Verifying Assembly of Multiple Assemblies

An Xtreme Algorithms Problem by Robert Schweller and Tim Wylie

1 High-level Model Overview

Here we give a high-level overview of the self-assembly models being used in order to motivate the problems posed, put it into context of the existing literature, and for clarity. The most common self-assembly models are explained conceptually in this section. For full detailed definitions, please see the referenced papers in each section. Some of these details will also be further explained in subsequent sections as needed.

1.1 The Abstract tile assembly model (aTAM)

The *abstract tile assembly model* (aTAM) is the first tile self-assembly model considered [7]. An aTAM system $\Gamma = (T, \tau, s \in T)$ consists of three parts: a tileset T, a bonding threshold τ called the *temperature*, and a seed tile $s \in T$. The set of producible assemblies are defined as the assemblies attained by attaching singleton tiles to the growing seed assembly one at a time, as long as each tile attachment bonds with a net strength of at least τ. A small example is provided in Figure 1a.

The 2-handed Assembly Model. *2-handed Assembly Model* (2HAM) [1, 3, 5], also referred to as *hierarchical* [2] self-assembly is one of the most well-known self-assembly models. In this model, the basic components are 4-sided square tiles with glue types assigned to each side. Each glue has some interaction strength (with other matching glues) defined by a *glue function*. An infinite supply each initial tile type is assumed, and assembly proceeds by combining any 2 tiles, or previously built assemblies, to create a new producible assembly as long as the combination meets a total net attachment strength, from the glue function, that meets some bonding threshold value called the *temperature*. A simple example is showin in Figure 1b.

1.2 Verification Complexity

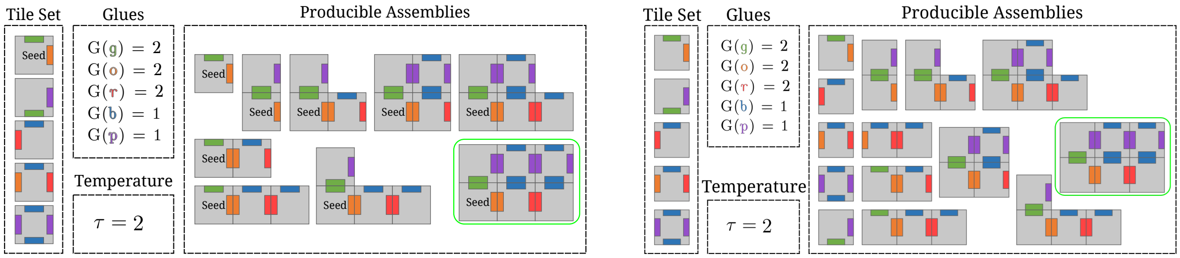
We are interested in the following problem which asks if a given tile system uniquely assembles a given assembly or set of assemblies:

Problem 1 (Unique Assembly Verification (UAV), k-Unique Assembly Verification (k-UAV))**.** *Given a tile system Γ (2HAM or aTAM) and an assembly A, determine if Γ uniquely assembles (is the unique terminally produced assembly) of Γ. More generally, given Γ and a set of k assemblies, determine if Γ uniquely produces this set (i.e. the input set is exactly the set of terminal assemblies for Γ). The problems are the UAV and k-UAV problem respectively.*

1.2.1 Single Assembly Verification in the 2HAM

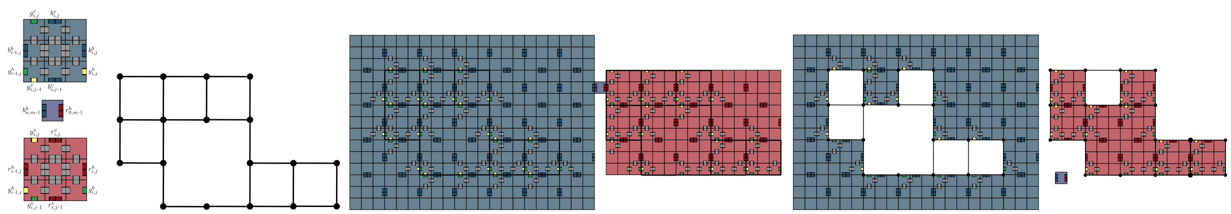
The unique assembly verification problem is in coNP [1] (Cannon et al. [1]). Partial lower-bound progress was also made by Cannon et al. [1], who proved that the problem is coNP-hard (and thus coNP-complete) if the model is extended to cubic tiles in three-dimensions, but the complexity in the standard 2D model was left open.

[1] A "No" answer to the UAV problem corresponds to a (polynomial-sized) witness assembly that is not a sub-assembly of A, whereas a "Yes" answer corresponds to a proof that no other terminal assemblies exist. Thus the problem naturally lies in coNP, but membership in NP remains unknown.



(a) aTAM Example **(b)** 2HAM Example

Figure 1: (a) An aTAM example with 5 tiles resulting in a 2×3 rectangle. The aTAM has seeded growth meaning every producible is begun from the same seed tile. Here there is only one unique terminal assembly. (b) A 2HAM example that uniquely builds a 2×3 rectangle. The top 4 tiles in the tile set all combine with strength-2 glues building the 'L' shape. The tile with blue and purple glues needs two tiles to cooperatively bind to the assembly with strength 2. All possible producibles are shown with the terminal assembly highlighted.



(a) **(b)** **(c)** **(d)**

Figure 2: (a) Blue and red 3×3 tile blocks (and a single connector tile). The center of each 3×3 block has bond strength of τ with its four neighbors. Each corner tile bonds to its horizontal and vertical neighbors with $\lceil \tau/2 \rceil$, $\lfloor \tau/2 \rfloor$ strength, respectively. (b) An example grid graph. (c) The unique terminal assembly of $\mathcal{T}$ if no Hamiltonian cycle exists. (d) Two producible assemblies C_{outer} (blue) and C_{inner} (red) are τ-combinable if they form the outside and inside of a Hamiltonian path.

Recent preliminary work [6] has resolved this open question, using high temperature to overcome difficulties with planarity encountered by previous attempts. We sketch a proof for this preliminary result to lead into a discussion of our proposed problems.

Theorem 1. *The unique assembly verification problem is* coNP*-complete in 2D.[6]*

The reduction is from the Hamiltonian cycle problem on grid graphs, proved NP-complete by [4]. Construct a tile set T_G from G as described in Figure 2a and consider the tile system $\mathcal{T} = (T_G, |V|)$. The tileset T_G consists of a collection of 3×3 blocks and a single connector tile. Each 3×3 block is connected by 4 distinct τ-strength glues unique to each block, along with unique cooperative $\tau - 1$ strength glues filling in block corners.

A blue and red block is constructed for every location. Red and blue glues have strength τ, while green and yellow glues have strength 1 or 0 as determined by the grid graph. The system $\mathcal{T}$ has a terminal assembly consisting of a pair of large rectangles of blue and red blocks, as shown in Figure 2c. If G has a Hamiltonian cycle, then there also exists a pair of producible assemblies C_{inner} and C_{outer} of red and blue 3×3 blocks corresponding to the interior and exterior of the cycle, respectively. By design, C_{inner} has exactly $\tau = |V|$ yellow and green glues exposed that can bond to a second assembly not found in the previous terminal assembly. See Figure 2d for such a pair combinable C_{inner} and C_{outer} and the grid graph they correspond to.

Given this reduction, we achieve coNP-hardness for UAV within the original 2D 2HAM model, in contrast to the previously shown coNP-completeness result of Cannon et al. [1] that applies to the three-dimensional model only. On the other hand, the 3D reduction works at the constant bounded temperature of 2, where as our reduction requires a larger temperature parameter. This leads to our first open question: Can both shortcomings be eliminated?

Problem 2. *What is the complexity of the unique assembly verification problem restricted to* $O(1)$*-*

temperature 2HAM systems (in 2D)?

1.2.2 Verification of Multiple Assemblies in the 2HAM

We now generalize As we already know that the UAV is hard in general, we restrict our consideration to the key scenarios for which the complexity of UAV is still unknown, i.e., for constant bounded temperature systems in 2D. Our approach is to relate the k-UAV problem to UAV by way of reduction. In particular, we focus on the following relationship:

Problem 3. *Is Unique k-Assembly Verification polynomially time reducible to Unique Assembly Verification in the 2HAM?*

Establishing a reduction such as this will provide a new avenue to establish hardness for UAV by utilizing the much more general problem inputs of k-UAV. Alternately, if UAV turns out to be in P, this result yields the surprising corollary that the seemingly harder k-UAV is also in P.

For instance, consider different types of assemblies as input such as ones with different external shapes or ones where only the internal tiles differ in the k assemblies.

References

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