Self-Assembly of Three-Dimensional DNA-based Structures

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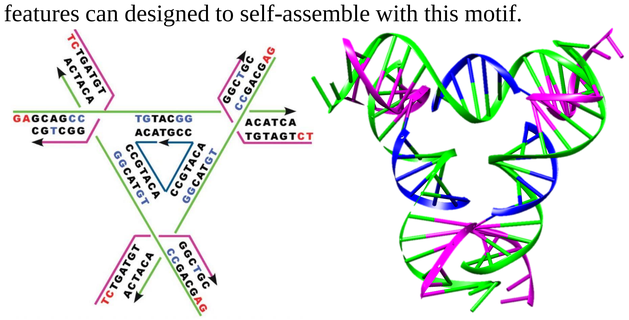
Abstract

We study the three-dimensional assembly of DNA-based structures. We present a design for the recursive growth of an aperiodic, self-similar, three-dimensional structure. A set of "cubic tiles," each comprised of a skewed triangular DNA motif, provides controllable building blocks for the continued self-assembly of the structure.

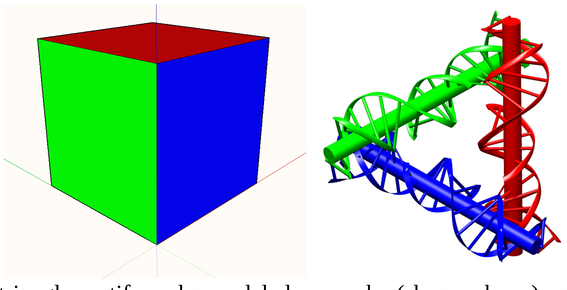
Background

At the center of our study is the "Tensegrity Triangle" DNA motif [1] featured below. Observe that the nucleobase subsequences in red of the motif are unpaired. Only a DNA strand with one of the matching subsequences (of unpaired nucleobases) can connect to this instance of the motif. These "sticky ends" [1] allow us to connect motifs together into 3D structures. Because we can design the sequence for each sticky end in each motif, we can design how the structures will assemble as well. Our goal is understand which structures and features can designed to self-assemble with this motif.



Tensegrity Triangle motif sequence [1] (left) and 3D representation (right).

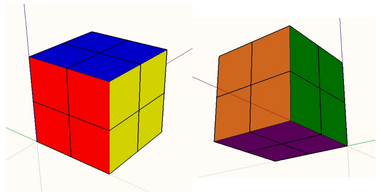
Mathematical Model



A triangle motif can be modeled as a cube (shown above), with faces representing sticky ends. So, we adopt a model wherein each motif is a "cubic tile" adhering to the same constraints:

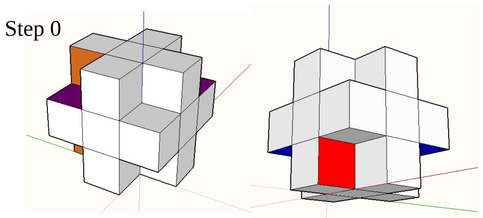
- Individual sticky end sequences in a motif correspond to "labels" in cubic tile. Because sticky ends come in complementary pairs, each label has a +/- polarity.
- Sticky ends have bond strength relative to an ambient temperature during synthesis. Structures whose unmatched sticky ends don't meet or exceed the temperature threshold will not bind. This is represented with "label strength" and "temperature" in the cubic tile model.

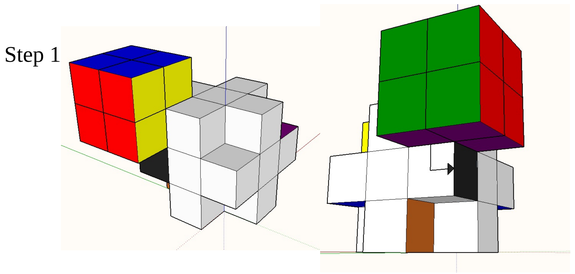
Cubic Tile Set for Recursive Assembly



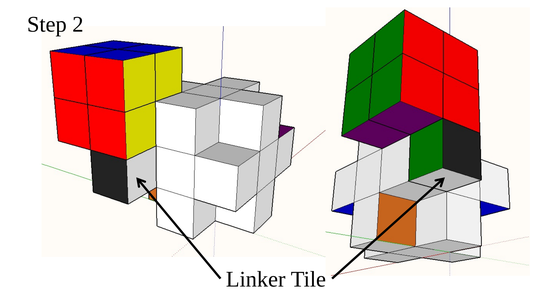
The triangle motifs which form the structure to the left enclose a cavity in the shape of a rhomohedron. We shall refer to this structure as the **seed cube**. We note that for the rest of the poster, distinct labels will correspond to distinct colors. Thus, the structure to the left has six distinct labels.

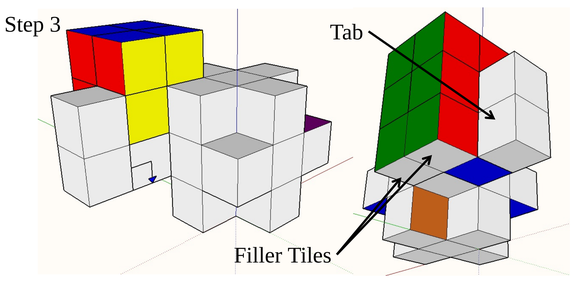
Our tile set is composed of eight distinct cubic tiles for the seed cube, nineteen for the **connector** structure (Step 0), seven **linker tiles** (Step 2), fourteen for seven distinct **tab** structures (Step 3) and eighteen edge and center **filler tiles** (Step 3).

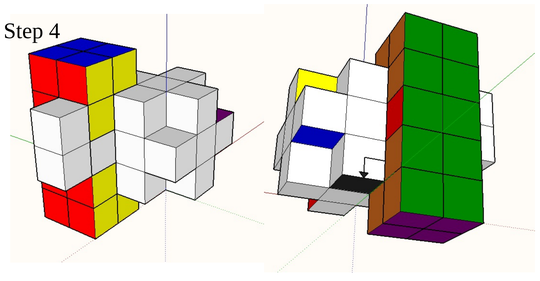


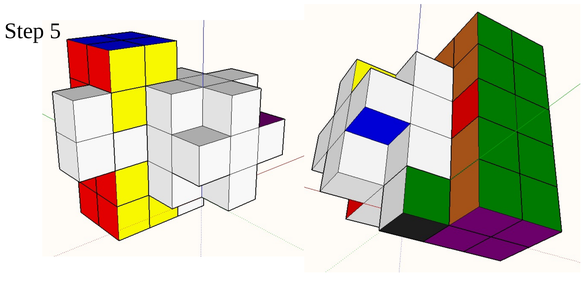


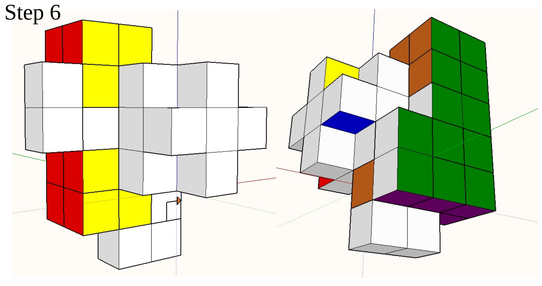
Additional strands with sticky ends can be attached to the structure of a DNA motif. These additional sticky ends can temporarily pair with the original sticky ends of a motif until they themselves are matched, causing the original sticky ends to become "inactive." The process of matching an additional strand to "activate" an original sticky end is used as "signal transmission" [2] in DNA motifs. This property is inherited in our cubic tile model, and the arrow in Step 1 represents a signal transmission which activates the label of cubic tile in the connector structure.

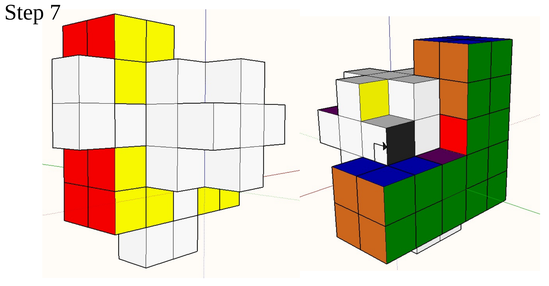






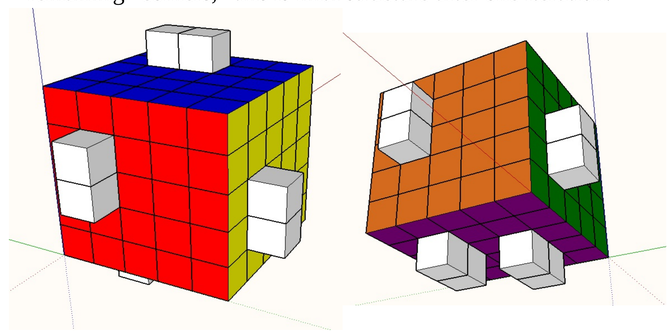






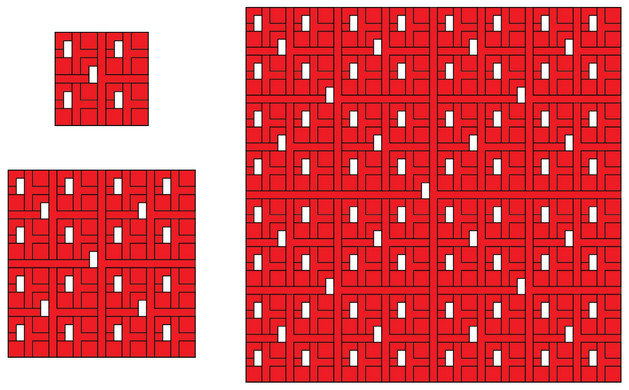
Results

After repeating the same linking and filling process for the remaining "corners," this is final structure after one iteration:



Our other goal was to demonstrate that the aperiodic, recursive growth of structures was possible with the our cubic tile model and thus the tensegrity triangle motif. Consider the "red face" of the structure above:

Focusing only on this "face," observe the aperiodicity of the structure after the next three iterations:



Acknowledgements

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References

[1]: J. Zheng, J. J. Birktoft, Y. Chen, T. Wang , R. Sha, P.E. Constantinou, S.L. Ginell, C. Mao & N.C. Seeman. From molecular to macroscopic via the rational design of a self-assembled 3D DNA crystal. *Nature* **461**, 74-77 (2009).

[2]: J.E. Padilla, J. Chen, N. Jonoska, & N.C. Seeman A Signal-Passing DNA Strand Exchange Mechanism for the Active Self-Assembly of DNA Nanostructures, in preparation.