Producibility in hierarchical self-assembly

David Doty[*]

Abstract

Three results are shown on producibility in the hierarchical model of tile self-assembly. It is shown that a simple greedy polynomial-time strategy decides whether an assembly α is producible. The algorithm can be optimized to use $O(|\alpha| \log^2 |\alpha|)$ time. Cannon, Demaine, Demaine, Eisenstat, Patitz, Schweller, Summers, and Winslow [5] showed that the problem of deciding if an assembly α is the unique producible terminal assembly of a tile system $\mathcal{T}$ can be solved in $O(|\alpha|^2|\mathcal{T}| + |\alpha||\mathcal{T}|^2)$ time for the special case of noncooperative "temperature 1" systems. It is shown that this can be improved to $O(|\alpha||\mathcal{T}| \log |\mathcal{T}|)$ time. Finally, it is shown that if two assemblies are producible, and if they can be overlapped consistently – i.e., if the positions that they share have the same tile type in each assembly – then their union is also producible.

1 Introduction

1.1 Background of the field

Winfree's abstract Tile Assembly Model (aTAM) [33] is a model of crystal growth through cooperative binding of square-like monomers called *tiles*, implemented experimentally (for the current time) by DNA [4, 35]. In particular, it models the potentially algorithmic capabilities of tiles that can be designed to bind if and only if the total strength of attachment (summed over all binding sites, called *glues* on the tile) is at least a parameter τ, sometimes called the *temperature*. In particular, when the glue strengths are integers and $\tau = 2$, this implies that two strength 1 glues must cooperate to bind the tile to a growing assembly. Two assumptions are key: 1) growth starts from a single specially designated *seed* tile type, and 2) only individual tiles bind to an assembly, never larger assemblies consisting of more than one tile type. We will refer to this model as the *seeded aTAM*. While violations of these assumptions are often viewed as errors in implementation of the seeded aTAM [28, 29], relaxing them results in a different model with its own programmable abilities. In the *hierarchical* (a.k.a. *multiple tile* [3], *polyomino* [23, 34], *two-handed* [5, 10, 14]) *aTAM*, there is no seed tile, and an assembly is considered producible so long as two producible assemblies are able to attach to each other with strength at least τ, with all individual tiles being considered as "base case" producible assemblies. In either model, an assembly is considered *terminal* if nothing can attach to it; viewing self-assembly as a computation, terminal assembly(ies) are often interpreted to be the output. See [12, 24] for an introduction to recent work in these models.

[*]California Institute of Technology, Pasadena, CA, USA, `ddoty@caltech.edu`. The author was supported by the Molecular Programming Project under NSF grant 0832824 and by NSF grants CCF-1219274 and CCF-1162589, and by a Computing Innovation Fellowship under NSF grant 1019343.

The hierarchical aTAM has attracted considerable recent attention. It is coNP-complete to decide whether an assembly is the unique terminal assembly produced by a hierarchical tile system [5]. There are infinite shapes that can be assembled in the hierarchical aTAM but not the seeded aTAM, and vice versa, and there are finite shapes requiring strictly more tile types to assemble in the seeded aTAM than the hierarchical aTAM, and vice versa [5]. Despite this incomparability between the models for exact assembly of shapes, with a small blowup in scale, any seeded tile system can be simulated by a hierarchical tile system [5], improving upon an earlier scheme that worked for restricted classes of seeded tile systems [23]. However, the hierarchical aTAM is not able to simulate itself from a single set of tile types, i.e., it is not *intrinsically universal* [10], unlike the seeded aTAM [13]. It is possible to assemble an $n \times n$ square in a hierarchical tile system with $O(\log n)$ tile types that exhibits a very strong form of fault-tolerance in the face of spurious growth via strength 1 bonds [14]. The parallelism of the hierarchical aTAM suggests the possibility that it can assemble shapes faster than the seeded aTAM, but it cannot for a wide class of tile systems [6].

Interesting variants of the hierarchical aTAM introduce other assumptions to the model. The *multiple tile* model retains a seed tile and places a bound on the size of assemblies attaching to it [3]. Under this model, it is possible to modify a seeded tile system to be *self-healing*, that is, it correctly regrows when parts of itself are removed, even if the attaching assemblies that refill the removed gaps are grown without the seed [34]. The model of *staged assembly* allows multiple test tubes to undergo independent growth, with excess incomplete assemblies washed away (e.g. purified based on size) and then mixed, with assemblies from each tube combining via hierarchical attachment [8, 9, 36]. The *RNase enzyme* model [1, 11, 25] assumes some tile types to be made of RNA, which can be digested by an enzyme called RNase, leaving only the DNA tiles remaining, and possibly disconnecting what was previously a single RNA/DNA assembly into multiple DNA assemblies that can combine via hierarchical attachment. Introducing negative glue strengths into the hierarchical aTAM allows for "fuel-efficient" computation [30]. Allowing tiles with more complex geometry than squares enables hierarchical assembly to use significantly fewer tile types for assembly of $n \times n$ squares [17].

1.2 Contributions of this paper

We show three results on producibility in the hierarchical aTAM.

1. In the seeded aTAM, there is an obvious linear-time algorithm to test whether assembly α is producible by a tile system: starting from the seed, try to attach tiles until α is complete or no more attachments are possible. We show that in the hierarchical aTAM, a similar greedy strategy correctly identifies whether a given assembly is producible, though it is more involved to prove that it is correct. The idea is to start with all tiles in place as they appear in α, but with no bonds, and then to greedily bind attachable assemblies until α is assembled. It is not obvious that this works, since it is conceivable that assemblies must attach in a certain order for α to form, but the greedy strategy may pick another order and hit a dead-end in which no assemblies can attach. The algorithm can be optimized to use $O(|\alpha| \log^2 |\alpha|)$ time. This is shown in Section 3.

2. The temperature 1 Unique Production Verification (UPV) problem studied by Cannon, Demaine, Demaine, Eisenstat, Patitz, Schweller, Summers, and Winslow [5] is the problem of determining whether assembly α is the unique producible terminal assembly of tile system $\mathcal{T}$, where $\mathcal{T}$ has temperature 1, meaning that all positive strength glues are sufficiently strong

to attach any two assemblies. They give an algorithm that runs in $O(|\alpha|^2|\mathcal{T}| + |\alpha||\mathcal{T}|^2)$ time. Cannon et al. proved their result by using an $O(|\alpha|^2 + |\alpha||\mathcal{T}|)$ time algorithm for UPV that works in the seeded aTAM [2], and then reduced the hierarchical temperature-1 UPV problem to $|\mathcal{T}|$ instances of the seeded UPV problem. We improve this result by showing that a faster $O(|\alpha| \log |\mathcal{T}|)$ time algorithm for the seeded UPV problem exists for the special case of temperature 1, and then we apply the technique of Cannon et al. relating the hierarchical problem to the seeded problem to improve the running time of the hierarchical algorithm to $O(|\alpha||\mathcal{T}| \log |\mathcal{T}|)$. This is shown in Section 4.

Part of the conceptual significance of this algorithm lies in the details of the proof. In particular, we show a relationship between deterministic seeded assembly at temperature 1 and biconnected decomposition of the binding graph of an assembly using the Hopcroft-Tarjan algorithm [21]. We hope that this will spur further insights in classifying the possible behaviors of deterministic temperature-1 systems. This model is conjectured to have only very simple behaviors [15]; it is known, for example, that the model cannot be intrinsically universal for the class of all tile systems [16].

3. We show that if two assemblies α and β are producible in the hierarchical model, and if they can be overlapped consistently (i.e., if the positions that they share have the same tile type in each assembly), then their union $\alpha \cup \beta$ is producible. This is trivially true in the seeded model, but it requires more care to prove in the hierarchical model. It is conceivable *a priori* that although β is producible, β must assemble $\alpha \cap \beta$ in some order that is inconsistent with how α assembles $\alpha \cap \beta$. This is shown in Section 5.

   This result is most interesting for the open question it raises: what happens if a tile system produces an assembly that overlaps consistently with a translation of *itself*? We conjecture, via a "pumping" argument, that this results in infinite producible assemblies, which would resolve an open question on lower bounds on the assembly time of hierarchical systems [6].

2 Informal definition of the abstract tile assembly model

We give an informal sketch of the seeded and hierarchical variants of the abstract Tile Assembly Model (aTAM). See Section A.1 for a formal definition.

A *tile type* is a unit square with four sides, each consisting of a *glue label* (often represented as a finite string) and a nonnegative integer *strength*. We assume a finite set T of tile types, but an infinite number of copies of each tile type, each copy referred to as a *tile*. If a glue has strength 0, we say it is *null*, and if a positive-strength glue facing some direction does not appear on some tile type in the opposite direction, we say it is *functionally null*. We assume that all tile sets in this paper contain no functionally null glues. An *assembly* is a positioning of tiles on the integer lattice $\mathbb{Z}^2$; i.e., a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$. We write $|\alpha|$ to denote $|\text{dom } \alpha|$. Write $\alpha \sqsubseteq \beta$ to denote that α is a *subassembly* of β, which means that $\text{dom } \alpha \subseteq \text{dom } \beta$ and $\alpha(p) = \beta(p)$ for all points $p \in \text{dom } \alpha$. In this case, say that β is a *superassembly* of α. We abuse notation and take a tile type t to be equivalent to the single-tile assembly containing only t (at the origin if not otherwise specified). Two adjacent tiles in an assembly *interact* if the glue labels on their abutting sides are equal and have positive strength. Each assembly induces a *binding graph*, a grid graph whose vertices are tiles, with an edge between two tiles if they interact. The assembly is τ-*stable* if every cut of its binding graph has strength at least τ, where the weight of an edge is the strength of the glue it represents.

A *seeded tile assembly system* (seeded TAS) is a triple $\mathcal{T} = (T, \sigma, \tau)$, where T is a finite set of tile types, $\sigma : \mathbb{Z}^2 \dashrightarrow T$ is a finite, τ-stable *seed assembly*, and τ is the *temperature*. If $\mathcal{T}$ has a single seed tile $s \in T$ (i.e., $\sigma(0,0) = s$ for some $s \in T$ and is undefined elsewhere), then we write $\mathcal{T} = (T, s, \tau)$. Let $|\mathcal{T}|$ denote $|T|$. An assembly α is *producible* if either $\alpha = \sigma$ or if β is a producible assembly and α can be obtained from β by the stable binding of a single tile. In this case write $\beta \to_1 \alpha$ (α is producible from β by the attachment of one tile), and write $\beta \to \alpha$ if $\beta \to_1^* \alpha$ (α is producible from β by the attachment of zero or more tiles). An assembly is *terminal* if no tile can be τ-stably attached to it.

A *hierarchical tile assembly system* (hierarchical TAS) is a pair $\mathcal{T} = (T, \tau)$, where T is a finite set of tile types and $\tau \in \mathbb{N}$ is the temperature. An assembly is *producible* if either it is a single tile from T, or it is the τ-stable result of translating two producible assemblies without overlap. Therefore, if an assembly α is producible, then it is produced via an *assembly tree*, a full binary tree whose root is labeled with α, whose $|\alpha|$ leaves are labeled with tile types, and each internal node is a producible assembly formed by the stable attachment of its two child assemblies. An assembly α is *terminal* if for every producible assembly β, α and β cannot be τ-stably attached. If α can grow into β by the attachment of zero or more assemblies, then we write $\alpha \to \beta$.

Our definitions imply only finite assemblies are producible. In either model, let $\mathcal{A}[\mathcal{T}]$ be the set of producible assemblies of $\mathcal{T}$, and let $\mathcal{A}_\Box[\mathcal{T}] \subseteq \mathcal{A}[\mathcal{T}]$ be the set of producible, terminal assemblies of $\mathcal{T}$. A TAS $\mathcal{T}$ is *directed* (a.k.a., *deterministic*, *confluent*) if $|\mathcal{A}_\Box[\mathcal{T}]| = 1$. If $\mathcal{T}$ is directed with unique producible terminal assembly α, we say that $\mathcal{T}$ *uniquely produces* α. It is easy to check that in the seeded aTAM, $\mathcal{T}$ uniquely produces α if and only if every producible assembly $\beta \sqsubseteq \alpha$. In the hierarchical model, a similar condition holds, although it is more complex since hierarchical assemblies, unlike seeded assemblies, do not have a "canonical translation" defined by the seed. $\mathcal{T}$ uniquely produces α if and only if for every producible assembly β, there is a translation β' of β such that $\beta' \sqsubseteq \alpha$. In particular, if there is a producible assembly $\beta \neq \alpha$ such that dom α = dom β, then α is not uniquely produced. Since dom β = dom α, every nonzero translation of β has some tiled position outside of dom α, whence no such translation can be a subassembly of α, implying α is not uniquely produced.

3 Efficient verification of production

Let S be a finite set. A *partition* of S is a collection $\mathcal{C} = \{C_1, \ldots, C_k\} \subseteq \mathcal{P}(S)$ such that $\bigcup_{i=1}^k C_i = S$ and for all $i \neq j$, $C_i \cap C_j = \varnothing$. A *hierarchical division* of S is a full binary tree Υ (a tree in which every internal node has exactly two children) whose nodes represent subsets of S, such that the root of Υ represents S, the $|S|$ leaves of Υ represent the singleton sets $\{x\}$ for each $x \in S$, and each internal node has the property that its set is the (disjoint) union of its two childrens' sets.

Lemma 3.1. *Let S be a finite set with $|S| \geq 2$. Let Υ be any hierarchical division of S, and let $\mathcal{C}$ be any partition of S other than $\{S\}$. Then there exist $C_1, C_2 \in \mathcal{C}$ with $C_1 \neq C_2$, and there exist $C_1' \subseteq C_1$ and $C_2' \subseteq C_2$, such that C_1' and C_2' are siblings in Υ.*

Proof. First, label each leaf $\{x\}$ of Υ with the unique element $C_i \in \mathcal{C}$ such that $x \in C_i$. Next, iteratively label internal nodes according to the following rule: while there exist two children of a node u that have the same label, assign that label to u. Notice that this rule preserves the invariant that each labeled node u (representing a subset of S) is a subset of the set its label represents. Continue until no node has two identically-labeled children. $\mathcal{C}$ contains only proper subsets of S, so the root (which is the set S) cannot be contained in any of them, implying the root will remain unlabeled. Follow any path starting at the root, always following an unlabeled child, until both children of the current internal node are labeled. (The path may vacuously end at the root.) Such a node is well-defined since at least all leaves are labeled. By the stopping condition stated previously, these children must be labeled differently. The children are the witnesses C'_1 and C'_2, with their labels having the values C_1 and C_2, testifying to the truth of the lemma. □

Lemma 3.1 will be useful when we view Υ as an assembly tree for some producible assembly α, and we view $\mathcal{C}$ as a partially completed attempt to construct another assembly tree for α, where each element of $\mathcal{C}$ is a subassembly that has been produced so far.

When we say "by monotonicity", this refers to the fact that glue strengths are nonnegative, which implies that if two assemblies α and β can attach, the addition of more tiles to either α or β cannot *prevent* this binding, so long as the additional tiles do not overlap the other assembly.

Algorithm 1 IS-PRODUCIBLE-ASSEMBLY(α, τ)

```
 1: input: assembly $\alpha$ and temperature $\tau$
 2: $\mathcal{C} \leftarrow \{\ \{v\}\ \mid v \in \mathrm{dom}\ \alpha\ \}$    // (positions defining) subassemblies of $\alpha$
 3: while $|\mathcal{C}| > 1$ do
 4:    if there exist $C_i, C_j \in \mathcal{C}$ with glues between $C_i$ and $C_j$ of total strength at least $\tau$ then
 5:       $\mathcal{C} \leftarrow (\mathcal{C} \setminus \{C_i, C_j\}) \cup \{C_i \cup C_j\}$
 6:    else
 7:       print "$\alpha$ is not producible" and exit
 8:    end if
 9: end while
10: print "$\alpha$ is producible"
```

We want to solve the following problem: given an assembly α and temperature τ, is α producible in the hierarchical aTAM at temperature τ?[1] The algorithm IS-PRODUCIBLE-ASSEMBLY (Algorithm 1) solves this problem.

Theorem 3.2. *There is an $O(|\alpha| \log^2 |\alpha|)$ time algorithm deciding whether an assembly α is producible at temperature τ in the hierarchical aTAM.*

Proof. **Correctness:** IS-PRODUCIBLE-ASSEMBLY works by building up the initially edge-free graph with the tiles of α as its nodes (the algorithm stores the nodes as points in $\mathbb{Z}^2$, but α would be used in step 4 to get the glues and strengths between tiles at adjacent positions), stopping when the graph becomes connected. The order in which connected components (implicitly representing assemblies) are removed from and added to $\mathcal{C}$ implicitly defines a particular assembly tree with α at the root (for every C_1, C_2 processed in line 5, the assembly $\alpha \upharpoonright (C_1 \cup C_2)$ is a parent of $\alpha \upharpoonright C_1$ and $\alpha \upharpoonright C_2$ in the assembly tree). Therefore, if the algorithm reports that α is producible,

[1]We do not need to give the tile set T as input because the tiles in α implicitly define a tile set, and the presence of extra tile types in T that do not appear in α cannot affect its producibility.

then it is. Conversely, suppose that α is producible via assembly tree Υ. Let $\mathcal{C} = \{C_1, \ldots, C_k\}$ be the set of assemblies at some iteration of the loop at line 3. It suffices to show that some pair of assemblies C_i and C_j are connected by glues with strength at least τ. By Lemma 3.1, there exist C_i and C_j with subsets $C_i' \subseteq C_i$ and $C_j' \subseteq C_j$ such that C_i' and C_j' are sibling nodes in Υ. Because they are siblings, the glues between C_i' and C_j' have strength at least τ. By monotonicity these glues suffice to bind C_i to C_j, so Is-Producible-Assembly is correct.
Running time: Let $n = |\alpha|$. The running time of the Is-Producible-Assembly (Algorithm 1) is polynomial in n, but the algorithm can be optimized to improve the running time to $O(n \log^2 n)$ by careful choice of data structures. Is-Producible-Assembly-Fast (Algorithm 2) shows pseudocode for this optimized implementation, which we now describe. Let $n = |\alpha|$. Instead of searching over all pairs of assemblies, only search those pairs of assemblies that are adjacent. This number is $O(n)$ since a grid graph has degree at most 4 (hence $O(n)$ edges) and the number of edges in the full grid graph of α is an upper bound on the number of adjacent assemblies at any time. This can be encoded in a dynamically changing graph G_c whose nodes are the current set of assemblies and whose edges connect those assemblies that are adjacent.

Each edge of G_c stores the total glue strength between the assemblies. Whenever two assemblies C_1 and C_2, with $|C_1| \geq |C_2|$ without loss of generality, are combined to form a new assembly, G_c is updated by removing C_2, merging its edges with those of C_1, and for any edges they already share (i.e., the neighbor on the other end of the edge is the same), summing the strengths on the edges. Each update of an edge (adding it to C_1, or finding it in C_1 to update its strength) can be done in $O(\log n)$ time using a tree set data structure to store neighbors for each assembly.

We claim that the total number of such updates of all edges is $O(n \log n)$ over all time, or amortized $O(\log n)$ updates per iteration of the outer loop. To see why, observe that the number of edges an assembly has is at most linear in its size, so the number of new edges that must be added to C_1, or existing edges in C_1 whose strengths must be updated, is at most (within a constant) the size of the smaller component C_2. The total number of edge updates is then, if Υ is the assembly tree discovered by the algorithm, $\sum_{\text{nodes } u \in \Upsilon} \min\{|\text{left}(u)|, |\text{right}(u)|\}$, where $|\text{left}(u)|$ and $|\text{right}(u)|$ respectively refer to the number of leaves of u's left and right subtrees. For a given number n of leaves, this sum is maximized with a balanced tree, and in that case (summing over all levels of the tree) is $\sum_{i=0}^{\log n} 2^i (n/2^i) = O(n \log n)$. So the total time to update all edges is $O(n \log^2 n)$.

As for actually finding C_1 and C_2, each iteration of the outer loop, we can look *any* pair of adjacent assemblies with sufficient connection strength. So in addition to storing the edges in a tree-backed set data structure, store them also in one of two linked lists: H and L in the algorithm, for "high" (strength $\geq \tau$) and "low" (strength $< \tau$), with each edge storing a pointer to its node in the linked list for $O(1)$ time removal (and also to its node in the tree-backed set for $O(\log n)$ time removal). We can simply choose an arbitrary edge from H to be the next pair of connected components to attach. We update the keys containing C_1 whose connection strength changed and removing those containing C_2 but not C_1. The edges whose connection strength changed correspond to precisely those neighbors that C_1 and C_2 shared before being merged. Therefore $|C_2|$ is an upper bound on the number of edge updates required. Thus the amortized number of linked list updates is $O(\log n)$ per iteration of the outer loop by the same argument as above. Since we can have each edge $\{C_1, C_2\}$ store a pointer to its node in the linked list to which it belongs, each list update can be done in $O(1)$ time. Thus each iteration takes amortized time $O(\log n)$.

The algorithm Is-Producible-Assembly-Fast (Algorithm 2) implements this optimized idea. The terminology for data structure operations is taken from [7]. Note that the way we remove C_1

and C_2 and add their union is to simply delete C_2 and then update C_1 to contain C_2's edges. The graph G_c discussed above is $G_c = (V_c, E_c)$ where V_c and E_c are variables in Is-Producible-Assembly-Fast.

Summarizing the analysis, each data structure operation takes time $O(\log n)$ with appropriate choice of a backing data structure. The two outer loops (lines 6 and 10) take $O(n)$ iterations. The inner loop (line 17) runs for amortized $O(\log n)$ iterations, and its body executes a constant number of $O(\log n)$ and $O(1)$ time operations. Therefore the total running time is $O(n \log^2 n)$. □

Algorithm 2 Is-Producible-Assembly-Fast(α, τ)

```
 1: input: assembly $\alpha$ and temperature $\tau$
 2: $V_c \leftarrow \{ \{v\} \mid v \in \text{dom}\,\alpha \}$   // (positions defining) subassemblies of $\alpha$
 3: $E_c \leftarrow \{\{\{u\},\{v\}\} \mid \{u\} \in V_c$ and $\{v\} \in V_c$ and $u$ and $v$ are adjacent and interact$\}$
 4: $H \leftarrow$ empty linked list   // pairs of subassemblies binding with strength $\geq \tau$
 5: $L \leftarrow$ empty linked list   // pairs of subassemblies binding with strength $< \tau$
 6: for all $\{\{u\},\{v\}\} \in E_c$ do
 7:   $w(\{u\},\{v\}) \leftarrow$ strength of glue binding $\alpha(u)$ and $\alpha(v)$
 8:   append $\{\{u\},\{v\}\}$ to $L$ if $w(\{u\},\{v\}) < \tau$, and append to $H$ otherwise
 9: end for
10: while $|V_c| > 1$ do
11:   if $H$ is empty then
12:     print "$\alpha$ is not producible" and exit
13:   end if
14:   $\{C_1, C_2\} \leftarrow$ first element of $H$   // assume $|C_1| \geq |C_2|$ without loss of generality
15:   remove $\{C_1, C_2\}$ from $H$
16:   remove $C_2$ from $V_c$
17:   for all neighbors $C$ of $C_2$ do
18:     remove $\{C_2, C\}$ from $E_c$ and $H$ or $L$
19:     if $\{C_1, C\} \in E_c$ then
20:       $w(C_1, C) \leftarrow w(C_1, C) + w(C_2, C)$
21:       if $w(C_1, C) \geq \tau$ and $\{C_1, C\} \in L$ then
22:         remove $\{C_1, C\}$ from $L$ and add it to $H$
23:       end if
24:     else
25:       $w(C_1, C) \leftarrow w(C_2, C)$
26:       add $\{C_1, C\}$ to $E_c$ and to $H$ if $w(C_1, C) \geq \tau$ and to $L$ otherwise
27:     end if
28:   end for
29: end while
30: print "$\alpha$ is producible"
```

4 Efficient verification of temperature 1 unique production

This section shows that there is an algorithm, faster than the previous known algorithm [5], that solves the temperature 1 *unique producibility verification* (UPV) problem: given an assembly α and a temperature-1 hierarchical tile system $\mathcal{T}$, decide if α is the unique producible, terminal assembly of $\mathcal{T}$. This is done by showing an algorithm for the temperature 1 UPV problem in the seeded model (which is faster than the general-temperature algorithm of [2]), and then applying the technique of [5] relating producibility and terminality in the temperature 1 seeded and hierarchical models.

Define the decision problems sUPV_1 and hUPV_1 by the language $\{ \ (\mathcal{T}, \alpha) \ \mid \mathcal{A}_{\Box}[\mathcal{T}] = \{\alpha\} \ \}$, where $\mathcal{T}$ is a temperature 1 seeded TAS in the former case and a temperature 1 hierarchical TAS in the latter case. To simplify the time analysis we assume $|\mathcal{T}| = O(|\alpha|)$. The following is the only result in this paper on the seeded aTAM.

Theorem 4.1. *There is an algorithm that solves the sUPV_1 problem in time $O(|\alpha| \log |\mathcal{T}|)$.*

Proof. Let $\mathcal{T} = (T, s, 1)$ and α be a instance of the sUPV_1 problem. We first check that every tile in α appears in T, which can be done in time $O(|\alpha| \log |T|)$ by storing elements of T in a data structure supporting $O(\log n)$ time access. In the seeded aTAM at temperature 1, α is producible if and only if it contains the seed s and its binding graph is connected, which can be checked in time $O(|\alpha|)$. We must also verify that α is terminal, which is true if and only if all glues on unbound sides are null, checkable in time $O(|\alpha|)$.

Once we have verified that α is producible and terminal, it remains to verify that $\mathcal{T}$ uniquely produces α. Adleman, Cheng, Goel, Huang, Kempe, Moisset de Espanés, and Rothemund [2] showed that this is true (at any temperature) if and only if, for every position $p \in \text{dom } \alpha$, if $\alpha_p \sqsubset \alpha$ is the maximal producible subassembly of α such that $p \notin \text{dom } \alpha_p$, then $\alpha(p)$ is the only tile type attachable to α_p at position p. They solve the problem by producing each such α_p and checking whether there is more than one tile type attachable to α_p at p. We use a similar approach, but we avoid the cost of producing each α_p by exploiting special properties of temperature 1 producibility.

Given $p, q \in \text{dom } \alpha$ such that $p \neq q$, write $p \prec q$ if, for every producible assembly β, $q \in \text{dom } \beta \implies p \in \text{dom } \beta$, i.e., the tile at position p must be present before the tile at position q can be attached. We must check each $p \in \text{dom } \alpha$ and each position $q \in \text{dom } \alpha$ adjacent to p such that $p \not\prec q$ to see whether a tile type $t \neq \alpha(p)$ shares a positive-strength glue with $\alpha(q)$ in direction $q - p$ (i.e., whether, if $\alpha(p)$ were not present, t could attach at p instead). If we know which positions q adjacent to p satisfy $p \not\prec q$, this check can be done in time $O(\log |T|)$ with appropriate choice of data structure, implying total time $O(|\alpha| \log |T|)$ over all positions $p \in \text{dom } \alpha$. It remains to show how to determine which adjacent positions $p, q \in \text{dom } \alpha$ satisfy $p \prec q$.

Recall that a *cut vertex* of a connected graph is a vertex whose removal disconnects the graph, and a subgraph is *biconnected* if the removal of any single vertex from the subgraph leaves it connected. Every graph can be decomposed into a tree of biconnected components, with cut vertices connecting different biconnected components (and belonging to all biconnected components that they connect). If p is not a cut vertex of the binding graph of α, then dom α_p is simply dom $\alpha \setminus \{p\}$ (i.e., it is possible to produce the entire assembly α except for position p) because, for all $q \in \text{dom } \alpha \setminus \{p\}$, $p \not\prec q$. If p is a cut vertex, then $p \prec q$ if and only if removing p from the binding graph of α places q and the seed position in two different connected components, since the connected component containing the seed after removing p corresponds precisely to α_p.

Run the linear time Hopcroft-Tarjan algorithm [21] for decomposing the binding graph of α into a tree of its biconnected components, which also identifies which vertices in the graph are cut vertices and which biconnected components they connect. Recall that the Hopcroft-Tarjan algorithm is an augmented depth-first search. Root the tree with s's biconnected component (i.e., start the depth-first search there), so that each component has a parent component and child components. In particular, each cut vertex p has a "parent" biconnected component and $k \geq 1$ "child" biconnected components. Removing such a cut vertex p will separate the graph into $k+1$ connected components: the k subtrees and the remaining nodes connected to the parent biconnected component of p. Thus $p \prec q$ if and only if p is a cut vertex and q is contained in the subtree rooted at p.

This check can be done for all positions p and their ≤ 4 adjacent positions q in linear time by "weaving" the checks into the Hopcroft-Tarjan algorithm. As the depth-first search executes, each vertex p is marked as either *unvisited*, *visiting* (meaning the search is currently in a subtree rooted at p), or *visited* (meaning the search has visited and exited the subtree rooted at p). If p is marked as visited or unvisited when q is processed, then q is not in the subtree under p. If p is marked as visiting when q is processed, then q is in p's subtree.

At the time q is visited during the Hopcroft-Tarjan algorithm, it may not yet be known whether p is a cut vertex. To account for this, simply run the Hopcroft-Tarjan algorithm first to label all cut vertices, then run a second depth-first search (visiting the nodes in the same order as the first depth-first search), doing the checks described previously and using the cut vertex information obtained from the Hopcroft-Tarjan algorithm. □

Theorem 4.2. *There is an algorithm that solves the* hUPV_1 *problem in time* $O(|\alpha||\mathcal{T}|\log|\mathcal{T}|)$.

Proof. Cannon, Demaine, Demaine, Eisenstat, Patitz, Schweller, Summers, and Winslow [5] showed that a temperature 1 hierarchical TAS $\mathcal{T} = (T, 1)$ uniquely produces α if and only if, for each $s \in T$, the seeded TAS $\mathcal{T}_s = (T, s, 1)$ uniquely produces α. Therefore, the hUPV_1 problem can be solved by calling the algorithm of Theorem 4.1 $|\mathcal{T}|$ times, resulting in a running time of $O(|\alpha||\mathcal{T}|\log|\mathcal{T}|)$. □

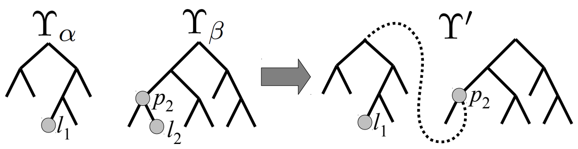
5 Consistent unions of producible assemblies are producible

Throughout this section, fix a hierarchical TAS $\mathcal{T} = (T, \tau)$. Let α, β be assemblies. We say α and β are *consistent* if $\alpha(p) = \beta(p)$ for all points $p \in \text{dom } \alpha \cap \text{dom } \beta$. If α and β are consistent, let $\alpha \cup \beta$ be defined as the assembly $(\alpha \cup \beta)(p) = \alpha(p)$ if α is defined, and $(\alpha \cup \beta)(p) = \beta(p)$ if $\alpha(p)$ is undefined. If α and β are not consistent, let $\alpha \cup \beta$ be undefined.

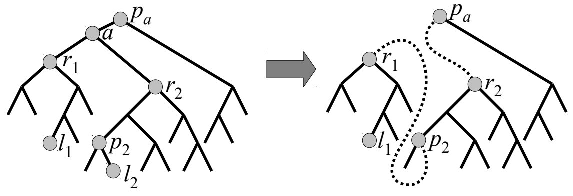
Theorem 5.1. *If* α, β *are producible assemblies that are consistent and* $\text{dom } \alpha \cap \text{dom } \beta \neq \varnothing$*, then* $\alpha \cup \beta$ *is producible. Furthermore,* $\alpha \to \alpha \cup \beta$*, i.e., it is possible to assemble exactly* α*, then to assemble the missing portions of* β*.*

Proof. If α and β are consistent and have non-empty overlap, then $\alpha \cup \beta$ is necessarily stable, since every cut of $\alpha \cup \beta$ is a superset of some cut of either α or β, which are themselves stable.

Let Υ_α and Υ_β be assembly trees for α and β, respectively. Define an assembly tree Υ for $\alpha \cup \beta$ by the following construction. Let l_1 be a leaf in Υ_α and let l_2 be a leaf in Υ_β representing the same position $x \in \text{dom } \alpha \cap \text{dom } \beta$, as shown in Figure 1(a). Remove l_2 and replace it with the entire tree Υ_α. Call the resulting tree Υ'. At this point, Υ' is not an assembly tree if α and β overlapped on more than one point, because every position in $\text{dom } \alpha \cap \text{dom } \beta \setminus \{x\}$ has



(a) First operation to combine the assembly trees for α and β. l_1 and l_2 are two leaves representing the same position in $\text{dom}\,\alpha \cap \text{dom}\,\beta$.



(b) Operation to eliminate one of two leaves l_1 and l_2 representing the same tile in the tree while preserving that all attachments are stable.

Figure 1: Constructing assembly tree for $\alpha \cup \beta$ from assembly trees for α and β.

duplicated leaves. Therefore the tree Υ' is not a hierarchical division of the set $\text{dom}\,\alpha \cup \text{dom}\,\beta$, since not all unions represented by each internal node are disjoint unions. However, each node does represent a stable assembly that is the union of the (possibly overlapping) assemblies represented by its two child nodes. We will show how to modify Υ' to eliminate each of these duplicates – at which point all unions represented by internal nodes will again be disjoint – while maintaining the invariant that each internal node represents a stable assembly, proving there is an assembly tree Υ for $\alpha \cup \beta$. Furthermore, the subtree Υ_α that was placed under p_2 will not change as a result of these modifications, which implies $\alpha \to \alpha \cup \beta$.

The process to eliminate one pair of duplicate leaves is shown in Figure 1(b). Let l_1 and l_2 be two leaves representing the same point in $\text{dom}\,\alpha \cap \text{dom}\,\beta$, and let a be their least common ancestor in Υ, noting that a is not contained in Υ_α since l_2 is not contained in Υ_α. Let p_a be the parent of a. Let r_1 be the root of the subtree under a containing l_1. Let r_2 be the root of the subtree under a containing l_2. Let p_2 be the parent of l_2. Remove the leaf l_2 and the node a. Set the parent of r_1 to be p_2. Set the parent of r_2 to be p_a.

Since we have replaced the leaf l_2 with a subtree containing the leaf l_1, the subtree rooted at r_1 is an assembly containing the tile represented by l_2, in the same position. Since the original attachment of l_2 to its sibling was stable, by monotonicity, the attachment represented by p_2 is still legal. The removal of a is simply to maintain that Υ is a full binary tree; leaving it would mean that it represents a superfluous "attachment" of the assembly r_2 to $\varnothing$. However, it is now legal for r_2 to be a direct child of p_a, since r_2 (due to the insertion of the entire r_1 subtree beneath a descendant of r_2, again by monotonicity) now has all the tiles necessary for its attachment to the old sibling of a to be stable. Since a was not contained in Υ_α, the subtree Υ_α has not been altered.

This process is iterated for all duplicate leaves. When all duplicates have been removed, Υ is a valid assembly tree with root $\alpha \cup \beta$. Since Υ contains Υ_α as a subtree, $\alpha \to \alpha \cup \beta$. □

It is worthwhile to observe that Theorem 5.1 does not immediately follow from Theorem 3.2. Theorem 3.2 implies that *if* $\alpha \cup \beta$ *is producible*, then this can be verified simply by attaching subassemblies until $\alpha \cup \beta$ is produced. Furthermore, since the hypothesis of Theorem 5.1 implies that α is producible, the greedy algorithm of Theorem 3.2 could potentially assemble α along the way to assembling $\alpha \cup \beta$, which implies that *if* $\alpha \cup \beta$ *is producible*, then it is producible from α. However, nothing in Theorem 3.2 guarantees that $\alpha \cup \beta$ is producible in the first place. There may be some additional details that could be added to the proof of Theorem 3.2 that would cause it to imply Theorem 5.1, but those details are likely to resemble the existing proof of Theorem 5.1, and it is conceptually cleaner to keep the two proofs separate.

6 Open Question

Theorem 5.1 shows that if assemblies α and β overlap consistently, then $\alpha \cup \beta$ is producible. What if $\alpha = \beta$? Suppose we have three copies of α, and label them each uniquely as $\alpha_1, \alpha_2, \alpha_3$. (See Figure 2 for an example.) Suppose further than α_2 overlaps consistently with α_1 when translated by some non-zero vector $\vec{v}$. Then we know that $\alpha_1 \cup \alpha_2$ is producible. Suppose that α_3 is α_2 translated by $\vec{v}$, or equivalently it is α_1 translated by $2\vec{v}$. Then $\alpha_2 \cup \alpha_3$ is producible, since this is merely a translated copy of $\alpha_1 \cup \alpha_2$. It seems intuitively that $\alpha_1 \cup \alpha_2 \cup \alpha_3$ should be producible as well. However, while α_1 overlaps consistently with α_2, and α_2 overlaps consistently with α_3, it could be the case that α_3 intersects α_1 inconsistently, i.e., they share a position but put a different tile type at that position. In this case $\alpha_1 \cup \alpha_2 \cup \alpha_3$ is undefined.

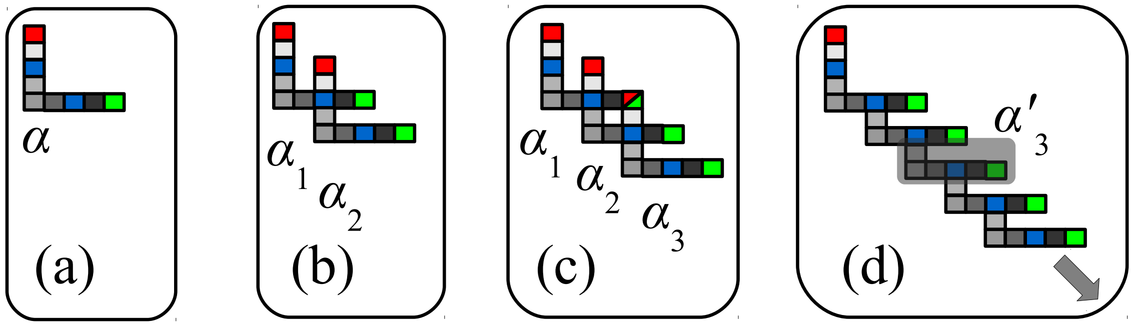


Figure 2: (a) A producible assembly α. Gray tiles are all distinct types from each other, but red, green, and blue each represent one of three different tile types, so the two blue tiles are the same type. (b) By Theorem 5.1, $\alpha_1 \cup \alpha_2$ is producible, where $\alpha_1 = \alpha$ and $\alpha_2 = \alpha_1 + (2, -2)$, because they overlap in only one position, and they both have the blue tile type there. (c) α_1 and α_3 both have a tile at the same position, but the types are different (red in the case of α_1 and green in the case of α_3). (d) However, a subassembly α'_i of each new α_i can grow, enough to allow the translated equivalent subassembly α'_{i+1} of α_{i+1} to grow from α'_i, so an infinite structure is producible.

In the example of Figure 2, although $\alpha_1 \cup \alpha_2 \cup \alpha_3$ is not producible (in fact, not even defined), "enough" of α_3 (say, $\alpha'_3 \sqsubset \alpha_3$) can grow off of $\alpha_1 \cup \alpha_2$ to allow a fourth copy α'_4 to begin to grow to an assembly to which a fifth copy α'_5 can attach, etc., so that an infinite assembly can grow by "pumping" additional copies of α'_3. Is this always possible? In other words, is it the case that if α is a producible assembly of a hierarchical TAS $\mathcal{T}$, and α overlaps consistently with some non-zero translation of itself, then $\mathcal{T}$ necessarily produces arbitrarily large assemblies? If true, this would imply that no hierarchical TAS producing such an assembly could be uniquely produce a finite assembly. This would settle an open question posed by Chen and Doty [6], who showed that as long as a hierarchical TAS does not produce assemblies that consistently overlap any translation of themselves, then the TAS cannot uniquely produce any shape in time sublinear in its diameter.

Acknowledgements. The author is very grateful to Ho-Lin Chen, David Soloveichik, Damien Woods, Matt Patitz, Scott Summers, Robbie Schweller, Ján Maňuch, and Ladislav Stacho for many insightful discussions.

References

[1] Zachary Abel, Nadia Benbernou, Mirela Damian, Erik D. Demaine, Martin L. Demaine, Robin Flatland, Scott Kominers, and Robert Schweller. Shape replication through self-assembly and RNase enzymes. In *SODA 2010: Proceedings of the Twenty-first Annual ACM-SIAM Symposium on Discrete Algorithms*, Austin, Texas, 2010. Society for Industrial and Applied Mathematics.

[2] Leonard M. Adleman, Qi Cheng, Ashish Goel, Ming-Deh A. Huang, David Kempe, Pablo Moisset de Espanés, and Paul W. K. Rothemund. Combinatorial optimization problems in self-assembly. In *STOC 2002: Proceedings of the Thirty-Fourth Annual ACM Symposium on Theory of Computing*, pages 23–32, 2002.

[3] Gagan Aggarwal, Qi Cheng, Michael H. Goldwasser, Ming-Yang Kao, Pablo Moisset de Espanés, and Robert T. Schweller. Complexities for generalized models of self-assembly. *SIAM Journal on Computing*, 34:1493–1515, 2005. Preliminary version appeared in SODA 2004.

[4] Robert D. Barish, Rebecca Schulman, Paul W. K. Rothemund, and Erik Winfree. An information-bearing seed for nucleating algorithmic self-assembly. *Proceedings of the National Academy of Sciences*, 106(15):6054–6059, March 2009.

[5] Sarah Cannon, Erik D. Demaine, Martin L. Demaine, Sarah Eisenstat, Matthew J. Patitz, Robert T. Schweller, Scott M. Summers, and Andrew Winslow. Two hands are better than one (up to constant factors). In *STACS 2013: Proceedings of the Thirtieth International Symposium on Theoretical Aspects of Computer Science*, pages 172–184, 2013.

[6] Ho-Lin Chen and David Doty. Parallelism and time in hierarchical self-assembly. In *SODA 2012: Proceedings of the 23rd Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1163–1182, 2012.

[7] Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein. *Introduction to Algorithms.* MIT Press, 2001.

[8] Erik D. Demaine, Martin L. Demaine, Sándor P. Fekete, Mashhood Ishaque, Eynat Rafalin, Robert T. Schweller, and Diane L. Souvaine. Staged self-assembly: Nanomanufacture of arbitrary shapes with $O(1)$ glues. *Natural Computing*, 7(3):347–370, 2008. Preliminary version appeared in DNA 2007.

[9] Erik D. Demaine, Sarah Eisenstat, Mashhood Ishaque, and Andrew Winslow. One-dimensional staged self-assembly. *Natural Computing*, 12(2):1–12, 2013. Preliminary version appeared in DNA 2011.

[10] Erik D. Demaine, Matthew J. Patitz, Trent Rogers, Robert T. Schweller, Scott M. Summers, and Damien Woods. The two-handed tile assembly model is not intrinsically universal. In *ICALP 2013: Proceedings of the 40th International Colloquium on Automata, Languages and Programming*, July 2013.

[11] Erik D. Demaine, Matthew J. Patitz, Robert T. Schweller, and Scott M. Summers. Self-assembly of arbitrary shapes using RNase enzymes: Meeting the Kolmogorov bound with

small scale factor. In *STACS 2011: Proceedings of the 28th International Symposium on Theoretical Aspects of Computer Science*, 2011.

[12] David Doty. Theory of algorithmic self-assembly. *Communications of the ACM*, 55(12):78–88, December 2012.

[13] David Doty, Jack H. Lutz, Matthew J. Patitz, Robert T. Schweller, Scott M. Summers, and Damien Woods. The tile assembly model is intrinsically universal. In *FOCS 2012: Proceedings of the 53rd Annual IEEE Symposium on Foundations of Computer Science*, pages 302–310. IEEE, 2012.

[14] David Doty, Matthew J. Patitz, Dustin Reishus, Robert T. Schweller, and Scott M. Summers. Strong fault-tolerance for self-assembly with fuzzy temperature. In *FOCS 2010: Proceedings of the 51st Annual IEEE Symposium on Foundations of Computer Science*, pages 417–426. IEEE, 2010.

[15] 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. Preliminary version appeared in DNA 2009.

[16] Pierre Étienne Meunier, Matthew J. Patitz, Scott M. Summers, Guillaume Theyssier, Andrew Winslow, and Damien Woods. Intrinsic universality in tile self-assembly requires cooperation. In *SODA 2014: Proceedings of the 25th Annual ACM-SIAM Symposium on Discrete Algorithms*, 2014. to appear.

[17] Bin Fu, Matthew J. Patitz, Robert T. Schweller, and Robert Sheline. Self-assembly with geometric tiles. In *ICALP 2012: Proceedings of the 39th International Colloquium on Automata, Languages and Programming*, pages 714–725, July 2012.

[18] Kei Goto, Yoko Hinob, Takayuki Kawashima, Masahiro Kaminagab, Emiko Yanob, Gaku Yamamotob, Nozomi Takagic, and Shigeru Nagasec. Synthesis and crystal structure of a stable S-nitrosothiol bearing a novel steric protection group and of the corresponding S-nitrothiol. *Tetrahedron Letters*, 41(44):8479–8483, 2000.

[19] Wilfried Heller and Thomas L. Pugh. "Steric protection" of hydrophobic colloidal particles by adsorption of flexible macromolecules. *Journal of Chemical Physics*, 22(10):1778, 1954.

[20] Wilfried Heller and Thomas L. Pugh. "Steric" stabilization of colloidal solutions by adsorption of flexible macromolecules. *Journal of Polymer Science*, 47(149):203–217, 1960.

[21] John Hopcroft and Robert Tarjan. Algorithm 447: efficient algorithms for graph manipulation. *Communications of the ACM*, 16(6):372–378, June 1973.

[22] James I. Lathrop, Jack H. Lutz, and Scott M. Summers. Strict self-assembly of discrete Sierpinski triangles. *Theoretical Computer Science*, 410:384–405, 2009. Preliminary version appeared in CiE 2007.

[23] Chris Luhrs. Polyomino-safe DNA self-assembly via block replacement. *Natural Computing*, 9(1):97–109, March 2010. Preliminary version appeared in DNA 2008.

[24] Matthew J. Patitz. An introduction to tile-based self-assembly. In *UCNC 2012: Proceedings of the 11th international conference on Unconventional Computation and Natural Computation*, pages 34–62, Berlin, Heidelberg, 2012. Springer-Verlag.

[25] Matthew J. Patitz and Scott M. Summers. Identifying shapes using self-assembly. *Algorithmica*, 64(3):481–510, 2012. Preliminary version appeared in ISAAC 2010.

[26] Paul W. K. Rothemund. *Theory and Experiments in Algorithmic Self-Assembly*. PhD thesis, University of Southern California, December 2001.

[27] Paul W. K. Rothemund and Erik Winfree. The program-size complexity of self-assembled squares (extended abstract). In *STOC 2000: Proceedings of the Thirty-Second Annual ACM Symposium on Theory of Computing*, pages 459–468, 2000.

[28] Rebecca Schulman and Erik Winfree. Synthesis of crystals with a programmable kinetic barrier to nucleation. *Proceedings of the National Academy of Sciences*, 104(39):15236–15241, 2007.

[29] Rebecca Schulman and Erik Winfree. Programmable control of nucleation for algorithmic self-assembly. *SIAM Journal on Computing*, 39(4):1581–1616, 2009. Preliminary version appeared in DNA 2004.

[30] Robert T. Schweller and Michael Sherman. Fuel efficient computation in passive self-assembly. In *SODA 2013: Proceedings of the 24th Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1513–1525, January 2013.

[31] Leroy G. Wade. *Organic Chemistry*. Prentice Hall, 2nd edition, 1991.

[32] Erik Winfree. *Algorithmic Self-Assembly of DNA*. PhD thesis, California Institute of Technology, June 1998.

[33] Erik Winfree. Simulations of computing by self-assembly. Technical Report CaltechCSTR:1998.22, California Institute of Technology, 1998.

[34] Erik Winfree. Self-healing tile sets. In Junghuei Chen, Natasa Jonoska, and Grzegorz Rozenberg, editors, *Nanotechnology: Science and Computation*, Natural Computing Series, pages 55–78. Springer, 2006.

[35] Erik Winfree, Furong Liu, Lisa A. Wenzler, and Nadrian C. Seeman. Design and self-assembly of two-dimensional DNA crystals. *Nature*, 394(6693):539–44, 1998.

[36] Andrew Winslow. Staged self-assembly and polyomino context-free grammars. In *DNA 2013: Proceedings of the 19th International Meeting on DNA Computing and Molecular Programming*, 2013.

A Formal definition of the abstract tile assembly model

A.1 Formal definition of the abstract tile assembly model

This section gives a terse definition of the abstract Tile Assembly Model (aTAM, [32]). This is not a tutorial; for readers unfamiliar with the aTAM, [27] gives an excellent introduction to the model.

Fix an alphabet Σ. Σ^* is the set of finite strings over Σ. Given a discrete object O, $\langle O \rangle$ denotes a standard encoding of O as an element of Σ^*. $\mathbb{Z}$, $\mathbb{Z}^+$, and $\mathbb{N}$ denote the set of integers, positive integers, and nonnegative integers, respectively. For a set A, $\mathcal{P}(A)$ denotes the power set of A. Given $A \subseteq \mathbb{Z}^2$, the *full grid graph* of A is the undirected graph $G^{\mathrm{f}}_A = (V, E)$, where $V = A$, and for all $u, v \in V$, $\{u, v\} \in E \iff \|u - v\|_2 = 1$; i.e., if and only if u and v are adjacent on the integer Cartesian plane. A *shape* is a set $S \subseteq \mathbb{Z}^2$ such that G^{f}_S is connected.

A *tile type* is a tuple $t \in (\Sigma^* \times \mathbb{N})^4$; i.e., a unit square with four sides listed in some standardized order, each side having a *glue label* (a.k.a. *glue*) $\ell \in \Sigma^*$ and a nonnegative integer *strength*, denoted $str(\ell)$. For a set of tile types T, let $\Lambda(T) \subset \Sigma^*$ denote the set of all glue labels of tile types in T. If a glue has strength 0, we say it is *null*, and if a positive-strength glue facing some direction does not appear on some tile type in the opposite direction, we say it is *functionally null*. We assume that all tile sets in this paper contain no functionally null glues.[2] Let $\{\mathsf{N}, \mathsf{S}, \mathsf{E}, \mathsf{W}\}$ denote the *directions* consisting of unit vectors $\{(0,1), (0,-1), (1,0), (-1,0)\}$. Given a tile type t and a direction $d \in \{\mathsf{N}, \mathsf{S}, \mathsf{E}, \mathsf{W}\}$, $t(d) \in \Lambda(T)$ denotes the glue label on t in direction d. We assume a finite set T of tile types, but an infinite number of copies of each tile type, each copy referred to as a *tile*. An *assembly* is a nonempty connected arrangement of tiles on the integer lattice $\mathbb{Z}^2$, i.e., a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$ such that $G^{\mathrm{f}}_{\mathrm{dom}\,\alpha}$ is connected and $\mathrm{dom}\,\alpha \neq \varnothing$. The *shape of* α is $\mathrm{dom}\,\alpha$. Write $|\alpha|$ to denote $|\mathrm{dom}\,\alpha|$. Given two assemblies $\alpha, \beta : \mathbb{Z}^2 \dashrightarrow T$, we say α is a *subassembly* of β, and we write $\alpha \sqsubseteq \beta$, if $\mathrm{dom}\,\alpha \subseteq \mathrm{dom}\,\beta$ and, for all points $p \in \mathrm{dom}\,\alpha$, $\alpha(p) = \beta(p)$.

Given two assemblies α and β, we say α and β are *equivalent up to translation*, written $\alpha \simeq \beta$, if there is a vector $\vec{x} \in \mathbb{Z}^2$ such that $\mathrm{dom}\,\alpha = \mathrm{dom}\,\beta + \vec{x}$ (where for $A \subseteq \mathbb{Z}^2$, $A + \vec{x}$ is defined to be $\{\ p + \vec{x} \mid p \in A\ \}$) and for all $p \in \mathrm{dom}\,\beta$, $\alpha(p + \vec{x}) = \beta(p)$. In this case we say that β is a *translation* of α. We have fixed assemblies at certain positions on $\mathbb{Z}^2$ only for mathematical convenience in some contexts, but of course real assemblies float freely in solution and do not have a fixed position.

Let α be an assembly and let $p \in \mathrm{dom}\,\alpha$ and $d \in \{\mathsf{N}, \mathsf{S}, \mathsf{E}, \mathsf{W}\}$ such that $p + d \in \mathrm{dom}\,\alpha$. Let $t = \alpha(p)$ and $t' = \alpha(p + d)$. We say that the tiles t and t' at positions p and $p + d$ *interact* if $t(d) = t'(-d)$ and $str(t(d)) > 0$, i.e., if the glue labels on their abutting sides are equal and have positive strength. Each assembly α induces a *binding graph* G^{b}_α, a grid graph $G = (V_\alpha, E_\alpha)$, where $V_\alpha = \mathrm{dom}\,\alpha$, and $\{p_1, p_2\} \in E_\alpha \iff \alpha(p_1)$ interacts with $\alpha(p_2)$.[3] Given $\tau \in \mathbb{Z}^+$, α is τ*-stable* if every cut of G^{b}_α has weight at least τ, where the weight of an edge is the strength of the glue it represents. That is, α is τ-stable if at least energy τ is required to separate α into two parts. When τ is clear from context, we say α is *stable*.

[2]This assumption does not affect the results of this paper. It is irrelevant for Theorem 5.1 or the correctness of the algorithms in the other theorems. It also does not affect the running time results for algorithms taking a TAS as input, because we can preprocess T in linear time to find and set to null any functionally null glues. The number of glues is $O(|T|)$, and we assume that each glue from glue set G is an integer in the set $\{0, \ldots, |G| - 1\}$. We can use a Boolean array of size $|G|$ to determine in time $O(|T|)$ which glues appear on the north that do not appear on the south of some tile type. Repeat this for each of the remaining three directions. Then replace all functionally null glues in T with null glues, which takes time $O(|T|)$. To do this replacement in an assembly α takes time $O(|\alpha|)$.

[3]For $G^{\mathrm{f}}_{\mathrm{dom}\,\alpha} = (V_{\mathrm{dom}\,\alpha}, E_{\mathrm{dom}\,\alpha})$ and $G^{\mathrm{b}}_\alpha = (V_\alpha, E_\alpha)$, G^{b}_α is a spanning subgraph of $G^{\mathrm{f}}_{\mathrm{dom}\,\alpha}$: $V_\alpha = V_{\mathrm{dom}\,\alpha}$ and $E_\alpha \subseteq E_{\mathrm{dom}\,\alpha}$.

A.2 Seeded aTAM

A *seeded tile assembly system* (seeded TAS) is a triple $\mathcal{T} = (T, \sigma, \tau)$, where T is a finite set of tile types, $\sigma : \mathbb{Z}^2 \dashrightarrow T$ is the finite, τ-stable *seed assembly*, and $\tau \in \mathbb{Z}^+$ is the *temperature*. Let $|\mathcal{T}|$ denote $|T|$. If $\mathcal{T}$ has a single seed tile $s \in T$ (i.e., $\sigma(0,0) = s$ for some $s \in T$ and is undefined elsewhere), then we write $\mathcal{T} = (T, s, \tau)$. Given two τ-stable assemblies $\alpha, \beta : \mathbb{Z}^2 \dashrightarrow T$, we write $\alpha \to_1^{\mathcal{T}} \beta$ if $\alpha \sqsubseteq \beta$ and $|\text{dom } \beta \setminus \text{dom } \alpha| = 1$. In this case we say α *$\mathcal{T}$-produces β in one step.*[4] If $\alpha \to_1^{\mathcal{T}} \beta$, $\text{dom } \beta \setminus \text{dom } \alpha = \{p\}$, and $t = \beta(p)$, we write $\beta = \alpha + (p \mapsto t)$.

A sequence of $k \in \mathbb{Z}^+$ assemblies $\vec{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_{k-1})$ is a *$\mathcal{T}$-assembly sequence* if, for all $1 \le i < k$, $\alpha_{i-1} \to_1^{\mathcal{T}} \alpha_i$. We write $\alpha \to^{\mathcal{T}} \beta$, and we say α *$\mathcal{T}$-produces* β (in 0 or more steps) if there is a $\mathcal{T}$-assembly sequence $\vec{\alpha} = (\alpha, \alpha_1, \alpha_2, \ldots, \alpha_{k-1} = \beta)$ of length $k = |\text{dom } \beta \setminus \text{dom } \alpha| + 1$. We say α is *$\mathcal{T}$-producible* if $\sigma \to^{\mathcal{T}} \alpha$, and we write $\mathcal{A}[\mathcal{T}]$ to denote the set of $\mathcal{T}$-producible assemblies. The relation $\to^{\mathcal{T}}$ is a partial order on $\mathcal{A}[\mathcal{T}]$ [22, 26].

An assembly α is *$\mathcal{T}$-terminal* if α is τ-stable and $\partial^{\mathcal{T}} \alpha = \varnothing$. We write $\mathcal{A}_{\Box}[\mathcal{T}] \subseteq \mathcal{A}[\mathcal{T}]$ to denote the set of $\mathcal{T}$-producible, $\mathcal{T}$-terminal assemblies.

A seeded TAS $\mathcal{T}$ is *directed (a.k.a., deterministic, confluent)* if the poset $(\mathcal{A}[\mathcal{T}], \to^{\mathcal{T}})$ is directed; i.e., if for each $\alpha, \beta \in \mathcal{A}[\mathcal{T}]$, there exists $\gamma \in \mathcal{A}[\mathcal{T}]$ such that $\alpha \to^{\mathcal{T}} \gamma$ and $\beta \to^{\mathcal{T}} \gamma$.[5] We say that $\mathcal{T}$ *uniquely produces* α if $\mathcal{A}_{\Box}[\mathcal{T}] = \{\alpha\}$.

A.3 Hierarchical aTAM

A *hierarchical tile assembly system* (hierarchical TAS) is a pair $\mathcal{T} = (T, \tau)$, where T is a finite set of tile types, and $\tau \in \mathbb{Z}^+$ is the *temperature*. Let $\alpha, \beta : \mathbb{Z}^2 \dashrightarrow T$ be two assemblies. Say that α and β are *nonoverlapping* if $\text{dom } \alpha \cap \text{dom } \beta = \varnothing$. If α and β are nonoverlapping assemblies, define $\alpha \cup \beta$ to be the assembly γ defined by $\gamma(p) = \alpha(p)$ for all $p \in \text{dom } \alpha$, $\gamma(p) = \beta(p)$ for all $p \in \text{dom } \beta$, and $\gamma(p)$ is undefined for all $p \in \mathbb{Z}^2 \setminus (\text{dom } \alpha \cup \text{dom } \beta)$. An assembly γ is *singular* if $\gamma(p) = t$ for some $p \in \mathbb{Z}^2$ and some $t \in T$ and $\gamma(p')$ is undefined for all $p' \in \mathbb{Z}^2 \setminus \{p\}$. Given a hierarchical TAS $\mathcal{T} = (T, \tau)$, an assembly γ is *$\mathcal{T}$-producible* if either 1) γ is singular, or 2) there exist producible nonoverlapping assemblies α and β such that $\gamma = \alpha \cup \beta$ and γ is τ-stable. In the latter case, write $\alpha + \beta \to_1^{\mathcal{T}} \gamma$. An assembly α is *$\mathcal{T}$-terminal* if for every producible assembly β such that α and β are nonoverlapping, $\alpha \cup \beta$ is not τ-stable.[6] Define $\mathcal{A}[\mathcal{T}]$ to be the set of all $\mathcal{T}$-producible assemblies. Define $\mathcal{A}_{\Box}[\mathcal{T}] \subseteq \mathcal{A}[\mathcal{T}]$ to be the set of all $\mathcal{T}$-producible, $\mathcal{T}$-terminal assemblies. A hierarchical TAS $\mathcal{T}$ is *directed (a.k.a., deterministic, confluent)* if $|\mathcal{A}_{\Box}[\mathcal{T}]| = 1$. We say that $\mathcal{T}$ *uniquely produces* α if $\mathcal{A}_{\Box}[\mathcal{T}] = \{\alpha\}$.

Let $\mathcal{T}$ be a hierarchical TAS, and let $\widehat{\alpha} \in \mathcal{A}[\mathcal{T}]$ be a $\mathcal{T}$-producible assembly. An *assembly tree* Υ of $\widehat{\alpha}$ is a full binary tree with $|\widehat{\alpha}|$ leaves, whose nodes are labeled by $\mathcal{T}$-producible assemblies, with $\widehat{\alpha}$ labeling the root, singular assemblies labeling the leaves, and node u labeled with γ having children u_1 labeled with α and u_2 labeled with β, with the requirement that $\alpha + \beta \to_1^{\mathcal{T}} \gamma$. That

[4]Intuitively $\alpha \to_1^{\mathcal{T}} \beta$ means that α can grow into β by the addition of a single tile; the fact that we require both α and β to be τ-stable implies in particular that the new tile is able to bind to α with strength at least τ. It is easy to check that had we instead required only α to be τ-stable, and required that the cut of β separating α from the new tile has strength at least τ, then this implies that β is also τ-stable.

[5]The following two convenient characterizations of "directed" are routine to verify. $\mathcal{T}$ is directed if and only if $|\mathcal{A}_{\Box}[\mathcal{T}]| = 1$. $\mathcal{T}$ is *not* directed if and only if there exist $\alpha, \beta \in \mathcal{A}[\mathcal{T}]$ and $p \in \text{dom } \alpha \cap \text{dom } \beta$ such that $\alpha(p) \neq \beta(p)$.

[6]The restriction on overlap is a model of a chemical phenomenon known as *steric hindrance* [31, Section 5.11] or, particularly when employed as a design tool for intentional prevention of unwanted binding in synthesized molecules, *steric protection* [18–20].

is, Υ represents one possible pathway through which $\widehat{\alpha}$ could be produced from individual tile types in $\mathcal{T}$. Let $\Upsilon(\mathcal{T})$ denote the set of all assembly trees of $\mathcal{T}$. If α is a descendant node of β in an assembly tree of $\mathcal{T}$, write $\alpha \to^{\mathcal{T}} \beta$. Say that an assembly tree is $\mathcal{T}$*-terminal* if its root is a $\mathcal{T}$-terminal assembly. Let $\Upsilon_{\Box}(\mathcal{T})$ denote the set of all $\mathcal{T}$-terminal assembly trees of $\mathcal{T}$. Note that even a directed hierarchical TAS can have multiple terminal assembly trees that all have the same root terminal assembly.

When $\mathcal{T}$ is clear from context, we may omit $\mathcal{T}$ from the notation above and instead write $\to_1$, $\to$, $\partial\alpha$, *assembly sequence*, *produces*, *producible*, and *terminal*.

A.4 Proofs omitted from main text

Lemma 3.1. Let S be a finite set with $|S| \geq 2$. Let Υ be any hierarchical division of S, and let $\mathcal{C}$ be any partition of S other than $\{S\}$. Then there exist $C_1, C_2 \in \mathcal{C}$ with $C_1 \neq C_2$, and there exist $C_1' \subseteq C_1$ and $C_2' \subseteq C_2$, such that C_1' and C_2' are siblings in Υ.

Proof. First, label each leaf $\{x\}$ of Υ with the unique element $C_i \in \mathcal{C}$ such that $x \in C_i$. Next, iteratively label internal nodes according to the following rule: while there exist two children of a node u that have the same label, assign that label to u. Notice that this rule preserves the invariant that each labeled node u (representing a subset of S) is a subset of the set its label represents. Continue until no node has two identically-labeled children. $\mathcal{C}$ contains only proper subsets of S, so the root (which is the set S) cannot be contained in any of them, implying the root will remain unlabeled. Follow any path starting at the root, always following an unlabeled child, until both children of the current internal node are labeled. (The path may vacuously end at the root.) Such a node is well-defined since at least all leaves are labeled. By the stopping condition stated previously, these children must be labeled differently. The children are the witnesses C_1' and C_2', with their labels having the values C_1 and C_2, testifying to the truth of the lemma. $\Box$