Size-Dependent Tile Self-Assembly: Constant-Height Rectangles and Stability

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Abstract. We introduce a new model of algorithmic tile self-assembly called *size-dependent assembly*. In previous models, supertiles are stable when the total strength of the bonds between any two halves exceeds some constant temperature. In this model, this constant temperature requirement is replaced by an nondecreasing *temperature function* $\tau : \mathbb{N} \rightarrow \mathbb{N}$ that depends on the size of the smaller of the two halves. This generalization allows supertiles to become unstable and break apart, and captures the increased forces that large structures may place on the bonds holding them together.

We demonstrate the power of this model in two ways. First, we give fixed tile sets that assemble constant-height rectangles and squares of arbitrary input size given an appropriate temperature function. Second, we prove that deciding whether a supertile is stable is coNP-complete. Both results contrast with known results for fixed temperature.

1 Introduction

In this paper, we introduce the *size-dependent tile self-assembly model*, a natural extension of the well-studied *two-handed tile assembly model* or *2HAM* [4]. As in the 2HAM, a size-dependent system consists of a collection of square Wang tiles [17, 21] with an associated *bond strength* assigned to each tile edge color. In the 2HAM, self-assembly proceeds by repeatedly combining any two previously assembled *supertiles* into a new *stable* supertile provided the total bond strength between the supertiles meets or exceeds some positive integer called the *temperature*.

Although the 2HAM is both simple and natural, the model does not capture the intuition that two large assemblies should require more bond strength to be stable than two very small assemblies. As an analogy, a single staple is sufficient to attach two pieces of paper or to attach a sheet of paper to the hull of a battleship. However, a staple is too weak to amalgamate together two battleships.

The size-dependent self-assembly model generalizes the 2HAM by replacing the fixed, integer temperature parameter τ of the 2HAM with a nondecreasing *temperature function* $\tau(n)$ that specifies a required threshold of bond strength when given the size of the smaller of two supertiles under consideration. A set of tile types and temperature function together define a size-dependent self-assembly system.

Our results. We first consider efficiently assembling fixed-height rectangles and squares in the size-dependent self-assembly model. We prove that there exists a fixed tile set assembling a $k \times 3$ rectangle for every $k \geq 7$ given an appropriate temperature function. This tile set is extended to obtain a matching result for $k \times k$ squares. These results demonstrate that size-dependent temperature functions can, in theory, direct assembly in the spirit of temperature programming [11, 20], concentration programming [3, 7, 12], and staging [5]. Unlike these other methods, size-dependence is present in all physical systems, but has not be demonstrated to be programmable. Thus these constructions demonstrate that this ubiquitous aspect of physical systems can (and likely already does) direct assembly in dramatic ways, regardless of whether they can be implemented physically.

In addition to the design of systems that assemble rectangles and squares, we consider the complexity of determining if a supertile is *stable*, i.e. cannot break apart due to insufficient bond strength. Determining the stability of an supertile is a fundamental problem for design, simulation, and analysis of tile self-assembly systems. This problem enjoys a straightforward, polynomial-time solution in the 2HAM. In contrast, we prove that the problem is coNP-complete in the size-dependent model, even for temperature functions with just two distinct temperatures.

Reversibility. A key feature of size-dependence is *reversibility*: the possibility of breaking bonds. Our rectangle and square constructions make critical use of reversibility to beat tile type lower bounds in similar models (see [18]), and our hardness result proves that this mechanism is capable of complex behaviors.

Reversibility has been more directly incorporated into a number of other self-assembly models via glues that repel [8, 16] or deactivate [10, 13, 14], tiles that dissolve [1], and temperatures that change over time [2, 20]. Reversibility in these models has yielded a number of new functionalities, including replication [1, 13], fuel-efficient computation [14, 19], shape identification [15], and efficient small-scale assembly of general shapes [6]. We believe that further study of the ubiquitous but indirect form of reversibility found in size-dependent self-assembly may yield similar functionality.

2 Definitions

The first three subsections define the 2HAM, giving definitions equivalent to those in prior work, e.g. [4]. The final section describes the differences between the two-handed and size-dependent models.

2.1 Tiles, assemblies, and supertiles

A *tile type* is a quadruple (g_N, g_E, g_S, g_W) of *glues* from a fixed alphabet Σ. Each glue $g_i \in \Sigma$ has an associated non-negative integer *strength*, denoted by $\mathrm{str}(g_i)$.[4] An instance of a tile type, called a *tile*, is an axis-aligned unit square with center in $\mathbb{Z}^2$. The edges of a tile are labeled with the glues of the tile's type (e.g. g_N, g_E, g_S, g_W) in clockwise order, starting with the edge with normal vector $\langle 0, 1\rangle$. Two tiles are *adjacent* if their centers have distance 1.

An *assembly* α is a partial mapping $\alpha : \mathbb{Z}^2 \to T$ from tile locations to a set of tile types T, also called a *tile set*. The domain of this partial function is denoted by $\mathrm{dom}(\alpha)$. Each assembly has a dual *bond graph*: a grid graph with vertex set $\mathrm{dom}(\alpha)$ and an edge between every pair of adjacent tiles that form a bond. An edge cut of the bond graph of an assembly is also called a *cut* of the assembly, and the total strength of the bonds of the edges in the cut is the *strength* of the cut. An assembly is *τ-stable* if every cut of the assembly has strength at least τ.

For an assembly $\alpha : \mathbb{Z}^2 \to T$ and vector $\vec{u} = \langle x, y\rangle$ with $x, y \in \mathbb{Z}^2$, the assembly $\alpha + \vec{u}$ denotes the assembly consisting of the tiles in α, each translated by $\vec{u}$. For two assemblies α and β, β is a *translation* of α, written $\beta \simeq \alpha$, provided that there exists a vector $\vec{u}$ such that $\beta = \alpha + \vec{u}$. The *supertile* of α is the set $\tilde{\alpha} = \{\beta : \alpha \simeq \beta\}$. A supertile $\tilde{\alpha}$ is *τ-stable* provided that the assemblies it contains are τ-stable. The *size* of a supertile is denoted by $|\tilde{\alpha}|$ and is equal to the size of an assembly in $\tilde{\alpha}$ (and not the cardinality of $\tilde{\alpha}$, which is always $\aleph_0$).

2.2 The assembly process

Two assemblies α and β are *disjoint* if $\mathrm{dom}(\alpha) \cap \mathrm{dom}(\beta) = \varnothing$. The *union* of two disjoint assemblies α and β, denoted by $\alpha \cup \beta$, is the partial function $\alpha \cup \beta : \mathbb{Z}^2 \to T$ defined as $(\alpha \cup \beta)(x, y) = \alpha(x, y)$ if $(x, y) \in \mathrm{dom}(\alpha)$ and $(\alpha \cup \beta)(x, y) = \beta(x, y)$ if $(x, y) \in \mathrm{dom}(\beta)$. Two supertiles $\tilde{\alpha}$ and $\tilde{\beta}$ can *combine* into a supertile $\tilde{\gamma}$ provided:

- There exist disjoint assemblies $\alpha \in \tilde{\alpha}$ and $\beta \in \tilde{\beta}$.
- $\alpha \cup \beta = \gamma \in \tilde{\gamma}$ and the cut partioning $\mathrm{dom}(\gamma)$ into $\mathrm{dom}(\alpha)$ and $\mathrm{dom}(\beta)$ has strength at least τ (equivalently, γ is τ-stable).

The set of all combinations of $\tilde{\alpha}$ and $\tilde{\beta}$ at temperature τ is denoted by $C^{\tau}_{\tilde{\alpha},\tilde{\beta}}$.

2.3 Two-handed tile assembly systems

A *two-handed tile assembly system* or *two-handed system* is a pair $\mathcal{T} = (T, \tau)$, where T is a *tile set* and $\tau \in \mathbb{N}$ is a *temperature*. Given a system $\mathcal{T} = (T, \tau)$, a supertile $\tilde{\alpha}$ is *producible*, written $\tilde{\alpha} \in \mathcal{A}[\mathcal{T}]$, provided that either $|\tilde{\alpha}| = 1$ or $\tilde{\alpha}$ is a combination of two other producible supertiles of $\mathcal{T}$. A supertile $\tilde{\alpha}$ is *terminal* provided that for all producible supertiles $\tilde{\beta}$, $C^{\tau}_{\tilde{\alpha},\tilde{\beta}} = \varnothing$. A system is *directed* or *deterministic* provided that it has only one terminal supertile.

[4] In later sections, glues with strength 0 are treated as non-existent.

Given a *shape* $P \subseteq \mathbb{Z}^2$, we say a system $\mathcal{T}$ *self-assembles* P, provided that every terminal supertile $\tilde{\alpha}$ of $\mathcal{T}$ has an assembly $\alpha \in \tilde{\alpha}$ such that $\mathrm{dom}(\alpha) = P$. That is, every terminal supertile has shape P, up to translation. A shape P is a $w \times h$ *rectangle* provided that $P = \{x+1, x+2, \dots, x+w\} \times \{y+1, y+2, \dots, y+h\}$ for some $x, y, w, h \in \mathbb{Z}$. If $w = h$, then the rectangle is a *square*.

2.4 Size-dependent systems

A *size-dependent two-handed tile assembly system* or *size-dependent system* $\mathcal{S} = (T, \tau)$ is a generalization of a two-handed tile assembly system. Two-handed and size-dependent systems are identical, except for the definition of τ. Recall that in two-handed systems, $\tau \in \mathbb{N}$ determines the bond strength needed for two supertiles to combine and for a supertile to be τ-stable.

In size-dependent systems, τ is not an integer temperature, but rather a non-decreasing *temperature function* $\tau : \mathbb{N} \to \mathbb{N}$. An assembly γ is *τ-stable* provided any cut partioning $\mathrm{dom}(\gamma)$ into two assemblies $\mathrm{dom}(\alpha)$, $\mathrm{dom}(\beta)$ has strength at least $\tau(\min(|\alpha|, |\beta|))$. A supertile $\tilde{\gamma}$ is *τ-stable* provided the assemblies in $\tilde{\gamma}$ are τ-stable. Also, two supertiles $\tilde{\alpha}$ and $\tilde{\beta}$ can *combine* into a supertile $\tilde{\gamma}$ provided that:

- There exist disjoint assemblies $\alpha \in \tilde{\alpha}$ and $\beta \in \tilde{\beta}$.
- $\alpha \cup \beta = \gamma \in \tilde{\gamma}$ and the cut partioning $\mathrm{dom}(\gamma)$ into $\mathrm{dom}(\alpha)$ and $\mathrm{dom}(\beta)$ has strength at least $\tau(\min(|\alpha|, |\beta|))$.

For a given temperature function $\tau : \mathbb{N} \to \mathbb{N}$, the set of all combinations of $\tilde{\alpha}$ and $\tilde{\beta}$ is denoted by $C^{\tau}_{\tilde{\alpha},\tilde{\beta}}$. Note that the second condition is not equivalent to γ being τ-stable. Figure 1 illustrates an example: a cut in a supertile has sufficient strength, but combining with another supertile causes increased size that causes the cut to become insufficiently strong. So $\tilde{\alpha}$, $\tilde{\beta}$ may be τ-stable while their combination $\tilde{\gamma}$ is *τ-unstable*.

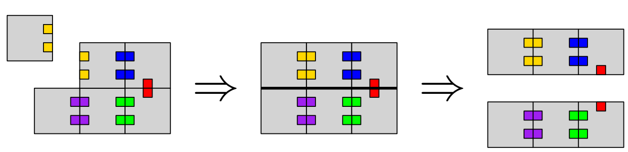

Fig. 1. Three steps of size-dependent self-assembly with glue function $\tau(n) = n - 1$. The addition of a new tile (left) causes the supertile to have a strength-1 cut partioning it into two supertiles of 3 tiles each (center). Because $\tau(3) = 2 > 1$, the supertile can then break (right).

Supertiles that are τ-unstable can also "break" into smaller supertiles. A supertile $\tilde{\gamma}$ can *break* into $\tilde{\alpha}$ and $\tilde{\beta}$ provided that:

- There exist disjoint assemblies $\alpha \in \tilde{\alpha}$ and $\beta \in \tilde{\beta}$ with connected bond graphs.

– $\alpha \cup \beta = \gamma \in \tilde{\gamma}$ and the strength of the cut partioning γ into α and β is less than $\tau(\min(|\alpha|, |\beta|))$.

A cut between two supertiles resulting from a break is called a *break cut*. For a given temperature function $\tau : \mathbb{N} \rightarrow \mathbb{N}$, the set of all supertiles resulting from breaks of $\tilde{\gamma}$ is denoted by $B^{\tau}_{\tilde{\gamma}}$. Given a size-dependent system $\mathcal{T} = (T, \tau)$, a supertile $\tilde{\alpha}$ is *producible* provided either:

– $|\tilde{\alpha}| = 1$.
– $\tilde{\alpha}$ is the combination of two other producible supertiles.
– $\tilde{\alpha}$ is the result of a break of a producible supertile.

A producible supertile $\tilde{\alpha}$ is *terminal* provided $C^{\tau}_{\tilde{\alpha},\tilde{\beta}} = \varnothing$ and $B^{\tau}_{\tilde{\alpha}} = \varnothing$.

Note that the conditions on supertiles combining and breaking do *not* imply that combining supertiles or supertiles resulting from a break are τ-stable. This allows for systems with an infinite number of producible supertiles and a unique terminal supertile, including those described in this work.

3 Constant-Height Rectangles

Here we prove that there exists a single set of tiles that can be used to self-assemble constant-height rectangles of arbitrary width using an appropriate choice of temperature function. Such a result contrasts with the polynomial number of tiles required to assemble a constant-height rectangle in an assembly system with constant temperature [2].

Theorem 1. *There exists a tile set T such that for every $k \geq 7$, there exists a size-dependent system with tile set T that self-assembles a $k \times 3$ rectangle.*

Proof. The temperature function used is:

$$\tau(n) = \begin{cases} 3 : n \leq k-6 \\ 4 : k-5 \leq n \leq k+3 \\ 5 : k+4 \leq n \leq 2k-2 \\ 8 : \text{otherwise} \end{cases}$$

The tile set consists of three tile types and two *blocks*: supertiles with unique internal glues and strength 8, the maximum temperature of the system. The tiles and blocks are listed and named in Figure 2.

The system works by assembling a unique terminal $k \times 3$ supertile in three phases. First, top filler tiles and top bases combine into arbitrarily wide height-2 supertiles. These undergo at least two breaks to form *top half* supertiles of size $2k-3$. Second and separately, bottom filler tiles and bottom bases combine to form *bottom half* supertiles of size approximately $k+3$. Finally, these two halves combine into a terminal $k \times 3$ supertiles shown in Figure 3. It can easily be verified that this supertile is a terminal supertile of the system; it remains to be shown that no other terminal supertiles of the system exist (necessary for the system to *self-assemble* a $k \times 3$ rectangle).

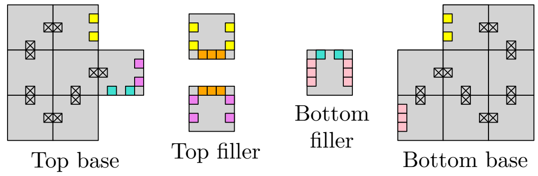

Fig. 2. The tile types and blocks for the constant-height rectangle construction. The gray glues are unique and strength at least 8.

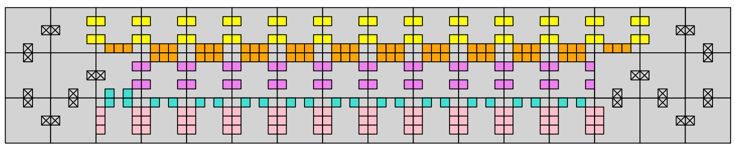

Fig. 3. The unique terminal supertile of the constant-height rectangle construction.

Top filler supertiles. To start, consider the producible supertiles consisting of only top filler tiles, called *top filler* supertiles. Because $\tau(n) > 2$ for all n, upper and lower top filler tiles must first combine into size-2 supertiles before combining with other top filler supertiles into height-2 rectangular supertiles (lower right supertile in Figure 4). These rectangular supertiles break along 2-edge and 3-edge cuts into the remaining supertiles seen in Figure 4.

Because $k \geq 7$, any partition of the lower right supertile in Figure 4 either has a part that is a single tile or uses a strength-4 cut of at least 2 edges and thus both parts have size at least $k + 3 \geq 10$. Therefore, the remaining 8 types of supertiles in Figure 4 have at least 4 columns of 2 tiles each.

The width bounds seen in the figure are computed by considering how the supertiles are created. If the supertile is the result of a break, it must satisfy the size bound for the strength of the cut used in the break. If it is the result of a combination, it must be larger than the total sizes of the combined supertiles.[5]

We designate three types of top filler supertiles as seen in Figure 4. As already proven, breaks only result in single tiles or supertiles of size 10 and larger. Any two-tab (one-tab) supertile can break into a one-tab (tabless) supertile and a single tile, and these are the only breaks that use cuts of strength at most 3. Then any other break uses a cut of strength 4 or more, and so results in supertiles of size at least $k + 4$. Thus any combination of two-tab and one-tab supertiles has size at least $2(k + 4)$. A two-tab supertile can also be the result of a break using a cut of strength 7 and thus have size at least $2k - 3$ and, because two-tab supertiles have even size, $2k - 2$. Because $\min(2(k + 4), 2k - 2) - 1 = 2k - 3$ and $k \geq 7$, $2k - 3 \geq k + 4$ and a break of a two-tab supertile into a single tile and one-tab supertile cannot yield a one-tab supertile smaller than $k + 4$. In conclusion, one-tab and two-tab supertiles have size at least $k + 4$ and $2k - 2$, respectively, implying the bounds seen in Figure 4.

[5] An upper bound is also implied by τ, but this is ignored here.

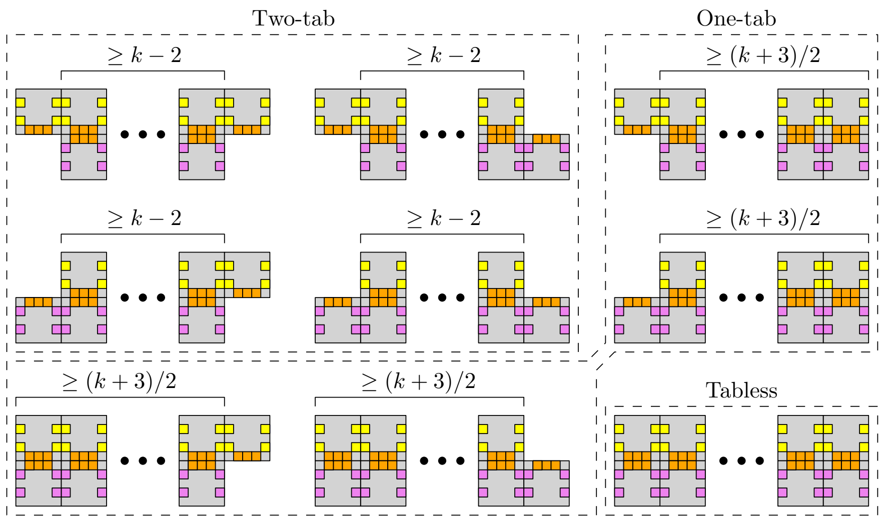

Fig. 4. The producible top filler supertiles.

Top and bottom halves. Top filler supertiles cannot combine with other supertiles, except for a complete top base to form a *top half* supertile (upper supertile in Figure 5). Top half supertiles may combine with top filler supertiles and break into top half and top filler supertiles. A top half supertile with a single upper filler tile in the rightmost column is *ready*. Because ready top half supertiles are two-tab top filler supertiles that have combined with a top base, they have size at least $2k-3$ and thus width at least $k-2$.

Independently of top halves, bottom filler tiles combine into arbitrarily wide height-1 supertiles called a *bottom filler* supertile. These supertiles also combine with bottom bases at various stages of assembly. A *bottom half* supertile contains bottom filler tiles and a completed bottom base. If the number of bottom filler tiles in a bottom half is at least $2k-18$ (and there exists a 1-edge strength-3 cut partitioning the supertile into two of size at least $k-5$), the bottom half can break into a bottom half and bottom filler supertile.

Combining halves. The only shared glues between top and bottom tiles are the strength-2 glues on the south of the top base and west of the bottom base (turquoise and yellow in Figure 2). Thus a supertile consisting of bottom tiles cannot combine with a supertile consisting of top tiles, unless the supertiles are bottom and top halves.

A bottom half and top half can combine, provided they have the same width and the top half is ready (and thus has width at least $k-2$. Moreover, because the maximum strength of the bonds between the bottom and top halves is 4, they can only combine only if the smaller supertile, necessarily the bottom half, has size at most $k+3$ and thus width at most $k-2$. Thus, the bottom and top halves combine provided they both have width exactly $k-2$, forming a terminal supertile of width exactly k.

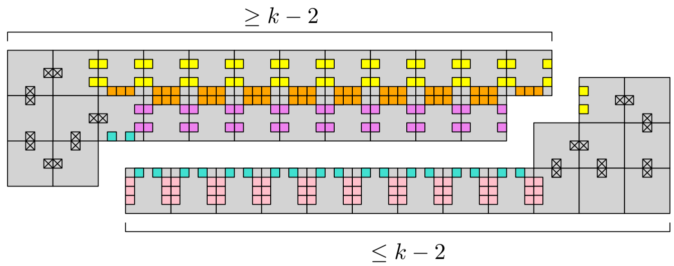

Fig. 5. The top half and bottom half supertiles. The bottom half λ can be arbitrarily large, but the upper bound follows from the requirement that to combine, $\tau(|\lambda|) \leq 4$ and thus $|\lambda| \leq k$.

No waste. Although it is not required by the definition of self-assembly, this system also has the property that every supertile may undergo a sequence of breaks and combinations to become terminal. In other words, the system has no "waste" supertiles. This can be seen by noting that supertiles not found within the (unique) terminal supertile, i.e. top filler supertiles wider than $k-4$, top halves wider than $k-2$, bottom filler supertiles of width more than $k-5$, and bottom halves of width more than $k-2$ can repeatedly break into smaller supertiles that *are* found in the terminal supertile. □

The temperature functions used in the previous construction all have a maximum bounded above by the constant 8. Next, we prove that any set of temperature functions used to assemble arbitrarily large constant-height rectangles are similarly bounded above by a constant.

Theorem 2. *Let T be a tile set and $\tau_1, \tau_2, \ldots$ be an infinite sequence of temperature functions such that the size-dependent system (T, τ_i) assembles a $k_i \times O(1)$ rectangle and all k_i are distinct. Let $f(n) = \min_{i \in \mathbb{N}}(\tau_i(n))$. Then $f(n) = O(1)$.*

Proof. Let $c \in \mathbb{N}$ be the maximum height of a rectangle assembled by a system (T, τ_i). Let $g_{\max}$ be the maximum strength of a glue in T. Let $\tilde{\gamma}$ be a terminal assembly of (T, τ_i) and thus a rectangle with width k_i. For any $n \leq k_i/2$, there exists a cut of $\tilde{\gamma}$ into supertiles $\tilde{\alpha}, \tilde{\beta}$ such that $n = |\tilde{\alpha}| \leq |\tilde{\beta}|$ and the cut contains at most $c+1$ edges. Then since $\tilde{\gamma}$ is stable, $f(n) \leq \tau_i(n) \leq (c+1)g_{\max}$ for all $n \leq k_i/2$. Because there exist infinitely many k_i, every n has $n \leq k_i/2$ for large enough k_i and we conclude that $f(n) \leq (c+1)g_{\max}$ for all $n \in \mathbb{N}$. □

4 Squares

Here we extend the constant-height rectangle construction in the last section to assemble squares. The temperature function, tile types, and blocks from the constant-height rectangle construction are used to form the base of the square; additional tile types and blocks are used to "fill in" the remainder of the square once the base is complete.

Theorem 3. *There exists a tile set T such that, for every $k \geq 7$, there exists a size-dependent system with tile set T that self-assembles a $k \times k$ square.*

The constant-height rectangle construction used as the basis for the construction of Theorem 3 result in temperature functions that are bounded above by a constant. We conjecture that there exists a square construction that uses temperature functions that all scale as $\Omega(\sqrt{n})$, and prove that no better lower bound is possible:

Theorem 4. *Let T be a tile set and $\tau_1, \tau_2, \ldots$ be an infinite sequence of temperature functions such that the size-dependent system (T, τ_i) assembles a $k_i \times k_i$ square and k_i are all distinct. Let $f(n) = \min_{i \in \mathbb{N}}(\tau_i(n))$, the minimum of all temperature functions for size n. Then $f(n)$ is not $\omega(\sqrt{n})$.*

5 τ-stabilility is coNP-complete

In two-handed tile assembly systems that are not size-dependent, determining whether a supertile is τ-stable amounts to determining if there exists a cut of the bond graph of weight less than τ, a problem decidable in polynomial time. In contrast, we prove that the same problem is coNP-complete for size-dependent systems, even when restricted to constant-time-computable temperature functions with just two distinct temperatures.

The reduction is from maximum independent set in Hamiltonian cubic (3-regular) planar graphs, proved NP-hard in [9]. The constructed assembly contains vertex gadgets arranged horizontally along a line bisecting the assembly. Gadgets are connected by zero-strength cuts mirroring the edges of the input graph, and have two possible cuts through them: *include* or *exclude*. The include path has slightly lower strength, but intersects the zero-strength cuts connecting the vertex gadget to the gadgets of adjacent vertices in the input graph. The temperature function requires that any cut passes through all vertex gadgets, does not use the include cuts of the gadgets of two adjacent vertices in the graph, and does not use too many exclude paths. Thus an independent set of at least some size exists if and only if there exists a sufficiently larger independent set of vertices.

Theorem 5. *Given a temperature function $\tau : \mathbb{N} \to \mathbb{N}$ and supertile, determining whether the supertile is τ-stable is* coNP*-complete.*

6 Open Problems

The rectangle and square constructions in this work use artificial temperature functions engineered in tandem with the tile sets. A central open question is whether physically implementable families of temperature functions (e.g. $\tau(n) = cn^\delta$ for varying $c, \delta > 0$) are similarly capable of such control. We conjecture that the design of such systems is possible but difficult; consider the lengthy analysis of the construction in Section 3 with just 5 components. Alternatively, temperature functions may be given as input along with shapes, with the goal of designing systems that assemble shapes *despite* the temperature functions.

The difficulty of system design is supported by the coNP-hardness of determining stability. Proving the PSPACE-hardness of predicting a system outcomes, such as whether a unique terminal supertile exists, would give even further evidence of this difficulty.

As previously discussed, *reversibility* is a key feature of size-dependent systems. Reversibility has been more directly incorporated into algorithmic design in other tile assembly models, leading to functionality not found in irreversible models. For instance, *replication* of shapes and patterns [1, 13], *fuel-efficient* systems [14, 19], and assembly of arbitrary shapes using a small, bounded scale factor [6]. Can any of these be achieved with size-dependent systems?

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