

# The Two-Handed Tile Assembly Model Is Not Intrinsically Universal\*

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**Abstract.** In this paper, we study the intrinsic universality of the well-studied Two-Handed Tile Assembly Model (2HAM), in which two “supertile” assemblies, each consisting of one or more unit-square tiles, can fuse together (self-assemble) whenever their total attachment strength is at least the global temperature  $\tau$ . Our main result is that for all  $\tau' < \tau$ , each temperature- $\tau'$  2HAM tile system cannot simulate at least one temperature- $\tau$  2HAM tile system. This impossibility result proves that the 2HAM is not intrinsically universal, in stark contrast to the simpler abstract Tile Assembly Model which was shown to be intrinsically universal (*The tile assembly model is intrinsically universal*, FOCS 2012). On the positive side, we prove that, for every fixed temperature  $\tau \geq 2$ , temperature- $\tau$  2HAM tile systems are intrinsically universal: for each  $\tau$  there is a single universal 2HAM tile set  $U$  that, when appropriately initialized, is capable of simulating the behavior of any temperature  $\tau$  2HAM tile system. As a corollary of these results we find an infinite set of infinite hierarchies of 2HAM systems with strictly increasing power within each hierarchy. Finally, we show how to construct, for

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\* A full version of this paper will appear on the arXiv.

\*\* This author’s research was supported in part by National Science Foundation Grant CCF-1117672.

\*\*\* This author’s research was supported by National Science Foundation grants 0832824 (The Molecular Programming Project), CCF-1219274, and CCF-1162589.

each  $\tau$ , a temperature- $\tau$  2HAM system that simultaneously simulates all temperature- $\tau$  2HAM systems.

## 1 Introduction

Self-assembly is the process through which unorganized, simple, components automatically coalesce according to simple local rules to form some kind of target structure. It sounds simple, but the end result can be extraordinary. For example, researchers have been able to self-assemble a wide variety of structures experimentally at the nanoscale, such as regular arrays [28], fractal structures [13,24], smiling faces [23], DNA tweezers [29], logic circuits [21], neural networks [22], and molecular robots [18]. These examples are fundamental because they demonstrate that self-assembly can, in principle, be used to manufacture specialized geometrical, mechanical and computational objects at the nanoscale. Potential future applications of nanoscale self-assembly include the production of smaller, more efficient microprocessors and medical technologies that are capable of diagnosing and even treating disease at the cellular level.

Controlling nanoscale self-assembly for the purposes of manufacturing atomically precise components will require a bottom-up, hands-off strategy. In other words, the self-assembling units themselves will have to be “programmed” to direct themselves to do the right thing—efficiently and correctly. Thus, it is necessary to study the extent to which the process of self-assembly can be controlled in an algorithmic sense.

In 1998, Erik Winfree [27] introduced the abstract Tile Assembly Model (aTAM), an over-simplified discrete mathematical model of algorithmic DNA nanoscale self-assembly pioneered by Seeman [25]. The aTAM essentially augments classical Wang tiling [26] with a mechanism for sequential “growth” of a tiling (in Wang tiling, only the existence of a valid, mismatch-free tiling is considered and not the order of tile placement). In the aTAM, the fundamental components are un-rotatable, but translatable square “tile types” whose sides are labeled with (alpha-numeric) glue “colors” and (integer) “strengths”. Two tiles that are placed next to each other *interact* if the glue colors on their abutting sides match, and they *bind* if the strengths on their abutting sides match and sum to at least a certain (integer) “temperature”. Self-assembly starts from a “seed” tile type and proceeds nondeterministically and asynchronously as tiles bind to the seed-containing-assembly. Despite its deliberate over-simplification, the aTAM is a computationally expressive model. For example, Winfree [27] proved that it is Turing universal, which implies that self-assembly can be directed by a computer program.

In this paper, we work in a generalization of the aTAM, called the *two-handed* [3] (a.k.a., hierarchical [5], q-tile [6], polyomino [17]) abstract Tile Assembly Model (2HAM). A central feature of the 2HAM is that, unlike the aTAM, it allows two “supertile” assemblies, each consisting of one or more tiles, to fuse together. For two such assemblies to bind, they should not “sterically hinder” each other, and they should have a sufficient number of matching glues distributed along the interface

where they meet. Hence the model includes notions of local interactions (individual glues) and non-local interactions (large assemblies coming together). In the 2HAM, an assembly of tiles is producible if it is either a single tile, or if it results from the stable combination of two other producible assemblies.

We study the *intrinsic universality* in the 2HAM. Intrinsic universality uses a special notion of simulation, where the simulator preserves the dynamics of the simulated system. In the field of cellular automata, the topic of intrinsic universality has given rise to a rich theory [2, 4, 7, 8, 12, 19, 20] and indeed has also been studied in Wang tiling [14–16] and tile self-assembly [10, 11]. The aTAM has been shown to be intrinsically universal [10], meaning that there is a single set of tiles  $U$  that works at temperature 2, and when appropriately initialized, is capable of simulating the behavior of an arbitrary aTAM tile assembly system. Modulo rescaling, this single tile set  $U$  represents the full power and expressivity of the entire aTAM model, at any temperature. Here, we ask whether there such a universal tile set for the 2HAM.

The theoretical power of non-local interaction in the 2HAM has been the subject of recent research. For example, Doty and Chen [5] proved that, surprisingly,  $N \times N$  squares do not self-assemble any faster in so-called *partial order* 2HAM systems than they do in the aTAM, despite being able to exploit massive parallelism. More recently, Cannon, et al. [3], while comparing the abilities of the 2HAM and the aTAM, proved three main results, which seem to suggest that the 2HAM is at least as powerful as the aTAM: (1) non-local binding in the 2HAM can dramatically reduce the tile complexity (i.e., minimum number of unique tile types required to self-assemble a shape) for certain classes of shapes; (2) the 2HAM can simulate the aTAM in the following sense: for any aTAM tile system  $\mathcal{T}$ , there is a corresponding 2HAM tile system  $\mathcal{S}$ , which simulates the exact behavior—modulo connectivity—of  $\mathcal{T}$ , at scale factor 5; (3) the problem of verifying whether a 2HAM system uniquely produces a given assembly is coNP-complete (for the aTAM this problem is decidable in polynomial time [1]).

**Main results.** In this paper, we ask if the 2HAM is *intrinsically universal*: does there exist a “universal” 2HAM tile set  $U$  that, when appropriately initialized, is capable of simulating the behavior of an arbitrary 2HAM tile system? A positive answer would imply that such a tile set  $U$  has the ability to model the capabilities of all 2HAM systems.<sup>1</sup> Our first main result, Theorem 1, says that the 2HAM is *not* intrinsically universal, which means that the 2HAM is incapable of simulating itself. This statement stands in stark contrast to the case of the aTAM, which was recently shown to be intrinsically universal by Doty, Lutz, Patitz, Schweller, Summers and Woods [10]. Specifically, we show that for any temperature  $\tau$ , there is a temperature  $\tau$  2HAM system that cannot be simulated by any temperature  $\tau' < \tau$  2HAM system. It is worthy of note that, in order to prove this result, we use a simple, yet novel combinatorial argument, which as

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<sup>1</sup> Note that the above simulation result of Cannon et al. does not imply that the 2HAM is intrinsically universal because (a) it is for 2HAM simulating aTAM, and (b) it is an example of a “for all, there exists...” statement, whereas intrinsic universality is a “there exists, for all...” statement.

far as we are aware of, is the first lower bound proof in the 2HAM that does not use an information-theoretic argument. In our proof of Theorem 1 we show that the 2HAM cannot simulate massively cooperative binding, where the number of cooperative bindings is larger than the temperature of the simulator).

Our second main result, Theorem 3, is positive: we show, via constructions, that the 2HAM *is* intrinsically universal for fixed temperature, that is, the temperature  $\tau$  2HAM can simulate the temperature  $\tau$  2HAM. So although our impossibility result tells us that the 2HAM can not simulate “too much” cooperative binding, our positive result tells us it can indeed simulate *some* cooperative binding: an amount exactly equal to the temperature of the simulator.

As an immediate corollary of these results, we get a separation between classes of 2HAM tile systems based on their temperatures. That is, we exhibit an infinite hierarchy of 2HAM systems, of strictly-increasing temperature, that cannot be simulated by lesser temperature systems but can downward simulate lower temperature systems. Indeed, we exhibit an infinite number of such hierarchies in Theorem 4. Thus, as was suggested as future work in [10], and as has been shown in the theory of cellular automata [8], we use the notion of intrinsic universality to classify, and separate, 2HAM systems via their simulation ability.

As noted above, we show that temperature  $\tau$  2HAM systems are intrinsically universal. We actually show this for two different, seemingly natural, notions of simulation (called *simulation* and *strong simulation*), showing trade-offs between, and even within, these notions of simulation. For both notions of simulation, we show tradeoffs between scale factor, number of tile types, and complexity of the initial configuration. Finally, we show how to construct, for each  $\tau$ , a temperature- $\tau$  2HAM system that simultaneously simulates all temperature- $\tau$  2HAM systems. We finish with a conjecture:

*Conjecture 1.* There exists  $c \in \mathbb{N}$ , such that for each  $\tau \geq c$ , temperature  $\tau$  2HAM systems do not strongly simulate Temperature  $\tau - 1$  2HAM systems.

## 2 Definitions

### 2.1 Informal Definition of 2HAM

The 2HAM [6, 9] is a generalization of the aTAM in that it allows for two assemblies, both possibly consisting of more than one tile, to attach to each other. Since we must allow that the assemblies might require translation before they can bind, we define a *supertile* to be the set of all translations of a  $\tau$ -stable assembly, and speak of the attachment of supertiles to each other, modeling that the assemblies attach, if possible, after appropriate translation. We now give a brief, informal, sketch of the 2HAM.

A *tile type* is a unit square with four sides, each having a *glue* consisting of a *label* (a finite string) and *strength* (a non-negative integer). 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*. A *supertile* is (the set of all translations of) a positioning of tiles on the integer lattice  $\mathbb{Z}^2$ . Two adjacent tiles in a supertile

*interact* if the glues on their abutting sides are equal and have positive strength. Each supertile induces a *binding graph*, a grid graph whose vertices are tiles, with an edge between two tiles if they interact. The supertile is  $\tau$ -*stable* if every cut of its binding graph has strength at least  $\tau$ , where the weight of an edge is the strength of the glue it represents. That is, the supertile is stable if at least energy  $\tau$  is required to separate the supertile into two parts. A 2HAM *tile assembly system* (TAS) is a pair  $\mathcal{T} = (T, \tau)$ , where  $T$  is a finite tile set and  $\tau$  is the *temperature*, usually 1 or 2. Given a TAS  $\mathcal{T} = (T, \tau)$ , a supertile is *producible*, written as  $\alpha \in \mathcal{A}[\mathcal{T}]$  if either it is a single tile from  $T$ , or it is the  $\tau$ -stable result of translating two producible assemblies without overlap. A supertile  $\alpha$  is *terminal*, written as  $\alpha \in \mathcal{A}_{\square}[\mathcal{T}]$  if for every producible supertile  $\beta$ ,  $\alpha$  and  $\beta$  cannot be  $\tau$ -stably attached. A TAS is *directed* if it has only one terminal, producible supertile.<sup>2</sup>

### 2.2 Definitions for Simulation

In this subsection, we formally define what it means for one 2HAM TAS to “simulate” another 2HAM TAS. For a tileset  $T$ , let  $A^T$  and  $\tilde{A}^T$  denote the set of all assemblies over  $T$  and all supertiles over  $T$  respectively. Let  $A^T_{<\infty}$  and  $\tilde{A}^T_{<\infty}$  denote the set of all finite assemblies over  $T$  and all finite supertiles over  $T$  respectively.

In what follows, let  $U$  be a tile set. An  $m$ -*block assembly*, or *macrotile*, over tile set  $U$  is a partial function  $\gamma : \mathbb{Z}_m \times \mathbb{Z}_m \dashrightarrow U$ , where  $\mathbb{Z}_m = \{0, 1, \dots, m - 1\}$ . Let  $B^U_m$  be the set of all  $m$ -block assemblies over  $U$ . The  $m$ -block with no domain is said to be *empty*. For an arbitrary assembly  $\alpha \in A^U$  define  $\alpha^m_{x,y}$  to be the  $m$ -block defined by  $\alpha^m_{x,y}(i, j) = \alpha(mx + i, my + j)$  for  $0 \leq i, j < m$ .

For a partial function  $R : B^U_m \dashrightarrow T$ , define the *assembly representation function*  $R^* : A^U \dashrightarrow A^T$  such that  $R^*(\alpha) = \beta$  if and only if  $\beta(x, y) = R(\alpha^m_{x,y})$  for all  $x, y \in \mathbb{Z}^2$ . Further,  $\alpha$  is said to map *cleanly* to  $\beta$  under  $R^*$  if either (1) for all non empty blocks  $\alpha^m_{x,y}$ ,  $(x + u, y + v) \in \text{dom } \beta$  for some  $u, v \in \{-1, 0, 1\}$  such that  $u^2 + v^2 < 2$ , or (2)  $\alpha$  has at most one non-empty  $m$ -block  $\alpha^m_{x,y}$ . In other words, we allow for the existence of simulator “fuzz” directly north, south, east or west of a simulator macrotile, but we exclude the possibility of diagonal fuzz.

For a given *assembly representation function*  $R^*$ , define the *supertile representation function*  $\tilde{R} : \tilde{A}^U \dashrightarrow \mathcal{P}(A^T)$  such that  $\tilde{R}(\tilde{\alpha}) = \{R^*(\alpha) \mid \alpha \in \tilde{\alpha}\}$ .  $\tilde{\alpha}$  is said to *map cleanly* to  $\tilde{R}(\tilde{\alpha})$  if  $\tilde{R}(\tilde{\alpha}) \in \tilde{A}^T$  and  $\alpha$  maps cleanly to  $R^*(\alpha)$  for all  $\alpha \in \tilde{\alpha}$ .

In the following definitions, let  $\mathcal{T} = (T, S, \tau)$  be a 2HAM TAS and, for some initial configuration  $S_{\mathcal{T}}$ , that depends on  $\mathcal{T}$ , let  $\mathcal{U} = (U, S_{\mathcal{T}}, \tau')$  be a 2HAM TAS, and let  $R$  be an  $m$ -block representation function  $R : B^U_m \dashrightarrow T$ .

**Definition 1.** *We say that  $\mathcal{U}$  and  $\mathcal{T}$  have equivalent productions (at scale factor  $m$ ), and we write  $\mathcal{U} \Leftrightarrow_R \mathcal{T}$  if the following conditions hold:*

1.  $\{\tilde{R}(\tilde{\alpha}) \mid \tilde{\alpha} \in \mathcal{A}[\mathcal{U}]\} = \mathcal{A}[\mathcal{T}]$ .

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<sup>2</sup> We do not use this definition in this paper but have included it for the sake of completeness.

2. For all  $\tilde{\alpha} \in \mathcal{A}[\mathcal{U}]$ ,  $\tilde{\alpha}$  maps cleanly to  $\tilde{R}(\tilde{\alpha})$

**Definition 2.** We say that  $\mathcal{T}$  follows  $\mathcal{U}$  (at scale factor  $m$ ), and we write  $\mathcal{T} \dashv_R \mathcal{U}$  if, for any  $\tilde{\alpha}, \tilde{\beta} \in \mathcal{A}[\mathcal{U}]$  such that  $\tilde{\alpha} \rightarrow_{\mathcal{U}}^1 \tilde{\beta}$ ,  $\tilde{R}(\tilde{\alpha}) \rightarrow_{\tilde{\mathcal{T}}}^{\leq 1} \tilde{R}(\tilde{\beta})$ .

**Definition 3.** We say that  $\mathcal{U}$  weakly models  $\mathcal{T}$  (at scale factor  $m$ ), and we write  $\mathcal{U} \models_{\tilde{R}}^- \mathcal{T}$  if, for any  $\tilde{\alpha}, \tilde{\beta} \in \mathcal{A}[\mathcal{T}]$  such that  $\tilde{\alpha} \rightarrow_{\mathcal{T}}^1 \tilde{\beta}$ , for all  $\tilde{\alpha}' \in \mathcal{A}[\mathcal{U}]$  such that  $\tilde{R}(\tilde{\alpha}') = \tilde{\alpha}$ , there exists an  $\tilde{\alpha}'' \in \mathcal{A}[\mathcal{U}]$  such that  $\tilde{R}(\tilde{\alpha}'') = \tilde{\beta}$ ,  $\tilde{\alpha}' \rightarrow_{\mathcal{U}} \tilde{\alpha}''$ , and  $\tilde{\alpha}'' \rightarrow_{\mathcal{U}}^1 \tilde{\beta}'$  for some  $\tilde{\beta}' \in \mathcal{A}[\mathcal{U}]$  with  $\tilde{R}(\tilde{\beta}') = \tilde{\beta}$ .

**Definition 4.** We say that  $\mathcal{U}$  strongly models  $\mathcal{T}$  (at scale factor  $m$ ), and we write  $\mathcal{U} \models_{\tilde{R}}^+ \mathcal{T}$  if for any  $\tilde{\alpha}, \tilde{\beta} \in \mathcal{A}[\mathcal{T}]$  such that  $\tilde{\gamma} \in C_{\tilde{\alpha}, \tilde{\beta}}^{\tau}$ , then for all  $\tilde{\alpha}', \tilde{\beta}' \in \mathcal{A}[\mathcal{U}]$  such that  $\tilde{R}(\tilde{\alpha}') = \tilde{\alpha}$  and  $\tilde{R}(\tilde{\beta}') = \tilde{\beta}$ , it must be that there exist  $\tilde{\alpha}'', \tilde{\beta}'', \tilde{\gamma}' \in \mathcal{A}[\mathcal{U}]$ , such that  $\tilde{\alpha}' \rightarrow_{\mathcal{U}} \tilde{\alpha}'', \tilde{\beta}' \rightarrow_{\mathcal{U}} \tilde{\beta}'', \tilde{R}(\tilde{\alpha}'') = \tilde{\alpha}, \tilde{R}(\tilde{\beta}'') = \tilde{\beta}, \tilde{R}(\tilde{\gamma}') = \tilde{\gamma}$ , and  $\tilde{\gamma}' \in C_{\tilde{\alpha}'', \tilde{\beta}''}^{\tau'}$ .

**Definition 5.** Let  $\mathcal{U} \Leftrightarrow_R \mathcal{T}$  and  $\mathcal{T} \dashv_R \mathcal{U}$ .

1.  $\mathcal{U}$  simulates  $\mathcal{T}$  (at scale factor  $m$ ) if  $\mathcal{U} \models_{\tilde{R}}^- \mathcal{T}$ .
2.  $\mathcal{U}$  strongly simulates  $\mathcal{T}$  (at scale factor  $m$ ) if  $\mathcal{U} \models_{\tilde{R}}^+ \mathcal{T}$ .

For simulation, we require that when a simulated supertile  $\tilde{\alpha}$  may grow, via one combination attachment, into a second supertile  $\tilde{\beta}$ , then any simulator supertile that maps to  $\tilde{\alpha}$  must also grow into a simulator supertile that maps to  $\tilde{\beta}$ . The converse should also be true.

For strong simulation, in addition to requiring that all supertiles mapping to  $\tilde{\alpha}$  must be capable of growing into a supertile mapping to  $\tilde{\beta}$  when  $\tilde{\alpha}$  can grow into  $\tilde{\beta}$  in the simulated system, we further require that this growth can take place by the attachment of *any* supertile mapping to  $\tilde{\gamma}$ , where  $\tilde{\gamma}$  is the supertile that attaches to  $\tilde{\alpha}$  to get  $\tilde{\beta}$ .

### 2.3 Intrinsic Universality

Let REPR denote the set of all  $m$ -block (or macrotile) representation functions. Let  $\mathfrak{C}$  be a class of tile assembly systems, and let  $U$  be a tile set. We say  $U$  is *intrinsically universal* for  $\mathfrak{C}$  if there are computable functions  $\mathcal{R} : \mathfrak{C} \rightarrow \text{REPR}$  and  $\mathcal{S} : \mathfrak{C} \rightarrow (A_{<\infty}^U \rightarrow \mathbb{N} \cup \{\infty\})$ , and a  $\tau' \in \mathbb{Z}^+$  such that, for each  $\mathcal{T} = (T, S, \tau) \in \mathfrak{C}$ , there is a constant  $m \in \mathbb{N}$  such that, letting  $R = \mathcal{R}(\mathcal{T})$ ,  $S_{\mathcal{T}} = \mathcal{S}(\mathcal{T})$ , and  $\mathcal{U}_{\mathcal{T}} = (U, S_{\mathcal{T}}, \tau')$ ,  $\mathcal{U}_{\mathcal{T}}$  simulates  $\mathcal{T}$  at scale  $m$  and using macrotile representation function  $R$ . That is,  $\mathcal{R}(\mathcal{T})$  gives a representation function  $R$  that interprets macrotiles (or  $m$ -blocks) of  $\mathcal{U}_{\mathcal{T}}$  as assemblies of  $\mathcal{T}$ , and  $\mathcal{S}(\mathcal{T})$  gives the initial state used to create the necessary macrotiles from  $U$  to represent  $\mathcal{T}$  subject to the constraint that no macrotile in  $S_{\mathcal{T}}$  can be larger than a single  $m \times m$  square.

### 3 The 2HAM Is Not Intrinsically Universal

In this section, we prove the main result of this paper: there is no universal 2HAM tile set that, when appropriately initialized, is capable of simulating an arbitrary 2HAM system. That is, we prove that the 2HAM, unlike the aTAM, is not intrinsically universal.

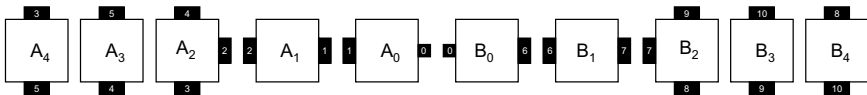
**Theorem 1.** *The 2HAM is not intrinsically universal.*

In order to prove Theorem 1, we prove Theorem 2, which says that, for any claimed 2HAM simulator  $\mathcal{U}$ , that runs at temperature  $\tau'$ , there exists a 2HAM system, with temperature  $\tau > \tau'$ , that cannot be simulated by  $\mathcal{U}$ .

**Theorem 2.** *Let  $\tau \in \mathbb{N}, \tau \geq 2$ . For every tile set  $U$ , there exists a 2HAM TAS  $\mathcal{T} = (T, S, \tau)$  such that for any initial configuration  $S_{\mathcal{T}}$  and  $\tau' \leq \tau - 1$ , the 2HAM TAS  $\mathcal{U} = (U, S_{\mathcal{T}}, \tau')$  does not simulate  $\mathcal{T}$ .*

**The basic idea** of the proof of Theorem 2 is to use Definitions 3 and 1 in order to exhibit two producible supertiles in  $\mathcal{T}$ , that do not combine in  $\mathcal{T}$  because of a lack of total binding strength, and show that the supertiles that simulate them in  $\mathcal{U}$  do combine in the (lower temperature) simulator  $\mathcal{U}$ . Then we argue that Definition 2 says that, because the simulating supertiles can combine in the simulator  $\mathcal{U}$ , then so too can the supertiles being simulated in the simulated system  $\mathcal{T}$ , which contradicts the fact that the two originally chosen supertiles from  $\mathcal{T}$  do not combine in  $\mathcal{T}$ .

*Proof.* Our proof is by contradiction. Therefore, suppose, for the sake of obtaining a contradiction, that there exists a universal tile set  $U$  such that, for any 2HAM TAS  $\mathcal{T} = (T, S, \tau)$ , there exists an initial configuration  $S_{\mathcal{T}}$  and  $\tau' \leq \tau - 1$ , such that  $\mathcal{U} = (U, S_{\mathcal{T}}, \tau')$  simulates  $\mathcal{T}$ . Define  $\tilde{\mathcal{T}} = (T, \tau)$  where  $T$  is the tile set defined in Figure 1, the default initial state is used, and  $\tau > 1$ . Let  $\tilde{\mathcal{U}} = (U, S_{\tilde{\mathcal{T}}}, \tau')$  be the temperature  $\tau' \leq \tau - 1$  2HAM system, which uses tile set  $U$  and initial configuration  $S_{\tilde{\mathcal{T}}}$  (depending on  $\tilde{\mathcal{T}}$ ) to simulate  $\tilde{\mathcal{T}}$  at scale factor  $m$ . Let  $\tilde{R}$  denote the assembly replacement function that testifies to the fact that  $\tilde{\mathcal{U}}$  simulates  $\tilde{\mathcal{T}}$ .



**Fig. 1.** The tile set for the proof of Theorem 2. Black rectangles represent strength- $\tau$  glues (labeled 1-8), and black squares represent the strength-1 glue (labeled 0).

We say that a supertile  $\tilde{l} \in \mathcal{A}[\mathcal{T}]$  is a *left half-ladder* of height  $h \in \mathbb{N}$  if it contains  $h$  tiles of the type A2 and  $h - 1$  tiles of type A3, arranged in a vertical column, plus  $\tau$  tiles of each of the types A1 and A0. (An example of a left half-ladder is shown on the left in Figure 2. The dotted lines show positions at which

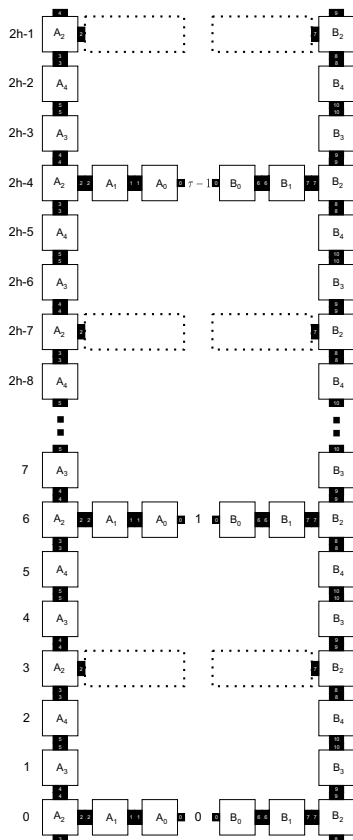


Fig. 2. Example half-ladders with  $\tau$  rungs

tiles of type A1 and A0 could potentially attach, but since a half-ladder has exactly  $\tau$  of each, only  $\tau$  such locations have tiles.) Essentially, a left half-ladder consists of a single-tile-wide vertical column of height  $2h - 1$  with an A2 tile at the bottom and top, and those in between alternating between A3 and A2 tiles. To the east of exactly  $\tau$  of the A2 tiles, an A1 tile is attached and to the east of each A1 tile, an A0 tile type is attached. These A1-A0 pairs, collectively, form the  $\tau$  rungs of the left half-ladder. We can define right half-ladders similarly. A right half-ladder of height  $h$  is defined exactly the same way but using the tile types B3, B2, B1, and B0 and with rungs growing to the left of the vertical column. The east glue of A0 is a strength-1 glue matching the west glue of B0.

Let  $LEFT \subseteq \mathcal{A}[T]$  and  $RIGHT \subseteq \mathcal{A}[T]$  be the set of all left and right half-ladders of height  $h$ , respectively. Note that there are  $\binom{h}{\tau}$  half-ladders of height  $h$  in  $LEFT$  ( $RIGHT$ ). Define, for each  $\tilde{l} \in LEFT$ , the mirror image of  $\tilde{l}$  as the supertile  $\bar{\tilde{l}} \in RIGHT$  such that  $\bar{\tilde{l}}$  has rungs at the same positions as  $\tilde{l}$ .

For some  $\tilde{l} \in LEFT$ , we say that  $\tilde{\tilde{l}} \in \mathcal{A}[U]$  is a simulator left half-ladder of height  $h$  if  $\tilde{R}(\tilde{\tilde{l}}) = \tilde{l}$ . Note that  $\tilde{\tilde{l}}$  need not be unique. (One could even imagine



$\tilde{l}$  and  $\tilde{l}'$  satisfying  $\tilde{R}(\tilde{l}) = \tilde{l}$  and  $\tilde{R}(\tilde{l}') = \tilde{l}$  but  $\tilde{l}$  and  $\tilde{l}'$  only differ by a single tile!) The notation  $C_{\tilde{\alpha}, \tilde{\beta}}^\tau$  is defined as the set of all supertiles that result in the  $\tau$ -stable combination of the supertiles  $\tilde{\alpha}$  and  $\tilde{\beta}$ .

For some  $\tilde{r} \in \mathcal{A}[\mathcal{U}]$ , we say that  $\tilde{r}$  is a *mate* of  $\tilde{l}$  if  $\tilde{R}(\tilde{r}) = \tilde{r} \in \text{RIGHT}$ , where  $\tilde{r} = \tilde{l}$ ,  $C_{\tilde{l}, \tilde{r}}^\tau \neq \emptyset$  (they combine in  $\mathcal{T}$ ), and  $C_{\tilde{l}, \tilde{r}}^{\tau-1} \neq \emptyset$  (they combine in  $\mathcal{U}$ ). For a simulator left half-ladder  $\tilde{l}$ , we say that  $\tilde{l}$  is *combinable* if  $\tilde{l}$  has a mate. Part 1 of Definition 5 guarantees the existence of at least one combinable simulator left half-ladder for each left half-ladder. It is easy to see from Part 1 of Definition 5 that an arbitrary simulator left half-ladder need not be combinable, since by Definition 3, it may be a half-ladder  $\hat{l} \in \mathcal{A}[\mathcal{U}]$ , which must first “grow into” a combinable left half-ladder  $\tilde{l}'$  (analogous to  $\tilde{\alpha}' \rightarrow_{\mathcal{U}} \tilde{\alpha}''$  in Definition 3).

Denote as  $LEFT'$  some set that contains exactly one combinable simulator left half-ladder for each  $\tilde{l} \in LEFT$ . Note that, by Definitions 1 and 3, there must be at least one combinable simulator left half-ladder  $\tilde{l}$  for each  $\tilde{l}$ , but that there also may be more than one, so the set  $LEFT'$ , while certainly not empty, need not be unique. By the definition of  $LEFT'$ , it is easy to see that  $|LEFT'| = \binom{h}{\tau}$ . We know that each combinable simulator left half-ladder  $\tilde{l}$  has exactly  $\tau$  rungs, and furthermore, since glue strengths in the 2HAM cannot be fractional, it is the case that  $\tau'$  of these rungs bind to (the corresponding rungs of) a mate with a combined total strength of at least  $\tau'$ . (Note that some, but not all, of these  $\tau'$  rungs may be redundant in the sense that they do not interact with positive strength.)

There are  $\binom{h}{\tau'}$  ways to position/choose  $\tau'$  rungs on a (simulator) half-ladder of height  $h$ . (Note that a rung on a simulator half-ladder need not be a  $m \times m$  block of tiles but merely a collection of rung-like blocks that map to rungs in the input system  $\mathcal{T}$  via  $\tilde{R}$ .) Now consider the size  $\binom{h}{\tau'}$  set of all possible rung positions, each denoted by a subset  $X \subset \{0, 1, \dots, h - 1\}$ , and the size  $\binom{h}{\tau}$  set  $LEFT'$ . For each simulated half-ladder  $\tilde{l} \in LEFT'$ , there must exist a set of  $\tau'$  rungs  $X$  such that  $\tilde{l}$  binds to a mate via the rungs specified by  $X$ , with total strength at least  $\tau'$ . As there are  $\binom{h}{\tau}$  elements of  $LEFT'$  and only  $\binom{h}{\tau'}$  choices for  $X$ , the Generalized Pigeonhole Principle implies that there must be some set  $LEFT'' \subset LEFT'$  with  $|LEFT''| \geq \frac{\binom{h}{\tau}}{\binom{h}{\tau'}}$  such that every simulator left half-ladder in  $LEFT''$  binds to a mate via the  $\tau'$  rungs specified by a single choice of  $X$ , with total strength at least  $\tau'$ . In the case that  $h \geq 2\tau$ , we have that  $|LEFT''| \geq \frac{\binom{h}{\tau}}{\binom{h}{\tau'}} \geq \frac{\binom{h}{\tau}}{\binom{h}{\tau-1}} = \frac{h-\tau+1}{\tau}$ .

Let  $k = |U|^{4m^2}$ , which is the number of ways to tile a neighborhood of four  $m \times m$  squares from a set of  $|U|$  distinct tile types. If  $h = \tau(k^{\tau-1} + \tau)$ , then  $|LEFT''| \geq k^{\tau-1} + 1$ . There are  $k^{\tau'} \leq k^{\tau-1}$  ways to tile  $\tau'$  neighborhoods that map to tiles of type A0 (plus any additional simulator fuzz that connects to simulated A0 tiles), under  $\tilde{R}$ , at the ends of the  $\tau'$  rungs of a simulator left half-ladder. This tells us that there are at least two (combinable) simulator left

half-ladders  $\tilde{l}_1, \tilde{l}_2 \in LEFT''$  such that  $\tilde{l}_1$  binds to a mate via the rungs specified by  $X$ , with total strength at least  $\tau'$ ,  $\tilde{l}_2$  binds to a mate via the rungs specified by  $X$ , with total strength at least  $\tau'$  and the rungs (along with any surrounding fuzz) specified by  $X$  of  $\tilde{l}_1$  are tiled exactly the same as the rungs specified by  $X$  of  $\tilde{l}_2$  are tiled. Thus, we can conclude that  $\tilde{r}$ , a mate of  $\tilde{l}_1$ , is a mate of  $\tilde{l}_2$ . We can conclude this because, while  $\tilde{l}_1$  and  $\tilde{l}_2$  agree exactly along  $\tau'$  of their rungs, they also each have one rung in a unique position and since consecutive rungs in  $\mathcal{T}$  have at least two empty spaces between them, the offset simulator rungs (and even their fuzz) cannot prevent  $\tilde{l}_2$  from matching up with the mate of  $\tilde{l}_1$ .

However,  $\tilde{R}(\tilde{r}) = \tilde{r} \in R$ ,  $\tilde{R}(\tilde{l}_2) = \tilde{l}_2 \in L$  but  $C_{\tilde{r}, \tilde{l}_2}^\tau = \emptyset$  because  $\tilde{r}$  and  $\tilde{l}_2$  differ from each other in one rung location and therefore interact in  $\mathcal{T}$  with total strength at most  $\tau - 1$ . This is a contradiction to Definition 2, which implies  $C_{\tilde{r}, \tilde{l}_2}^\tau \neq \emptyset$ . □

**Corollary 1.** *There is no universal tile set  $U$  for the 2HAM, i.e., there is no  $U$  such that, for all 2HAM tile assembly systems  $\mathcal{T} = (T, S, \tau)$ , there exists an initial configuration  $S_{\mathcal{T}}$  and temperature  $\tau'$  such that  $\mathcal{U} = (U, S_{\mathcal{T}}, \tau')$  simulates  $\mathcal{T}$ .*

*Proof.* Our proof is by contradiction, so assume that  $U$  is a universal tile set. Denote as  $g$  the strength of the strongest glue on any tile type in  $U$ . Let  $\mathcal{T}' = (T', 4g + 1)$  be a modified version of the TAS  $\mathcal{T} = (T, \tau)$  from the proof of Theorem 2 with each  $\tau$ -strength glue in  $T$  converted to a strength  $4g + 1$  glue in  $T'$  (all other glues and labels are unmodified). For any initial configuration  $S_{\mathcal{T}}$ , we know that  $\mathcal{U} = (U, S_{\mathcal{T}}, \tau')$  does not simulate  $\mathcal{T}$  for any  $\tau' < 4g + 1$ . If  $\tau' \geq 4g + 1$ , then the size of the largest supertile in  $\mathcal{A}[\mathcal{U}]$  is 1, whence  $U$  is not a universal tile set. □

## 4 The Temperature- $\tau$ 2HAM Is Intrinsically Universal

In this section we state our second main result, which states that for fixed temperature  $\tau \geq 2$  the class of 2HAM systems at temperature  $\tau$  is intrinsically universal. In other words, for such  $\tau$  there is a tile set that, when appropriately initialized, simulates any temperature  $\tau$  2HAM system. Denote as 2HAM( $k$ ) the set of all 2HAM systems at temperature  $k$ .

**Theorem 3.** *For all  $\tau \geq 2$ , 2HAM( $\tau$ ) is intrinsically universal.*

In the full version of this paper we prove this theorem for two different, but seemingly natural notions of simulation. The first, simply called *simulation*, is where we require that when a simulated supertile  $\tilde{\alpha}$  may grow, via one attachment, into a second supertile  $\tilde{\beta}$ , then any simulator supertile that maps to  $\tilde{\alpha}$  must also grow into a simulator supertile that maps to  $\tilde{\beta}$ . The converse should also be true. The second notion, called *strong simulation*, is a stricter definition where in addition to requiring that all supertiles mapping to  $\tilde{\alpha}$  must be capable of growing into a supertile mapping to  $\tilde{\beta}$  when  $\tilde{\alpha}$  can grow into  $\tilde{\beta}$  in the simulated

system, we further require that this growth can take place by the attachment of *any* supertile mapping to  $\tilde{\gamma}$ , where  $\tilde{\gamma}$  is the supertile that attaches to  $\tilde{\alpha}$  to get  $\tilde{\beta}$ . Theorem 3 is proven for both notions of simulation. For each notion we provide three results, and in all cases we provide lower scale factor for simulation relative to strong simulation.

When we combine our negative and positive results, we get a separation between classes of 2HAM tile systems based on their temperatures.

**Theorem 4.** *There exists an infinite number of infinite hierarchies of 2HAM systems with strictly-increasing power (and temperature) that can simulate downward within their own hierarchy.*

*Proof.* Our first main result (Theorem 2) tells us that the temperature  $\tau$  2HAM cannot be simulated by any temperature  $\tau' < \tau$  2HAM. Hence we have, for all  $i > 0, c \geq 4$ ,  $2\text{HAM}(c^i) \succ 2\text{HAM}(c^{i-1})$ , where  $\succ$  is the relation “cannot be simulated by”. Moreover, Theorem 3 tells us that temperature  $\tau$  2HAM is intrinsically universal for fixed temperature  $\tau$ . Suppose that  $\tau' < \tau$  such that  $\tau/\tau' \in \mathbb{N}$ . Then temperature  $\tau$  2HAM can simulate temperature  $\tau'$  (by simulating strength  $g \leq \tau'$  attachments in the temperature  $\tau'$  system with strength  $g(\tau/\tau')$  attachments in the temperature  $\tau$  system). Thus, for all  $0 < i' \leq i$ ,  $2\text{HAM}(c^i)$  can simulate, via Theorem 3,  $2\text{HAM}(c^{i'})$ . The theorem follows by noting that our choice of  $c$  was arbitrary.  $\square$

We have shown that for each  $\tau \geq 2$  there exists a single set of tile types  $U_\tau$ , and a set of input supertiles over  $U_\tau$ , such that the 2HAM system strongly simulates any 2HAM TAS  $\mathcal{T}$ . A related question is: does there exist a tile set that can simulate, or strongly simulate, all temperature  $\tau$  2HAM TASs simultaneously? Surprisingly, the answer is yes!

**Theorem 5.** *For each  $\tau > 1$ , there exists a 2HAM system  $\mathcal{S} = (U_\tau, \tau)$  which simultaneously strongly simulates all 2HAM systems  $\mathcal{T} = (T, \tau)$ .*

## References

1. Adleman, L.M., Cheng, Q., Goel, A., Huang, M.-D.A., Kempe, D., de Espanés, P.M., Rothmund, P.W.K.: Combinatorial optimization problems in self-assembly. In: Proceedings of the Thirty-Fourth Annual ACM Symposium on Theory of Computing, pp. 23–32 (2002)
2. Arrighi, P., Schabanel, N., Theyssier, G.: Intrinsic simulations between stochastic cellular automata. arXiv preprint arXiv:1208.2763 (2012)
3. Cannon, S., Demaine, E.D., Demaine, M.L., Eisenstat, S., Patitz, M.J., Schweller, R., Summers, S.M., Winslow, A.: Two hands are better than one (up to constant factors). In: Proceedings of the Thirtieth International Symposium on Theoretical Aspects of Computer Science (to appear, 2013)
4. Chacc, E.G., Meunier, P.-E., Rapaport, I., Theyssier, G.: Communication complexity and intrinsic universality in cellular automata. *Theor. Comput. Sci.* 412(1-2), 2–21 (2011)

5. Chen, H.-L., Doty, D.: Parallelism and time in hierarchical self-assembly. In: SODA 2012: Proceedings of the 23rd Annual ACM-SIAM Symposium on Discrete Algorithms, pp. 1163–1182. SIAM (2012)
6. Cheng, Q., Aggarwal, G., Goldwasser, M.H., Kao, M.-Y., Schweller, R.T., de Españés, P.M.: Complexities for generalized models of self-assembly. *SIAM Journal on Computing* 34, 1493–1515 (2005)
7. Delorme, M., Mazoyer, J., Ollinger, N., Theyssier, G.: Bulking I: an abstract theory of bulking. *Theoretical Computer Science* 412(30), 3866–3880 (2011)
8. Delorme, M., Mazoyer, J., Ollinger, N., Theyssier, G.: Bulking II: Classifications of cellular automata. *Theor. Comput. Sci.* 412(30), 3881–3905 (2011)
9. Demaine, E.D., Demaine, M.L., Fekete, S.P., Ishaque, M., Rafalin, E., Schweller, R.T., Souvaine, D.L.: Staged self-assembly: nanomanufacture of arbitrary shapes with  $O(1)$  glues. *Natural Computing* 7(3), 347–370 (2008)
10. Doty, D., Lutz, J.H., Patitz, M.J., Schweller, R.T., Summers, S.M., Woods, D.: The tile assembly model is intrinsically universal. In: Proceedings of the 53rd Annual IEEE Symposium on Foundations of Computer Science, pp. 439–446 (October 2012)
11. Doty, D., Lutz, J.H., Patitz, M.J., Summers, S.M., Woods, D.: Intrinsic universality in self-assembly. In: Proceedings of the 27th International Symposium on Theoretical Aspects of Computer Science, pp. 275–286 (2009)
12. Durand, B., Róka, Z.: The game of life: universality revisited. In: Delorme, M., Mazoyer, J. (eds.) *Cellular Automata*. Kluwer (1999)
13. Fujibayashi, K., Hariadi, R., Park, S.H., Winfree, E., Murata, S.: Toward reliable algorithmic self-assembly of DNA tiles: A fixed-width cellular automaton pattern. *Nano Letters* 8(7), 1791–1797 (2007)
14. Lafitte, G., Weiss, M.: Universal tilings. In: Thomas, W., Weil, P. (eds.) *STACS 2007*. LNCS, vol. 4393, pp. 367–380. Springer, Heidelberg (2007)
15. Lafitte, G., Weiss, M.: Simulations between tilings. In: Conference on Computability in Europe (CiE 2008), Local Proceedings, pp. 264–273 (2008)
16. Lafitte, G., Weiss, M.: An almost totally universal tile set. In: Chen, J., Cooper, S.B. (eds.) *TAMC 2009*. LNCS, vol. 5532, pp. 271–280. Springer, Heidelberg (2009)
17. Luhrs, C.: Polyomino-safe DNA self-assembly via block replacement. In: Goel, A., Simmel, F.C., Sosik, P. (eds.) *DNA 14*. LNCS, vol. 5347, pp. 112–126. Springer, Heidelberg (2009)
18. Lund, K., Manzo, A.T., Dabby, N., Micholotti, N., Johnson-Buck, A., Nangreave, J., Taylor, S., Pei, R., Stojanovic, M.N., Walter, N.G., Winfree, E., Yan, H.: Molecular robots guided by prescriptive landscapes. *Nature* 465, 206–210 (2010)
19. Ollinger, N.: Intrinsically universal cellular automata. In: The Complexity of Simple Programs, in *Electronic Proceedings in Theoretical Computer Science*, vol. 1, pp. 199–204 (2008)
20. Ollinger, N., Richard, G.: Four states are enough? *Theoretical Computer Science* 412(1), 22–32 (2011)
21. Qian, L., Winfree, E.: Scaling up digital circuit computation with DNA strand displacement cascades. *Science* 332(6034), 1196 (2011)
22. Qian, L., Winfree, E., Bruck, J.: Neural network computation with DNA strand displacement cascades. *Nature* 475(7356), 368–372 (2011)
23. Rothmund, P.: Folding DNA to create nanoscale shapes and patterns. *Nature* 440(7082), 297–302 (2006)
24. Rothmund, P.W., Papadakis, N., Winfree, E.: Algorithmic self-assembly of DNA Sierpinski triangles. *PLoS Biology* 2(12), 2041–2053 (2004)

25. Seeman, N.C.: Nucleic-acid junctions and lattices. *Journal of Theoretical Biology* 99, 237–247 (1982)
26. Wang, H.: Proving theorems by pattern recognition – II. *The Bell System Technical Journal* XL(1), 1–41 (1961)
27. Winfree, E.: Algorithmic Self-Assembly of DNA. PhD thesis, California Institute of Technology (June 1998)
28. Winfree, E., Liu, F., Wenzler, L.A., Seeman, N.C.: Design and self-assembly of two-dimensional DNA crystals. *Nature* 394(6693), 539–544 (1998)
29. Yurke, B., Turberfield, A., Mills Jr., A., Simmel, F., Neumann, J.: A DNA-fuelled molecular machine made of DNA. *Nature* 406(6796), 605–608 (2000)