New Geometric Algorithms for Staged Self-Assembly

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Abstract

We consider *staged self-assembly*, in which square-shaped Wang tiles can be added to bins in several stages. Within these bins the tiles may connect to each other, depending on the *glue types* of their edges. In general, self-assembly constructs complex (polyomino-shaped) structures from a limited set of square tiles. Previous work by Demaine et al. considered a setting in which assembly proceeds in stages. It was shown that a relatively small number of tile types suffices to produce arbitrary shapes; however, these constructions were only based on a spanning tree of the geometric shape, so they did not produce full connectivity of the underlying grid graph. We present new systems for stages assembly to assemble a fully connected polyomino in $O(\log^2 n)$ stages. Our construction works even for shapes with holes and uses only a constant number of glues and tiles.

1 Introduction

In *self-assembly*, a set of simple *tiles* form complex structures without any active or deliberate handling of individual components. Instead, the overall construction is governed by a simple set of rules, which describe how mixing the tiles leads to bonding between them and eventually a geometric shape.

The leading theoretical model for self-assembly is the *abstract tile-assembly model* (aTAM). It was first introduced by Winfree [12, 9]. The *tiles* used in this model are building blocks called *Wang tiles* [11], which are unrotatable squares with a specific glue on each side. Equal glues have a connection strength and may stick together. If two partial assemblies ("supertiles") want to assemble, then the sum of the glue strength along the linkage needs to be at least some minimum value τ, which is called the *temperature*. While assembling some shapes we consider the minimum number of distinct tiles to uniquely assemble this shape; this is called the *tile complexitiy* t. Apart from that we also consider a minimum number of glues, which is the *glue complexitiy* g. Clearly, $g \leq t \leq g^4$.

In this paper we consider the *staged tile assembly model* introduced by Demaine et al. [3]. In this model the assembly process is split into sequential stages that are kept in separate bins, with supertiles from earlier stages mixed together consecutively to gain some new supertiles. We can either add a new tile to an existing bin, or we pour one bin into another bin, such that the content of both get mixed. Hence, there are bins at each stage. Unassembled parts get removed. The overall number of necessary stages and bins are the *stage complexity* and the *bin complexity*. Demaine et al. [3] achieved a number of results that are summarized in Table 1. Most notably, they were able to come up with a system (based on utilizing a spanning tree) that can produce arbitrary shapes in $O(\textit{diameter})$ many stages, $O(\log n)$ bins and a constant number of glues; the downside is that the resulting shapes are not fully connected.

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1.1 Our results

We show that there is a staged assembly system for an arbitrary polyomino with the following properties:

1. polylogarithmic stage complexity
2. constant glue and tile complexity
3. constant scale factor
4. full connectivity

We show how to assemble an arbitrary polyomino even with holes. Most methods of Demaine et al. using a constant number of glues and tiles have either a big stage complexity or the build polyomino is not fully connected. We use a polylogarithmic number of stages with full connectivity and still use a constant number of glues and tiles. On the other hand, we use a small constant scale factor for the assembled shapes. Table 1 gives an overview of the methods which uses a constant number of glues and tiles.

1.2 Related work

As mentioned above, we stick to the aTAM. For other models, see [1]. Other related geometric work by Cannon et al. [2] and Demaine et al. [4] considers reductions between different systems, often based on geometric properties. Fu et al. [6] use geometric tiles in a generalized tile assembly model to assemble shapes [6]. Fekete et al. [5] study the power of using more complicated polyominoes as tiles.

Lines and Squares	Glues	Tiles	Bins	Stages	τ	Scale	Conn.	Planar
Line [3] (sect. 2.1)	3	6	7	$O(\log n)$	1	1	full	yes
Square — Jigsaw techn. [3] (sect. 2.2)	9	$O(1)$	$O(1)$	$O(\log n)$	1	1	full	yes
Square — $\tau = 2$ (sect. 2.3)	4	$O(1)$	$O(1)$	$O(\log n)$	2	1	full	yes

Arbitrary Shapes	Glues	Tiles	Bins	Stages	τ	Scale	Conn.	Planar
Spanning Tree Method [3]	2	16	$O(\log n)$	$O(diameter)$	1	1	partial	no
Simple Shapes [3]	8	$O(1)$	$O(n)$	$O(n)$	1	2	full	no
Simple Shapes (sect. 3.2)	18	$O(1)$	$O(\|V\|)$	$O(\log^2 n)$	1	4	full	no
Monotone Shapes [3] (sect. 3.1)	9	$O(1)$	$O(n)$	$O(\log n)$	1	1	full	yes
Shape with holes (sect. 3.3)	7	$O(1)$	$O(\|V\|)$	$O(\log^2 n)$	2	3	full	no

Table 1: Overview of some results from Demaine et al. [3] and us using a constant number of glues and tiles. Also pictured are bin complexity, stage complexity, temperature, scale factor, connectivity and planarity. n is the side length of a smalles bounding square and V are the vertices of the polyomino.

Using stages has received attention in DNA self assembly. Reif [8] uses a step-wise model for parallel computing. Park et al. [7] consider assembly techniques with hierarchies to assemble DNA lattices. Somei et al. [10] use a stepwise assembly of DNA tiles. None of these works considers complexity aspects.

2 Lines and Squares

We start with staged assembly for lines and squares. While the results of Section 2.1 and 2.2 are due to [3], Section 2.3 states a new result.

2.1 $1 \times n$ lines

Theorem 1 *A $1 \times n$-line can be assembled with a $\tau = 1$ staged assembly system using $O(\log n)$ stages, 3 glues, 6 tiles and 7 bins.*

2.2 $n \times n$ squares (divide and conquer)

Making use of a "jigsaw" technique, Demaine et al. [3] were able to come up with an efficient method that is

Theorem 2 *An $n \times n$-square can be assembled with full connectivity in $O(\log n)$ stages with 9 glues, $O(1)$ tiles, $O(1)$ bins, and $\tau = 1$.*

2.3 $n \times n$ squares with $\tau = 2$

For $\tau = 2$ assembly systems, it is possible to come up with more efficient ways of constructing a square. The construction is based on an idea by Rothemund and Winfree (see [9]), which we adapt to staged assembly. Basically, it consists of connecting two lines by a corner tile, before filling up this frame; see Figure 1.

Theorem 3 *There exists a $\tau = 2$ assembly system for a fully connected $n \times n$ square with $O(\log n)$ stages, 4 glues, 14 tiles and 7 bins.*

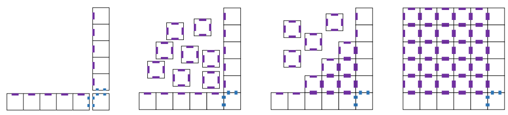

Figure 1: First: Construction for square assembly. Second: Filling up the square. Third: Intermediate Result: some tiles have been assembled to the backbone. Fourth: Fully assembled square.

Proof. First we need to construct the $1 \times (n-1)$ lines with strength 2 glues. We know from Theorem 1 that a line can be constructed in $O(\log n)$ stages, 3 glues, 6 tiles and 7 bins. Because both lines are perpendicular they will not connect. Therefore we can use all 7 bins to construct both lines parallel. For each line we use tiles such that the side, which is directed to the inner side of the square, has a strength 1 glue. In the next stage we mix together the single corner tile with the two lines. In the last step we add a tile with the strength 1 glues on all four sides. When the square is filled no further tile will be connecting because every connection would have a strength sum of 1.

Overall we needed $O(\log n)$ stages with 4 glues (3 for the construction, 1 for filling up the square), 14 tiles (6 for each line, 1 for the corner tile, 1 for filling up the square) and 7 bins for the parallel construction of the two lines. ☐

3 Assembling Polyominoes

Now we describe approaches for assembling arbitrary polyominoes.

3.1 Monotone shapes

For monotone shapes, [3] showed the following.

Theorem 4 *A monotone polyomino can be assembled with full connectivity in a $\tau = 1$ staged assembly system in $O(\log n)$ stages using 9 glues, $O(1)$ tiles and $O(n)$ bins.*

3.2 Simple shapes

We present a system for building simple polyominoes. The main idea comes from [3], i.e., splitting the polyomino into strips. Then an arbitrary strip gets assembled piece by piece and if there is a component which can assemble to the currently strip then we create the component and attach it to the strip.

Our new staged assembly system partitions the polyomino into rectangles and uses them to assemble the whole polyomino. We may use more bins than the old method, but we have an improvement in the stage complexity. We first consider a building block, see Figure 2. Details are omitted due to limited space.

Lemma 1 *A $2n \times 2n$ square which has at most two tabs each top or left side and at most two pockets each bottom or right side (see Figure 2) can be assembled with $O(\log n)$ stages, 9 glues, $O(1)$ tiles and $O(1)$ bins at $\tau = 1$.*

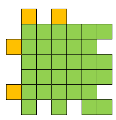

Figure 2: A square (green) with tabs on top and left side (yellow) and pockets on bottom and right side.

This construction works equally well for modified $2n \times 2m$ rectangles. Hence, we can search for a decomposition of a simple polyomino into components of this type.

Theorem 5 *Let V be the set of vertices of the polyomino. There exists a $\tau = 1$ staged assembly system that constructs a fully connected simple polyomino in $O(\log^2 n)$ stages with 18 glues, $O(1)$ tiles, $O(|V|)$ bins and scale factor 4.*

Proof. Details are omitted for lack of space. The main idea is to cut the polyomino into rectangles. These rectangles are recursively divided into subsets, and assembled making use of jigsaw techniques.

Overall we have $O(\log n)$ stages to assemble the $O(|V|)$ rectangles with $O(1)$ bins for each rectangle plus $O(\log^2 n)$ stages to assemble the polyomino from the rectangles which are in total $O(\log^2 n)$ stages and $O(|V|)$ bins. For the rectangles we need 9 glues and 9 glues for the remaining assemblage, hence, in total 18 glues and with it $O(1)$ tiles. To uniquely assemble the polyomino we need to scale it by a factor of 4 in total (scaled by 2 two times). That is, we replace each tile by a 4×4 supertile. □

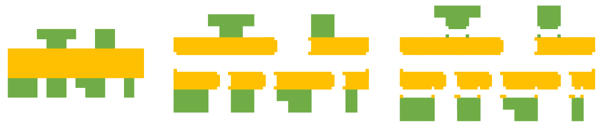

Figure 3: Left: A chosen rectangle (orange) which splits the polyomino into components (green). Middle: Decomposition of splitting rectangle. Right: Decomposition of the components.

3.3 Temperature $\tau = 2$ assembly

The idea for assembling polyominoes with holes at $\tau = 2$ is similar to squares. To this end, we construct a **backbone**. For an arbitrary polyomino scaled by a factor 3, this is a spanning construct formed with the following line types:

1. the lines on the **left** boundary of the polyomino or **right** boundary of a hole,
2. the lines on the **right** boundary of the polyomino or **left** boundary of a hole,
3. the lines on the **upper** boundary of the polyomino or **lower** boundary of a hole,
4. the lines on the **lower** boundary of the polyomino or **upper** boundary of a hole.
5. the lines that connect two components along the first row of an 3×3 supertile.

In order to avoid cycle in this construction, we leave out the lowest leftmost line on the boundary of the polyomino and the highest rightmost line on the boundary of each hole. Moreover, the fifth line type can be found by moving left from a leftmost (and lowest in case of ties) tile of each hole until a line gets hit. Hence, the construction yields a simple shape. An example for a backbone can be found in Figure 4.

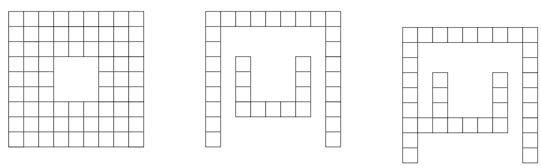

Figure 4: Left: A scaled polyomino with one hole. Middle: Backbone without the fifth type of lines. Right: Complete Backbone of the shape.

Lemma 2 *Let V be the set of vertices of a polyomino P. After scaling P by a factor of 3, the corresponding backbone can be assembled in $O(\log^2 n)$ stages with 4 glues, $O(1)$ tiles and $O(|V|)$ bins.*

Proof. The backbone consists of two types: lines and connection tiles (see Figure 5). Observe that each connection tile has either two or three adjacent lines. Hence, in the adjacency graph they would have degree two and three respectively.

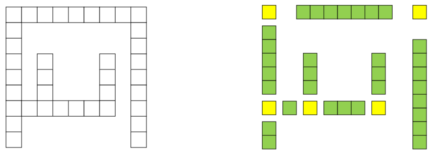

Figure 5: Left: A backbone of a polyomino. Right: A backbone decomposed into lines (green) and connection tiles (yellow).

The construction proceeds in three steps. Details are omitted due to space constraints. In total we use 4 glues, $O(1)$ tiles and $O(|V|)$ bins to assemble a backbone for a given polyomino within $O(\log^2 n + 2 \cdot \log n) = O(\log^2 n)$ stages. □

We can now use this idea to construct any polyomino by assembling its backbone and then filling up:

Theorem 6 *Let V be the set of vertices of the polyomino. Then there is a $\tau = 2$ staged assembly system that constructs a fully connected arbitrary polyomino in $O(\log^2 n)$ stages, 7 glues, $O(1)$ tiles, $O(|V|)$ bins and scale factor 3.*

Proof. The construction proceeds in two parts; again, we have to omit details. For the first part we present a construction such that no tile gets to an unwanted position while filling up the polyomino.

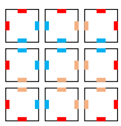

Figure 6: Glue chart for 3×3 tiles to fill up the shape. Blue glue $\triangleq g1$, orange glue $\triangleq g2$ and red glue $\triangleq g3$.

To fill up the polyomino we mix the nine kinds of tiles (see Figure 6) plus the backbone in one bin. In total we need $O(\log^2 n)$ stages, 7 glues, $O(1)$ tiles and $O(|V|)$ bins to assemble a fully connected polyomino, scaled by a factor 3 from the target shape. □

4 Future Work

Our new methods have the same stage and bin complexity and use quite a small number of glues. Because the bin complexity is in $O(|V|)$ for some polyomino with V as the set of vertices, we may need many bins if the polyomino has many vertices. Hence, both methods are good for slightly branched polyominoes. This raises the question for a staged assembly system with the same complexities but a better bin complexity for polyominoes with many vertices, i.e., if $|V| \in O(n^2)$?

Another interesting challenge is to come up with a more efficient system for an arbitrary polyomino. Is there a staged assembly system of stage complexity $o(\log^2 n)$ without increasing the other complexities? In total we think that both methods are a good approach to assemble a polyomino although the number of bins may be a really big value.

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