Reducing Tile Complexity for the Self-assembly of Scaled Shapes Through Temperature Programming

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Received: 16 September 2009 / Accepted: 24 April 2011 / Published online: 6 May 2011 © Springer Science+Business Media, LLC 2011

Abstract This paper concerns the self-assembly of scaled-up versions of arbitrary finite shapes. We work in the multiple temperature model that was introduced by Aggarwal, Cheng, Goldwasser, Kao, and Schweller (Complexities for Generalized Models of Self-Assembly, SIAM J. Comput. 2005). The multiple temperature model is a natural generalization of Winfree’s abstract tile assembly model, where the temperature of a tile system is allowed to be shifted up and down as self-assembly proceeds. We first exhibit two constant-size tile sets in which scaled-up versions of arbitrary shapes self-assemble. Our first tile set has the property that each scaled shape self-assembles via an asymptotically “Kolmogorov-optimum” temperature sequence but the scaling factor grows with the size of the shape being assembled. In contrast, our second tile set assembles each scaled shape via a temperature sequence whose length is proportional to the number of points in the shape but the scaling factor is a constant independent of the shape being assembled. We then show that there is no constant-size tile set that can uniquely assemble an arbitrary (non-scaled, connected) shape in the multiple temperature model, i.e., the scaling is necessary for self-assembly. This answers an open question of Kao and Schweller (Proceedings of the 17th Annual ACM-SIAM Symposium on Discrete Algorithms (SODA 2006), pp. 571–580, 2006), who asked whether such a tile set exists.

Keywords Temperature programming · Kolmogorov complexity · Self-assembly · Bio-molecular computation

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1 Introduction

Self-assembly is a process by which a small number of fundamental components automatically coalesce to form a target structure. In 1998, Winfree [22] introduced the abstract Tile Assembly Model (aTAM) as an over-simplified discrete mathematical model of the DNA tile self-assembly pioneered by Seeman [17]. The aTAM is an “effectivization” of classical Wang tiling [20, 21] 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 aTAM were given by Rothemund and Winfree in [13, 15].

Despite its deliberate over-simplification, the aTAM is a computationally expressive model in the sense that Winfree [22] proved it is Turing-universal in two (or more) spatial dimensions. This suggests that it is possible, in principle, to algorithmically direct the process of self-assembly. The aTAM has also been studied from the perspective of computational complexity theory. A problem that has received substantial attention is that of finding “small” tile sets that assemble \( N \times N \) squares in the aTAM. For instance, Adleman, Cheng, Goel, and Huang [1] proved that \( N \times N \) squares self-assemble with \( O\left(\frac{\log N}{\log \log N}\right) \) distinct tile types, matching the Kolmogorov-dictated lower bound that was established in [15]. The more general problem of the self-assembly of arbitrary shapes in the aTAM has also been considered. Most notably, Soloveichik and Winfree [18] discovered a beautiful connection between the Kolmogorov complexity of an arbitrary scaled shape and the minimum number of tile types required to assemble it.

In addition to being an elegant and powerful theoretical tool, there is also experimental justification for the aTAM. For example, using DNA double-crossover molecules to construct tiles only a few nanometers long, Rothemund, Papadakis and Winfree [16] implemented the molecular self-assembly of the well-known fractal structure called the discrete Sierpinski triangle with low enough error rates to achieve correct placement of 100 to 200 tiles. Moreover, Barish, Schulman, Rothemund and Winfree [2] have recently used Rothemund’s DNA origami [14] as a seed structure to which subsequent “computation” DNA tiles can attach and assemble computationally interesting patterns with error rates less than .2%! Note that this technique, although robust, is not general-purpose in the sense that all of the information about the to-be-assembled shape (or pattern) is encoded into the DNA tiles and origami seed.

In fact, a central problem in algorithmic self-assembly is that of providing input to a tile assembly system (e.g., the size of a square, the description of a shape, etc.). In real-world laboratory implementations, as well as theoretical constructions, input to a tile system in the aTAM is provided via a (possibly large) collection of “hard-coded” seed tile types [1, 2, 15, 18]. Unfortunately in practice, it is more expensive to manufacture many different types of tiles, as opposed to creating several copies of each tile type. This suggests that it might be advantageous to be able to provide input to a tile system without having to resort to hard-coding the input into a large number its own tiles. As a result, several natural generalizations of the aTAM have...