Signal Transmission across Tile Assemblies: 3D Static Tiles Simulate Active Self-assembly by 2D Signal-Passing Tiles

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Abstract. The 2-Handed Assembly Model (2HAM) is a tile-based self-assembly model in which, typically beginning from single tiles, arbitrarily large aggregations of static tiles combine in pairs to form structures. The Signal-passing Tile Assembly Model (STAM) is an extension of the 2HAM in which the tiles are dynamically changing components which are able to alter their binding domains as they bind together. In this paper, we prove that there exists a 3D tile set in the 2HAM which is intrinsically universal for the class of all 2D STAM$^+$ systems at temperature 1 and 2 (where the STAM$^+$ does not make use of the STAM's power of glue deactivation and assembly breaking, as the tile components of the 2HAM are static and unable to change or break bonds). This means that there is a single tile set U in the 3D 2HAM which can, for an arbitrarily complex STAM$^+$ system S, be configured with a single input configuration which causes U to exactly simulate S at a scale factor dependent upon S. Furthermore, this simulation uses only 2 planes of the third dimension.

To achieve this result, we also demonstrate useful techniques and transformations for converting an arbitrarily complex STAM$^+$ tile set into an STAM$^+$ tile set where every tile has a constant, low amount of complexity, in terms of the number and types of "signals" they can send, with a trade off in scale factor.

While the first result is of more theoretical interest, showing the power of static tiles to simulate dynamic tiles when given one extra plane in 3D, the second is of more practical interest for the experimental implementation of STAM tiles, since it provides potentially useful strategies for developing powerful STAM systems while keeping the complexity of individual tiles low, thus making them easier to physically implement.

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1 Introduction

Self-assembling systems are those in which large, disorganized collections of relatively simple components autonomously, without external guidance, combine to form organized structures. Self assembly drives the formation of a vast multitude of naturally forming structures, across a wide range of sizes and complexities (from the crystalline structure of snowflakes to complex biological structures such as viruses). Recognizing the immense power and potential of self-assembly to manufacture structures with precision down to the molecular level, researchers have been pursuing the creation and study of artificial self-assembling systems. This research has led to steadily increasing sophistication of both the theoretical models (from the Tile Assembly Model (TAM) [21], to the 2-Handed Assembly Model (2HAM) [4, 8], and many others [1–3, 8, 12]) as well as experimentally produced building blocks and systems (a mere few of which include [5, 13, 15, 16, 19, 20]). While a number of models exist for passive self-assembly, as can be seen above, research into modeling active self-assembly is just beginning [18, 22]. Unlike passive self-assembly where structures bind and remain in one state, active self-assembly allows for structures to bind and then change state.

A newly developed model, the Signal-passing Tile Assembly Model (STAM) [18], is based upon the 2HAM but with a powerful and important difference. Tiles in the aTAM and 2HAM are static, unchanging building blocks which can be thought of as analogous to write-once memory, where a location can change from empty to a particular value once and then never change again. Instead, the tiles of the STAM each have the ability to undergo some bounded number of transformations as they bind to an assembly and while they are connected. Each transformation is initiated by the binding event of a tile's glue, and consists of some other glue on that tile being turned either "on" or "off". By chaining together sequences of such events which propagate across the tiles of an assembly, it is possible to send "signals" which allow the assembly to adapt during growth. Since the number of transitions that any glue can make is bounded, this doesn't provide for "fully reusable" memory, but even with the limited reuse it has been shown that the STAM is more powerful than static models such as the aTAM and 2HAM (in 2D), for instance being able to strictly self-assemble the Sierpinski triangle [18]. A very important feature of the STAM is its asynchronous nature, meaning that there is no timeframe during which signals are guaranteed to fully propagate, and no guaranteed ordering to the arrival of multiple signals. Besides providing a useful theoretical framework of asynchronous behavior, the design of the STAM was carefully aligned to the physical reality of implementation by DNA tiles using cascades of strand-displacement. Capabilities in this area are improving, and now include the linear transmission of signals, where one glue binding event can activate one other glue on a DNA tile [17].

Although the STAM is intended to provide both a powerful theoretical framework and a solid basis for representing possible physical implementations, often those two goals are at odds. In fact, in the STAM it is possible to define tiles which have arbitrary *signal complexity* in terms of the numbers of glues that they have on any given side and the number of signals that each tile can initiate. Clearly, with increasing complexity of individual tiles, the ease of making them in the laboratory diminishes. Therefore, in this paper our first set of results provide a variety of methods for simplifying the tiles in STAM systems. Besides reducing just the general signal complexity of tiles, we also seek to reduce and/or remove certain patterns of signals which may be more difficult to build into DNA-based tiles, namely *fan-out* (which occurs when a single signal must split into multiple paths and have multiple destinations), *fan-in* (which occurs when multiple signals must converge and join into one path to arrive at a single glue), and *mutual activation* (which occurs when both of the glues participating in a particular binding event initiate their own signals). By trading signal complexity for tile complexity and scale factor, we show how to use some simple primitive substitutions to reduce STAM tile sets to those with much simpler tiles. Note that while in the general STAM it is possible for signals to turn glues both "on" and "off", our results pertain only to systems which turn glues "on" (which we call $STAM^+$ systems).

In particular, we show that the tile set for any temperature 1 STAM$^+$ system, with tiles of arbitrary complexity, can be converted into a temperature 1 STAM$^+$ system with a tile set where no tile has greater then 2 signals and either fan-out or mutual activation are completely eliminated. We show that any temperature 2 STAM$^+$ system can be converted into a temperature 2 STAM$^+$ system where no tile has greater than 1 signal and both fan-out and mutual activation are eliminated. Importantly, while both conversions have a worst case scale factor of $|T^2|$, where T is the tile set of the original system, and worst case tile complexity of $|T^2|$, those bounds are required for the extremely unrealistic case where *every* glue is on *every* edge of some tile and also sends signals to *every* glue on *every* side of that tile. Converting from a more realistic tile set yields factors which are on the order of the square of the maximum signal complexity for each side of a tile, which is typically much smaller. Further, the techniques used to reduce signal complexity and remove fan-out and mutual activation are likely to be useful in the original design of tile sets rather than just as brute force conversions of completed tile sets.

We next consider the topic of intrinsic universality, which was initially developed to aid in the study of cellular automata [6, 7]. The notion of intrinsic universality was designed to capture a strong notion of simulation, in which one particular automaton is capable of simulating the *behavior* of any automaton within a class of automata. Furthermore, to simulate the behavior of another automaton, the simulating automaton must evolve in such a way that a translated rescaling (rescaled not only with respect to rectangular blocks of cells, but also with respect to time) of the simulator can be mapped to a configuration of the simulated automaton. The specific rescaling depends on the simulated automaton and gives rise to a global rule such that each step of the simulated automaton's evolution is mirrored by the simulating automaton, and vice versa via the inverse of the rule.

In this way, it is said that the simulator captures the dynamics of the simulated system, acting exactly like it, modulo scaling. This is in contrast to a computational simulation, for example when a general purpose digital computer runs a program to simulate a cellular automata while the processor's components don't actually arrange themselves as, and behave like, a grid of cellular automata. In [11], it was shown that the aTAM is intrinsically universal, which means that there is a single tile set U such that, for any aTAM tile assembly system $\mathcal{T}$ (of any temperature), the tiles of U can be arranged into a seed structure dependent upon $\mathcal{T}$ so that the resulting system (at temperature 2), using only the tiles from U, will faithfully simulate the behaviors of $\mathcal{T}$. In contrast, in [9] it was shown that no such tile set exists for the 2HAM since, for every temperature, there is a 2HAM system which cannot be simulated by any system operating at a lower temperature. Thus no tile set is sufficient to simulate 2HAM systems of arbitrary temperature.

For our main result, we show that there is a 3D 2HAM tile set U which is intrinsically universal (IU) for the class $\mathfrak{C}$ of all STAM$^+$ systems at temperature 1 and 2. For every $\mathcal{T} \in \mathfrak{C}$, a single input supertile can be created, and using just copies of that input supertile and the tiles from U, at temperature 2 the resulting system with faithfully simulate $\mathcal{T}$. Furthermore, the simulating system will use only 2 planes of the third dimension. (The signal tile set simplification results are integral in the construction for this result, especially in allowing it to use only 2 planes.) This result is noteworthy especially because it shows that the dynamic behavior of signal tiles (excluding glue deactivation) can be *fully duplicated* by static tile systems which are allowed to "barely" use three dimensions. Furthermore, for every temperature $\tau > 1$ there exists a 3D 2HAM tile set which can simulate the class of all STAM$^+$ systems at temperature τ.

2 Preliminaries

Here we provide informal descriptions of the models and terms used in this paper. Due to space limitations, the formal definitions can be found in [14].

2.1 Informal Definition of the 2HAM

The 2HAM [4,8] is a generalization of the abstract Tile Assembly Model (aTAM) [21] 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 τ-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 d-dimensional 2HAM, for $d \in \{2, 3\}$, which is normally defined as a 2D model but which we extend to 3D as well, in the natural and intuitive way.

A *tile type* is a unit square if $d = 2$, and cube if $d = 3$, with each side 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 $\mathbb{Z}^d$. 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 *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. That is, the supertile is stable if at least energy τ 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 τ is the *temperature*, usually 1 or 2. (Note that this is considered the "default" type of 2HAM system, while a system can also be defined as a triple (T, S, τ), where S is the *initial configuration* which in the default case is just infinite copies of all tiles from T, but in other cases can additionally or instead consist of copies of pre-formed supertiles.) 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 τ-stable result of translating two producible assemblies without overlap. Note that if $d = 3$, or if $d = 2$ but it is explicitly mentioned that *planarity* is to be preserved, it must be possible for one of the assemblies to start infinitely far from the other and by merely translating in d dimensions arrive into a position such that the combination of the two is τ-stable, without ever requiring overlap. This prevents, for example, binding on the interior of a region completely enclosed by a supertile. A supertile α is *terminal*, written as $\alpha \in \mathcal{A}_{\Box}[\mathcal{T}]$, if for every producible supertile β, α and β cannot be τ-stably attached. A TAS is *directed* if it has only one terminal, producible supertile.

2.2 Informal Description of the STAM

In the STAM, tiles are allowed to have sets of glues on each edge (as opposed to only one glue per side as in the TAM and 2HAM). Tiles have an initial state in which each glue is either "`on`" or "`latent`" (i.e. can be switched `on` later). Tiles also each implement a transition function which is executed upon the binding of any glue on any edge of that tile. The transition function specifies, for each glue g on a tile, a set of glues (along with the sides on which those glues are located) and an action, or *signal* which is *fired* by g's binding, for each glue in the set. The actions specified may be to: 1. turn the glue `on` (only valid if it is currently `latent`), or 2. turn the glue `off` (valid if it is currently `on` or `latent`). This means that glues can only be `on` once (although may remain so for an arbitrary amount of time or permanently), either by starting in that state or being switched `on` from `latent` (which we call *activation*), and if they are ever switched to `off` (called *deactivation*) then no further transitions are allowed for that glue. This essentially provides a single "use" of a glue (and the signal sent by its binding). Note that turning a glue `off` breaks any bond that that glue may have formed with a neighboring tile. Also, since tile edges can have multiple active glues, when tile edges with multiple glues are adjacent, it is assumed that all matching glues in the `on` state bind (for a total binding strength equal to the sum of the strengths of the individually bound glues). The transition function defined for each tile type is allowed a unique set of output actions for the binding event of each glue along its edges, meaning that the binding of any particular glue on a tile's edge can initiate a set of actions to turn an arbitrary set of the glues on the sides of the same tile either `on` or `off`.

As the STAM is an extension of the 2HAM, binding and breaking can occur between tiles contained in pairs of arbitrarily sized supertiles. In order to allow for physical mechanisms which implement the transition functions of tiles but are arbitrarily slower or faster than the average rates of (super)tile attachments and detachments, rather than immediately enacting the outputs of transition functions, each output action is put into a set of "pending actions" which includes all actions which have not yet been enacted for that glue (since it is technically possible for more than one action to have been initiated, but not yet enacted, for a particular glue). Any event can be randomly selected from the set, regardless of the order of arrival in the set, and the ordering of either selecting some action from the set or the combination of two supertiles is also completely arbitrary. This provides fully asynchronous timing between the initiation, or firing, of signals (i.e. the execution of the transition function which puts them in the pending set) and their execution (i.e. the changing of the state of the target glue), as an arbitrary number of supertile binding events may occur before any signal is executed from the pending set, and vice versa.

An STAM system consists of a set of tiles and a temperature value. To define what is producible from such a system, we use a recursive definition of producible assemblies which starts with the initial tiles and then contains any supertiles which can be formed by doing the following to any producible assembly: 1. executing any entry from the pending actions of any one glue within a tile within that supertile (and then that action is removed from the pending set), 2. binding with another supertile if they are able to form a τ-stable supertile, or 3. breaking into 2 separate supertiles along a cut whose total strength is $< \tau$.

The STAM, as formulated, is intended to provide a model based on experimentally plausible mechanisms for glue activation and deactivation. However, while the model allows for the placement of an arbitrary number of glues on each tile side and for each of them to signal an arbitrary number of glues on the same tile, this is (currently quite) limited in practice. Therefore, each system can be defined to take into account a desired threshold for each of those parameters, not exceeding it for any given tile type, and so we have defined the notion of *full-tile signal complexity* as the maximum number of signals on any tile in a set (see [14]) to capture the maximum complexity of any tile in a given set.

Definition 1. *We define the* STAM$^+$ *to be the STAM restricted to using only glue activation, and no glue deactivation. Similarly, we say an STAM$^+$ tile set is one which contains no defined glue deactivation transitions, and an STAM$^+$ system $\mathcal{T} = (T, \tau)$ is one in which T is an STAM$^+$ tile set.*

As the main goal of this paper is to show that self-assembly by systems using active, signalling tiles can be simulated using the static, unchanging tiles of the 3D 2HAM, since they have no ability to break apart after forming τ-stable structures, all of our results are confined to the STAM$^+$.

A detailed, technical definition of the STAM model is provided in [14].

2.3 Informal Definitions for Simulation

Here we informally describe what it means for one 2HAM or STAM TAS to "simulate" another. Formal definitions, adapted from those of [9], can be found in [14] .

Let $\mathcal{U} = (U, S_U, \tau_U)$ be the system which is simulating the system $\mathcal{T} = (T, S_T, \tau_T)$. There must be some scale factor $c \in \mathbb{N}$ at which $\mathcal{U}$ simulates $\mathcal{T}$, and we define a *representation function* R which maps each $c \times c$ square (sub)assembly in $\mathcal{U}$ to a tile in $\mathcal{T}$ (or empty space if it is incomplete). Each such $c \times c$ block is referred to as a *macrotile*, since that square configuration of tiles from set U represent a single tile from set T. We say that $\mathcal{U}$ simulates $\mathcal{T}$ under representation function R at scale c.

To properly simulate $\mathcal{T}$, $\mathcal{U}$ must have 1. *equivalent productions*, meaning that every supertile producible in $\mathcal{T}$ can be mapped via R to a supertile producible in $\mathcal{U}$, and vice versa, and 2. *equivalent dynamics*, meaning that when any two supertiles α and β, which are producible in $\mathcal{T}$, can combine to form supertile γ, then there are supertiles producible in $\mathcal{U}$ which are equivalent to α and β which can combine to form a supertile equivalent to γ, and vice versa. Note that especially the formal definitions for equivalent dynamics include several technicalities related to the fact that multiple supertiles in $\mathcal{U}$ may map to a single supertile in $\mathcal{T}$, among other issues. Please see [14] for details.

We say that a tile set U is *intrinsically universal* for a class of tile assembly systems if, for every system in that class, a system can be created for which 1. U is the tile set, 2. there is some initial configuration which consists of supertiles created from tiles in U, where those "input" supertiles are constructed to encode information about the system being simulated, and perhaps also singleton tiles from U, 3. a representation function which maps macrotiles in the simulator to tiles in the simulated system, and 4. under that representation function, the simulator has equivalent productions and equivalent dynamics to the simulated system. Essentially, there is one tile set which can simulate any system in the class, using only custom configured input supertiles.

3 Transforming STAM$^+$ Systems from Arbitrary to Bounded Signal Complexity

In this section, we demonstrate methods for reducing the signal complexity of STAM$^+$ systems with $\tau = 1$ or $\tau > 1$ and results related to reducing signal complexity. First, we define terms related to the complexity of STAM systems, and then state our results for signal complexity reduction.

We now provide informal definitions for fan-out and mutual activation. For more rigorous definitions, see [14].

Definition 2. *For an STAM system $\mathcal{T} = (T, \sigma, \tau)$, we say that $\mathcal{T}$ contains* **fan-out** *iff there exists a glue g on a tile $t \in T$ such that whenever g binds, it triggers the activation or deactivation of more than* 1 *glue on t.*

Definition 3. *For an STAM system $\mathcal{T} = (T, \sigma, \tau)$, we say that $\mathcal{T}$ contains* **mutual activation** *iff $\exists t_1, t_2 \in T$ with glue g on adjacent edges of t_1 and t_2 such that whenever t_1 and t_2 bind by means of glue g, the binding of g causes the activation or deactivation of other glues on both t_1 and t_2.*

3.1 Impossibility of Eliminating Both Fan-Out and Mutual Activation at $\tau = 1$

We now discuss the impossibility of completely eliminating both fan-out and mutual activation at temperature 1. Consider the signal tiles in Figure 1 and let $\mathcal{T} = (T, 1)$ be the STAM$^+$ system where T consists of exactly those tiles. Theorem 1 shows that at temperature 1, it is impossible to completely eliminate both fan-out and mutual activation. In other words, any STAM$^+$ simulation of $\mathcal{T}$ must contain some instance of either fan-out or mutual activation. The intuitive idea is that the only mechanism for turning on glues is binding, and at temperature 1 we cannot control when glues in the `on` state bind. Hence any binding pair of glues that triggers some other glue must do so by means of a sequence of glue bindings leading from the source of the signal to the signal to be turned `on`. Hence there must be paths to both of the triggered glues from the single originating glue where at some point a single binding event fires two signals. We will see that this is not the case at temperature 2 since we can control glue binding through cooperation there.

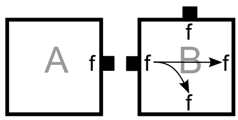

Fig. 1. An example of a tile set where fan-out and mutual activation cannot be completely removed. The glue f on the west edge of tile type B signals two other glues.

Theorem 1. *At temperature 1, there exists an STAM$^+$ system $\mathcal{T}$ such that any STAM$^+$ system $\mathcal{S}$ that simulates $\mathcal{T}$ contains fan-out or mutual activation.*

The proof of Theorem 1 can be found in [14].

3.2 Eliminating Either Fan-Out or Mutual Activation

In this section we will discuss the possibility of eliminating fan-out from an STAM$^+$ system. We do this by simulating a given STAM$^+$ system with a simplified STAM$^+$ system that contains no fan-out, but does contain mutual activation. A slight modification to the construction that we provide then shows that mutual activation can be swapped for fan-out.

Definition 4. *An n-*simplified STAM tile set *is an STAM tile set which has the following properties: (1) the full-tile signal complexity is limited to a fixed constant $n \in \mathbb{N}$, (2) there is no fan-out, and (3) fan-in is limited to 2. We say that an STAM system $\mathcal{T} = (T, \sigma, \tau)$ is n-simplified if T is n-simplified.*

Theorem 2. *For every STAM$^+$ system $\mathcal{T} = (T, \sigma, \tau)$, there exists a 2-simplified STAM$^+$ system $\mathcal{S} = (S, \sigma', \tau)$ which simulates $\mathcal{T}$ with scale factor $O(|T|^2)$ and tile complexity $O(|T|^2)$.*

To prove Theorem 2, we construct a macrotile such that every pair of signal paths that run in parallel are never contained on the same tile. This means that at most two signals are ever on one tile since it is possible for a tile to contain at most two non-parallel (i.e. crossing) signals. In place of fan-out, we use mutual activation gadgets (see Figure 3) within the *fan-out zone*. Similarly, we use a *fan-in zone* consisting of tiles that merge incoming signals two at a time, in order to reduce fan-in. For examples of these zones, see Figure 2. Next, we print a circuit (a system of signals) around the perimeter of the macrotile which ensures that the external glues (the glues on the edges of the macrotiles that cause macrotiles to bind to one another) are not turned on until a macrotile is fully assembled. More details of the construction can be found in [14] .

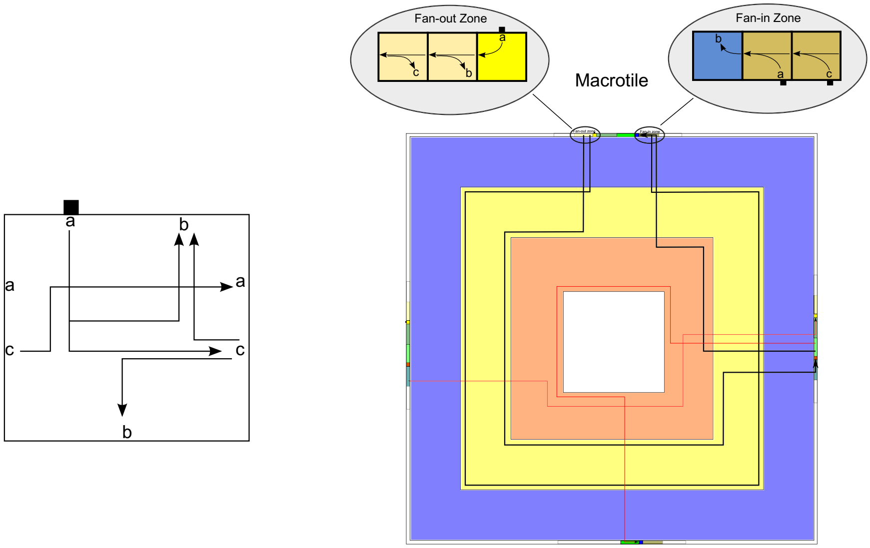

Fig. 2. A tile with 5 signals (left) and the STAM$^+$ macrotile that simulates it (right). Here, the yellow squares represent glue a, the blue square represents glue b and the orange squares represent glue c. The color of each frame corresponds to the glue of the same color. For example on the tile to be simulated (left) there is a signal that runs from glue a to glue c. In order to simulate this signaling, a signal runs from the fan-out zone of glue a (the yellow glue) to the frame associated with glue a on the north edge. The signal then wraps around the frame until it reaches the east side on which glue c lies. Then the signal enters the fan-in zone of glue c.

To further minimize the number of signals per tile at $\tau > 1$, cooperation allows us to reduce the number of signals per tile required to just 1. To achieve this result, we modify the construction used to show Theorem 2, and prove Theorem 3. The details of the modification are in [14] .

Theorem 3. *For every STAM$^+$ system $\mathcal{T} = (T, \sigma, \tau)$ with $\tau > 1$, there exists a* 1*-simplified STAM$^+$ system $\mathcal{S} = (S, \sigma', \tau)$ which simulates $\mathcal{T}$ with scale factor $O(|T|^2)$ and tile complexity $O(|T|^2)$.*

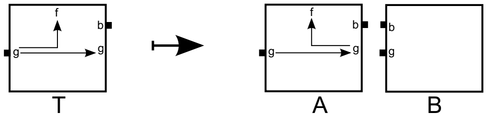

Fig. 3. An example of a mutual activation gadget consisting of tiles A and B without fan-out simulating, at $\tau = 1$, the functionality of tile T which has fan-out. The glue b represents the generic glues which holds the macrotile together. The idea is to "split" the signals from the west glue g on tile A into two signals without using fan-out. Once the west glue g on tile A binds, it turns on the east glue g on tile A. Then, when the east glue g on tile A binds to tile B, it triggers glue f. Thus, the east glue g triggers both the west glue g and glue f without fan-out.

3.3 Summary of Results

At temperature 1, the minimum signal complexity obtainable in general is 2 and while it is possible to eliminate either fan-in or mutual activation, it is impossible to eliminate both. For temperatures greater than 1, cooperation allows for signal complexity to be reduced to just 1 and for both fan-in and mutual activation to be completely eliminated. Table 1 gives a summary of these two cases of reducing signal complexity and shows the cost of such reductions in terms of scale factor and tile complexity.

Table 1. The cost of reducing signal complexity at $\tau = 1$ and at $\tau > 1$

Temperature	Signal per Tile	Scale Factor	Tile Complexity	Contains Fan-In / Mutual Activation
1	2	$O(\|T\|^2)$	$O(\|T\|^2)$	one or the other
> 1	1	$O(\|T\|^2)$	$O(\|T\|^2)$	neither

4 A 3D 2HAM Tile Set Which Is IU for the STAM$^+$

In this section we present our main result, namely a 3D 2HAM tile set which can be configured to simulate any temperature 1 or 2 STAM$^+$ system, at temperature 2. It is notable that although three dimensions are fundamentally required by the simulations, only two planes of the third dimension are required.

Theorem 4. *There is a 3D tile set U such that, in the 2HAM, U is intrinsically universal at temperature* 2 *for the class of all 2D STAM$^+$ systems where $\tau \in \{1, 2\}$. Further, U uses no more than* 2 *planes of the third dimension.*

To prove Theorem 4, we let $\mathcal{T}' = (T', S', \tau)$ be an arbitrary STAM$^+$ system where $\tau \in \{1, 2\}$. For the first step of our simulation, we define $\mathcal{T} = (T, S, \tau)$ as a 2-simplified STAM$^+$ system which simulates $\mathcal{T}'$ at scale factor $m' = O(|T'|^2)$, tile complexity $O(|T'|^2)$, as given by Theorem 2, and let the representation function for that simulation be $R' : B^T_{m'} \dashrightarrow T'$. We now show how to use tiles from a single, universal tile set U to form an initial configuration $S_\mathcal{T}$ so that the 3D 2HAM system $\mathcal{U}_\mathcal{T} = (U, S_\mathcal{T}, 2)$ simulates $\mathcal{T}$ at scale factor $m = O(|T| \log |T|)$ under representation function $R : B^U_m \dashrightarrow T$. This results in $\mathcal{U}_\mathcal{T}$ simulating $\mathcal{T}'$ at a scale factor of $O(|T'|^4 \log(|T'|^2))$ via the composition of R and R'. Note that throughout this section, τ refers to the temperature of the simulated systems $\mathcal{T}$ and $\mathcal{T}'$, while the temperature of $\mathcal{U}_{\mathcal{T}'}$ is always 2.

4.1 Construction Overview

In this section, due to restricted space we present the 3D 2HAM construction at a very high level. Please see [14] for more details.

Assuming that T is a 2-simplified STAM$^+$ tile set derived from T', we note that for each tile in T: 1. glue deactivation is not used, 2. it has ≤ 2 signals, 3. it has no fan-out, and 4. fan-in is limited to 2. To simulate $\mathcal{T}$, we create an input supertile $\sigma_\mathcal{T}$ from tiles in U so that $\sigma_\mathcal{T}$ fully encodes $\mathcal{T}$ in a rectangular assembly where each row fully encodes the definition of a single tile type from T. Beginning with an initial configuration containing an infinite count of that supertile and the individual tile types from U, assembly begins with the growth of a row on top of (i.e. in the $z = 1$ plane) each copy of $\sigma_\mathcal{T}$. The tiles forming this row nondeterministically select a tile type $t \in T$ for the growing supertile to simulate, allowing each supertile the possibility of simulating exactly one $t \in T$, and each such t to be simulated. Once enough tiles have attached, that supertile maps to the selected t via the representation function R, and at this point we call it a *macrotile*.

Each such macrotile grows as an extension of $\sigma_\mathcal{T}$ in $z = 0$ to form a square ring with a hole in the center. The growth occurs clockwise from $\sigma_\mathcal{T}$, creating the west, north, east, then south sides, in that order. As each side grows, the information from the definition of t which is relevant to that side is rotated so that it is presented on the exterior edge of the forming macrotile. The second to last stage of growth for each side is the growth of geometric "bumps and dents" near the corners, which ensure that any two macrotiles which attempt to combine along adjacent edges must have their edges in perfect alignment for any binding to occur. The final stage of growth for each side is to place the glues which face the exterior of the macrotile and are positioned correctly to represent the glues which begin in the `on` state for that side.

Once the first side of a macrotile completes (which is most likely to be the west side, but due to the nondeterministic ordering of tile additions it could potentially be any side), that macrotile can potentially bind to another macrotile, as long as the tiles that they represent would have been able to do so in $\mathcal{T}$. Whenever macrotiles do bind to each other, the points at which any binding glues exist allow for the attachment of duples (supertiles consisting of exactly 2

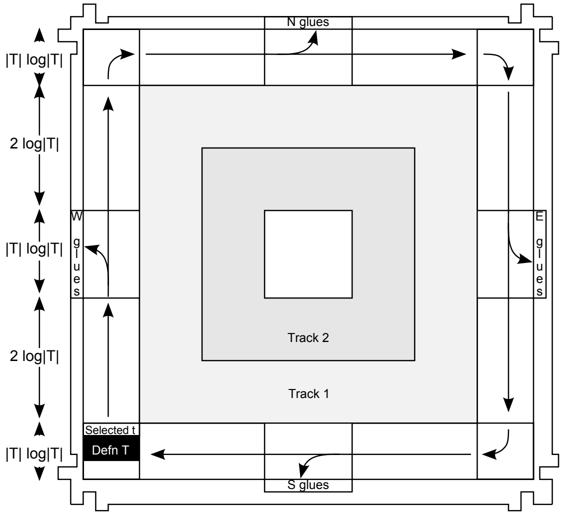

Fig. 4. A high level sketch of the components and formation of a macrotile, including dimensions, not represented to scale

tiles) on top of the two binding tiles (in $z = 1$). These duples initiate the growth of rows in $z = 1$ which move inward on each macrotile to determine if there is information encoded which specifies a signal for that simulated glue to fire. If not, that row terminates. If so, it continues growth by reading the information about that signal (i.e. the destination side and glue), and then growth continues which carries that information inward to the hole in the center of the macrotile. Once there, it grows clockwise in $z = 0$ until arriving at the correct side and glue, where it proceeds to initiate the growth of a row in $z = 1$ out to the edge of the macrotile in the position representing the correct glue. Once it arrives, it initiates the addition of tiles which effectively change the state of the glue from `latent` to `on` by exposing the necessary glue(s) to the exterior of the macrotile.

The width of the center hole is carefully specified to allow for the maximum necessary 2 "tracks" along which fired signals can travel, and growth of the signal paths is carefully designed to occur in a zig-zag pattern such that there are well-defined "points of competition" which allow two signals which are possibly using the same track to avoid collisions, with the second signal to arrive growing over the first, rotating toward the next inward track, and then continuing along that track. Further, the positioning of the areas representing the glues on each edge is such that there is always guaranteed to be enough room for the signals to perform the necessary rotations, inward, and outward growth. If it is the case that both signals are attempting to activate the same glue on the same side, when the second signal arrives, the row growing from the innermost track toward the edge of the macrotile will simply run into the "activating" row from the first signal and halt, since there is no need for both to arrive and in the STAM such a situation simply entails that signal being discarded. (Note that this construction can be modified to allow for any arbitrary full-tile signal complexity n for a given tile set by simply increasing the number of tracks to n, and all growth will remain correct and restricted to $z \in \{0, 1\}$.)

This construction allows for the faithful simulation of $\mathcal{T}$ by exploiting the fact that the activation of glues by fired signals is completely asynchronous in the STAM, as is the attachment of any pair of supertiles, and both processes are being represented through a series of supertile binding events which are similarly asynchronous in the 2HAM. Further, since the signals of the STAM$^+$ only ever activate glues (i.e. change their states from `latent` to `on`), the constantly "forward" direction of growth (until terminality) in both models ensures that the simulation by $\mathcal{U}_{\mathcal{T}}$ can eventually produce representations of all supertiles in $\mathcal{T}$, while never generating supertiles that don't correctly map to supertiles in $\mathcal{T}$ (equivalent production), and also that equivalent dynamics are preserved.

Theorem 5. *For every $\tau > 1$, there is a 3D tile set U_τ such that, in the 2HAM, U_τ is IU at temperature τ for the class of all 2D STAM$^+$ systems where of temperature τ. Further, U uses no more than 2 planes of the third dimension.*

To prove Theorem 5, we create a new tile set U_τ for each τ from the tile set of Theorem 4 by simply creating $O(\tau)$ new tile types which can encode the value of the strength of the glues of T in $\sigma_{\mathcal{T}}$, and which can also be used to propagate that information to the edges of the macrotiles. For the exterior glues of the macrotiles, just as strength 2 glues were split across two tiles on the exterior of the macrotiles, so will τ-strength glues, with one being of strength $\lceil \tau/2 \rceil$ and the other $\lfloor \tau/2 \rfloor$. All glues which appear on the interior of the macrotile are changed so that, if they were strength 1 glues they become strength $\lceil \tau/2 \rceil$, and if they were strength 2 they become strength τ. In this way, the new tile set U_τ will form macrotiles exactly as before, while correctly encoding glues of strengths 1 through τ on their exteriors, and the systems using it will correctly simulate STAM$^+$ systems at temperature τ.

5 Conclusion

We have shown how to transform STAM$^+$ systems (at temperature 1 or > 1) of arbitrary signal complexity into STAM$^+$ systems which simulate them while having signal complexity no greater than 2 and 1, respectively. However, if the original tile set being simulated is T, the scale factor and tile complexity of the simulating system are approximately $O(|T|^2)$. It seems that these factors cannot be reduced in the worst case, i.e. when a tile of T has a copy of every glue of the tile set on each side, and each copy of each glue on the tile activates every other, yielding a signal complexity of $O(|T|^2)$. However, whether or not this is a true lower bound remains open, as well as what factors can be achieved for more "typical" systems with much lower signal complexity.

A significant open problem which remains is that of generalizing both constructions (the signal reduction and the 3D 2HAM simulation) to the unrestricted STAM. Essentially, this means correctly handling glue deactivation and possible subassembly dissociation. While this can't be handled within the standard 3D 2HAM where glue bonds never change or break, it could perhaps be possible if negative strength (i.e. repulsive) glues are allowed (see [10] for a discussion of various formulations of models with negative strength glues). However, it appears that since both constructions use scaled up macrotiles to represent individual tiles of the systems being simulated, there is a fundamental barrier. The STAM assumes that whenever two tiles are adjacent, all pairs of matching glues across the adjacent edge which are both currently `on` will immediately bind (which is in contrast to other aspects of the model, which are asynchronous). Since both constructions trade the ability of individual tile edges in the STAM to have multiple glues with scaled up macrotiles which distribute those glues across individual tiles of the macrotile edges, it appears to be difficult if not impossible to maintain the correct simulation dynamics. Basically, a partially formed side of a macrotile could have only a subset of its initially `on` glues in place, but enough to allow it to bind to another macrotile. At that point, if glue deactivations are initiated which result in the dissociation of the macrotile before the remaining glues of the incomplete macrotile side assemble, then in the simulating system, those additional glues won't ever bind. However, in the simulated system they would have. This results in a situation where, after the dissociation, the simulated system would potentially have additional pending glue actions (initiated by the bindings of the additional glues) which the simulating system would not, breaking the simulation.

Overall, laboratory experiments continue to show the plausibility of physically implementing signalling tiles [17], while previous theoretical work [18] shows some of their potential, and the results in this paper demonstrate how to obtain much of that power with simplified tiles. We feel that research into self-assembly with active components has a huge amount of potential for future development, and continued studies into the various tradeoffs (i.e. complexity of components, number of unique component types, scale factor, etc.) between related models provide important context for such research. We hope that our results help to contribute to continued advances in both theoretical and experimental work along these lines.

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