naturvidenskapelig klasse. *Akademi i Oslo I. Matematisk naturvidenskapelig klasse*, 7:1–28, 1931.
  47. Hao Wang. Proving theorems by pattern recognition ii. *Bell Systems Technical Journal*, 40:1–41, 1961.
  48. Erik Winfree. *Algorithmic self-assembly of DNA*. Ph.D. thesis. California Institute of Technology, June 1998.
  49. Erik Winfree. Simulation of computing by self-assembly. *Technical Report 1998.22, Caltech*, 1998.
  50. H. Yan, L. Feng, T.H. LaBean, and J.H. Reif. Parallel molecular computations of pairwise exclusive-or (xor) using dna string tile self-assembly. *Journal of the American Chemical Society*, 125(47):14246–14247, Nov 2003.
  51. P. Young. Godel theorems, exponential difficulty and undecidability of arithmetic theories: an exposition. In A. Nerode and R. Shore, editors, *Recursion Theory*, pages 503–522. American Mathematical Society, 1985.