

Self-Assembly of Infinite Structures¹

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Abstract

We review some recent results related to the self-assembly of infinite structures in the Tile Assembly Model. These results include impossibility results, as well as novel tile assembly systems in which shapes and patterns that represent various notions of computation self-assemble. Several open questions are also presented and motivated.

1 Introduction

The simplest mathematical model of nanoscale self-assembly is the Tile Assembly Model (TAM), an effectivization of Wang tiling [24, 25] that was introduced by Winfree [27] and refined by Rothmund and Winfree [18, 19]. (See also [1, 17, 22].) As a basic model for the self-assembly of matter, the TAM has allowed researchers to explore an assortment of avenues into both laboratory-based and theoretical approaches to designing systems that self-assemble into desired shapes or autonomously coalesce into patterns that, in doing so, perform computations.

Actual physical experimentation has driven lines of research involving kinetic variations of the TAM to deal with molecular concentrations, reaction rates, etc. as in [26], as well as work focused on error prevention and error correction [6, 21, 28]. For examples of the impressive progress in the physical realization of self-assembling systems, see [20, 23].

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Divergent from, but supplementary to, the laboratory work, much theoretical research involving the TAM has also been carried out. Interesting questions concerning the minimum number of tile types required to self-assemble shapes have been addressed in [2, 4, 19, 22]. Different notions of running time and bounds thereof were explored in [5, 7, 14]. Variations of the model where temperature values are intentionally fluctuated and the ensuing benefits and tradeoffs can be found in [4, 10]. Systems for generating randomized shapes or approximations of target shapes were investigated in [5, 11]. This is just a small sampling of the theoretical work in the field of algorithmic self-assembly.

However, as different as they may be, the above mentioned lines of research share a common thread. They all tend to focus on the self-assembly of *finite* structures. Clearly, for experimental research, this is a necessary limitation. Further, if the eventual goal of most of the theoretical research is to enable the development of fully functional, real world self-assembly systems, a valid question is: “Why care about anything other than finite structures?” This is the question that we address in this paper.

This paper surveys a collection of recent findings related to the self-assembly of *infinite* structures in the TAM. As a theoretical exploration of the TAM, this collection of results seeks to define absolute limitations on the classes of shapes that self-assemble. These results also help to explore how fundamental aspects of the TAM, such as the inability of spatial locations to be reused and their immutability, affect and limit the constructions and computations that are achievable.

In addition to providing concise statements and intuitive descriptions of results, we also define and motivate a set of open questions in the hope of furthering this line of research. First, we begin with some preliminary definitions and constructions that will be referenced throughout this paper.

2 Preliminaries

2.1 The Tile Assembly Model

This section provides a very brief overview of the TAM. See [13, 18, 19, 27] for other developments of the model. Our notation is that of [13]. We work in the 2-dimensional discrete space \mathbb{Z}^2 . We write U_2 for the set of all *unit vectors*, i.e., vectors of length 1 in \mathbb{Z}^2 . We write $[X]^2$ for the set of all 2-element subsets of a set X . All *graphs* here are undirected graphs, i.e., ordered pairs $G = (V, E)$, where V is the set of *vertices* and $E \subseteq [V]^2$ is the set of *edges*.

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 $\vec{a} - \vec{b} \in U_2$. The *full grid graph* on a set $V \subseteq \mathbb{Z}^2$ is the graph $G_V^\# = (V, E)$ in which E contains *every* $\{\vec{a}, \vec{b}\} \in [V]^2$ such 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” of “color” $\text{col}_t(\vec{u})$ - a string over some fixed alphabet Σ - and “strength” $\text{str}_t(\vec{u})$ - a natural number - 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 $(\text{col}_t(\vec{u}), \text{str}_t(\vec{u})) = (\text{col}_{t'}(-\vec{u}), \text{str}_{t'}(-\vec{u}))$.

Given a set T of tile types, an *assembly* is a partial function $\alpha : \mathbb{Z}^2 \dashrightarrow T$. An assembly is τ -*stable*, where $\tau \in \mathbb{N}$, if it cannot be broken up into smaller assemblies without breaking bonds whose strengths sum to at least τ .

Self-assembly begins with a *seed assembly* σ and proceeds asynchronously and nondeterministically, with tiles adsorbing one at a time to the existing assembly in any manner that preserves stability at all times. 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. An *assembly sequence* in a TAS $\mathcal{T} = (T, \sigma, 1)$ 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. We write $\mathcal{A}[\mathcal{T}]$ for the *set of all producible assemblies of \mathcal{T}* . An assembly α is *terminal*, and we write $\alpha \in \mathcal{A}_\square[\mathcal{T}]$, if no tile can be stably added to it. We write $\mathcal{A}_\square[\mathcal{T}]$ for the *set of all terminal assemblies of \mathcal{T}* . A TAS \mathcal{T} is *directed*, or *produces a unique assembly*, if it has exactly one terminal assembly i.e., $|\mathcal{A}_\square[\mathcal{T}]| = 1$. The reader is cautioned that the term “directed” has also been used for a different, more specialized notion in self-assembly [3].

A set $X \subseteq \mathbb{Z}^2$ *weakly self-assembles* if there exists a TAS $\mathcal{T} = (T, \sigma, 1)$ and a set $B \subseteq T$ such that $\alpha^{-1}(B) = X$ holds for every assembly $\alpha \in \mathcal{A}_\square[\mathcal{T}]$. A set X *strictly self-assembles* if there is a TAS \mathcal{T} for which every assembly $\alpha \in \mathcal{A}_\square[\mathcal{T}]$ satisfies $\text{dom } \alpha = X$. The reader is encouraged to consult [22] for a detailed discussion of *local determinism* - a general and powerful method for proving the correctness of tile assembly systems.

2.2 Discrete Self-Similar Fractals

In this subsection we introduce discrete self-similar fractals, and zeta-dimension.

Definition Let $1 < c \in \mathbb{N}$, and $X \subseteq \mathbb{N}^2$. We say that X is a *c-discrete self-similar fractal*, if there is a (non-trivial) set $V \subseteq \{0, \dots, c-1\} \times \{0, \dots, c-1\}$

such that $X = \bigcup_{i=0}^{\infty} X_i$, where X_i is the i^{th} stage satisfying $X_0 = \{(0,0)\}$, and $X_{i+1} = X_i \cup (X_i + c^i V)$. In this case, we say that V generates X .

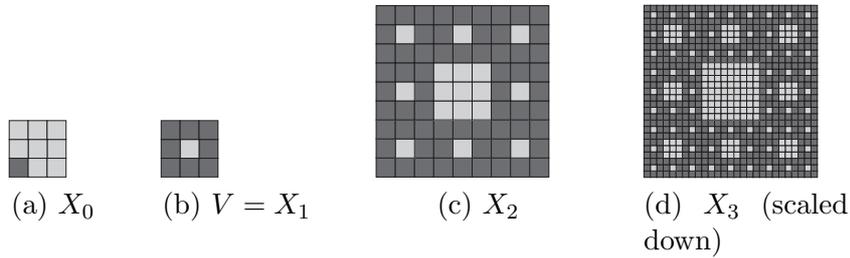


Fig. 1. Example of a c -discrete self-similar fractal ($c = 3$), the Sierpinski carpet

The most commonly used dimension for discrete fractals is zeta-dimension, which we refer to in this paper.

Definition [8] For each set $A \subseteq \mathbb{Z}^2$, the *zeta-dimension* of A is

$$\text{Dim}_\zeta(A) = \limsup_{n \rightarrow \infty} \frac{\log |A_{\leq n}|}{\log n},$$

where $A_{\leq n} = \{(k, l) \in A \mid |k| + |l| \leq n\}$. It is clear that $0 \leq \text{Dim}_\zeta(A) \leq 2$ for all $A \subseteq \mathbb{Z}^2$.

2.3 The Wedge Construction

In order to perform universal computation in the TAM, we make use of a particular TAS called the “wedge construction” [15]. The wedge construction, based on Winfree’s proof of the universality of the TAM [27], is used to simulate an arbitrary Turing machine $M = (Q, \Sigma, \Gamma, \delta, q_0, q_A, q_R)$ on a given input string $w \in \Sigma^*$ in a temperature 2 TAS.

The wedge construction works as follows. Every row of the assembly specifies the complete configuration of M at some time step. M starts in its initial state with the tape head on the leftmost tape cell and we assume that the tape head never moves left off the left end of the tape. The

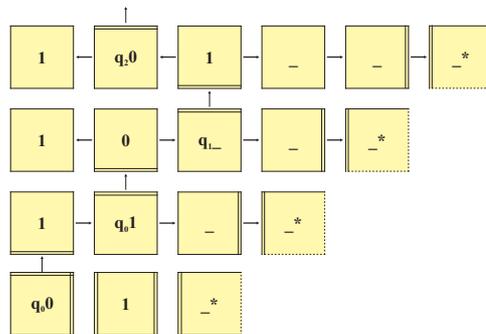


Fig. 2: Example of the first four rows of a sample wedge construction which is simulating a Turing machine M on the input string ‘01’

seed row (bottommost) encodes the initial configuration of M . There is a special tile representing a blank tape symbol as the rightmost tile in the seed row. Every subsequent row grows by one additional cell to the right. This gives the assembly the wedge shape responsible for its name. Figure 2 shows the first four rows of a wedge construction for a particular TM, with arrows depicting a possible assembly sequence.

3 Strict Self-Assembly

The self-assembly of shapes (i.e., subsets of \mathbb{Z}^2) in the TAM is most naturally characterized by strict self-assembly. In searching for absolute limitations of strict self-assembly in the TAM, it is necessary to consider infinite shapes because any finite, connected shape strictly self-assembles via a spanning tree construction in which there is a unique tile type created for each point. In this section we discuss (both positive and negative) results pertaining to the strict self-assembly of infinite shapes in the TAM.

3.1 Pinch-point Discrete Self-Similar Fractals Do Not Strictly Self-Assemble

In [16], Patitz and Summers defined a class \mathcal{C} of (non-tree) “pinch-point” discrete self-similar fractals, and proved that if $X \in \mathcal{C}$, then X does not strictly self-assemble.

Definition A *pinch-point discrete self-similar fractal* is a discrete self-similar fractal satisfying (1) $\{(0, 0), (0, c - 1), (c - 1, 0)\} \subseteq V$, (2) $V \cap (\{1, \dots, c - 1\} \times \{c - 1\}) = \emptyset$, (3), $V \cap (\{c - 1\} \times \{1, \dots, c - 1\}) = \emptyset$, and $G_V^\#$ is connected

A famous example of a pinch-point fractal is the standard discrete Sierpinski triangle \mathbf{S} . The impossibility of the strict self-assembly of \mathbf{S} was first shown in [13]. Figure 3 shows another example of a pinch-point discrete self-similar fractal. Note that any fractal X such that $G_X^\#$ is a tree is necessarily a pinch-point discrete self-similar fractal.

The following (slight) generalization to [13] was shown in [16].

Theorem 3.1 *If $X \subsetneq \mathbb{N}^2$ is a pinch-point discrete self-similar fractal, then X does not strictly self-assemble in the TAM.*

The idea behind the proof of Theorem 3.1 can be seen in Figure 3. Note that the black points are pinch-points in the sense that arbitrarily large aperiodic sub-structures appear on the far-side of the black tile from the origin.

Theorem 3.1 motivates the following question.

Open Problem 3.2 *Does any non-trivial discrete self-similar fractal strictly self-assemble in the TAM? We conjecture that the answer is ‘no’, for any temperature $\tau \in \mathbb{N}$. However, proving that there exists a (non-trivial) discrete self-similar fractal that does strictly self-assemble would likely involve a novel and useful algorithm for directing the behavior self-assembly.*

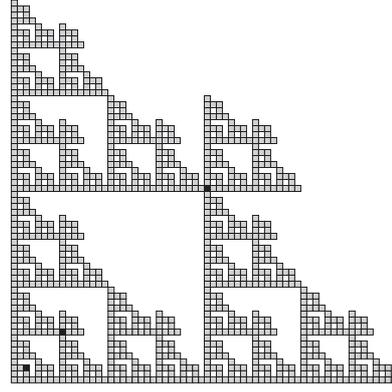


Fig. 3: An example of the first four stages of pinch-point fractal with the first three pinch-points highlighted in black.

3.2 Strict Self-Assembly of Nice Discrete Self-Similar Fractals

As shown above, there is a class of discrete self-similar fractals that do not strictly self-assemble (at any temperature) in the TAM. However, in [16], Patitz and Summers introduced a particular set of “nice” discrete self-similar fractals that contains some but not all pinch-point discrete self-similar fractals. Further, they proved that any element of the former class has a “fibered” version that strictly self-assembles.

3.2.1 Nice Discrete Self-Similar Fractals

Definition A nice discrete self-similar fractal is a discrete self-similar fractal such that $(\{0, \dots, c-1\} \times \{0\}) \cup (\{0\} \times \{0, \dots, c-1\}) \subseteq V$, and $G_V^\#$ is connected.

See Figure 4 for examples of both nice, and non-nice discrete self-similar fractals.

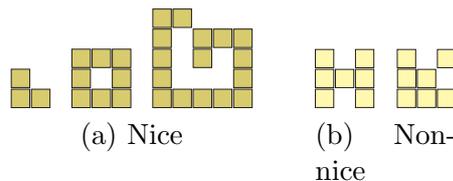


Fig. 4. Stage 2 of some discrete self-similar fractals.

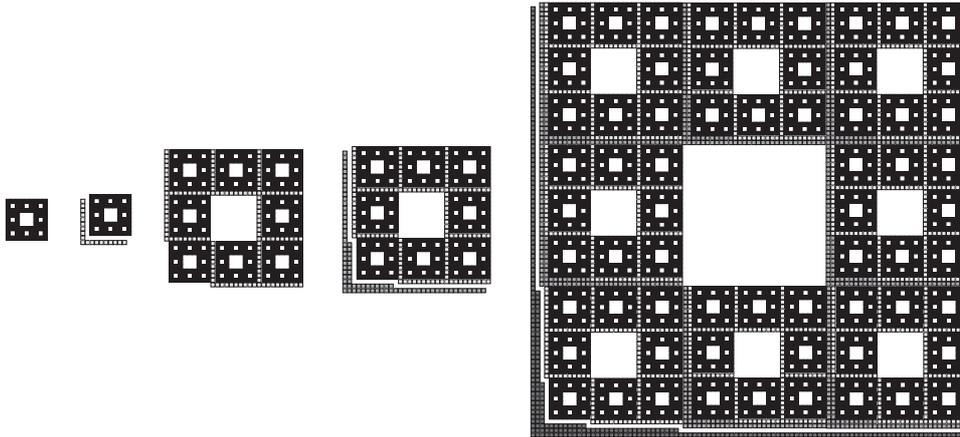


Fig. 5. Construction of the fibered Sierpinski carpet

3.2.2 Nice Fractals Have Fibered Versions

The inability of pinch-point fractals (and the conjectured inability of any discrete self-similar fractal) to strictly self-assemble in the TAM is based on the intuition that the necessary amount of information cannot be transmitted through available connecting tiles during self-assembly.

Thus, for any nice discrete self-similar fractal X , Patitz and Summers [16] defined a fibered operator $\mathcal{F}(X)$ (a routine extension of [13]) which adds, in a zeta-dimension-preserving manner, additional bandwidth to X . Strict self-assembly of $\mathcal{F}(X)$ is achieved via a “modified binary counter” algorithm that is embedded into the additional bandwidth of $\mathcal{F}(X)$.

For any nice discrete self-similar fractal X , $\mathcal{F}(X)$ is defined recursively. Figure 5 shows an example of the construction of $\mathcal{F}(X)$, where X is the discrete Sierpinski carpet. Note that $\mathcal{F}(X)$ is only defined if X is a nice discrete self-similar fractal. Moreover, it appears non-trivial to extend \mathcal{F} to other discrete self-similar fractals such as the ‘H’ fractal (the second-to-the-right most image in Figure 4).

Open Problem 3.3 *Does there exist a zeta-dimension-preserving fibered operator \mathcal{F} for a class of discrete self-similar fractals which is a superset of the nice discrete self-similar fractals (e.g. it also includes the ‘H’ fractal)? The above open question is intentionally vague. Not only should \mathcal{F} preserve zeta-dimension, but $\mathcal{F}(X)$ should also “look” like X in some reasonable visual sense.*

4 Weak Self-Assembly

Weak self-assembly is a natural way to define what it means for a tile assembly system to compute. There are examples of (decidable) sets that weakly self-assemble but do not strictly self-assemble (i.e., the discrete Sierpinski triangle [13]). However, if a set X weakly self-assembles, then X is necessarily computably enumerable. In this section, we discuss results that pertain to the weak self-assembly of (1) discrete self-similar fractals [16], (2) decidable sets [15], and (3) computably enumerable sets [12].

4.1 Discrete Self-Similar Fractals

Recall that pinch-point discrete self-similar fractals do not strictly self-assemble (at any temperature). Furthermore, Patitz and Summers [16] proved that *no* (non-trivial) discrete self-similar fractal weakly self-assembles in a locally deterministic [22] temperature 1 tile assembly system.

Theorem 4.1 *If $X \subsetneq \mathbb{N}^2$ is a discrete self-similar fractal, and X weakly self-assembles in the locally deterministic TAS $\mathcal{T}_X = (T, \sigma, \tau)$, where σ consists of a single tile placed at the origin, then $\tau > 1$.*

Intuitively, the proof relies on the aperiodic nature of discrete self-similar fractals and the fact that the binding (a.k.a. adjacency) graph of the terminal assembly of \mathcal{T}_X is an infinite tree, and every infinite branch is composed of an infinite, periodically repeating sequence of tile types.

Open Problem 4.2 *Does Theorem 4.1 hold for any directed (not necessarily locally deterministic) TAS? We conjecture that it does, and that such a proof would provide useful new tools for impossibility proofs in the TAM.*

4.2 Decidable Sets

We now shift gears and discuss the weak self-assembly of sets at temperature 2.

4.2.1 A Characterization of Decidable Sets of Natural Numbers

In [15], Patitz and Summers exhibited a novel characterization of decidable sets of positive integers in terms of weak self-assembly in the TAM, where they proved the following theorem.

Theorem 4.3 *Let $A \subseteq \mathbb{N}$. Then $A \subseteq \mathbb{N}$ is decidable if and only if $A \times \{0\}$ and $A^c \times \{0\}$ weakly self-assemble.*

Theorem 4.3 is the “self-assembly version” of the classical theorem, which says that a set $A \subseteq \mathbb{N}$ is decidable if and only if A and A^c are computably enumerable. The following lemma makes the proof of the reverse direction of Theorem 4.3 straight-forward.

Lemma 4.4 *Let $X \subseteq \mathbb{Z}^2$. If X weakly self-assembles, then X is computably enumerable.*

The proof of Lemma 4.4 constructs a self-assembly simulator to enumerate X .

To prove the forward direction of Theorem 4.3, it suffices to construct an infinite stack of wedge constructions and simply propagate the halting signals down to the negative y -axis. This is illustrated in Figure 6.

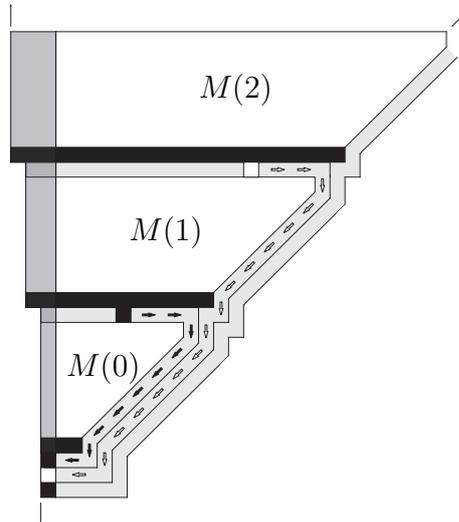


Fig. 6. The left-most (dark grey) vertical bars represent a binary counter that is embedded into the tile types of the TM; the darkest (black) rows represent the initial configuration of M on inputs 0, 1, and 2; and the (light grey) horizontal rows that contain a white/black tile represent halting configurations of M . Although this image seems to imply that the embedded binary counter increases its width (to the left) each time it increments, this is not true in the construction. This image merely depicts the general shape of the counter as it increments.

4.2.2 Quadrant Optimality

In addition to their positive result, Patitz and Summers [15] established that any tile assembly system \mathcal{T} that “row-computes” a decidable language $A \subseteq \mathbb{N}$ having sufficient space complexity must place at least one tile in each of two adjacent quadrants. A TAS \mathcal{T} is said to *row-compute* a language $A \subseteq \mathbb{N}$ if \mathcal{T} simulates a TM M with $L(M) = A$ on every input $n \in \mathbb{N}$, one row at a

time, and uses single-tile-wide paths of tiles to propagate the answer to the question, “does M accept input n ?” to the x -axis. Figure 6 depicts the essence of what it means for a TAS to row-compute some language. This result, stated precisely, is as follows.

Theorem 4.5 *Let $A \subseteq \mathbb{N}$. If $A \notin \text{DSPACE}(2^n)$, and \mathcal{T} is any TAS that “row-computes” A , then every terminal assembly of \mathcal{T} places at least one tile in each of two adjacent quadrants.*

Open Problem 4.6 *Let $A \subseteq \mathbb{N}$ with $A \notin \text{DSPACE}(2^n)$. Is it possible to construct a directed TAS \mathcal{T} in which the sets $A \times \{0\}$ and $A^c \times \{0\}$ weakly self-assemble, and every terminal assembly $\alpha \in \mathcal{A}_\square[\mathcal{T}]$ is contained in the first quadrant? We conjecture that the answer is ‘no’, and any proof would account for all, possibly exotic methods of computation in the TAM, not only by row-computing.*

4.2.3 There Exists a Decidable Set That Does Not Weakly Self-Assemble

In contrast to Theorem 4.3, Lathrop, Lutz, Patitz, and Summers [12] proved that there are decidable sets $D \subseteq \mathbb{Z}^2$ that do not weakly self-assemble. To see this, for each $r \in \mathbb{N}$, define

$$D_r = \{(m, n) \in \mathbb{Z}^2 \mid |m| + |n| = r\}.$$

This set is a “diamond” in \mathbb{Z}^2 with radius r and center at the origin. For each $A \subseteq \mathbb{N}$, let

$$D_A = \bigcup_{r \in A} D_r.$$

This set is the “system of concentric diamonds” centered at the origin with radii in A . Using Lemma 4.4, one can establish the following result.

Lemma 4.7 *Let $A \in \mathbb{N}$. If D_A weakly self-assembles, then there exists an algorithm that, given $r \in \mathbb{N}$, halts and accepts in time $O(2^{4n})$, where $n = \lfloor \lg r \rfloor + 1$, if and only if $r \in A$.*

The proof of Lemma 4.7 is based on the simple observation that each diamond is finite, and once a tile is placed at some point, it cannot be removed. The time hierarchy theorem [9] can be employed to show that there exists a set $A \in \mathbb{N}$ such that $A \in \text{DTIME}(2^{5n}) - \text{DTIME}(2^{4n})$. Lemma 4.7 with $D = D_A$ is sufficient to prove the following theorem.

Theorem 4.8 *There is a decidable set $D \subseteq \mathbb{Z}^2$ that does not weakly self-assemble.*

It is easy to see that if $A \subseteq \mathbb{N}$, then $D_A \in \text{DTIME}(2^{\text{linear}})$ because you can simulate self-assembly with a Turing machine. Is it possible to do better?

Open Problem 4.9 [12] *Is there a polynomial-time decidable set $D \in \mathbb{Z}^2$ such that D does not weakly self-assemble?*

4.3 Computationally Enumerable Sets

The characterization of decidable sets in terms of weak self-assembly [15] is closely related to the characterization of computably enumerable sets in terms of weak self-assembly due to Lathrop, Lutz, Patitz and Summers [12].

Let $f : \mathbb{Z}^+ \rightarrow \mathbb{Z}^+$ be a function such that for all $n \in \mathbb{N}$, $f(n) \geq n$ and $f(n) = O(n^2)$. For each set $A \subseteq \mathbb{Z}^+$, the set

$$X_A = \{(f(n), 0) \mid n \in A\}$$

is thus a straightforward representation of A as a set of points on the positive x -axis. The first main result of [12] is stated as follows.

Theorem 4.10 *If $f : \mathbb{Z}^+ \rightarrow \mathbb{Z}^+$ is a function as defined above, then, for all $A \subseteq \mathbb{Z}^+$, A is computably enumerable if and only if the set $X_A = \{(f(n), 0) \mid n \in A\}$ self-assembles.*

The reverse direction of the proof follows easily from Lemma 4.4. To prove the forward direction, it is sufficient to exhibit, for any TM M , a directed TAS \mathcal{T}_M that correctly simulates M on all inputs $x \in \mathbb{Z}^+$ in \mathbb{Z}^2 . A snapshot of the main construction of [12] is shown in Figure 7.

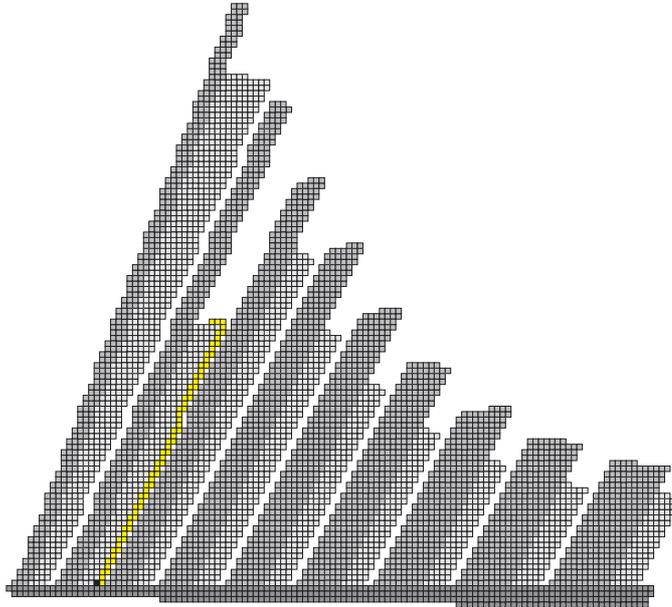


Fig. 7. Simulation of M on every input $x \in \mathbb{N}$. Notice that $M(2)$ halts - indicated by the black tile along the x -axis.

Intuitively, \mathcal{T}_M self-assembles a “gradually thickening bar” immediately below the positive x -axis with upward growths emanating from well-defined intervals of points. For each $x \in \mathbb{Z}^+$, there is an upward growth, in which a modified wedge construction carries out a simulation of M on x . If M halts on x , then (a portion of) the upward growth associated with the simulation of $M(x)$ eventually stops, and sends a signal down along the right side of the upward growth via a one-tile-wide-path of tiles to the point $(f(x), 0)$, where a black tile is placed.

Note that Theorem 4.3 is exactly Theorem 4.10 with “computably enumerable” replaced with “decidable,” and $f(n) = n$.

Open Problem 4.11 [12] *Does Theorem 4.10 hold for any f such that $f(n) = O(n)$? We conjecture that the answer is “no”, and that the construction of [12] is effectively optimal. If the answer to this question is “yes,” then the proof would require a novel construction which manages to provide an infinite amount of space for each of an infinite number of perhaps non-halting computations in a more compact way than [12].*

5 Conclusion

This paper surveyed a subset of recent theoretical results in algorithmic self-assembly relating to the self-assembly of infinite structures in the TAM. Specifically, in this paper we reviewed impossibility results with respect to the strict/weak self-assembly of various classes of discrete self-similar fractals [16], impossibility results for the weak self-assembly of exponential-time decidable sets [12], characterizations of particular classes of languages in terms of weak self-assembly [12, 15], and the strict self-assembly of fractal-like structures. Finally, we believe that the benefit of continued research along these lines has the potential to shed light on the elusive relationship between geometry and computation.

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