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New geometric algorithms for fully connected staged self-assembly ☆

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We consider *staged self-assembly systems*, in which square-shaped 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. Previous work by Demaine et al. showed that a relatively small number of tile types suffices to produce arbitrary shapes in this model. 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 in the case of shapes with holes; self-assembly of fully connected assemblies with a polylogarithmic number of stages was left as a major open problem. We resolve this challenge by presenting new systems for staged assembly that produce fully connected polyominoes in $\mathcal{O}(\log^2 n)$ stages, for various scale factors and temperature $\tau = 2$ as well as $\tau = 1$. Our constructions work even for shapes with holes and use only a constant number of glues and tiles. Moreover, the underlying approach is more geometric in nature, implying that it promises to be more feasible for shapes with compact geometric description.

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 classic theoretical model for self-assembly is the *abstract tile-assembly model* (aTAM). It was first introduced by Winfree [15,13]. The *tiles* used in this model are building blocks, which are unrotatable squares with a specific glue on each side. Equal glues have a connection strength and may stick together. The *glue complexity* of a tile set T is the number of different glues on all the tiles in T, while the *tile complexity* of T is the number of different tile types in T. If an additional tile wants to attach to the existing assembly by making use of matching glues, the sum of corresponding glue strengths needs to be at least some minimum value τ, which is called the *temperature*.

A generalization of the aTAM called the *two-handed assembly model* (2HAM) was introduced by Demaine et al. [4]. While in the aTAM, only individual tiles can be attached to an existing intermediate assembly, the 2HAM allows attaching other

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Table 1
Overview of results from [4] and this paper. The number of pixels of P is denoted by $N \in \mathcal{O}(n^2)$, n is the side length of a smallest bounding square, while k is the number of vertices of the polyomino, with $k \in \Omega(1)$ and $k \in \mathcal{O}(N)$. The *diameter* is the maximum of all shortest paths between any two pixels in the adjacency graph of the corresponding shape.

Lines and squares	Glues	Tiles	Bins	Stages	τ	Scale	Conn.	Planar
Line [4]	3	6	7	$\mathcal{O}(\log n)$	1	1	full	yes
Square – Jigsaw techn. [4]	9	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(\log n)$	1	1	full	yes
Square – $\tau = 2$ (Sect. 3.1)	4	$\mathcal{O}(1)$	$\mathcal{O}(1)$	$\mathcal{O}(\log n)$	2	1	full	yes

Arbitrary shapes	Glues	Tiles	Bins	Stages	τ	Scale	Conn.	Planar
Spanning tree method [4]	2	16	$\mathcal{O}(\log n)$	$\mathcal{O}(diameter)$	1	1	partial	no
Monotone shapes [4]	9	$\mathcal{O}(1)$	$\mathcal{O}(n)$	$\mathcal{O}(\log n)$	1	1	full	yes
Hole-free shapes [4]	8	$\mathcal{O}(1)$	$\mathcal{O}(N)$	$\mathcal{O}(N)$	1	2	full	no
Shape with holes (Sect. 3.2)	6	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(\log^2 n)$	2	3	full	no
Hole-free shapes (Sect. 3.2)	6	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(\log n)$	2	3	full	no
Hole-free shapes (Sect. 4.1)	18	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(\log^2 n)$	1	4	full	no
Shape with holes (Sect. 4.2)	20	$\mathcal{O}(1)$	$\mathcal{O}(k)$	$\mathcal{O}(\log^2 n)$	1	6	full	no

partial assemblies. If two partial assemblies ("supertiles") want to assemble, then the sum of the glue strength along the whole common boundary needs to be at least τ.

In this paper we consider the *staged tile assembly model* introduced in [4], which is based on the 2HAM. 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 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 gets mixed; afterwards, unassembled parts get removed. The overall number of stages and bins of a system are the *stage complexity* and the *bin complexity*. Demaine et al. [4] achieved several results summarized in Table 1. Most notably, they presented a system (based on a spanning tree) that can produce arbitrary polyomino shapes P in $\mathcal{O}(diameter)$ many stages, $\mathcal{O}(\log N) = \mathcal{O}(\log n)$ bins and a constant number of glues, where N is the number of unit squares, called *pixels*, whose union forms P, n is the size of the bounding box, i.e., a smallest square containing P, and the diameter is measured by the maximum length of a shortest path between any two pixels in the adjacency graph of the pixels in P; this can be as big as N. The downside is that the resulting supertiles are not fully connected. For achieving full connectivity, only the special case of monotone shapes was resolved by a system with $\mathcal{O}(\log n)$ stages; for hole-free shapes, Demaine et al. [4] were able to give a system with full connectivity, scale factor 2, but $\mathcal{O}(n)$ stages. This left a major open problem: designing a staged assembly system with full connectivity, polylogarithmic stage complexity and constant scale factor for general shapes.

Our results. We show that for any polyomino, even with holes, there is a staged assembly system with the following properties, both for $\tau = 2$ and $\tau = 1$.

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

See Table 1 for an overview. The main novelty of our method is to focus on the underlying geometry of a constructed shape P, instead of just its connectivity graph. This results in bin complexities that are a function of k, the number of vertices of P: while k can be as big as $\Theta(n^2)$, n can be arbitrarily large for fixed k, implying that our approach promises to be more suitable for constructing natural shapes with a clear geometric structure.

Related work. As mentioned above, our work is based on the 2HAM. There is a variety of other models, e.g., see [2]. A variation of the staged 2HAM is the *Staged Replication Assembly Model* by Abel et al. [1], which aims at reproducing supertiles by using *enzyme self assembly*. Another variant is the *Signal-passing Tile Assembly Model* introduced by Padilla et al. [10].

Other related geometric work by Cannon et al. [3] and Demaine et al. [5] considers reductions between different systems, often based on geometric properties. Fu et al. [8] use geometric tiles in a generalized tile assembly model to assemble shapes. Fekete et al. [7] study the power of using more complicated polyominoes as tiles.

Using stages has also received attention in DNA self assembly. Reif [12] uses a stepwise model for parallel computing. Park et al. [11] consider assembly techniques with hierarchies to assemble DNA lattices. Somei et al. [14] use a stepwise assembly of DNA tiles. Padilla et al. [9] include active signaling and glue activation in the aTAM to control hierarchical assembly of Robinson patterns. None of these works considers complexity aspects.

2. The staged assembly model

In this section, we present basic definitions common to most assembly models, followed by a description of the staged assembly model, and finally we define various metrics to measure the efficiency of a staged assembly system. Staged assem-