Designing a set of non-square tiles that self-assembles into a desired shape

Yuta Matsumura[1], Ibuki Kawamata[1], Satoshi Murata[1]

[1]Department of Robotics, Graduate School of Engineering, Tohoku University, Japan

Recent progress in nano-engineering enables us to build a nanostructure by using self-assembly of material molecules. Especially, structural units called *DNA tile* have great potential to self-assemble into a two-dimentional nanostructure with a specific shape and pattern based on sequence-specific binding rules [1]. When constructing a complex nanostructure using DNA tile, the number of tile types with different binding rules should be minimized in order to improve yield of the structure, and also to reduce production cost. However, there are vast combinatorial possibilities in the tile binding rules, which make it difficult to design tile sets by human trial and error. Therefore, methods for automatically designing tile sets to form a desired pattern have been proposed [2]. However, methods reported so far focus on designing tile sets with square shape, and cannot handle tiles with other shapes. On the other hand, the number of tile types can be reduced by using DNA tiles with various shapes. For example, Hamada and Murata showed that one type of S-shape or U-shape DNA tile can produce complex periodic patterns [3].

In this research, we propose an automatic design method for a set of tiles with various shapes. Here, automatic design means finding a tile set which self-assembles into a target shape as shown in Figure 1(a). To realize this, we propose a new tile model in which the shape of a tile is determined by a combination of square shapes (called "combined tile model"), a self-assembly simulator based on the model, and an optimization algorithm to search for the best tile set. As a result of automatic design, the algorithm was able to find a tile set, which self-assembles into target shape (Figure 1). Extending this method will enable us to automatically design a tile set that forms a large scale structure.

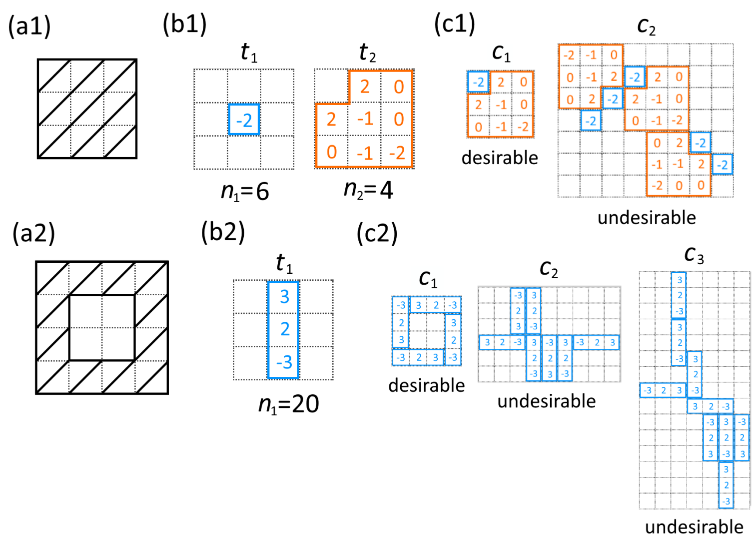

Figure 1: (a) The target shape. (b) Examples of a tile set generated by the algorithm. (c) Structures formed by self-assembly represented by (b). 1st row: An example of a 3×3 square. 2nd row: An example of a 4×4 hollow square.

[1] P. W. K Rothemund et al. PLoS Biol 2 (12) e424 (2004)

[2] Xiaojun M., Fabrizio L. IEEE Transactions on Circuits, 27 (5) 963–967 (2008)

[3] Shogo H., Satoshi M. Angew. Chem. Int. Ed. 48 (37) 6820-6823 (2009)