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INTRINSIC UNIVERSALITY IN SELF-ASSEMBLY

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Abstract. We show that the Tile Assembly Model exhibits a strong notion of universality where the goal is to give a single tile assembly system that simulates the behavior of any other tile assembly system. We give a tile assembly system that is capable of simulating a very wide class of tile systems, including itself. Specifically, we give a tile set that simulates the assembly of any tile assembly system in a class of systems that we call *locally consistent*: each tile binds with exactly the strength needed to stay attached, and that there are no glue mismatches between tiles in any produced assembly.

Our construction is reminiscent of the studies of *intrinsic universality* of cellular automata by Ollinger and others, in the sense that our simulation of a tile system T by a tile system U represents each tile in an assembly produced by T by a $c \times c$ block of tiles in U, where c is a constant depending on T but not on the size of the assembly T produces (which may in fact be infinite). Also, our construction improves on earlier simulations of tile assembly systems by other tile assembly systems (in particular, those of Soloveichik and Winfree, and of Demaine et al.) in that we simulate the actual process of self-assembly, not just the end result, as in Soloveichik and Winfree's construction, and we do not discriminate against infinite structures. Both previous results simulate only temperature 1 systems, whereas our construction simulates tile assembly systems operating at temperature 2.

Key words and phrases: Biological computing, Molecular computation, intrinsic universality, self-assembly.

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1. Introduction

The development of DNA tile self-assembly has moved nanotechnology closer to the goal of engineering useful systems that assemble themselves from molecular components. Since Seeman's pioneering work in the 1980s [18], many laboratory experiments have shown that DNA tiles can be designed to spontaneously assemble with one another into desired structures [17]. As physical and mathematical error-suppression techniques improve [3, 8, 11, 19, 21, 24], this molecular programming of matter will become practical at ever larger scales.

The Tile Assembly Model, developed by Winfree [16, 23], is a discrete mathematical model of DNA tile self-assembly that enables us to explore the potentialities and limitations of this kind of molecular programming. It is essentially an "effectivization" of classical Wang tiling [22] in which the fundamental components are un-rotatable, but translatable square "tile types" whose sides are labeled with glue "colors" and "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 strength on their abutting sides matches with total strength at least a certain ambient "temperature." Extensive refinements of the abstract Tile Assembly Model were given by Rothemund and Winfree in [15,16]. (Consult the technical appendix for full details of the abstract Tile Assembly Model.) The model deliberately oversimplifies the physical realities of self-assembly, but Winfree proved that it is Turing universal [23]. This implies that the process of self-assembly can be algorithmically directed.

In this paper we investigate whether the Tile Assembly Model is capable of a much stronger notion of universality where the goal is to give a single tile assembly system that simulates the behavior of any other tile assembly system. We give a tile assembly system that is capable of simulating a very wide class of tile systems, including itself. Our notion of simulation is inspired by, but somewhat stronger than, intrinsic universality in cellular automata [2, 7, 12, 13]. In our construction a simulated tile assembly system is encoded in a seed assembly of the simulating system. This encoding is done in a very simple (logspace computable) way. The seed assembly then grows to form an assembly that is a re-scaled (larger) version of the simulated assembly, where each tile in the latter is represented by a supertile (square of tiles) in the simulator. Not only this, but each of the possible (nondeterministically chosen) assembly sequences of the simulated tile system is modeled by a possible assembly sequence in the simulating system (also nondeterministically chosen). The latter property of our system is important and highlights one way in which this work distinguishes itself from other notions of intrinsic universality found in the cellular automata literature: not only do we want to simulate the final assembly but we also want the simulator to have the ability to dynamically simulate each of the valid growth processes that could lead to that final assembly.

A second distinguishing property of our universal tile set is that it simulates nondeterministic choice in a "fair" way. An inherent feature of the Tile Assembly Model is the fact there are often multiple (say k) tiles that can go into any one position in an assembly sequence, and one of these k is nondeterministically chosen. One way to simulate this feature is to nondeterministically choose which of k supertiles should grow in the analogous (simulated) position. However, due to the size blowup in supertiles caused by encoding an arbitrary-sized simulated tile set into a fixed-sized universal tile set, it seems that we need to simulate one nondeterministic choice by using a sequence of nondeterministic choices within the supertile. Interpreting the nondeterministic choice to be made according to uniform random selection, if the selection by the simulating tile set is implemented in a naïve way, this can lead to unfair selection: when selecting 1 supertile out of k, some supertiles are selected with extremely low probability. To get around this problem, our system uses a random number selector that chooses a random tile with probability $\Theta(1/k)$ and so we claim that we are simulating nondeterminism in a "fair" way.

Thirdly, the Tile Assembly Model has certain geometric constraints that are not seen in cellular automata, and this adds some difficulty to our construction. Existing techniques for constructing intrinsically universal cellular automata are not directly applicable to tile assembly. For example, when a tile is placed at a position, that position can not be reused for further "computation" and this presents substantial difficulties when trying to fit the various components of our construction into a supertile. Each supertile encodes the entire simulated tile set and has the functionality to propagate this information to other (yet to be formed) supertiles. Not only this, each supertile must decide which tile placement to simulate, whilst making (fair) nondeterministic choices if necessary. Finally, each supertile should correctly propagate (output) sides that are consistent with the chosen supertile. We give a number of figures to illustrate how these goals were met within the geometric constraints of the model.

Our main result presented in this paper is, in some sense, a continuation of some previous results in self-assembly. For instance, Soloveichik and Winfree [20] exhibit a beautiful connection between the Kolmogorov complexity of a finite shape X and the minimum number of tiles types needed to assemble X. It turns out that their construction can be made to be "universal" in the following sense: there exists a tile set T, such that for every "temperature 1" tile assembly system that produces a finite shape whose underlying binding graph (a.k.a., backbone graph) is a spanning tree, T simulates the given temperature 1 tile system with a corresponding blow-up in the scale. Note that this method restricts the simulated tile system to be temperature 1, i.e., a non-cooperative tile assembly system, which are conjectured [6] to produce only the "simplest" of shapes and patterns in the sense of Presburger arithmetic [14].

A similar result, recently discovered by Demaine, Demaine, Fekete, Ishaque, Rafalin, Schweller, and Souvaine [4], established the existence of a general-purpose "staged-assembly" system that is capable of simulating any temperature 1 tile assembly system that produces a "fully connected" finite shape. Note that, in this construction, the scaling factor is proportional to $O(\log |T|)$, where T is the simulated tile set. This construction has the desirable property that the set of tile types belonging to the simulator is general purpose (i.e., the size of the simulator tile set is independent of the to-be-simulated tile set) and all of the information needed to carry out the simulation is, in some sense, encoded in a sequence of laboratory steps. An open question in [4] is whether or not their construction can be augmented to handle temperature 2 tile assembly systems.

Our construction is general enough to be able to simulate powerful and interesting tile sets, yet sufficiently simple so that it actually belongs to the class of tile assembly systems that it can simulate. Modulo re-scaling, our universal tile set can be said to display the characteristics of the entire collection of tile sets in its class. Our construction is a *direct simulation* in that the technique does not involve the simulation of intermediate models (such as circuits or Turing machines), which have been used in intrinsically universal cellular automata constructions [13].

One of the nice properties of intrinsic universality [13] is that it provides a clear definition that facilitates proofs that a given tile set is not universal. We leave as an open problem the intrinsic universality status of the Tile Assembly Model in its full generality.

2. Intrinsic Universality in Self-Assembly

In this section, we define our notion of intrinsic universality of tile assembly systems. It is inspired by, but distinct from, similar notions for cellular automata [13]. Where appropriate, we identify where some part of our definition differs from the "corresponding" parts in [13], typically due to a fundamental difference between the abstract Tile Assembly Model and cellular automata models.

Intuitively, a tile set U is universal for a class $\mathfrak{C}$ of tile assembly systems if U can "simulate", through appropriate setting of the seed assembly to create a tile assembly system $\mathcal{U}$, any tile assembly system in $\mathfrak{C}$, and U is intrinsically universal if the simulation of $\mathcal{T}$ by $\mathcal{U}$ can be done according to a simple "block substitution scheme" where equal-size square blocks of tiles in assemblies produced by $\mathcal{U}$ represent tiles in assemblies produced by $\mathcal{T}$. Since we wish to simulate the entire process of self-assembly, and not only the final result, it is critical that the simulation of $\mathcal{T}$ by $\mathcal{U}$ be such that the "local transition rules" involving intermediate producible (and nonterminal) assemblies of $\mathcal{T}$ be faithfully represented in the simulation.

In the subsequent definitions, given two partial functions f, g, we write $f(x) = g(x)$ if f and g are both defined and equal on x, or if f and g are both undefined on x.

Let $c, c' \in \mathbb{N}$, let $[c : c']$ denote the set $\{c, c+1, \ldots, c'-1\}$, and let $[c]$ denote the set $[0 : c] = \{0, 1, \ldots, c-1\}$, so that $[c]^2$ is the set of c^2 points forming a $c \times c$ square with the origin as the lower-left corner.

The natural analog of a configuration of a cellular automaton is an assembly of a tile assembly system. However, unlike cellular automata in which every cell has a well-defined state, in tile assembly, there is a fundamental difference between a point being empty space and being occupied by a tile. Therefore we keep the convention of representing an assembly as a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$ (for some tile set T), rather than treating empty space as just another type of tile.

Let $\mathcal{T} = (T, \sigma_{\mathcal{T}}, \tau)$ and $\mathcal{S} = (S, \sigma_{\mathcal{S}}, \tau)$ be tile assembly systems. For simplicity, assume that $\sigma_{\mathcal{T}}(0,0)$ is defined, and $\sigma_{\mathcal{T}}$ is undefined on $\mathbb{Z}^2 - \{(0,0)\}$ (i.e., $\mathcal{T}$ is singly-seeded with the seed tile placed at the origin). We will use this assumption of a single seed throughout the paper, but it is not strictly necessary and is only used for simplicity of discussion. Define a *representation function* to be a partial function of the form $r : ([c]^2 \dashrightarrow S) \dashrightarrow T$. That is, r takes a pattern $p : [c]^2 \dashrightarrow S$ of tile types from S painted onto a $c \times c$ square (with locations at which p is undefined representing empty space), and (if r is defined for input p) gives a single tile type from T. Intuitively, r tells us how to interpret $c \times c$ blocks within assemblies of $\mathcal{S}$ as single tiles of T. We write REPR for the set of all representation functions.[1]

[1]Here, r is analogous to Ollinger's ϕ function for mixautomata which maps a state s of the simulated cellular automaton to a set of (blocks of) states in the simulating cellular automaton, however r is defined to map tile block patterns of the simulating tile system to the simulated tile system. So we have phrased our representation in "inverse" terms; i.e., a many-to-one function. In the case of cellular automata, every cellular automaton that is universal with multiple state representations ("intrinsically universal with respect to mixed bulking" in Ollinger's terminology) is known also to be universal with unique state representations ("intrinsically universal with respect to injective bulking"). In contrast, we do not know how to alter our construction so that each tile in the simulated TAS will have a unique representation as a block in the

We say $\mathcal{S}$ *(intrinsically) simulates* $\mathcal{T}$ *with resolution loss* c if there exists a representation function $r : ([c]^2 \dashrightarrow S) \dashrightarrow T$ such that the following conditions hold.

(1) $\operatorname{dom} \sigma_{\mathcal{S}} \subseteq [c]^2$ and $r(\sigma_{\mathcal{S}}) = \sigma_{\mathcal{T}}(0,0)$. That is, the seed assembly of $\mathcal{S}$ represents the seed tile of $\mathcal{T}$.

(2) For every producible assembly $\alpha_{\mathcal{T}} \in \mathcal{A}[\mathcal{T}]$ of $\mathcal{T}$, there is a producible assembly $\alpha_{\mathcal{S}} \in \mathcal{A}[\mathcal{S}]$ of $\mathcal{S}$ such that, for every $x, y \in \mathbb{Z}$,

$$r\left((\alpha_{\mathcal{S}} \upharpoonright ([cx : c(x+1)] \times [cy : c(y+1)])) + (-cx, -cy)\right) = \alpha_{\mathcal{T}}(x,y).$$

That is, the $c \times c$ block at (relative) position (x,y) (relative to the other $c \times c$ blocks; the absolute position is (cx, cy)) of assembly $\alpha_{\mathcal{S}}$ represents the tile type at (absolute) position (x,y) of assembly $\alpha_{\mathcal{T}}$. In this case, write $r^*(\alpha_{\mathcal{S}}) = \alpha_{\mathcal{T}}$; i.e., r induces a function $r^* : \mathcal{A}[\mathcal{S}] \to \mathcal{A}[\mathcal{T}]$.

(3) For all $\alpha_{\mathcal{T}}, \alpha'_{\mathcal{T}} \in \mathcal{A}[\mathcal{T}]$, it holds that $\alpha_{\mathcal{T}} \to_{\mathcal{T}} \alpha'_{\mathcal{T}}$ if and only if there exist $\alpha_{\mathcal{S}}, \alpha'_{\mathcal{S}} \in \mathcal{A}[\mathcal{S}]$ such that $r^*(\alpha_{\mathcal{S}}) = \alpha_{\mathcal{T}}$, $r^*(\alpha'_{\mathcal{S}}) = \alpha'_{\mathcal{T}}$ (in the sense of condition (2)), and $\alpha_{\mathcal{S}} \to_{\mathcal{S}} \alpha'_{\mathcal{S}}$. That is, every valid assembly sequence of $\mathcal{T}$ can be "mimicked" by $\mathcal{S}$, but no other assembly sequences can be so mimicked, so that the meaning of the relation $\to$ is preserved by r^*.[2]

Let $\mathfrak{C}$ be a class of singly-seeded tile assembly systems, and let U be a tile set (with tile assembly systems having tile set U not necessarily elements of $\mathfrak{C}$). Note that every element of $\mathfrak{C}$, REPR, and $\mathsf{FIN}(U)$ is a finite object, hence can be represented in a suitable format for computation in some formal system such as Turing machines. We say U is *(intrinsically) universal* for $\mathfrak{C}$ if there are computable functions $R : \mathfrak{C} \longrightarrow \mathsf{REPR}$ and $A : \mathfrak{C} \longrightarrow \mathsf{FIN}(U)$ such that, for each $\mathcal{T} = (T, \sigma_{\mathcal{T}}, \tau) \in \mathfrak{C}$, there is a constant $c \in \mathbb{N}$ such that, letting $r = R(\mathcal{T})$, $\sigma = A(\mathcal{T})$, and $\mathcal{U}_{\mathcal{T}} = (U, \sigma, \tau)$, $\mathcal{U}_{\mathcal{T}}$ simulates $\mathcal{T}$ with resolution loss c and representation function r. That is, $R(\mathcal{T})$ outputs a representation function that interprets assemblies of $\mathcal{U}_{\mathcal{T}}$ as assemblies of $\mathcal{T}$, and $A(\mathcal{T})$ outputs the seed assembly used to program tiles from U to represent the seed tile of $\mathcal{T}$.

3. An Intrinsically Universal Tile Set

In this section, we exhibit an intrinsically universal tile set for any "nice" tile assembly system. Before proceeding, we must first define the notion of a "nice" tile assembly system. Let $\mathcal{T} = (T, \sigma, 2)$ be a tile assembly system, and $\vec{\alpha}$ be an assembly sequence in $\mathcal{T}$ whose result is denoted as α. We say that $\mathcal{T}$ is *locally consistent* if the following conditions hold.

simulating TAS, since our block assembly depends on the direction(s) of the input sides of the tile, and a single tile type may not have have a unique set of input sides throughout the assembly process. This difference between tile assembly and cellular automata, in which tiles may not have a fixed "neighborhood", may imply that this difference is fundamental and not an artifact of our construction.

[2]Here is another fundamental difference between Ollinger's notion of a global transition function, and our notion of "transitioning" from one assembly to a larger assembly. Ollinger defines "rescaling" of a cellular automaton in such a way that it makes sense to talk about a global transition function that, in a single step, simulates multiple time steps of the simulating cellular automaton (enough of them to simulate a single time step of the simulated cellular automaton). The inherent nondeterminism of tile assembly, and in particular the choice of which frontier location should receive a tile in the next time step, makes such a related definition awkward and perhaps counterproductive, as the number of time steps before a new block is completed is variable, and in particular may be much more than the number of tiles that must be placed in the block before it is completed. Therefore, we keep the original "timescale" of the simulating TAS, rather than speed it up in an attempt to synchronize the time steps of the simulated and simulating TAS's.

(1) For all $\vec{m} \in \text{dom } \alpha - \text{dom } \sigma$,

$$\sum_{\vec{u} \in \text{IN}^{\vec{\alpha}}(\vec{m})} \text{str}_{\alpha(\vec{m})}(\vec{u}) = 2,$$

where $\text{IN}^{\vec{\alpha}}(\vec{m})$ is the set of sides on which the tile that $\vec{\alpha}$ places at location $\vec{m}$ initially binds. That is, every tile initially binds to the assembly with exactly bond strength equal to 2 (either a single strength 2 bond or two strength 1 bonds).

(2) For all producible assemblies $\alpha \in \mathcal{A}[\mathcal{T}]$, $\vec{u} \in U_2$, and $\vec{m} \in \text{dom } \alpha$, if $\alpha(\vec{m} + \vec{u})$ is defined, then the following condition holds:

$$\text{str}_{\alpha(\vec{m})}(\vec{u}) > 0 \Rightarrow \text{label}_{\alpha(\vec{m})}(\vec{u}) = \text{label}_{\alpha(\vec{m}+\vec{u})}(-\vec{u}) \text{ and } \text{str}_{\alpha(\vec{m})}(\vec{u}) = \text{str}_{\alpha(\vec{m}+\vec{u})}(-\vec{u}).$$

While condition (1) of the above definition is reminiscent of the first condition of local determinism [20], the second condition says that there are no (positive strength) label mismatches between abutting tiles. However, we must emphasize that a locally consistent tile assembly system need not be directed, and moreover, even a locally deterministic tile assembly system need not be locally consistent because of the lack of any kind of "determinism restriction" in the latter definition.

The main result of this paper is the following theorem.

Theorem 3.1 (Main theorem)**.** *Let $\mathfrak{C}$ be the set of all locally consistent tile assembly systems. There exists a finite tile set U that is intrinsically universal for $\mathfrak{C}$.*

In the remainder of this section, we prove Theorem 3.1, that is, we show that for every locally consistent tile assembly system $\mathcal{T} = (T, \sigma, 2)$, there exists a seed assembly $\sigma_{\mathcal{T}}$, such that the tile assembly system $\mathcal{S}_{\mathcal{T}} = (U, \sigma_{\mathcal{T}}, 2)$ simulates $\mathcal{T}$ with a resolution loss $c \in \mathbb{N}$ that depends only on the glue complexity of $\mathcal{T}$.

Intuitively, $\mathcal{S}$ simulates $\mathcal{T}$ by growing "supertiles" that correspond to tile types in T. In other words, every supertile is a $c \times c$ block of tiles that is mapped to a tile type $t \in T$. To do this, each supertile that assembles in $\mathcal{S}_{\mathcal{T}}$ contains the full specification of T as a lookup table (a long row of tiles that encodes all of the information in the set of tile types T), analogous to the genome of an organism being fully replicated in each cell of that organism, no matter how specialized the function of the cell. This lookup table is carefully propagated through each supertile in $\mathcal{S}_{\mathcal{T}}$ via a series of "rotation" and "copy" operations – both of which are well-known self-assembly primitives.

3.1. Construction of the Lookup Table

In order to simulate the behavior of $\mathcal{T}$ with $\mathcal{S}_{\mathcal{T}}$, we must first encode the definition of T using tiles from U. We will do this by constructing a "glue lookup table," denoted as $\mathbf{T}_{\mathcal{T}}$, and is essentially the self-assembly version of a kind of hash table. Informally, $\mathbf{T}_{\mathcal{T}}$ is a (very) long string (of tiles from U) consisting of two copies of the definition of the tile set T separated by a small group of spacer symbols. The left copy of the lookup table is the *reverse* of the right copy. The lookup table maps all possible sets of input sides for each tile type $t \in T$ to the corresponding sets of output sides.

3.1.1. *Addresses.* The lookup table $\mathbf{T}_{\mathcal{T}}$ consists of a contiguous sequence of "addresses," which are formed from the definition of T. Namely, for each tile type $t \in T$, we create a unique binary key for each combination of sides of t whose glue strengths sum to exactly 2. Each of these combinations represents a set of sides which *could* potentially serve as the input sides for a tile of type t in a producible assembly in $\mathcal{T}$.

We say that a *pad* is an ordered triple (g, d, s) where g is a glue label in T, $d \in \{North, South, East, West\} \approx \{N, S, E, W\}$ is an edge direction, and $s \in \{0, 1, 2\}$ is an allowable glue strength. Note that a set of four pads – one for each direction d – fully specifies a tile type. We use $\text{Pad}(t, d)$ to denote the pad on side d of the tile type $t \in T$

Let $\text{Bin}(p)$ be the binary encoding of a pad $p = (g, d, s)$, consisting of the concatenation of the following component binary strings:

(1) g (*glue specification*): Let G be the set of glue types from all edges with positive glue strengths in $T \cup \{g_{\text{null}}\}$ (a.k.a., the null glue). Fix some ordering $g_{\text{null}} \leq g_0 \leq g_1 \leq \cdots$ of the set G. The binary representation of g_i is the binary value of i padded with 0's to the left (as necessary) to ensure that the string is exactly $\lceil \log(|G| + 1) \rceil$ bits.
(2) d (*direction*): If $d = N$ (E, S, or W), append 00 (01, 10, or 11, respectively).
(3) s (*strength*): If $s = 1$ (2) append 0 (1).

Note that $\lceil \log(|G| + 1) \rceil + 2 + 1$ is the length of the binary string encoding an arbitrary pad p, and is a constant that depends only on T.

An *address* is a binary string that represents a set of pads which, themselves, can potentially serve as the input sides of some tile type $t \in T$. It can be composed of one of the two following binary strings:

(1) A prefix of zeros, $0^{\lceil \log(|G|+1) \rceil + 3}$, followed by $\text{Bin}(p)$ for $p = (g, d, 2)$, or
(2) the concatenation of $\text{Bin}(p_1)$ and $\text{Bin}(p_2)$ for $p_1 = (g_1, d_1, 1)$ and $p_2 = (g_2, d_2, 1)$. The ordering of $\text{Bin}(p_1)$ and $\text{Bin}(p_2)$ in an address must be consistent with the following orderings: EN, SE, WS, NW, NS, EW.

Note that it is possible for more than one tile type $t \in T$ to share a set of input pads and therefore an address.

3.1.2. *Encoding of T.* We will now construct the string $w_{\mathcal{T}}$, which will represent the definition of T. Intuitively, $w_{\mathcal{T}}$ will be composed of a series of "entries." Each entries is associated to exactly one address of a tile type $t \in T$ and specifies the pads for the output sides of t. In this way, once the input sides for a supertile have formed, the corresponding pads can be used to form an address specifying (a set of) appropriate output pads. Note that since more than one tile type may share an address in a nondeterministic tile assembly system, more than one tile type may share a single entry.

We define an *entry* to be a string beginning with '#' followed by zero or more "sub-entries", each corresponding to a different tile type, separated by semicolons. Let A be the set of all binary strings representing every address created for each $t \in T$. The string $w_{\mathcal{T}}$ will consist of $1 + \max A$ entries for addresses 0 to $\max A$. The i^{th} entry, denoted as e_i, corresponds to the i^{th} address, which may or may not be in A (if it is not, then e_i is empty).

We say that a *sub-entry* consists of a string specifying the pads for the output sides of a tile type $t \in T$. Let e_i be the entry containing a given sub-entry (note that i is the address of e_i), and $T_i \subseteq T$ be the set of tile types addressable by i (i.e., the set of tile types for which i is a valid address). The entry e_i will be comprised of exactly $|T_i|$ sub-entries. For $0 \leq k < j$, the k^{th} sub-entry in e_i, where $t_k \in T_i$ is the k^{th} element of T_i (relative to some fixed ordering), is the string $\mathrm{OUT}(N), \mathrm{OUT}(E), \mathrm{OUT}(S), \mathrm{OUT}(W)$ (the commas in the previous string are literal) with $\mathrm{OUT}(d) = \mathrm{Bin}(\mathrm{Pad}(t_k, d))^R$ if the glue for $\mathrm{Pad}(t_k, d)$ is not g_{null} and d is not a component of the address i, otherwise $\mathrm{OUT}(d) = \lambda$. Intuitively, a sub-entry is a comma-separated list of the (reversed) binary representations of the pads for an addressed tile type, but including only pads whose glues are not g_{null} and whose directions are not a part of the address (and therefore input sides).

We will now use the string $w_{\mathcal{T}}$ to construct the lookup table $\mathbf{T}_{\mathcal{T}}$.

3.1.3. *Full specification of* $\mathbf{T}_{\mathcal{T}}$. We now give the full specification for the lookup table $\mathbf{T}_{\mathcal{T}}$. First, define the following strings: $w_0 =$ '$>$', $w_1 =$ '$<$ %% $>$', $w_2 =$ '$<$'. Now let $\mathbf{T}_{\mathcal{T}}$ be as follows.

$$\mathbf{T}_{\mathcal{T}} = \mathrm{sb}(w_0 \circ w_{\mathcal{T}} \circ w_1 \circ (w_{\mathcal{T}})^R \circ w_2),$$

where, for strings x and y, $x \circ y$ is the concatenation of x and y, and $\mathrm{sb} : \Sigma^* \to \Sigma^*$ is defined to "splice blanks" into its input: between every pair of adjacent symbols in the string x, a single '$\sqcup$' (blank) symbol is inserted to create $\mathrm{sb}(x)$. This splicing of blanks is required to be able to read from the table without "locking it from view", when reading the table for operations that require growing a column of tiles in towards the table (as opposed to away from it), a blank column is used, and for growing a column away from the table, a symbol column is used so that the symbol can be propagated to the top of the column for later copying.

3.1.4. *The Lookup Procedure.* In our construction, when a supertile t^* that is simulating a tile type $t \in T$ forms, we must overcome the following problem: once we combine the input pads (given as the output pads of the supertiles to which t^* attaches), how do we use $\mathbf{T}_{\mathcal{T}}$ to lookup the output pads for t^*? In what follows, we briefly describe how we achieve this. In other words, we show how an address, a string of random bits, and a copy of $\mathbf{T}_{\mathcal{T}}$ are used to compute the pad values for the non-input sides of a supertile. A detailed figure and example of this procedure can be found in the technical appendix.

For ease of discussion and without loss of generality, we assume that the row of tiles encoding $\mathbf{T}_{\mathcal{T}}$ (assembled West to East) and the column of tiles encoding an address and a random string of bits (assembled North to South at the West end of $\mathbf{T}_{\mathcal{T}}$) are fully assembled, forming an 'L' shape with no tiles in the area between them. For other orientations of the table and address the logical behavior is identical, simply rotated.

Intuitively, the assembly of the lookup procedure assembles column wise in a zig-zag fashion from left to the right. In the "first phase," a counter initialized to 0 is incremented in each column where the value of the tile in the representation of $\mathbf{T}_{\mathcal{T}}$ is a ';', thus counting up at each entry contained in $\mathbf{T}_{\mathcal{T}}$. Once that number matches the value of the given address (which, along with the random bits is copied through this procedure), the entry e corresponding to that address has been reached and a new counter begins which counts the number of sub-entries n in that entry. Note that for directed tile systems, $n \leq 1$. Once the end of that entry is encountered, yet another counter, initialized to 0, begins and increments on each remaining entry until the end of the first copy of $w_{\mathcal{T}}$ is reached (the number n is propagated through to the right). This counts the number of entries, denoted as m, between e and the end of the lookup table. The "second phase" is used to perform, in some sense, an operation equivalent to calculating $p = b \mod n$, where b is the binary value of the string of random bits required for the lookup procedure (this is essentially how we simulate nondeterministic assemblies). This essentially selects the index of the sub-entry in e which will be used, thus completing the random selection of one of the possibly many tile types contained in entry e.

In the current version of our construction, we merely use a random number selection procedure reminiscent of the more involved (but more uniform) random selection procedures discussed in [5]. Although it is possible to incorporate these more advanced techniques into our construction (and thus achieve a higher degree of uniformity in the simulation of randomized tile systems), we choose not to do so for the sake of simplicity.

Next, a reverse counter, a.k.a., a subtractor, counts down at each entry from m to 0, and by the way we constructed $\mathbf{T}_{\mathcal{T}}$, this final counter obtains the value 0 at the entry e (in the reverse of $w_{\mathcal{T}}$). Now, another subtractor counts from p to 0 to locate the correct sub-entry that was selected randomly. Finally, each pad in the sub-entry is rotated "up and to the right," and the group of pads is propagated through the remainder of the lookup table, thus ending with the values of the non-input pads represented in the rightmost column.

3.2. Supertile design

A supertile s is a subassembly in $\mathcal{S}_{\mathcal{T}}$ consisting of a $c \times c$ block of tiles from T, where c depends on the glue complexity of T. Each s can be mapped to a unique tile type $t \in T$. In our construction there are two logical supertile designs. The first, denoted *type-0*, simulates tile additions in $\mathcal{T}$ in which there are 2 input sides, each with glue strength = 1. The second, denoted *type-1*, simulates the addition of tiles via a single strength 2 bond.

While there are several differences in the designs of *type-0* and *type-1* supertiles, one commonality is how their edges are defined. Namely each input or output edge of any supertile is defined by the same sequence of variable values. Since the edges for each direction are rotations of each other, we will discuss only the layout of the south side of a supertile. From left to right, the tiles along the south edge of a supertile will represent a string formed by the concatenation (in order) of the strings: $\mathbf{T}_{\mathcal{T}}$, $\mathrm{Bin}(\mathrm{Pad}(t, S))$, $0^{c'}$, $\mathrm{Bin}(\mathrm{Pad}(t, S))$, and $\mathbf{T}_{\mathcal{T}}$. Note that c' is a constant that depends on the glue complexity of T.

3.2.1. *Type-0 Supertiles (i.e., simulating tiles that attach via two single-strength bonds).*

When a tile binds to an assembly in $\mathcal{T}$ with two input sides whose glues are each single strength, there are $\binom{4}{2} = 6$ possible combinations of directions for those input sides: north and east (NE), north and south (NS), north and west (NW), east and south (ES), east and west (EW), and south and west (SW). These combinations can be divided into two categories, those in which the sides are opposite each other (NS and EW), and those in which the sides are adjacent to each other (NE, NW, ES, and SW).

Opposite Input Sides: Supertiles which represent tile additions with two opposite input sides, NS and EW, are logically identical to rotations of each other, so here we will only describe the details of a supertile with NS input sides. Figure 1 shows a detailed image depicting the formation of an NS supertile, with arrows giving the direction of growth for each portion and numbers specifying the order of growth. For ease of discussion and without loss of generality, we assume that the rows of tiles which form the input sides of a supertile have fully formed before any other part of the supertile assembles. The first portions to assemble are the center blocks to the interior of each input side, labeled 1. This subassembly forms a square in which a series of nondeterministic selections of tile types is used to generate a random sequence of bits. These bits are propagated to the left

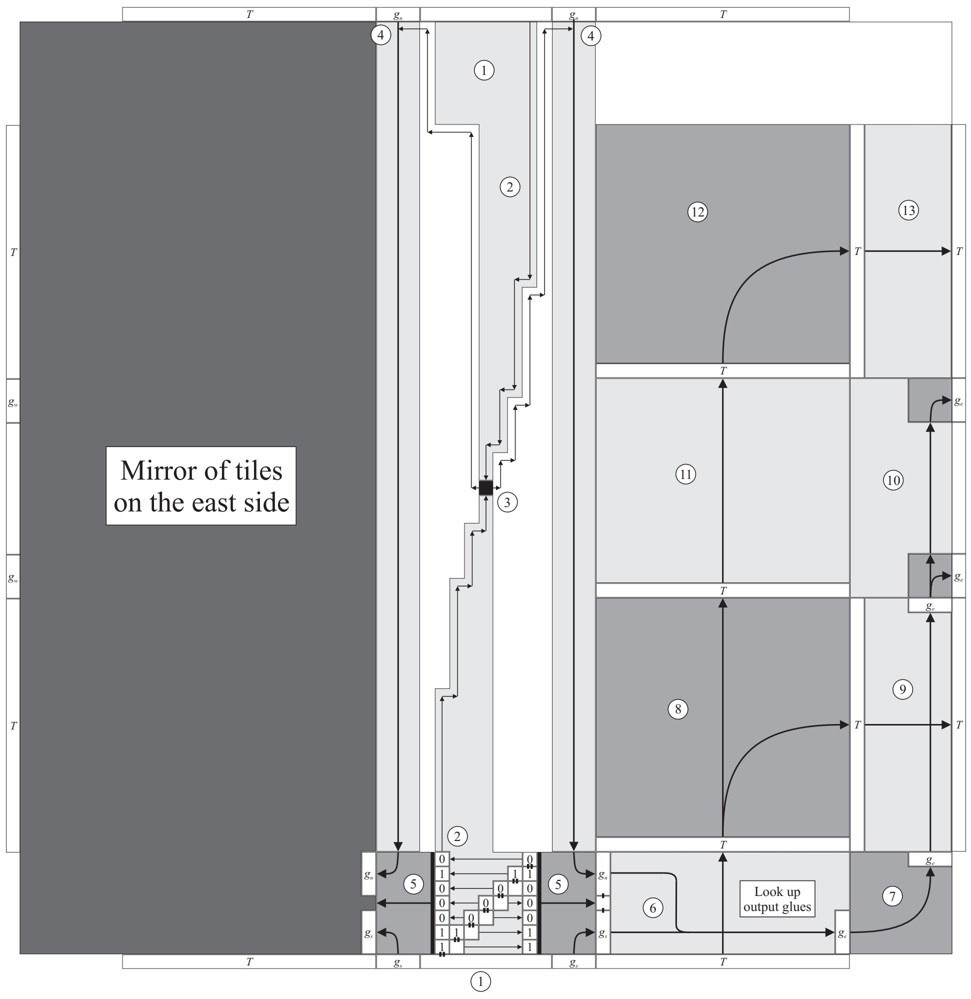

FIGURE 1. NS supertile

and right sides of the block, to ensure that each side uses the same random bits for the randomized selection after the sides have been "sealed off" from each other by "probes" described next. Once that block has completed, a log-width binary subtractor, which is half the width of the block, assembles. The subtractors from the north and south count down from a specified value (that depends on $\mathcal{T}$ and is encoded into the seed supertile) to 0, and shrink in width until they terminate at positions adjacent to the center square of the block. These subtractors are "probes" that grow to the center where the direction of the input sides (the *type*) is detected. It is at this point that the central (black in the figure) tile can attach. It is this tile which determines the *type* of the supertile (NS in this case) because it is unique to the combination of directions from which the inputs came. At this point, symmetry is broken and two paths of tiles assemble from the center back towards the north side. They in turn initiate the growth of subassemblies which propagate the value of the north input pad down towards the South of the supertile. Once that growth nears the southern side, the two input pads are rotated and brought together, with this combination of input pads forming an *address* in the lookup table. In the manner described previously,

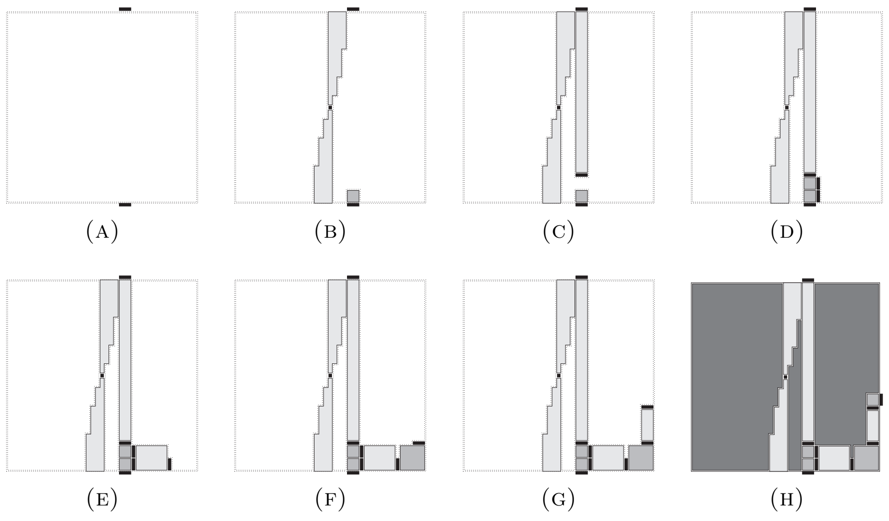

FIGURE 2. Intuitive depiction of (a portion of) the self-assembly of a type-0 supertile. Note that the lookup procedure is performed in (d) and (e).

this address along with the random bits generated within block 1 (which are also passed through block 5) is used to form the subassembly of block 6 whose southern row contains a representation of $\mathbf{T}_{\mathcal{T}}$ and results in the correct output pads being represented in the final column of that block. Note that Figure 1 only shows the details of the east side of the block since the West side is an identical but rotated version. Finally, subassemblies 7 through 13 form which rotate and pass the necessary information to the locations where it must be correctly deposited to form the output sides of the supertile. Every side of a supertile that is not an input side receives an output pad, even if it is for the null glue (in which case it does not initiate the growth of the input side of a possible adjacent supertile).

Additional details of our construction can be found in the technical appendix.

4. Conclusion

We have shown that there is a single tile set U in Winfree's abstract tile assembly model, which can be "programmed" through appropriate setting of a finite seed assembly, to simulate a scaled version of the assembly process of any in a wide class of *locally consistent* tile assembly systems, those that have the properties that each tile binds with exactly strength 2, and there are no glue mismatches in any producible assembly. This captures a wide class of tile assembly systems, including counters, square-builders and other shape-building tile assembly systems, and the tile assembly systems described in [1, 10, 16, 20].

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5. Appendix

5.1. The abstract Tile Assembly Model

All logarithms in this paper are base 2. We work in the 2-dimensional discrete space $\mathbb{Z}^2$. Define the set $U_2 = \{(0,1),(1,0),(0,-1),(-1,0)\}$ to be the set of all *unit vectors*, i.e., vectors of length 1 in $\mathbb{Z}^2$. All *graphs* in this paper are undirected. A *grid graph* is a graph $G = (V, E)$ in which $V \subseteq \mathbb{Z}^2$ and every edge $\{\vec{a}, \vec{b}\} \in E$ has the property that $\vec{a} - \vec{b} \in U_2$.

Intuitively, a tile type t is a unit square that can be translated, but not rotated, having a well-defined "side $\vec{u}$" for each $\vec{u} \in U_2$. Each side $\vec{u}$ of t has a "glue" with "label" $\text{label}_t(\vec{u})$ – a string over some fixed alphabet Σ – and "strength" $\text{str}_t(\vec{u})$ – a nonnegative integer – specified by its type t. Two tiles t and t' that are placed at the points $\vec{a}$ and $\vec{a}+\vec{u}$ respectively, *bind* with *strength* $\text{str}_t(\vec{u})$ if and only if $(\text{label}_t(\vec{u}), \text{str}_t(\vec{u})) = (\text{label}_{t'}(-\vec{u}), \text{str}_{t'}(-\vec{u}))$.

Given a set T of tile types, an *assembly* is a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$, with points $\vec{x} \in \mathbb{Z}^2$ at which $\alpha(\vec{x})$ is undefined interpreted to be empty space, so that $\text{dom}\ \alpha$ is the set of points with tiles. α is *finite* if $|\text{dom}\ \alpha|$ is finite. For assemblies α and α', we say that α is a *subassembly* of α', and write $\alpha \sqsubseteq \alpha'$, if $\text{dom}\ \alpha \subseteq \text{dom}\ \alpha'$ and $\alpha(\vec{x}) = \alpha'(\vec{x})$ for all $x \in \text{dom}\ \alpha$. α' is a *single-tile extension* of α if $\alpha \sqsubseteq \alpha'$ and $\text{dom}\ \alpha' - \text{dom}\ \alpha$ is a singleton set. In this case, we write $\alpha' = \alpha + (\vec{m} \mapsto t)$, where $\{\vec{m}\} = \text{dom}\ \alpha' - \text{dom}\ \alpha$ and $t = \alpha'(\vec{m})$

The *binding graph of* an assembly α is the grid graph $G_\alpha = (V, E)$, where $V = \text{dom}\ \alpha$, and $\{\vec{m}, \vec{n}\} \in E$ if and only if (1) $\vec{m} - \vec{n} \in U_2$, (2) $\text{col}_{\alpha(\vec{m})}(\vec{n} - \vec{m}) = \text{col}_{\alpha(\vec{n})}(\vec{m} - \vec{n})$, and (3) $\text{str}_{\alpha(\vec{m})}(\vec{n} - \vec{m}) > 0$. An assembly is *$\tau$-stable*, where $\tau \in \mathbb{N}$, if it cannot be broken up into smaller assemblies without breaking bonds of total strength at least τ; i.e., if every cut of G_α has weight at least τ, where the weight of an edge is the strength of the sides of tiles that it connects. In contrast to the model of Wang tiling, the nonnegativity of the strength function implies that glue mismatches between adjacent tiles do not prevent a tile from binding to an assembly, so long as sufficient binding strength is received from the (other) sides of the tile at which the glues match.

Self-assembly begins with a *seed assembly* σ (typically assumed to be finite and τ-stable) and proceeds asynchronously and nondeterministically,[3] with tiles adsorbing one at a time to the existing assembly in any manner that preserves stability at all times, formally modeled as follows.

A *tile assembly system* (*TAS*) is an ordered triple $\mathcal{T} = (T, \sigma, \tau)$, where T is a finite set of tile types, σ is a seed assembly with finite domain, and τ is the temperature. In subsequent sections of this paper, we assume that $\tau = 2$ unless explicitly stated otherwise. An *assembly sequence* of a TAS $\mathcal{T} = (T, \sigma, \tau)$ is a (possibly infinite) sequence $\vec{\alpha} = (\alpha_i \mid 0 \leq i < k)$ of assemblies in which $\alpha_0 = \sigma$ and each α_{i+1} is obtained from α_i by the "τ-stable" addition of a single tile.[4] The *result* of an assembly sequence $\vec{\alpha}$ is the unique assembly $\text{res}(\vec{\alpha})$ satisfying $\text{dom}\ \text{res}(\vec{\alpha}) = \bigcup_{0 \leq i < k} \text{dom}\ \alpha_i$ and, for each $0 \leq i < k$, $\alpha_i \sqsubseteq \text{res}(\vec{\alpha})$. For all assemblies

[3]There are multiple senses in which a tile system can be nondeterministic. A trivial sense is that the location of attachment, if there is more than one candidate, is selected nondeterministically. Such systems may still be deterministic in a stronger sense that they will lead to a unique final assembly. We employ a stronger version of nondeterminism in which the tile capable of binding to a *single* position of an assembly is not fixed.

[4]By "τ-stable addition", we mean the addition of a tile at a site where the sum of binding strengths of the tile to the assembly α_i is at least the temperature. It is easy to see that such additions preserve τ-stability; i.e., α_i is τ-stable $\implies$ α_{i+1} is τ-stable.

$\alpha, \alpha' : T \dashrightarrow \mathbb{Z}^2$, we write $\alpha \to_{\mathcal{T}} \alpha'$ (or $\alpha \to \alpha'$ when $\mathcal{T}$ is clear from context) to denote that there is an assembly sequence $\vec{\alpha} = (\alpha_i \mid 0 \leq i < k)$ such that $\alpha_0 = \alpha$ and $\mathrm{res}(\vec{\alpha}) = \alpha'$. It has been shown [15] that for all tile assembly systems $\mathcal{T}$, $\to_{\mathcal{T}}$ is a transitive, reflexive relation on assemblies of $\mathcal{T}$.

We write $\mathcal{A}[\mathcal{T}]$ to denote the set of all results of assembly sequences $\vec{\alpha} = (\alpha_i \mid 0 \leq i < k)$ of $\mathcal{T}$ such that $\alpha_0 = \sigma$, known as the *producible assemblies* of $\mathcal{T}$. A producible assembly α is *terminal*, and we write $\alpha \in \mathcal{A}_{\Box}[\mathcal{T}]$, if no tile can be stably added to it. Given a tile set T, let $\mathsf{FIN}(T)$ denote the set of all finite assemblies of T. $\mathcal{T}$ is *directed* (a.k.a., *deterministic*, *confluent*) if $|\mathcal{A}_{\Box}[\mathcal{T}]| = 1$.

For an assembly $\alpha : \mathbb{Z}^2 \dashrightarrow T$ and set of points $A \subseteq \mathbb{Z}^2$, define α *restricted to* A, written $\alpha \restriction A$ to be the assembly defined for all $\vec{m} \in \mathbb{Z}^2$ by $(\alpha \restriction A)(\vec{m}) = \alpha(\vec{m})$ if $\vec{m} \in A$ and $\alpha(\vec{m})$ is defined, and $(\alpha \restriction A)(\vec{m})$ is undefined otherwise. Given a vector $\vec{v} \in \mathbb{Z}^2$, define α *translated by* $\vec{v}$, written $\alpha + \vec{v}$, to be the assembly defined for all $\vec{m} \in \mathbb{Z}^2$ by $(\alpha + \vec{v})(\vec{m}) = \alpha(\vec{m} - \vec{v})$.

5.2. Lookup Example

We now consider an example tile assembly system $\mathcal{T} = (T, \sigma, 2)$ where T is the tile set defined in Figure 3 and σ is simply a single tile of type S located at point $(0, 0)$. In this section we will describe how $\mathcal{T}$ can be simulated using T_{univ}.

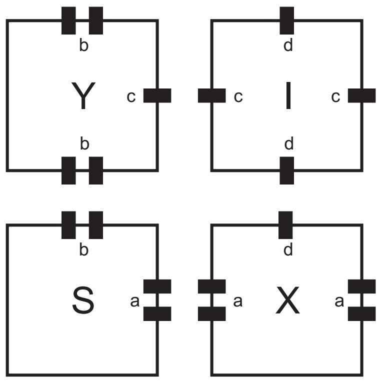


FIGURE 3. Example tile set T_{sim}

The set of glues, G, for T is (a, b, c, d), with binary representations $(001, 010, 011, 100)$, respectively, and 000 reserved for g_{null}.

The value for a_{max} will be the address for tile type I corresponding to '$(d, S, 1), (c, E, 1)$', namely 100100011010.

5.3. Additional Details

Adjacent Input Sides: Supertiles which represent tile additions with two adjacent input sides, NE, NW, ES, and SW, are logically identical to rotations of each other, so here we will only describe the details of a supertile with SW input sides.

Figure 5 shows a detailed image depicting the formation of an SW supertile. It is logically very similar to an NS supertile. However, once the center, black tile is placed then a row grows to the West, which initiates the growth of the subassemblies that propagate

Table 1. Pads and their binary representations (Note that there are no spaces in the actual binary representations, they've just been added to this table for convenience)

Pad	Bin(Pad)
$(b, N, 2)$	010 00 1
$(a, E, 2)$	001 01 1
$(g_{null}, S, 0)$	000 10 0
$(g_{null}, W, 0)$	000 11 0
$(c, E, 1)$	011 01 0
$(b, S, 2)$	010 10 1
$(a, W, 2)$	001 11 1
$(d, N, 1)$	100 00 0
$(d, S, 1)$	100 10 0
$(c, W, 1)$	011 11 0

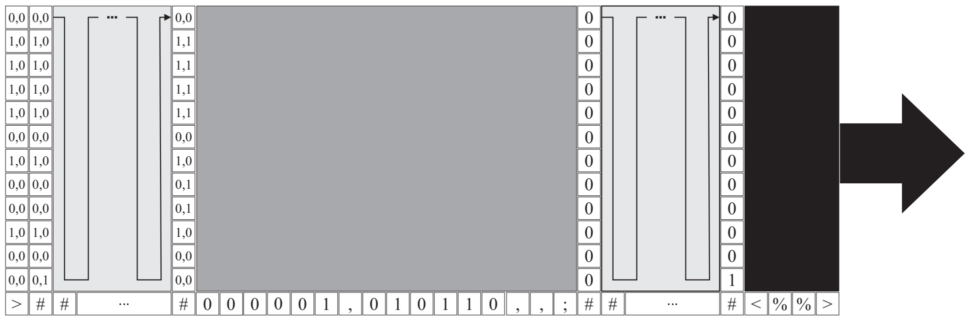
Table 2. Tile types, their possible addresses, and the binary representations of those addresses

Tile type	Addresses	Binary representations
S	$(b, N, 2)$	000 00 0 010 00 1
	$(a, E, 2)$	000 00 0 001 01 1
X	$(a, E, 2)$	000 00 0 001 01 1
	$(a, W, 2)$	000 00 0 001 11 1
Y	$(b, S, 2)$	000 00 0 010 10 1
	$(b, N, 2)$	000 00 0 010 00 1
I	$(c, E, 1), (d, N, 1)$	011 01 0 100 00 0
	$(d, N, 1), (d, S, 1)$	100 00 0 100 10 0
	$(d, N, 1), (c, W, 1)$	100 00 0 011 11 0
	$(d, S, 1), (c, E, 1)$	100 10 0 011 01 0
	$(c, E, 1), (c, W, 1)$	011 01 0 011 11 0
	$(c, W, 1), (d, S, 1)$	011 11 0 100 10 0

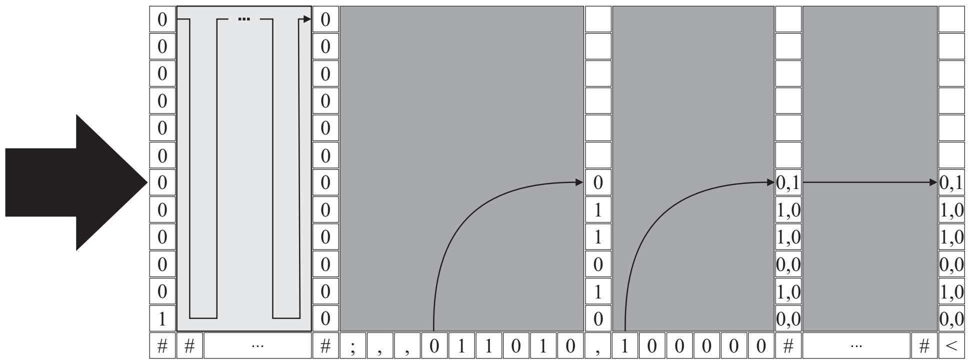
the west input pad to the proper location to be combined with the South pad. After the output pads are determined, then both the north and the east sides are assembled using the information from that single lookup table.

5.3.1. *Type-1 Supertiles, (i.e., simulating tiles that attach via a single double-strength bond).* Supertiles that represent tile additions with a single, strength 2, input side (N, S, E, or W) are logically identical to rotations of each other, so here we will only describe the details of a supertile with a south strength 2 input side.

Figure 6 shows a detailed image depicting the formation of an strength 2, South supertile. Notice that for supertiles of this type, the address for the lookup table is formed from only one pad, so as soon as the assembly of block 1 completes with the random string of bits, then the pad can be rotated up and the output pads computed. Finally, all three output pads are propagated around and "dropped off" in their respective locations.



(A) The initial phase of the lookup procedure. Notice the pairs of bits stored in the leftmost column. The leftmost bits represent the address of the desired set of output glues; the rightmost bits represent the counter used to "search" for appropriate entry in the table. The blank region is where we "randomly" select the output glues.



(B) The final phase of the lookup procedure. The subentries corresponding to the output glues are rotated up into column format and pass through the remainder of the table.

FIGURE 4. Example lookup of the output pads for address 011110100100 (or "$(c, W, 1), (d, S, 1)$"). Assume the sub-assembly begins with the bottom and left rows completely formed, and then proceeds column by column from left to right.

5.4. Constructing the Seed Supertile: $\sigma_{\mathcal{T}}$

Here we describe how the seed $\sigma_{\mathcal{T}}$ for $\mathcal{S}_{\mathcal{T}}$ is formed. First, using the procedure described previously, the lookup table $\mathbf{T}_T$ is generated. Then, using the value of $|\mathbf{T}_T|$ and the lengths of the binary representations of pads in T, the value to be used as the maximum value for the binary subtractors that grow to the center of type-0 supertiles can be calculated. Finally, tile types unique to the seed assembly are used to fill in the corners and interior of the the supertile that represents $\sigma_{\mathcal{T}}$.

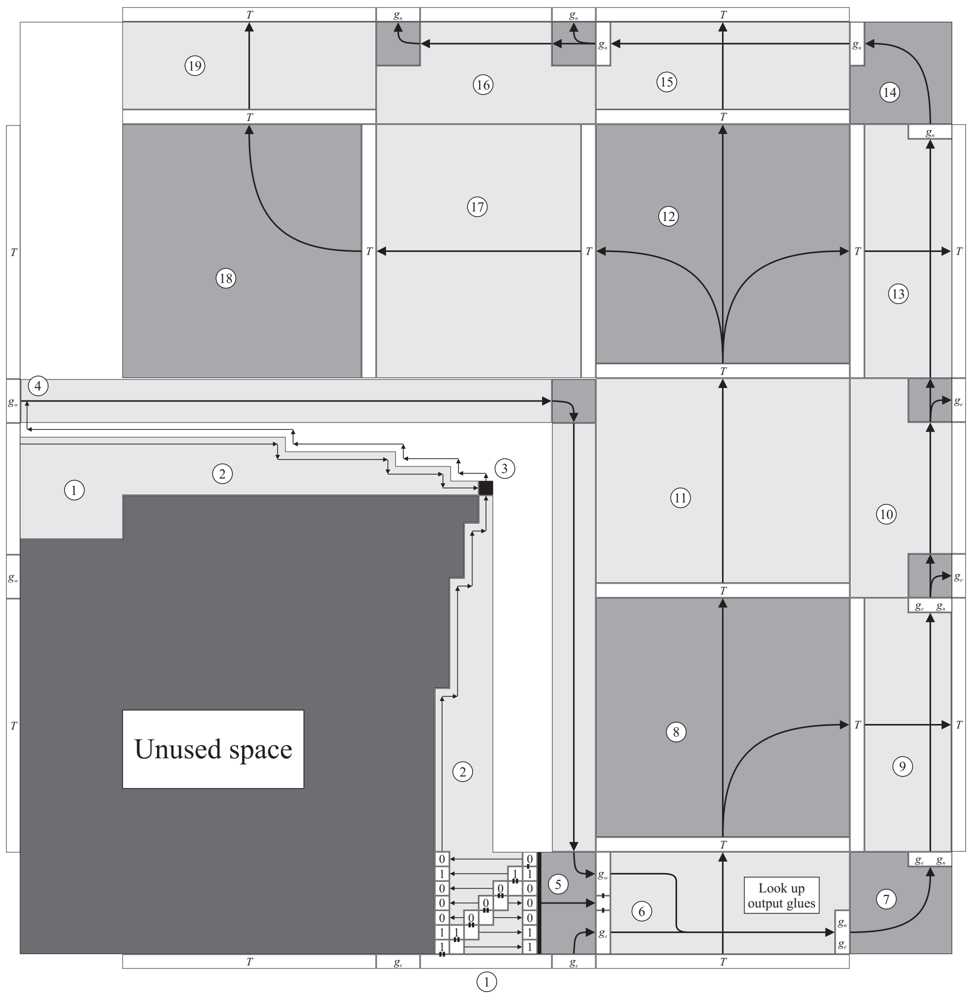


FIGURE 5. SW supertile

5.5. A Universal Computer Simulating Itself

We note that all the tile assembly systems produced using tiles from U by our construction satisfy the two properties of local consistency. We assumed for simplicity that the simulated system $\mathcal{T}$ is singly-seeded, whereas clearly $\mathcal{U}$ is not since the setting of a complex seed assembly is the means by which U is programmed. If we wish U to be able to simulate systems with larger seeds, say, k tiles in size, this can of course be done by programming the seed assembly of U to start with k blocks instead of a single block. But this does not imply U can simulate itself, as this construction can only simulate tile assembly systems with a strictly smaller seed assembly, if the resolution loss is 2 or greater.

The most theoretically striking reason to require a "universal computer" to be contained within the class of computers that it simulates is the idea that a computer can simulate itself. This result is used, with deep results, in the recursion theorem, and in Peter Gács' construction [9] of a fault-tolerant one-dimensional cellular automaton. While U (or more accurately tile assembly systems with U as the tile set) is in some sense contained in the

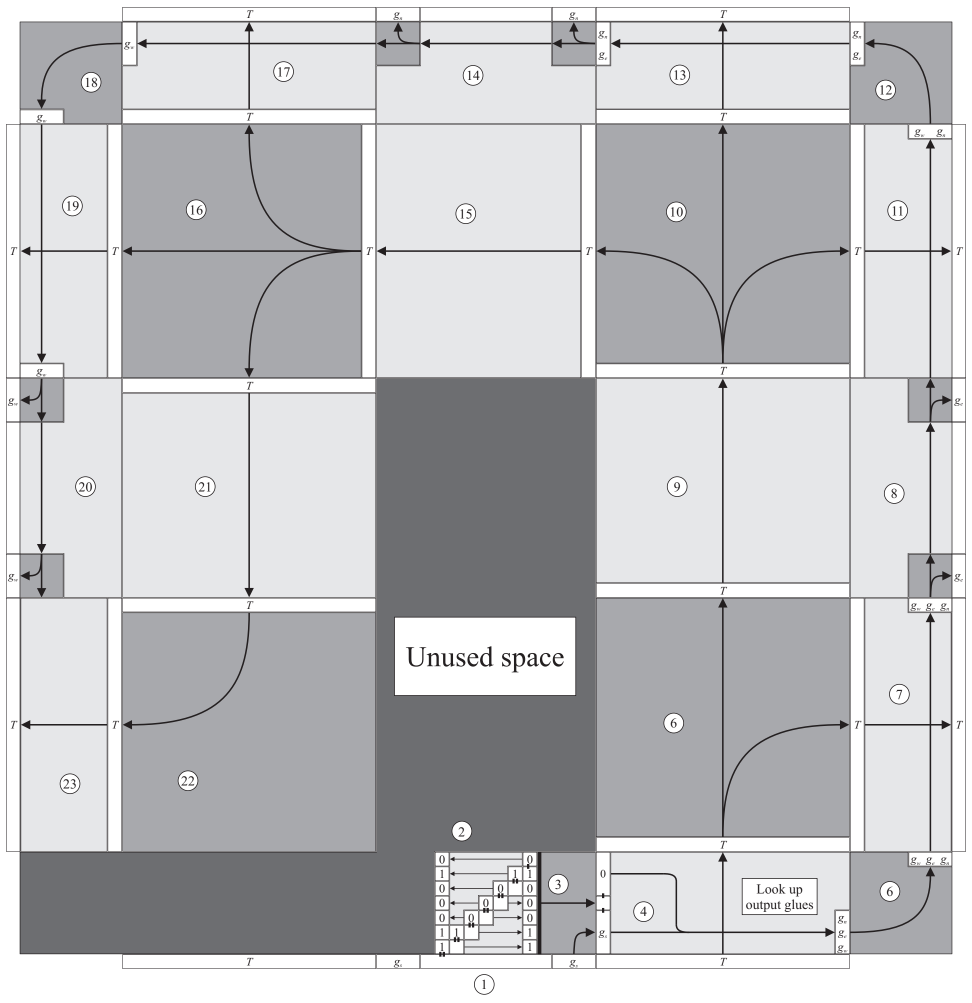


FIGURE 6. Strength 2 supertile

class of tile assembly systems that it simulates, it cannot simulate itself simulating itself simulating itself ... etc., as in Gács' construction. At some finite level, we must have "$\mathcal{U}$ simulates $\mathcal{U}$ simulating $\mathcal{U}$ ... simulating $\mathcal{U}$ simulating some other system $\mathcal{T}$".

5.6. Resolution Loss

We omit a formal analysis, but it is easy to bound the resolution loss of our construction in terms of the number of glues g in the system. In particular, the table used for lookup contains one entry for each pair of strength-1 glues in the system, and 1 entry for each strength-2 glue, and each entry consists of at most three output glues, each of which requires $\log g$ bits to represent. The size of this table asymptotically dominates the size of the blocks, so the resolution loss c is at most $O(g^2 \log g)$.

This is not tight for certain tile assembly systems. In particular, let G be the $g \times g$ Boolean matrix where entry (i, j) is 1 if the i^{th} and j^{th} glues ever function as inputs together[5], and 0 otherwise. If G is dense, then our resolution loss bound is tight, and if G is sparse, then it is not tight. It is not difficult to construct tile assembly systems to achieve either condition, implying in particular that our encoding of the table is inefficient for certain tile assembly systems.

An alternative encoding, which is more complicated to implement, is to store the table as key-value pairs, in which the input glues and output glues are encoded explicitly in each entry of the table, the input glues (addresses) serving as keys and the output glues serving as values. The tiles doing the lookup would then do a comparison between the address being searched and the keys stored in the table, rather than counting to the correct entry using the address as the start value for the counter. By storing only entries in which the addresses are actually used in some assembly sequence, the size of the table can be made $O(g' \log g)$, where g' is the number of pairs of input glues that are actually used. Since each glue that is an input for one tile type is an output for another, this implies $g' \geq g/2 = \Omega(g)$. Hence the savings is potentially up to a multiplicative factor of g.

[5]More precisely, if there exists an assembly sequence in which a tile type having those glues ever binds with positive strength on each of the glues