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| Name: | Damien Woods |
| Affil./Addr. | California Institute of Technology |
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# Intrinsic Universality in Self-Assembly

Damien Woods
California Institute of Technology

## Years aud Authors of Summarized Original Work

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Intrinsic universality, simulation, self-assembly, abstract Tile Assembly Model

## Problem Definition

Algorithmic self-assembly [11] is the idea that small self-assembling molecules can compute as they grow structures. It gives programmers a set of theoretical models in which to specify and design target structures while trying to optimise resources such as number of molecule types or even construction time. The abstract Tile Assembly Model [11] is one such model. An instance of the model is called a tile assembly system and is a triple $\mathcal{T} = (T, \sigma, \tau)$ consisting of a finite set $T$ of square tiles, a seed assembly $\sigma$ (one or more tiles stuck together), and a temperature $\tau \in \{1, 2, 3, \ldots\}$, as shown in Figure 1(a). Each side of a square tile has a glue (or colour) $g$ which in turn has a strength $s \in \{0, 1, 2, \ldots\}$. Growth occurs on the integer plane and begins from a seed assembly (or a seed tile) placed at the origin, as shown in Figure 1(b). A tile sticks to a partially-formed assembly if it can be placed next to the assembly in such a way that enough of its glues match the glues of the adjacent tiles on the assembly and the sum of the matching glue strengths is at least the temperature. Growth proceeds one tile at a time, asynchronously and nondeterministically.

Here, we discuss recent results, and suggest open questions, on intrinsic universality and simulation as a method to compare self-assembly models. Figure 2 gives an overview of these and other results. For a more thorough overview see [12].

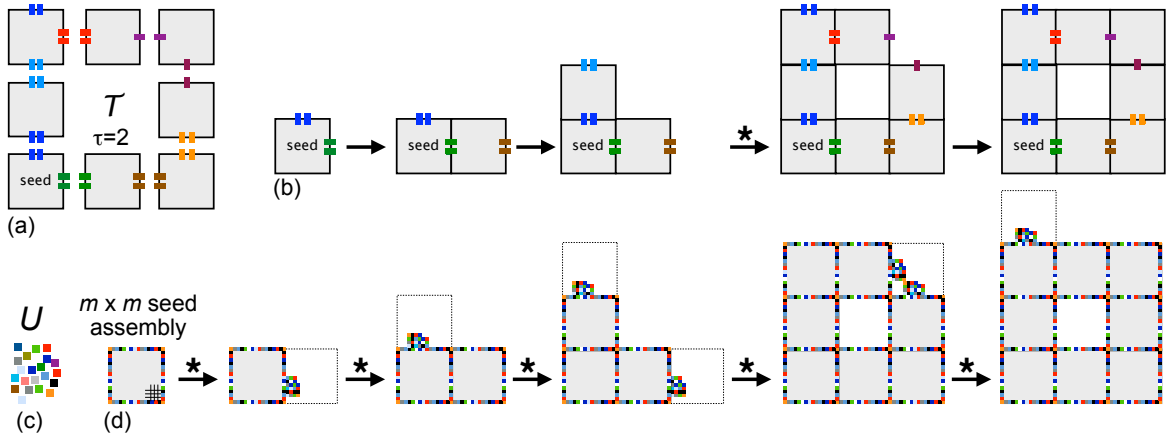


**Fig. 1.** An instance of the abstract Tile Assembly Model, and an example showing simulation and intrinsic universality. (a) A tile assembly system $\mathcal{T}$ consists of a tile set, seed tile and a temperature $\tau \in \mathbb{N}$. Coloured glues on the tiles' sides have a natural number strength (shown here as 0, 1 or 2 coloured tabs). (b) Growth begins from the seed with tiles sticking to the growing assembly if the sum of the strengths of the matching glues is at least $\tau$. (c) An intrinsically universal tile set $U$. (d) When initialised with a seed assembly (that encodes $\mathcal{T}$) and at temperature 2, the intrinsically universal tile set simulates the dynamics of $\mathcal{T}$ with each tile placement in $\mathcal{T}$ being simulated by the growth of an $m \times m$ block of tiles. Single tile attachment is denoted by $\rightarrow$ and $\stackrel{*}{\rightarrow}$ denotes multiple tile attachments. Note that both systems have many other growth dynamics that are not shown.

***Simulation and intrinsic universality*** Intuitively, one self-assembly model simulates another if they grow the same structures, via the same dynamical growth processes, possibly with some spatial scaling. Let $\mathcal{S}$ and $\mathcal{T}$ be tile assembly systems of the abstract Tile Assembly Model described above. $\mathcal{S}$ is said to *simulate* $\mathcal{T}$ if the following conditions hold: (1) each tile of $\mathcal{T}$ is represented by one or more $m \times m$ blocks of tiles in $\mathcal{S}$ called *supertiles*, (2) the seed assembly of $\mathcal{T}$ is represented by the *seed assembly* of $\mathcal{S}$ (one or more connected $m \times m$ supertiles), and (3) via supertile representation every sequence of tile placements in the simulated system $\mathcal{T}$ has a corresponding sequence of supertile placements in the simulator system $\mathcal{S}$, and vice versa. It is worth pointing out that although the intuitive idea of one assembly system simulating another is fairly simple, the formal definition of simulation [10] gets a little technical as the filling out of supertiles in the simulator is an asynchronous and nondeterministic distributed process with many supertiles growing independently and in parallel in the simulator system.

## Key Results

***The abstract Tile Assembly Model is intrinsically universal*** A class of tile assembly systems $C$ is said to be *intrinsically universal* if there exists a single set of tiles $U$ that simulates any instance of $C$. For each such simulation, $U$ should be appropriately initialised as an instance (i.e. a tile assembly system) of $C$ itself. Figure 1(d) illustrates the concept. For example, the abstract Tile Assembly Model has been shown to be intrinsically universal [5]. Specifically, this means that there is a single set of tiles $U$ that when appropriately initialised, is capable of simulating an arbitrary tile assembly system $\mathcal{T}$. To program such a simulation, tiles from $\mathcal{T}$ are

represented as $m \times m$ supertiles (built from tiles in $U$) and the seed assembly of $\mathcal{T}$ is represented as a connected assembly $\sigma_{\mathcal{T}}$ of such supertiles. Furthermore, the entire tile assembly system $\mathcal{T}$ (a finite object) is itself encoded in the supertiles of $\sigma_{\mathcal{T}}$ of $\mathcal{U}$. Then if we watch all possible growth dynamics in both $\mathcal{T} = (T, \sigma, \tau)$ and $\mathcal{U} = (U, \sigma_{\mathcal{T}}, 2)$ we get that both systems produce the same set of assemblies via the same dynamics where we use a supertile representation function to map from supertiles over $U$ to tiles from $T$. It is worth pointing out that in this particular construction [5] the simulating system is always (merely) at temperature $\tau = 2$ no matter how large the temperature ($\tau \geq 1$) of the simulated system.

This intrinsically universal tile set $U$ has the ability to simulate both the geometry and growth order of any tile assembly system. Modulo spatial rescaling, $U$ represents the full power and expressivity of the entire abstract Tile Assembly Model.

***Noncooperative assembly is weaker than cooperative assembly*** The temperature 1, or noncooperative, model is a restriction of the abstract Tile Assembly Model. 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 it matches on at *least one side*. Separating the power of the noncooperative and cooperative models has presented significant challenge to the community.

Recently it has been shown that the noncooperative model is provably weaker than the full model [10] in that sense that it is not capable of *simulating* arbitrary tile assembly systems. This is the first fully general negative result about temperature 1 that does not assume restrictions on the model nor unproven hypotheses.

An interesting aspect of this result is that it holds for 3D noncooperative systems, they too can not simulate arbitrary tile assembly systems. This seems quite shocking, given that 3D noncooperative systems are Turing-universal [1]! So in particular, 3D noncooperative systems can simulate 2D (or 3D) cooperative systems by simulating a Turing machine that in turn simulates the cooperative system, but this loose style of simulation ends up destroying the geometry and dynamics of tile assembly by encoding everything as "geometry-less" strings. Hence, Turing-universal algorithmic behaviour in self-assembly does not imply the ability to simulate, in a direct geometric fashion, arbitrary algorithmic self-assembly processes.

***One tile to rule them all*** As an example of a simulation result on a very different model of self-assembly, Demaine, Demaine, Fekete, Patitz, Schweller, Winslow, and Woods [3] describe a sequence of simulations that route from squares tiles, to the intrinsically universal tile set, to hexagons (with strength $< \tau$, or weak, glues) to a *single* polygon that is translatable, rotatable and flipable. Their fixed-sized polygon, when appropriately seeded, simulates any tile assembly system from the abstract Tile Assembly Model. They also show that with translation only (i.e. no rotation), such results are not possible with a small (size $\leq 3$) seed (although with larger seeds a single translation-only polyomino simulates the space-time diagram of a 1D cellular automaton). In the simpler setting of Wang plane tilling, they give an easy method to "compile" any tile set $T$ (on the square or hexagonal lattice) to a single regular polygon that simulates exactly the tilings of $T$, except with tiny gaps between the polygons.

***Two-hands*** 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 [4]. Specifically there is no tile set that, in the two-handed model, can simulate all two-handed systems for all temperatures. However, for each $\tau \in \{2, 3, 4, \ldots\}$ there is a tileset $U_\tau$ that is intrinsically universal for the class of two-handed systems that work at temperature $\tau$. Also, there is an infinite hierarchy of

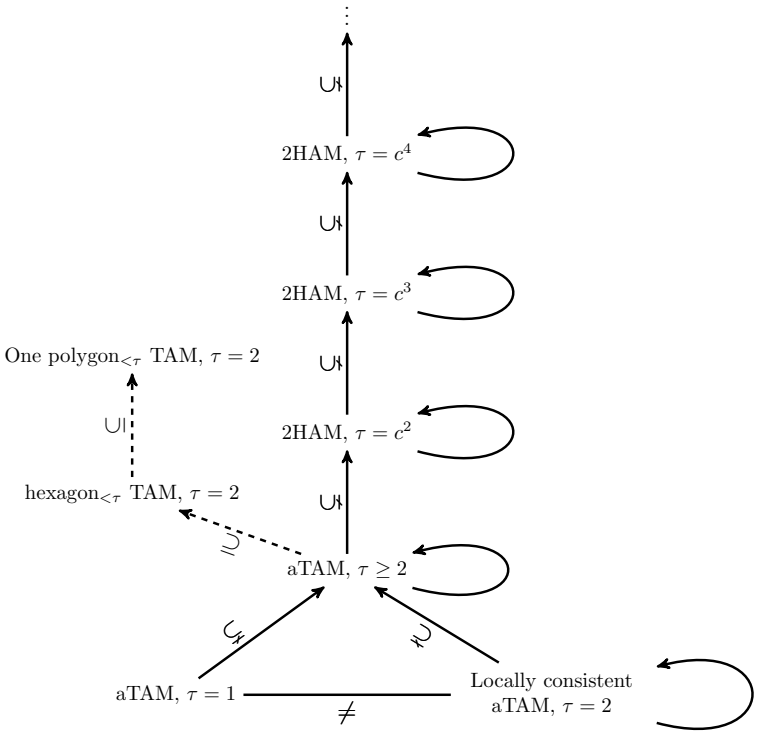


**Fig. 2.** Classes of tile assembly systems, and their relationship with respect to simulation. There is an arrow from $B$ to $A$ if $A$ contains $B$ with respect to simulation: that is for each tile assembly system $\mathcal{B} \in B$ there is a tile assembly system $\mathcal{A}_\mathcal{B} \in A$ that simulates $\mathcal{B}$. Dashed arrows denote containment, solid arrows denote strict containment and a self-loop denotes the existence of an intrinsically universal tile set for a class and its omission implies that the existence of such a tile set is an open problem. 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 (assemblies of tiles stick together in 2D). A 2HAM temperature hierarchy is shown for some $c \in \{2, 3, 4, \ldots\}$ and, in fact, for each such $c$ the set of temperatures $\{c^i | i \in \{2, 3, \ldots\}\}$ gives an infinite hierarchy of classes of strictly increasing simulation power in the 2HAM.

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 2. These results give a formalisation of the intuition that multiple long range interactions are more powerful than fewer long range interactions in the two-handed model.

# Open Problems

Gaps in Figure 2 (i.e. missing solid arrows and missing models) suggest a variety of open questions. Also, it remains as future work to further tease apart the power of restrictions of the abstract Tile Assembly Model, for example, it remains open whether 2D noncooperative systems are intrinsically universal for themselves.

It is an open question whether or not the hexagonal Tile Assembly Model [3], various polygonal Tile Assembly Models [3, 6], the Nubot model [13] and Signal-Passing Tile Assembly Model [7, 9] are intrinsically universal. Furthermore, simulation could be used to tease apart the power of subclasses of these models.

Gilbert et al [6] investigate the computational power of various kinds of polygonal tile assembly systems, showing that regular polygon tiles with $> 6$ sides simulate Turing machines. What is the relationship between tile geometry and simulation power? Do more sides give strictly more simulation power?

A desirable feature of a simulator is not only that it simulates all possible dynamics of some simulated system, but that the probability of a given dynamics is roughly equal in both the simulated system and the simulator. Is there an intrinsically universal tile set with that property? Here, the probability of seeing a given dynamics or assembly in a simulator should be close to that of the simulated system, where "close" means, say, within a factor proportional to the spatial scaling.

Does there exist a tile set $U$ for the abstract Tile Assembly Model, 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 non-trivial class $S$. $U$ is a tile set that can do one thing and nothing else: simulate tile assembly systems from the class $S$. This question about $U$ is inspired by the factor simulation question in CA [2].

Many algorithmic tile assembly systems use cooperative self-assembly to simulate Turing machines in a "zig-zag" fashion, as do a number of experimentally implemented systems. Can the negative result of [10] be extended to show 2D temperature 1 abstract Tile Assembly Model systems do not simulate zig-zag tile assembly systems?

There are a number of future research directions for the two-handed, or hierarchical, self-assembly model. One open question [4, 8] asks whether or not temperature $\tau$ two-handed systems can simulate temperature $\tau - 1$ two-handed systems. Another direction involves finding which aspects of the model (e.g. mismatches, excess binding strength, geometric blocking) are required for intrinsic universality at a given temperature, to better understand the intricacies of this very powerful, but natural, model.

Of course, there are many other ways to compare the power of self-assembly models: shape and pattern building, tile complexity, time complexity, determinism versus nondeterminism, and randomised (coin-flipping) algorithms in self-assembly. 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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## Cross-References

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Combinatorial Optimization and Verification in Self-Assembly
Patterned Self-Assembly Tile Set Synthesis
Randomized Self-Assembly
Robustness in Self-Assembly
Self-Assembly at Temperature 1
Self-Assembly of Fractals
Self-Assembly of Squares and Scaled Shapes
Self-Assembly with Active Components
Self-Assembly with General Shaped Tiles
Temperature Programming in Self-Assembly
Two Handed Self-Assembly

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