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Combinatorial Optimization and Verification in Self-Assembly

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Years and Authors of Summarized Original Work

2002; Adleman, Cheng, Goel, Huang, Kempe, Moisset, Rothemund
2013; Cannon, Demaine, Demaine, Eisenstat, Patitz, Schweller, Summers, Winslow

Problem Definition

Tile Assembly Models

Two of the most studied tile self-assembly models in the literature are the abstract Tile Assembly Model (aTAM) [7] and the Two-Handed Tile Assembly Model (2HAM) [4]. Both models constitute a mathematical model of self-assembly in which system components are four-sided Wang tiles with glue types assigned to each tile edge. Any pair of glue types are assigned some nonnegative interaction strength denoting how strongly the pair of glues bind. The models differ in their rules for growth in that the aTAM allows singleton tiles to attach one at a time to a growing seed, whereas the 2HAM permits any two previously built assemblies to combine given enough affinity for attachment.

In more detail, an aTAM system is an ordered triplet (T, τ, σ) consisting of a set of tiles T, a positive integer threshold parameter τ called the system's *temperature*, and a special tile $\sigma \in T$ denoted as the *seed* tile. Assembly proceeds by attaching copies of tiles from T to a growing seed assembly whenever the placement of a tile on the 2D grid achieves a total strength of attachment from abutting edges, determined by the sum of pairwise glue interactions, that meets or exceeds the temperature parameter τ. An additional twist that is often considered is the ability to specify a relative concentration distribution on the tiles in T. The growth from the initial seed then proceeds randomly with higher concentrated tile types attaching more quickly than lower concentrated types. Even when the final assembly is deterministic, adjusting concentration profiles may substantially alter the expected time to reach the unique terminal state.

The Two-Handed Tile Assembly Model (2HAM) [4] is similar to the aTAM, but removes the concept of a seed tile. Instead, a 2HAM system (T, τ) *produces* a new assembly whenever any two previously built (and potentially large) assemblies may translate together into a new stable assembly based on glue interactions and temperature. The distinction between the 2HAM and the aTAM is that the 2HAM allows large assemblies to grow independently and attach as large, pre-

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built assemblies, while the aTAM grows through the step-by-step attachment of singleton tiles to a growing seed.

A typical goal in tile self-assembly is to design an *efficient* tile system that uniquely assembles a target shape. Two primary efficiency metrics are (1) the number of distinct tile types used to self-assemble the target shape and (2) the expected time the system takes to self-assemble the target shape. Toward minimizing the number of tiles used to build a shape, the Minimum Tile Set Problem is considered. Toward the goal of minimizing assembly time, the problem of selecting an optimal concentration distribution over the tiles of a given set is considered in the Tile Concentration Problem. Finally, the computational problem of simply verifying whether a given system correctly and uniquely self-assembles a target shape is considered in the Unique Assembly Verification Problem. Formally, the problems are as follows:

Problem 1 (The Minimum Tile Set Problem [2]). Given a shape, find the tile system with the minimum number of tile types that uniquely self-assembles into this shape.

Problem 2 (The Tile Concentration Problem [2]). Given a shape and a tile system that uniquely produces the given shape, assign concentrations to each tile type so that the expected assembly time for the shape is minimized.

Problem 3 (The Unique Assembly Verification Problem [2, 4]). Given a tile system and an assembly, determine if the tile system uniquely self-assembles into the assembly.

Key Results

Minimum Tile Set Problem

The NP-completeness of the Minimum Tile Set Problem within the aTAM is proven in [2] by a reduction from 3CNF-SAT. The proof is notable in that the polynomial time reduction relies on the polynomial time solution of the Minimum Tile Set Problem for tree shapes, which the authors show is polynomial time solvable. The authors also show that the Minimum Tile Set Problem is polynomial time solvable for $n \times n$ squares by noting that since the optimal solution has at most $O(\log n)$ tile types [7], a brute force search of candidate tile sets finishes in polynomial time as long as the temperatures of the systems under consideration are all a fixed constant. Extending the polynomial time solution to find the minimum tile system over any temperature is achieved in [5].

Theorem 1. *The Minimum Tile Set Problem is NP-complete within the aTAM. For the restricted classes of shapes consisting of squares and trees, the Minimum Tile Set Problem is polynomial time solvable.*

Concentration Optimization

The next result provides an approximation algorithm for the Tile Concentration Problem for a restricted class of aTAM tile system called *partial order* systems. Partial order systems are systems in which a unique assembly is constructed, and for any pair of adjacent tiles in the final assembly

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which have positive bonding strength, there is a strict order in which the two tiles are placed with respect to each other for all possible assembly sequences. For such systems, a $O(\log n)$-approximation algorithm is presented [2].

Theorem 2. *For any partial order aTAM system* (T, τ, σ) *that uniquely self-assembles a size-n assembly, there exists a polynomial time* $O(\log n)$*-approximation algorithm for the Tile Concentration Problem.*

Assembly Verification

The next result provides an important distinction in verification complexity between the aTAM and the 2HAM. In [2] a straightforward quadratic time algorithm for assembly verification is presented. In contrast, the problem is shown to be co-NP-complete in [4] through a reduction from 3CNF-SAT. The hardness holds for a 3D generalization of the 2HAM, but requires only 1 step into the third dimension. To achieve this reduction, the exponentially many candidate 3CNF-SAT solutions are engineered into the order in which the system might grow while maintaining that these candidate paths all collapse into a single polynomial-sized final assembly in the case that no satisfying solution exists. This reduction fundamentally relies on the third dimension and thus leaves open the complexity of 2D verification in the 2HAM.

Theorem 3. *The Unique Assembly Verification Problem is co-NP-complete for the 3D 2HAM and solvable in polynomial time* $O(|A|^2 + |A||T|)$ *in the aTAM.*

Open Problems

A few open problems in this area are as follows. The Minimum Tile Set Problem has an efficient solution for squares which stems from a logarithmic upper bound on the complexity of assembling such shapes. This holds more generally for thick rectangles, but this ceases to be true when the width of the rectangle becomes sufficiently thin [3]. The complexity of the Minimum Tile Set Problem is open for this class of simple geometric shapes. For the Tile Concentration Problem, an exact solution is conjectured to be #P-hard for partial order systems [2], but this has not been proven. More generally, little is known about the Tile Concentration Problem for non-partial order systems. Another direction within the scope of minimizing assembly time is to consider optimizing over the tiles used, as well as the concentration distribution over the tile set. Some work along these lines has been done with respect to the fast assembly of $n \times n$ squares [1] and the fast implementation of basic arithmetic primitives in self-assembly [6]. In the case of the Unique Assembly Verification Problem, the complexity of the problem for the 2HAM in 2D is still unknown. For the aTAM, it is an open question as to whether the quadratic run time of verification can be improved.

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Cross References

- ▸ Active Self-Assembly and Molecular Robotics with the Nubot Model
- ▸ Combinatorial Optimization and Verification in Self-Assembly
- ▸ Intrinsic Universality in Self-Assembly
- ▸ Patterned Self-Assembly Tile Set Synthesis
- ▸ Randomized Self-Assembly
- ▸ Robustness in Self-Assembly
- ▸ Self-Assembly at Temperature 1
- ▸ Self-Assembly of Fractals
- ▸ Self-Assembly of Squares and Scaled Shapes
- ▸ Self-Assembly with General Shaped Tiles
- ▸ Temperature Programming in Self-Assembly
- ▸ Two Handed Self-Assembly

Recommended Reading

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