Samson Petrosyan Grigory Tikhomirov

NANOFRAME.ORG

A WEB-BASED DNA WIREFRAME DESIGN TOOL

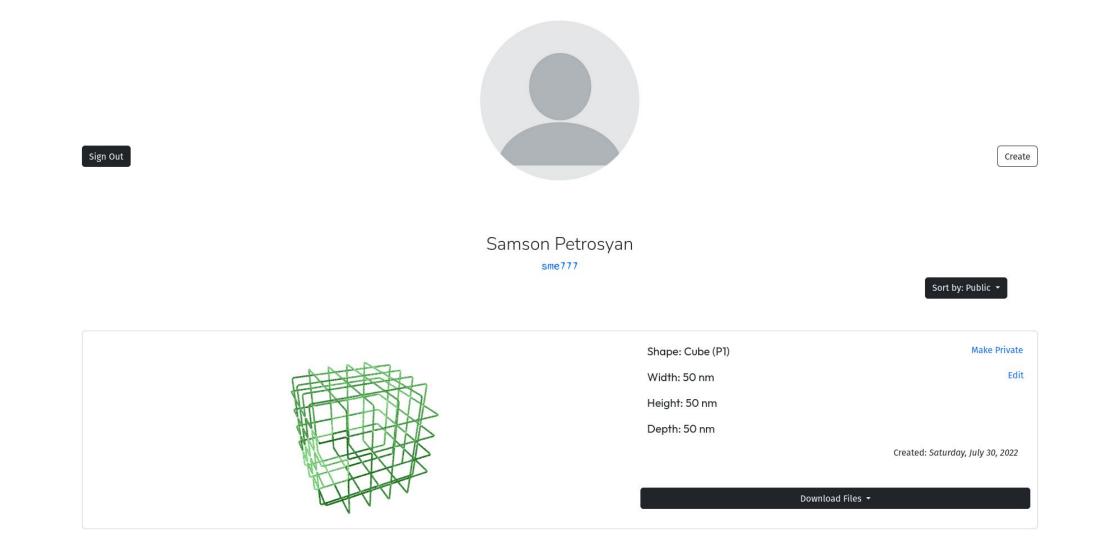
University of California, Berkeley Electrical Engineering & Computer Science

INTRODUCTION

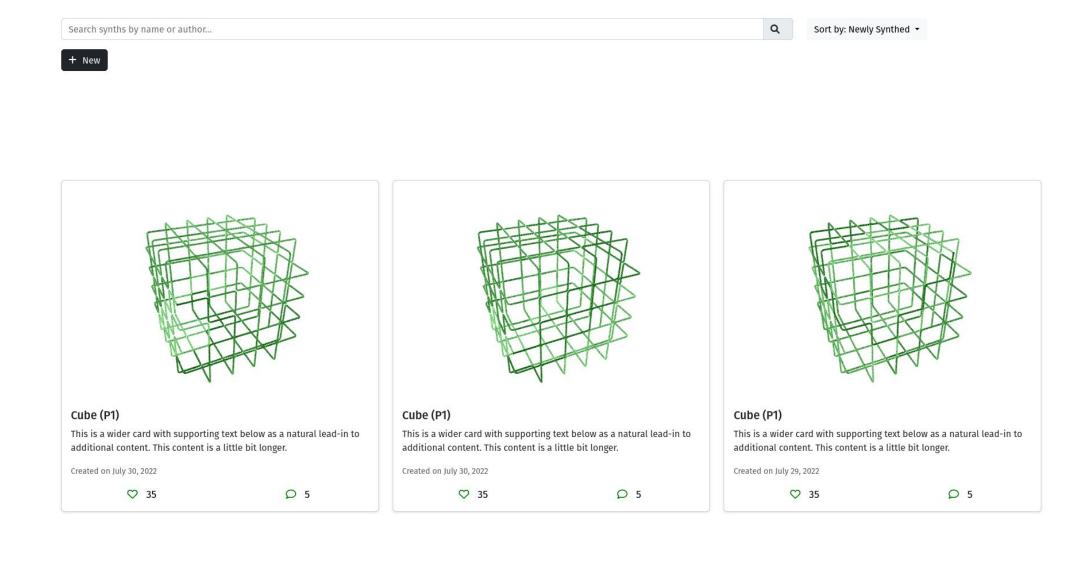
- nanoframe.org is an open-source web-based DNA wireframe design application built as "software as a service".
- nanoframe.org's focus is on wireframes because compared to close-packed DNA origamis, wireframes cover larger surface area, which we need for embedding molecular recognition capabilities of DNA into non-DNA materials.
- nanoframe.org allows creation of multi-origami nanostructures by combining single-origami "blocks" in the playground mode.
- nanoframe.org provides a free-of-charge storage for saving work in the cloud, and enables viewing and working with projects with a user-friendly graphical user interface.
- nanoframe.org has a feed system where public user-generated projects can be shared and discussed.

HOME & FEED

Authentication with nanoframe.org provides many advantages including free storage of generates shapes.



nanoframe.org's feed system helps keep track of latest nano innovations and designs while providing a forum for discussion.



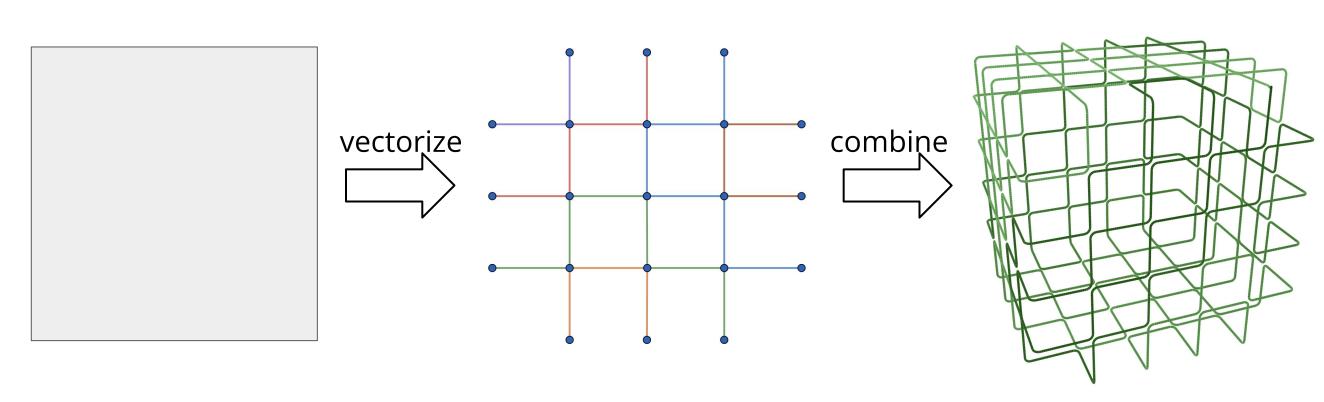
MODEL & METHODS

We develop scaffold routing, staple breaking, and cage opening algorithms for synthesizing polyhedra.

While nanoframe.org currently only supports cuboids, the algorithms can be extended to any-non cuboid polyhedra.

Scaffold Routing

Polyhedra are broken down to a collection of polygons, and a randomized DFS is run on each plane. The polygons are combined through an iterative greedy algorithm to reconstruct the desired polyhedron.



Staple Breaking

Staple breaking is an iterative process and can be divided into 3 stages.

Stage 1: Stapes are broken into 3 categories: staples that jump across edges (reflections), staples that jump across planes (refractions), and staples that stay on one edge (protractions).

Stage 2: Reflection staples are broken down across boundary edges (more below) to have a toe-like shape. Refractions are broken down into pairs – matching each side.

Stage 3: Staples are extended towards interior and exterior for particle capturing and self-assembly.

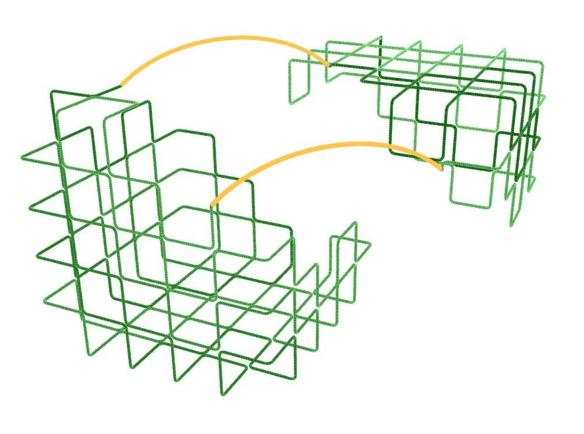
Cage Opening

We built algorithms for detecting strongest connected components of the structure and establishing edge boundaries.

Staples are broken to have a toe-like shape among the boundary edges to facilitate opening upon annealing at low temperatures.

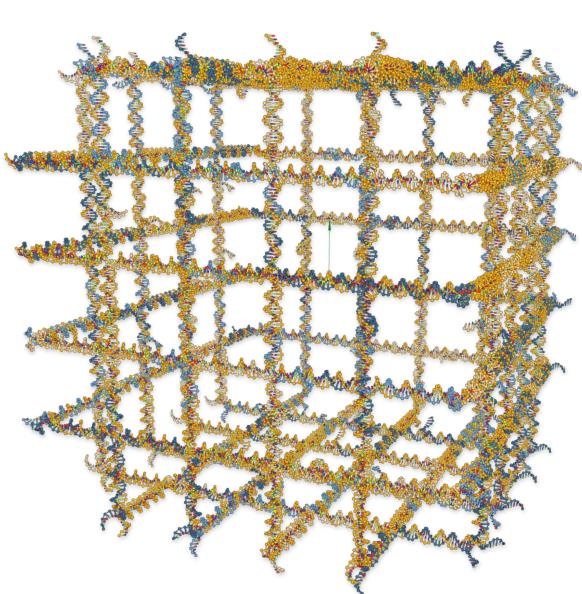
The length of the toe can be adjusted by the user, default value is 3 nucleotides.





SELF-ASSEMBLY

- → We develop special types of staples extending towards the interior and exterior of the wireframe enabling particle capture and mult-origami assembly.
- → Interior staples can be programmed to be complementary with sequences present in the nanoparticle.
- → Exterior staples are automatically computed to match neighboring structures for hierarchical self-assembly.
- → MD can be run on all nanoframe.org structures by exporting them to other nucleic acid formats (i.e. oxDNA, PDB).
- → All nanoframe.org structures are stored in native JSON like .nfr format.



PLAYGROUND

In playground mode of nanoframe.org, one can combine single-origami wireframes to generate more complex multi-origami structures.

In the GUI, when objects are within close proximity, their exterior extension will automatically bind, bringing the two structures together.

It the scriptable format, one can provide a geometric specifications of the nanostructure, and the building blocks would be added automatically.

Users can choose to include payload in the full or partial structure. Playground work can be saved to user's account or exported to nucleic acid formats.

