

# Intrinsic universality and the computational power of self-assembly

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This short survey of recent work in tile self-assembly discusses the use of simulation to classify and separate the computational and expressive power of self-assembly models. The journey begins with the result that there is a single universal tile set that, with proper initialization and scaling, simulates any tile assembly system. This universal tile set exhibits something stronger than Turing universality: it captures the geometry and dynamics of any simulated system. From there we find that there is no such tile set in the noncooperative, or temperature 1, model, proving it weaker than the full tile assembly model. In the two-handed or hierarchical model, where large assemblies can bind together on one step, we encounter an infinite set, of infinite hierarchies, each with strictly increasing simulation power. Towards the end of our trip, we find one tile to rule them all: a single rotatable flipable polygonal tile that can simulate any tile assembly system. It seems this could be the beginning of a much longer journey, so directions for future work are suggested.

## Introduction

Self-assembly is the process by which small pieces of matter coalesce according to simple rules to form some kind of target structure. Theoretical models of self-assembly have been used to design a variety of DNA nanoscale structures that have been experimentally implemented, and indeed many view it as imperative to have a theory of self-assembly to guide this rapidly developing engineering field. Self-assembly models are capable of Turing-universality, and so of an infinite variety of interesting computational behaviours.

The abstract Tile Assembly Model, put forward by Winfree [26], is one such model. It is a kind of asynchronous nondeterministic cellular automaton that models crystal growth processes. Put another way, the abstract Tile Assembly Model restricts classical square Wang tiling [25] to use a mechanism for crystal-like growth of a tiling, one tile at a time, starting from a special seed tile. Of course individual tiles need not be square, indeed triangles [16], hexagons [27, 8, 16] and arbitrary polygons have been considered [8]. Other models of self-assembly allow for non-local rules and large-scale interactions. One such model is the two-handed (or hierarchical) model [3, 9] which allows large structures to stick together if enough of their tiles' edge colours match. Another is the Nubots model [27] where large assemblies of molecules can grow and then move relative to each other, implementing a kind of molecular robotics. Although some forms of self-assembly can be thought of as generalizations of cellular automata, or effectivisations of Wang tiling, these models are quite distinct from each other both in terms of questions that can be asked and results that can be obtained.

Here we discuss the relative computational and expressive power of self-assembly models, with much of the discussion summarized in Figure 1. Specifically, we seek to classify tile assembly models based upon their ability to simulate each other, or not. To do this, tile assemblers have borrowed a powerful

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idea from the cellular automata community: intrinsic universality. The topic of intrinsic universality, with its tight notion of simulation, has given rise to a rich theory in cellular automata [6, 7, 20, 21, 4, 2] and Wang tiling [17, 18]. This short survey attempts to show that we are beginning to see this in self-assembly too [11, 12, 8, 9, 19, 13, 14].

### **The abstract Tile Assembly Model is intrinsically universal**

An instance of the abstract Tile Assembly Model [26] is called a tile assembly system and is a triple consisting of a set of square tiles, a seed assembly (one or more tiles stuck together), and a temperature  $\tau \in \{1, 2, 3, \dots\}$ . Each side of a square tile has a glue (or colour)  $g$  and strength  $s \in \{0, 1, 2, \dots\}$ . Growth begins from the seed assembly. A tile sticks to a partially-formed assembly if it can be positioned so that enough of its glues match those of adjacent tiles on the assembly and the sum of the matching glue strengths exceeds the temperature. Growth proceeds one tile at a time, asynchronously and nondeterministically. (Tiles may not overlap nor rotate, and unlike Wang tiling, adjacent glues (colours) may mismatch in an assembly.) This is a formal model of a crystal-like growth process.

Recently, the abstract Tile Assembly Model has been shown to be intrinsically universal [11], meaning that there is a single set of tiles  $U$  that when appropriately initialized, is capable of simulating the behavior of an arbitrary tile assembly system  $\mathcal{T}$ , up to rescaling. Specifically, this means that (1) each tile of  $\mathcal{T}$  is represented by a “supertile” of  $U$ , that is, by a  $k \times k$  block of tiles (where  $k$  depends on the size of  $\mathcal{T}$ ’s tile set, but is independent of what  $\mathcal{T}$  does), (2) the simulated system  $\mathcal{T}$  is encoded in a  $k \times k$  “seed supertile” of the simulator, and (3) every sequence of tile placements in the simulated system is simulated by a sequence of supertile placements in the universal simulator system, and vice-versa. In other words, this intrinsically universal tile set has the ability to simulate both the geometry and growth order of any tile assembly system. Modulo rescaling, this universal tile set  $U$  represents the full power and expressivity of the entire abstract Tile Assembly Model.

### **Temperature 1: negative results in intrinsic universality**

It has been known for some time that the temperature 2 tile assembly model, where at least *some* of the tiles are required to match on *two or more* sides, i.e. *cooperative growth*, leads to highly non-trivial behavior. Turing machine simulation [23], efficient production of  $n \times n$  squares and other simple shapes using  $\Theta(\log n / \log \log n)$  tile types [1], efficient production of arbitrary finite connected shapes using a number of tile types within a log factor of the Kolmogorov complexity of the shape [24], and even intrinsic universality [11] (as mentioned above) can all be achieved with cooperative, or temperature 2, growth.

The fact that the abstract Tile Assembly Model is intrinsically universal suggests an obvious question: can we show that some subclasses of the model are provably weaker than the full model, by showing that these subclasses are not universal for the full model?

The most notorious such subclass is called temperature 1. Despite its esoteric name, it models a fundamental and ubiquitous form of growth: asynchronous growing and branching tips in Euclidian space where each new tile is added if matches on at *least one side*. Since temperature 1 binding requires matching glues on only one or more sides, it is called noncooperative binding. In 2D, its like snakes on a plane.

Recently, ideas from intrinsic universality have been used to show that the Temperature 1 Tile Assembly Model (i.e. noncooperative binding) is provably weaker than the full tile assembly model [19]: in particular, temperature 1 tile assembly is not capable of *simulating* arbitrary tile assembly systems. In fact, there is a very simple cooperative tile assembly system that can not be simulated by any noncooperative tile

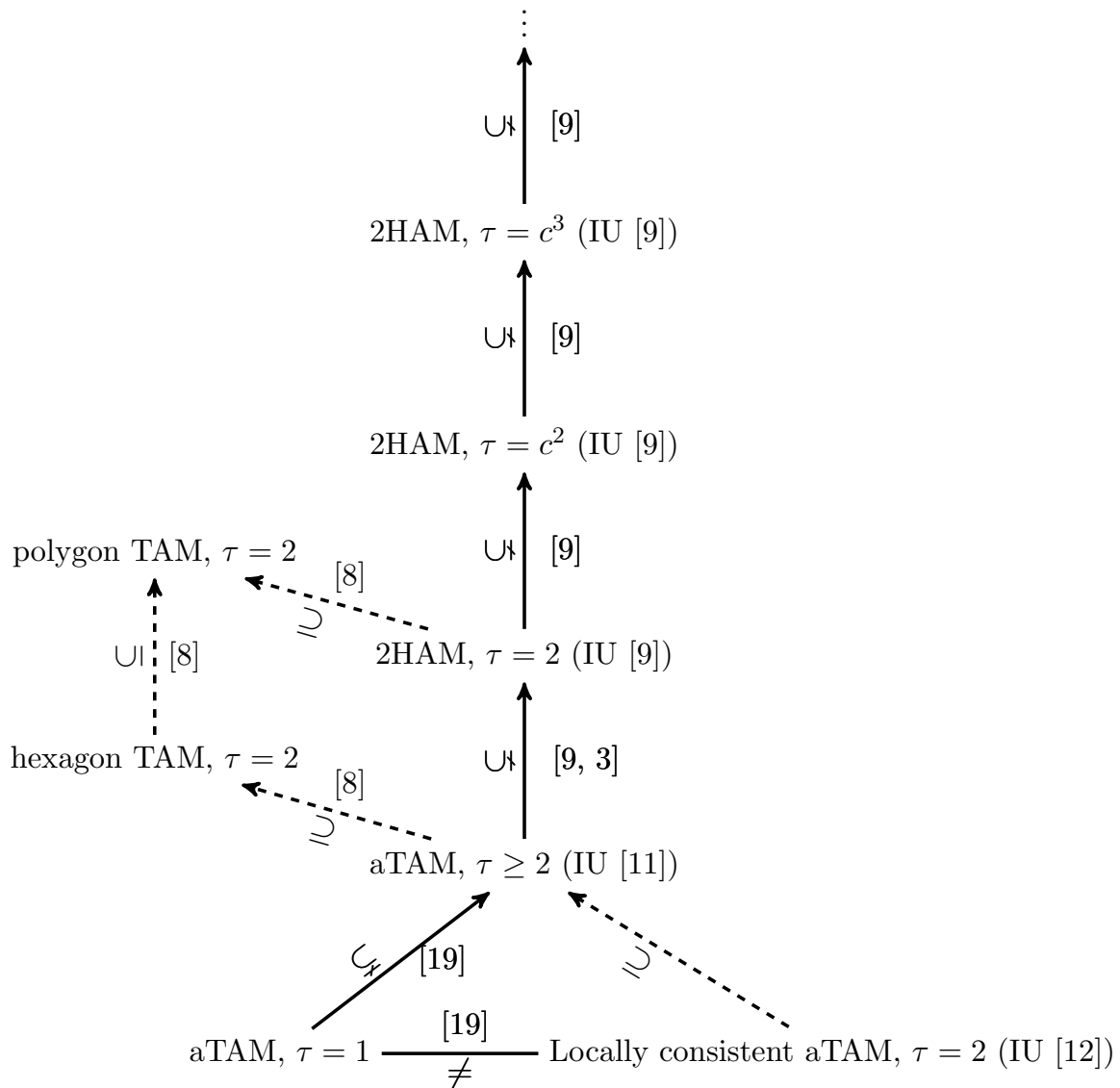


Figure 1: Classes of tile assembly systems, and their relationship with respect to simulation. aTAM: abstract Tile Assembly Model (growth from a seed assembly by single tile addition in 2D),  $\tau$  denotes “temperature”. 2HAM: Two-Handed Tile Assembly Model (individual tiles and large assemblies stick together in 2D). Class  $A$  contains class  $B$  if there is a tile set  $U$  that simulates any member of  $B$  and does so in a tile assembly system from  $A$ . Solid arrows denote strict containment, dashed arrows denote containment. A 2HAM temperature hierarchy is shown for some  $c \in \{2, 3, 4, \dots\}$ . In fact, for each such  $c$  the set  $\{c^i | i \in \{1, 2, 3, \dots\}\}$  gives an infinite hierarchy of classes of strictly increasing simulation power in the 2HAM. The letters “IU” denote the existence of an intrinsically universal tile set for a class, and omission of “IU” implies that the existence of such a tile set is an open problem for that class. Citations are given in square brackets. Simulation results for a number of other models are described in the main text.

assembly system. This is the first fully general negative result about temperature 1 that does not assume restrictions on the model nor unproven hypotheses. (However, it tantalizingly leaves open the question of whether 2D deterministic temperature 1 systems are Turing universal, or whether they can efficiently assemble  $n \times n$  squares with less than  $2n - 1$  tile types.) An interesting aspect of this negative result is that it holds for 3D noncooperative systems, they too can not simulate arbitrary tile assembly systems. This is quite shocking, given that 3D noncooperative systems are Turing-universal [5]! Hence, the negative result in [19] can be interpreted to mean that Turing-universal algorithmic behavior in self-assembly does not imply the ability to simulate arbitrary algorithmic self-assembly processes.

What about other subclasses of the abstract tile assembly model? It was shown that 3D noncooperative systems can simulate 2D noncooperative systems [19]. The same paper contains the conjecture that there is no 2D noncooperative tile set that can simulate all 2D noncooperative tile assembly systems.

The first intrinsic universality result in tile assembly showed that locally consistent tile assembly systems (a restriction of the general model where binding uses at most two sides, with bonds that are not “too strong”) have an intrinsically universal tile set [12]. It turns out that even these locally consistent systems can not be simulated by noncooperative systems [19]. As observed in [12], Soloveichik and Winfree’s construction [24] gives a tile set that, when suitably seeded, simulates any temperature 1 tile assembly system whose underlying binding graph is a spanning tree.

It remains as future work to further characterize the power of interesting subclasses of the abstract Tile Assembly Model, and in particular, to separate such subclasses.

### **Simulation and intrinsic universality in other models of self-assembly**

What about other models of self assembly besides the abstract Tile Assembly Model? It has been shown that the two-handed, or hierarchical, model of self-assembly (where large assemblies of tiles may come together in a single step) is not intrinsically universal [9]. Specifically there is no tile set that can simulate all two-handed systems for all temperatures. However, the same paper shows that for each temperature  $\tau \in \{2, 3, 4, \dots\}$  there is a tileset that is intrinsically universal for the class of two-handed systems that work at temperature  $\tau$ . Also, there is an infinite hierarchy of classes of such systems with each level strictly more powerful than the one below. In fact there are an infinite set of such hierarchies, as described in the caption of Figure 1. These results [9] formalize the intuition that multiple long range interactions are more powerful than fewer long range interactions in the two-handed model.

By combining results from [3] and [11], we get that there is a tile set for the two-handed model that (at temperature 2) simulates any instance (assembly system) of the abstract Tile Assembly Model, as shown in Figure 1.

The Signal-passing Tile Assembly Model has tiles with molecular (DNA) wires on their surface. Essentially there is a “use once” circuit sitting on the assembly itself! These wires use an experimentally plausible DNA strand displacement mechanism. Recently, Hendricks, Padilla, Patitz and Rogers [13] have shown that in the two-handed model there is a single 3D tile set, that can simulate any 2D signal-passing tile assembly system. Their result shows that a constant number of planes (in the third dimension) is sufficient to handle wire crossings and asynchronous signal passing.

As mentioned above, the Tile Assembly Model can be thought of as an asynchronous and nondeterministic cellular automaton (CA), that models the notion of a crystal growth frontier. Hendricks and Patitz [14] formally relate the abstract Tile Assembly Model and CA: they give a single CA that simulates any tile assembly system, as well as a single tile set that simulates any nondeterministic CA with a finite initial configuration. The methods of updating configurations in both models are quite different (CA are infinite, synchronous and deterministic, while tile assembly is finite, asynchronous and nondeterministic),

and so their constructions need to handle this. Their work opens the possibility of further comparing and contrasting the CA and tile assembly models.

## The One

Demaine, Demaine, Fekete, Patitz, Schweller, Winslow, and Woods [8] take the existence of an intrinsically universal tile set for the abstract Tile Assembly Model [11] as merely the first in a sequence of simulations that routes from squares tiles, to the intrinsically universal tile set, to (low-strength) hexagons to a *single* polygon that is translatable, rotatable and flipable. Their fixed-sized polygon, when appropriately seeded, simulates any tile assembly system. This polygon, *The One*, captures the power of the entire abstract Tile Assembly Model: to simulate a tile assembly system  $\mathcal{T}$  one simply puts together a seed assembly of polygons that encodes  $\mathcal{T}$  and just lets it go! Likewise, Turing machines can be simulated with this single tile. They also show [8] that with translation only, such results are not possible with a small (size  $\leq 3$ ) seed. In the simpler setting of Wang plane tiling, they show [8] how to take any tile set  $T$  (on the square or hexagonal lattice) and “compile” it to get a single regular polygon that simulates exactly the tilings of  $T$ , except with tiny gaps between the polygons. In particular, if one starts with any aperiodic square or hexagon tile set, that set can be easily compiled to a *single regular polygonal tile*, all of whose tilings are aperiodic, with tiny gaps between the polygons.

## Future work

As Figure 1 shows, we are beginning to classify the power of tile assembly models using intrinsic universality. Indeed gaps in the figure suggest obvious future directions. It is an open question whether or not the hexagonal Tile Assembly Model [8], polygonal Tile Assembly Model [8], Nubots model [27] and Signal-passing Tile Assembly Model [13, 15] are intrinsically universal. And independent of whether or not these models turn out to be intrinsic universal, we suggest that simulation can be used to tease apart their computational and expressive power, as well as the power of subclasses of these models.

A more technical question: Does there exist a tile set  $U$  for the aTAM, such that for any (adversarially chosen) seed assembly  $\sigma$ , at temperature 2, this tile assembly system simulates some tile assembly system  $\mathcal{T}$ ? Moreover,  $U$  should be able to simulate all such members  $\mathcal{T}$  of some (hopefully, non-trivial) class  $S$ .  $U$  is a tile set that can do one thing and nothing else: simulate tile assembly systems from  $S$ . This question about  $U$  is inspired by the factor simulation question in CA [7], although it differs in the details.

Many cooperative “algorithmic” tile assembly systems (temperature 2 and above) simulate Turing machines in a “zig-zag” fashion. Can the technique of [19] be extended to show that no 2D temperature 1 aTAM system simulates zig-zag aTAM tile assembly systems? This would be a non-trivial extension as [19] holds for the 3D temperature 1 aTAM, which can indeed simulate zig-zag systems, and would show that no deterministic 2D temperature 1 system can simulate Turing machines in the “usual way”.

Of course, there are many other ways to compare the power of self-assembly models [22, 10]: researchers have looked at shape and pattern building, tile complexity, time complexity, determinism versus nondeterminism, and randomization in self-assembly, and it remains as important future work to find relationships between these notions on the one hand, and intrinsic universality and simulation on the other hand. Can ideas from intrinsic universality be used to answer questions about these notions?

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