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Applications of Euler Circuits in DNA Self-Assembly

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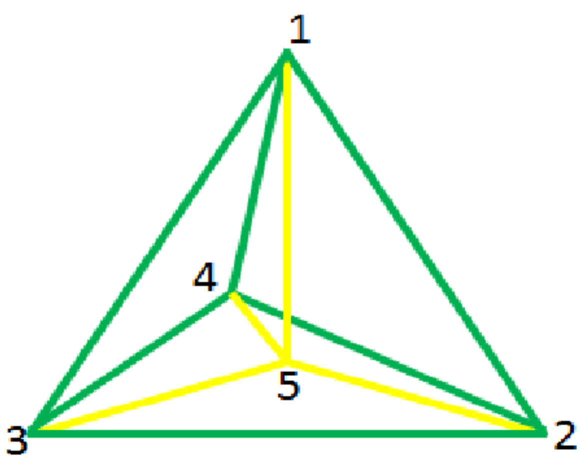
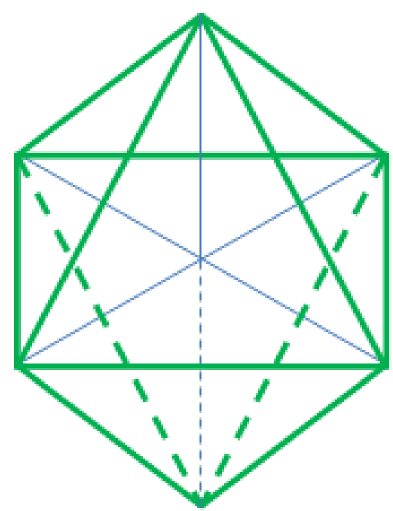
Our Project

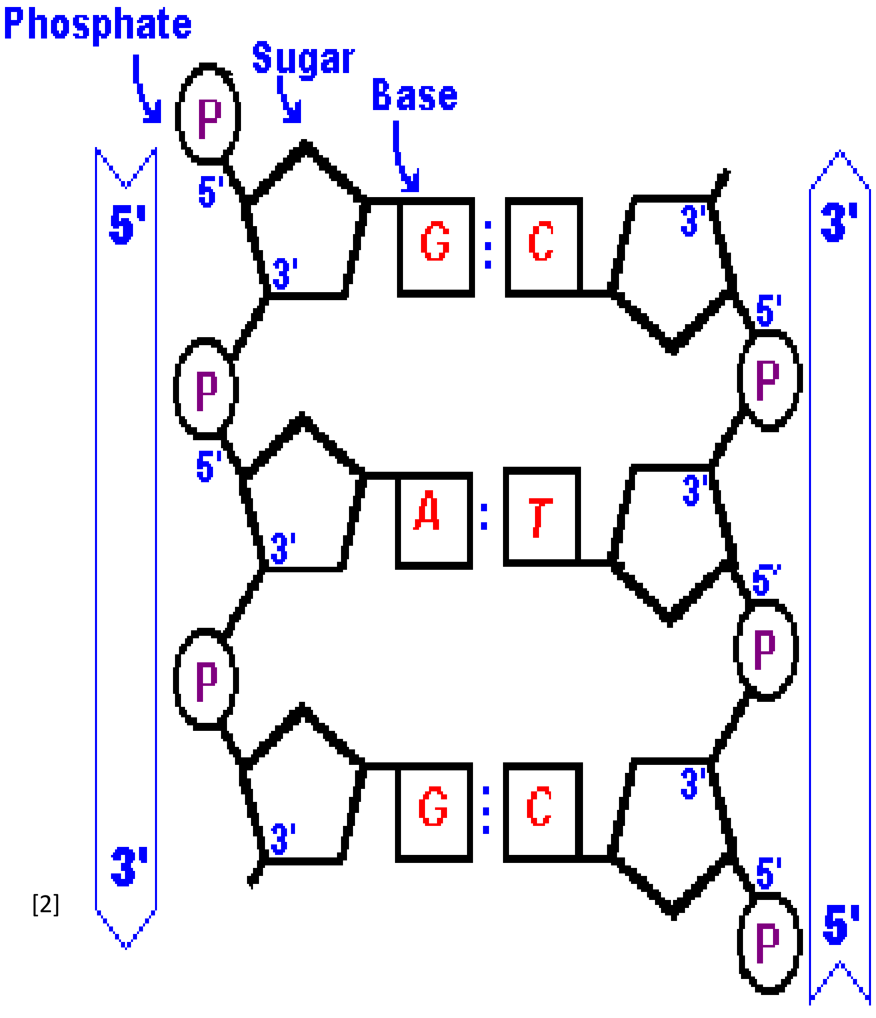
- Design self-assembling DNA nano-structures using DNA origami and graph theory
- Specifically look at skeletons of Platonic Archimedean solids (e.g. octahedron, tetrahedron, cuboctahedron with central vertices
- We thank Ned Seeman from Seeman’s Lab at NYU, who is the source of our design problems.





Recalling DNA structure

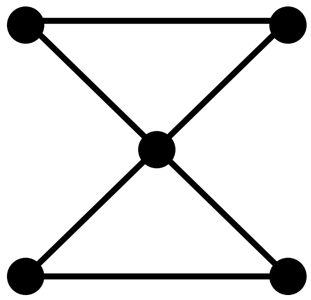
- DNA's 3, 5 sugar backbone
- Nucleotides



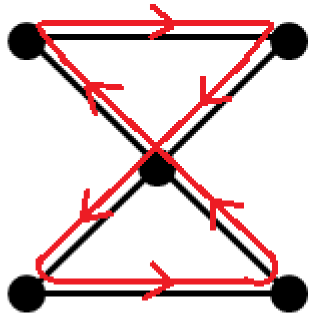
[2]

Graph Theory

- Euler Circuit – A path beginning and ending at the same vertex, which traces every edge of the graph once.
  - Vertices can be reused
  - All vertices must be of even degree



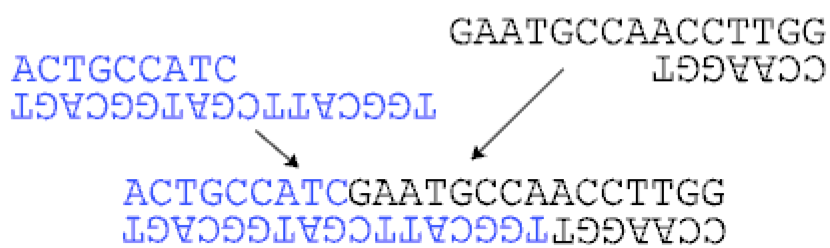
Eulerian Graph



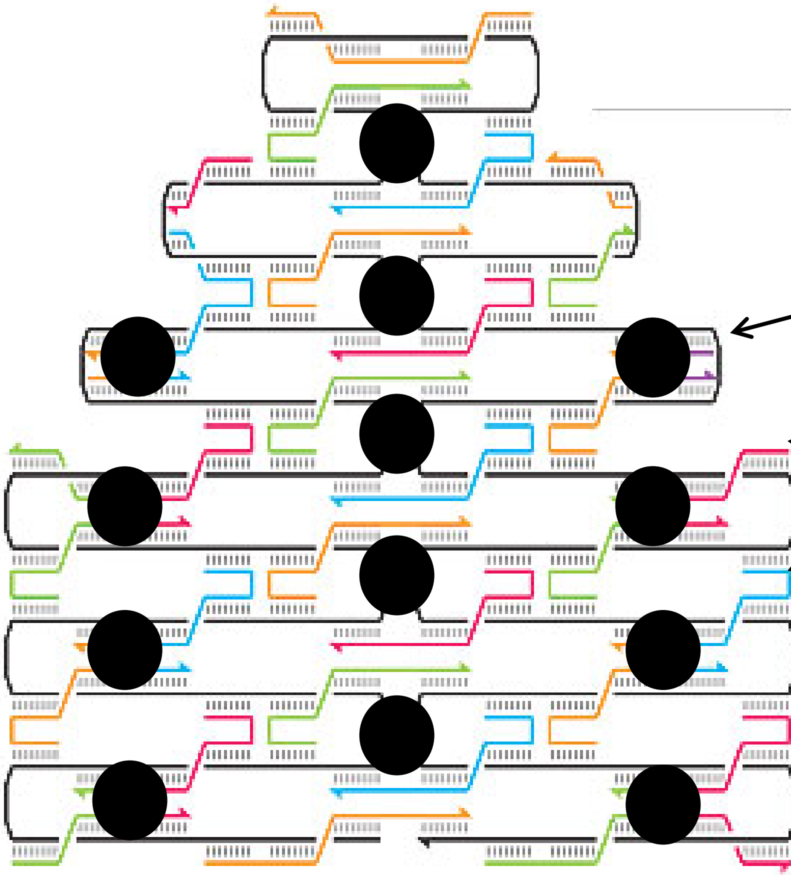
Eulerian Circuit

What is Self-Assembly?

- A chemical process where DNA strands with desired base configurations are put into a solution, and those with complementary configurations will attach to each other (think Velcro) and (hopefully) assemble into a structure.



DNA Origami



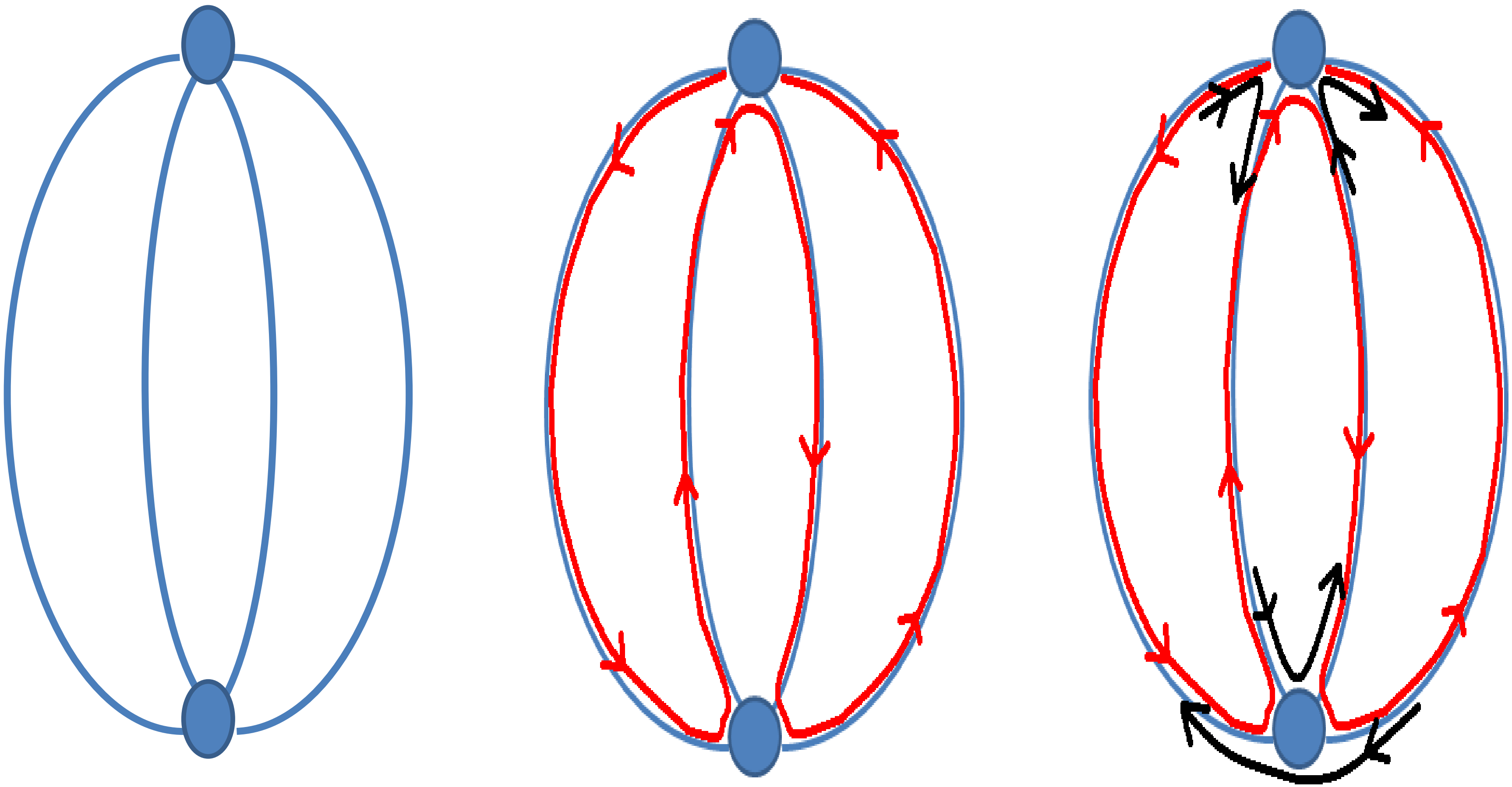
[1] DNA Origami [4]

A scaffolding strand traces the edges of a construct, and staple strands fold and hold the scaffolding strand in place.

Goals

- Find symmetric Euler circuits of certain structures given chemical and geometric constraints
  - Euler circuit will be used as the route for the scaffolding strand
- Attach staples to the scaffolding strand in a way that coincides with the geometric and chemical constraints
- Attach *receiving staples* to the scaffolding strand in a way that will enable larger structures to be built
- Achieve a minimal amount of different vertex configurations

Small Example



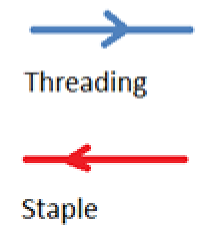
Graph with 2 vertices and 4 edges

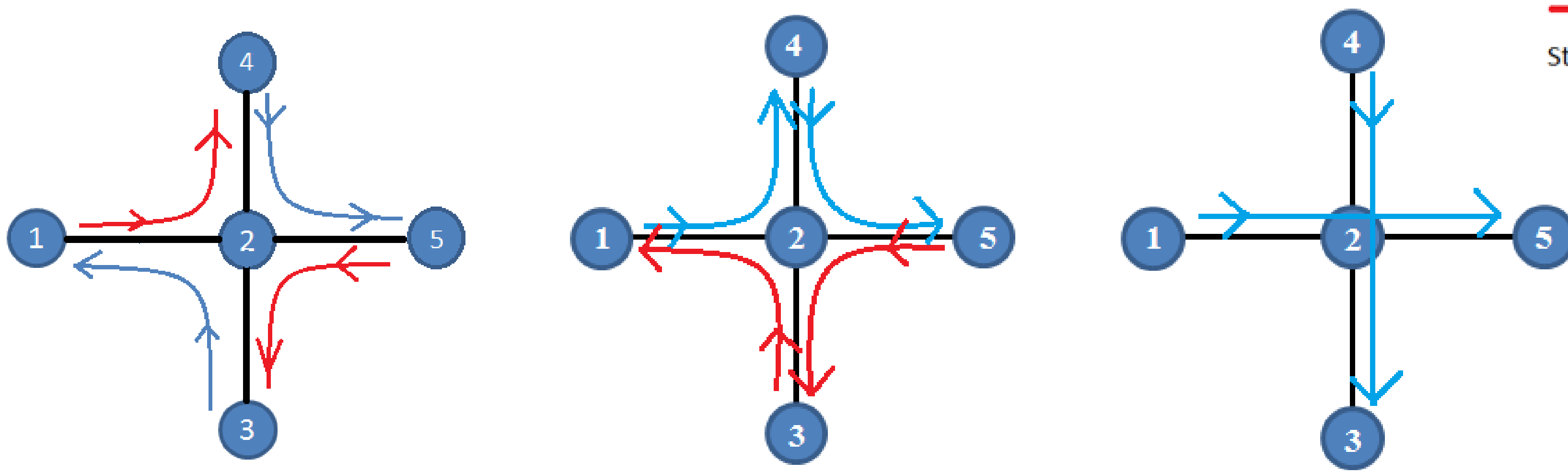
Euler Circuit or Threading

Possible Staples

Threading and Staples

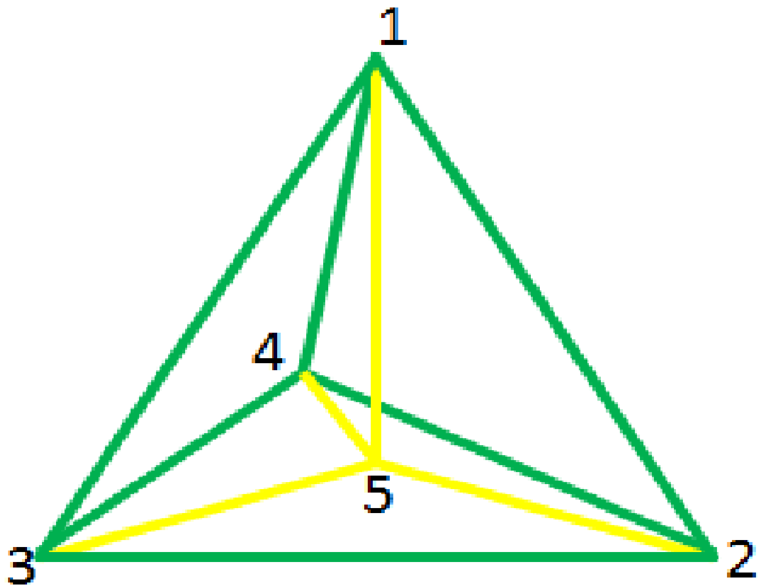
a) Threading and staples must run the opposite direction of each other.
b) A staple cannot occupy consecutive edges in the threading.
c) Staples and threading cannot cross over each other or the outside of any vertex.

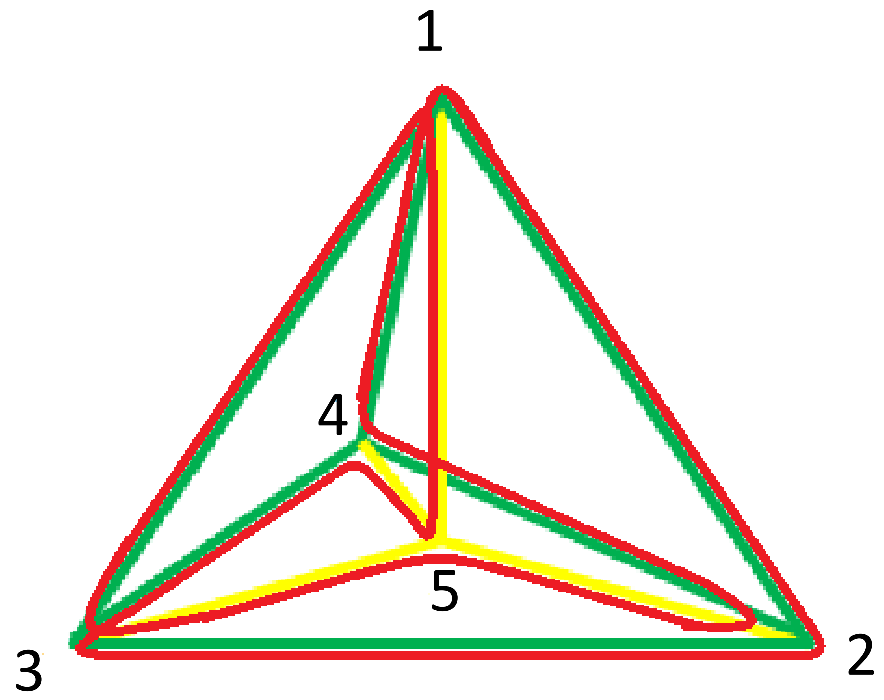




(a) Good (b) Bad (c) Bad

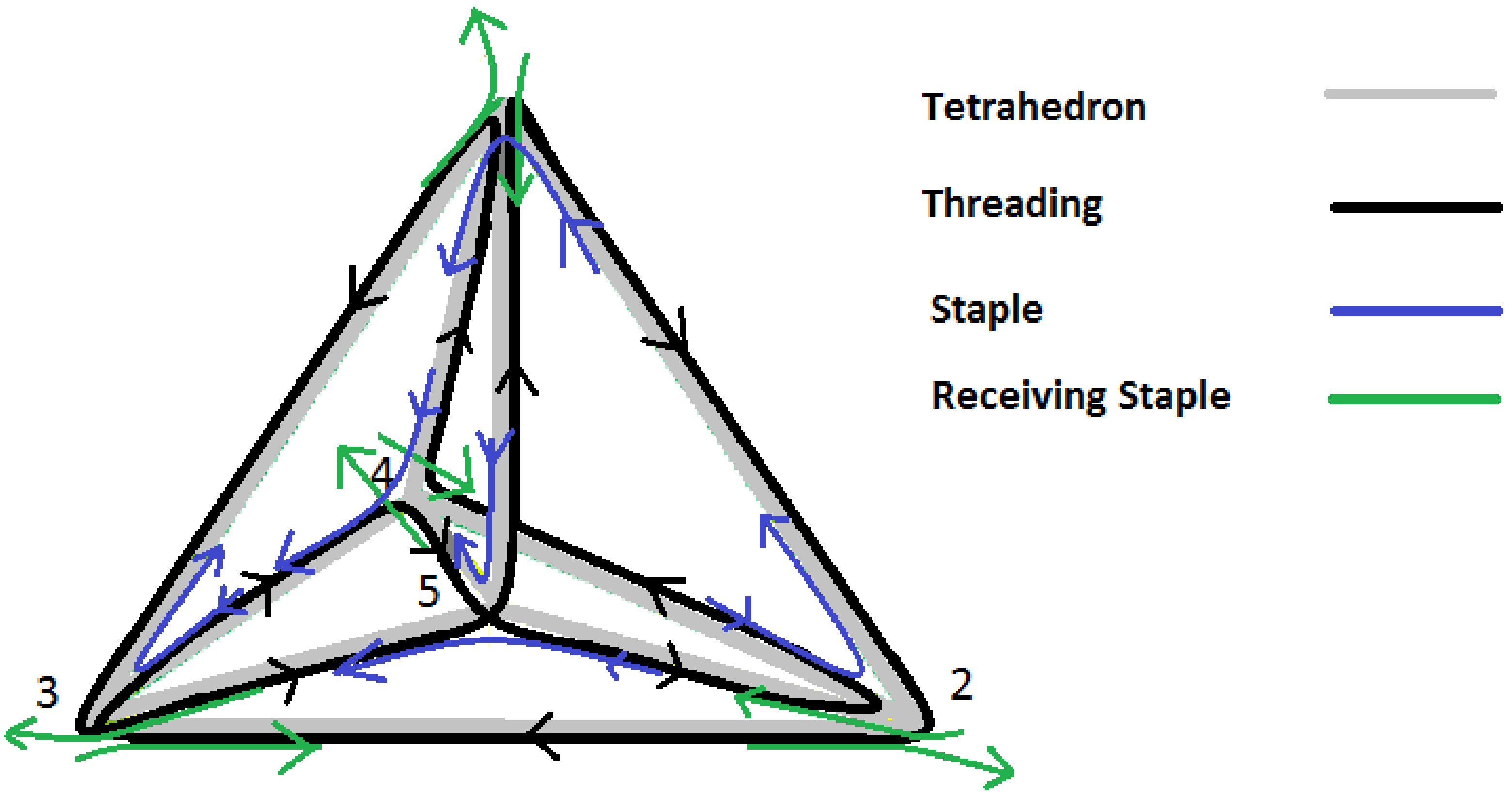
The Tetrahedron with Central Vertex



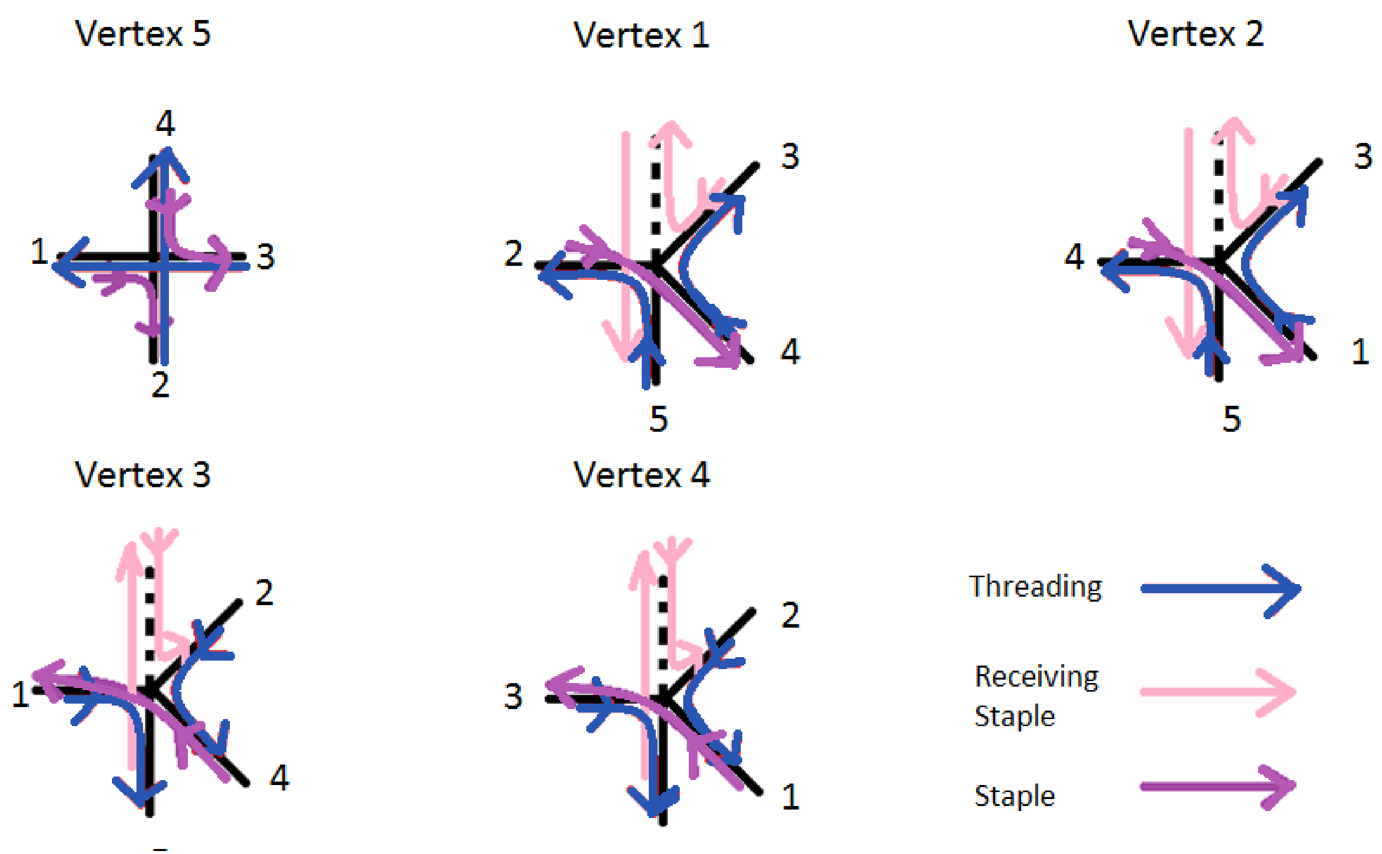


The threading of the tetrahedron.

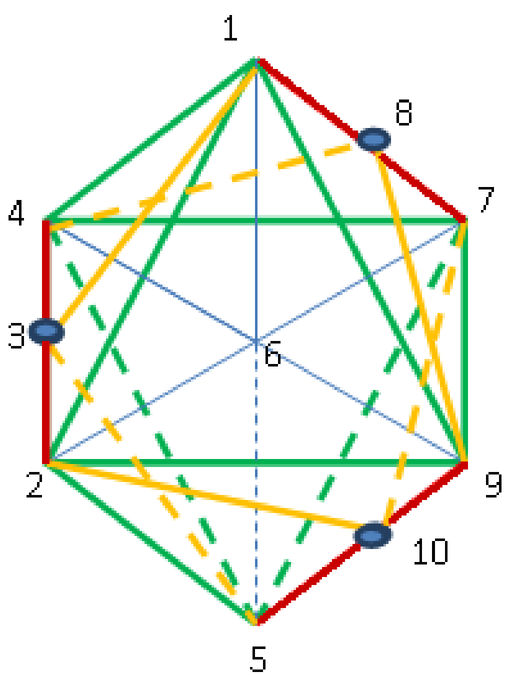
Tetrahedron Threading and Staples

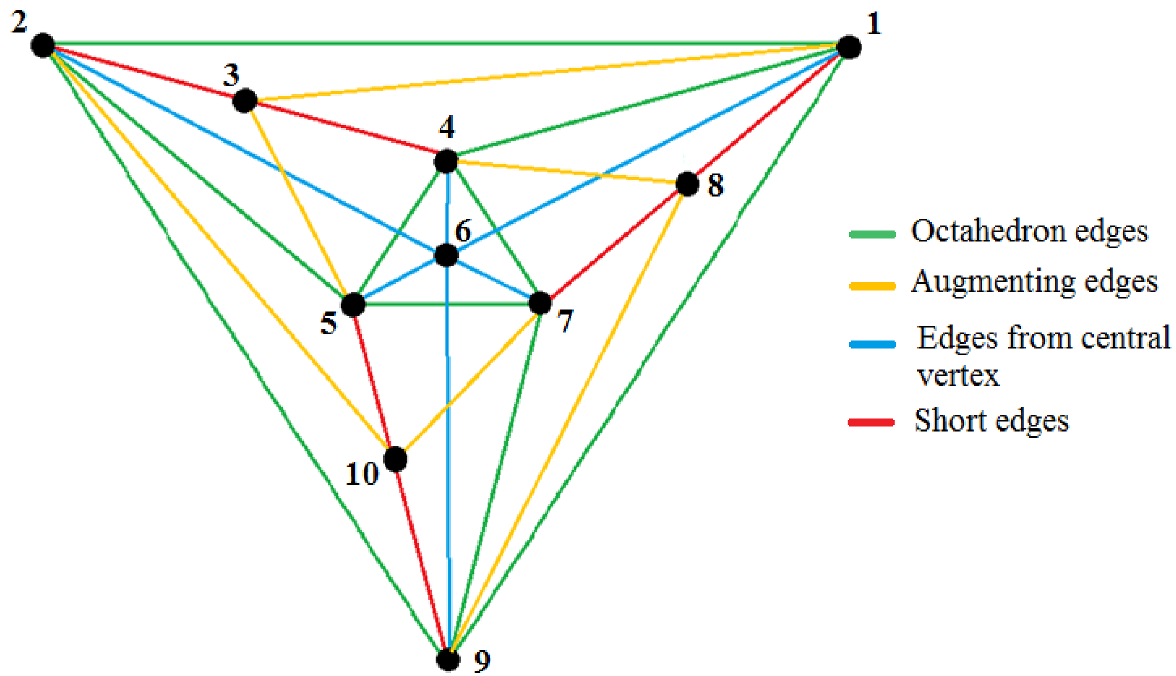


Vertex Configurations

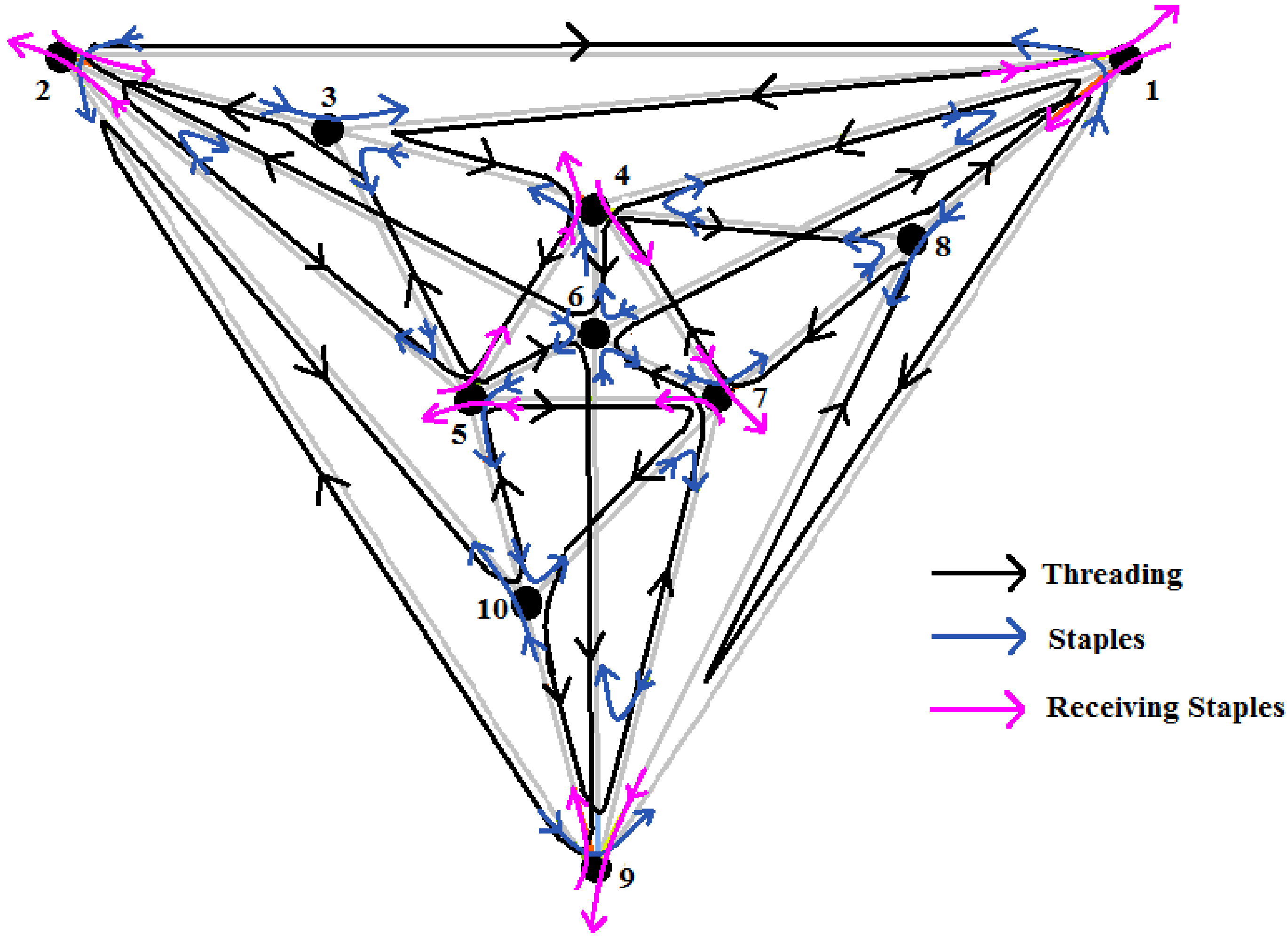


The Octahedron with Central Vertex and Augmenting Edges

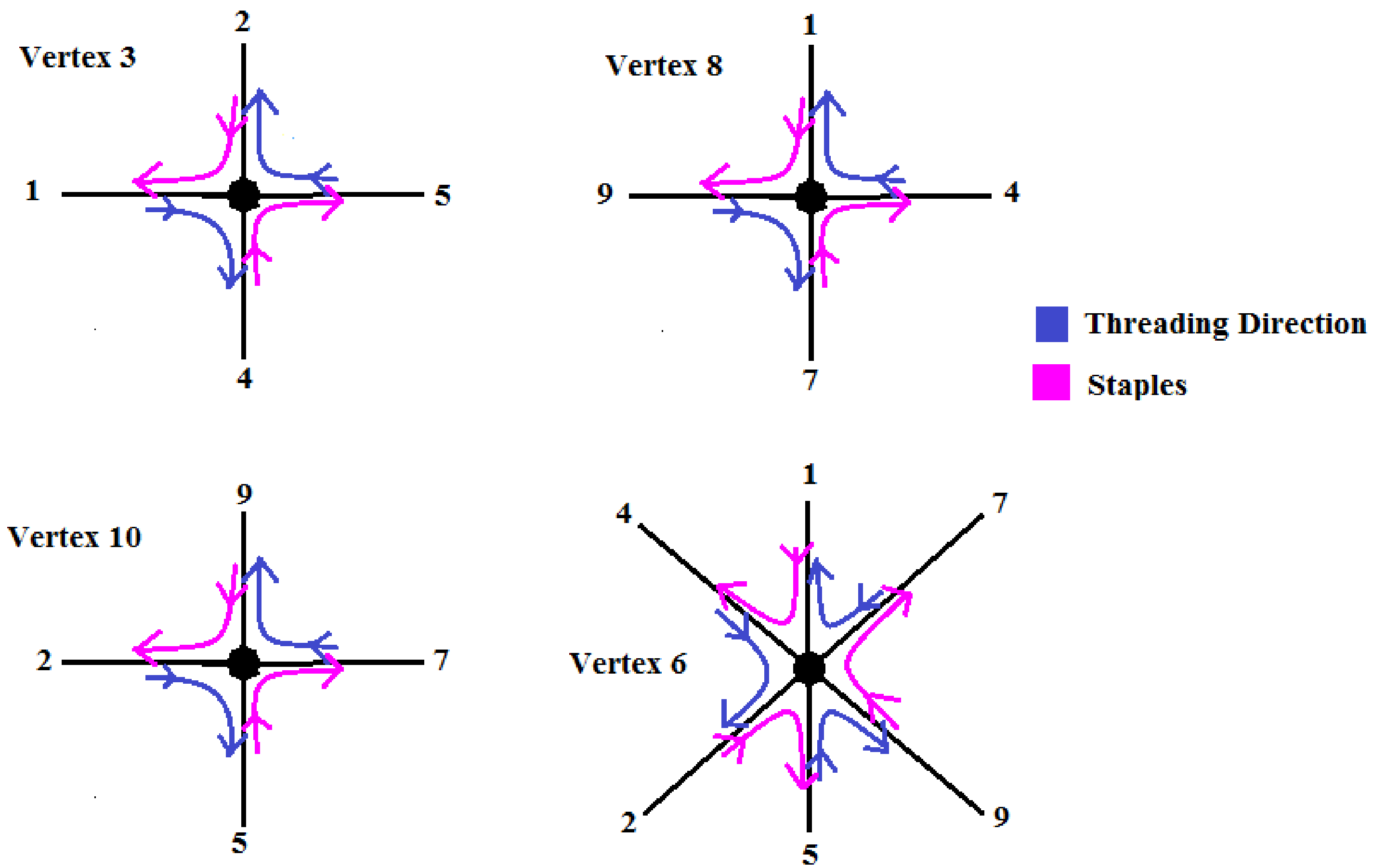




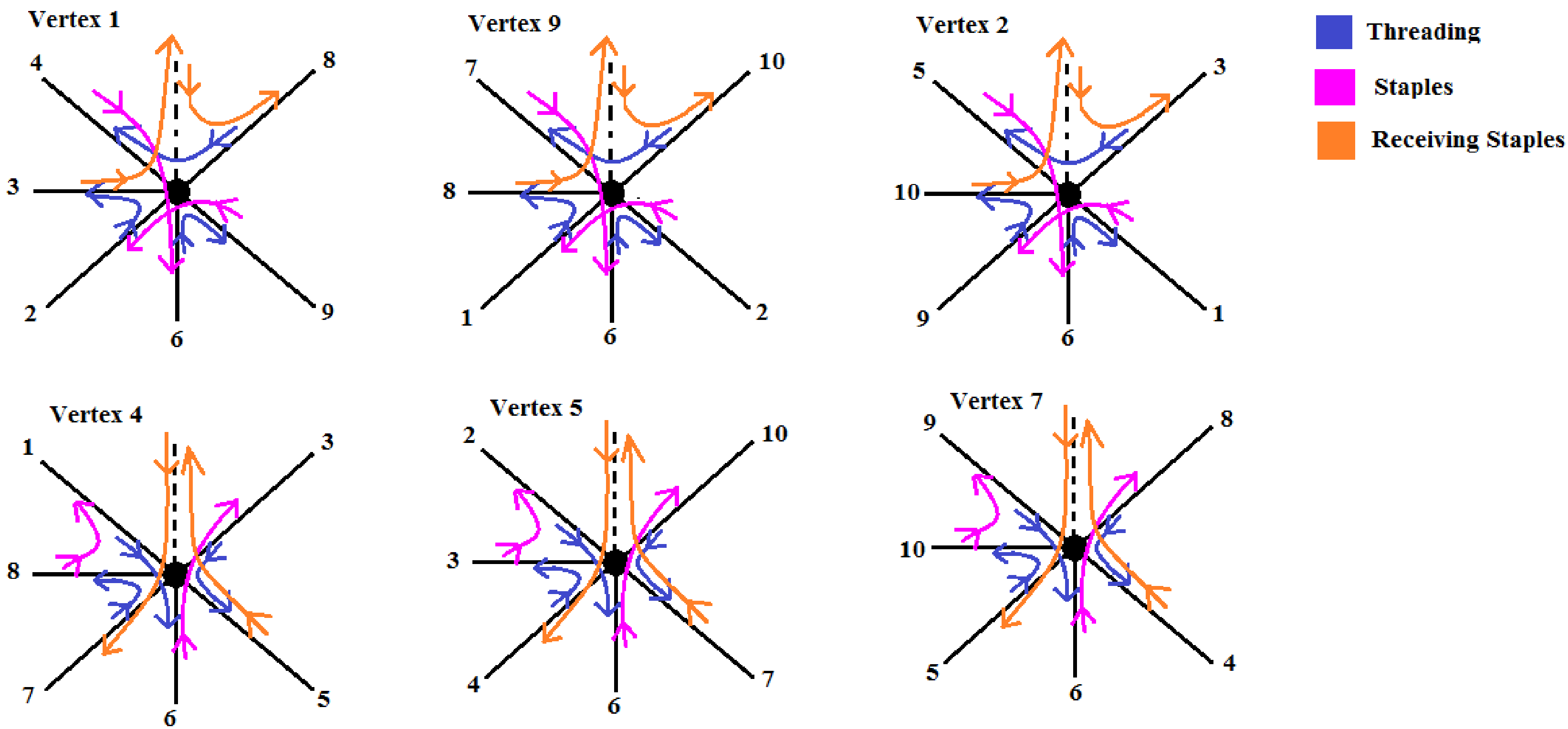
Octahedron With Threading and Staples



Vertex Configurations



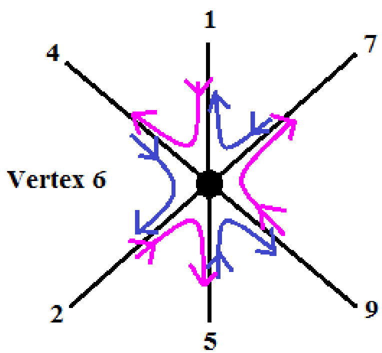
Vertex Configurations Cont.



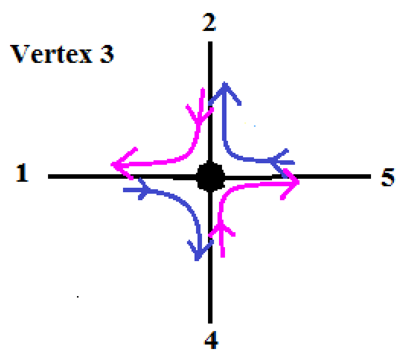
Proof

Claim: This threading of the ModOc uses four symmetrically oriented vertex types.

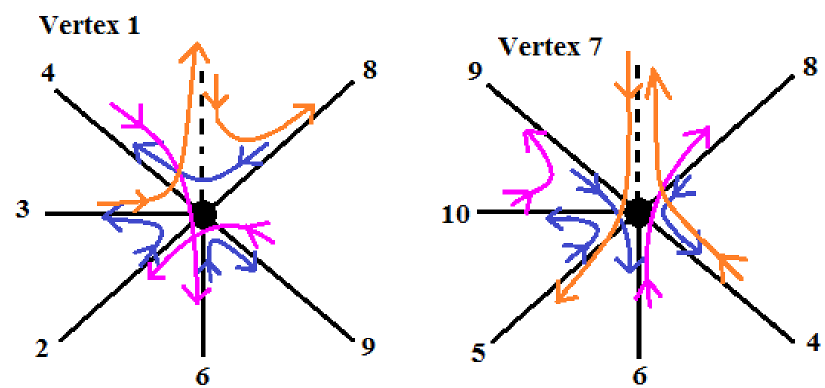
Type 1



Type 2



Type 3 and 4

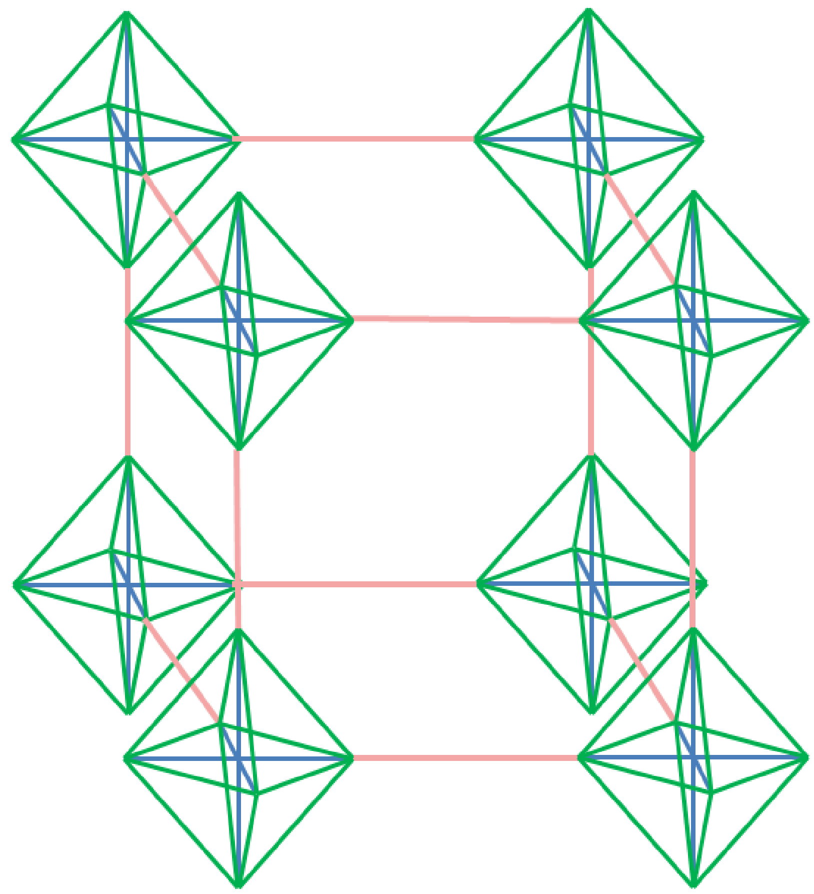


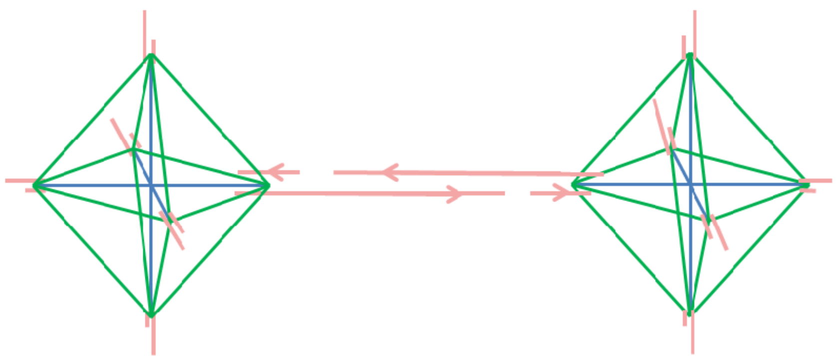
We conclude ModOc has 2 types of outer configurations, the inner vertex configuration, and th
degree 4 vertex configurations requiring a minimum of 4 different vertex configurations.

Receiving Staples

• Receiving staples have one end attached to their construct, and one end which floats freely.

•Ideally, constructs will be able to connect to other constructs to create complete complexes of polyhedra.

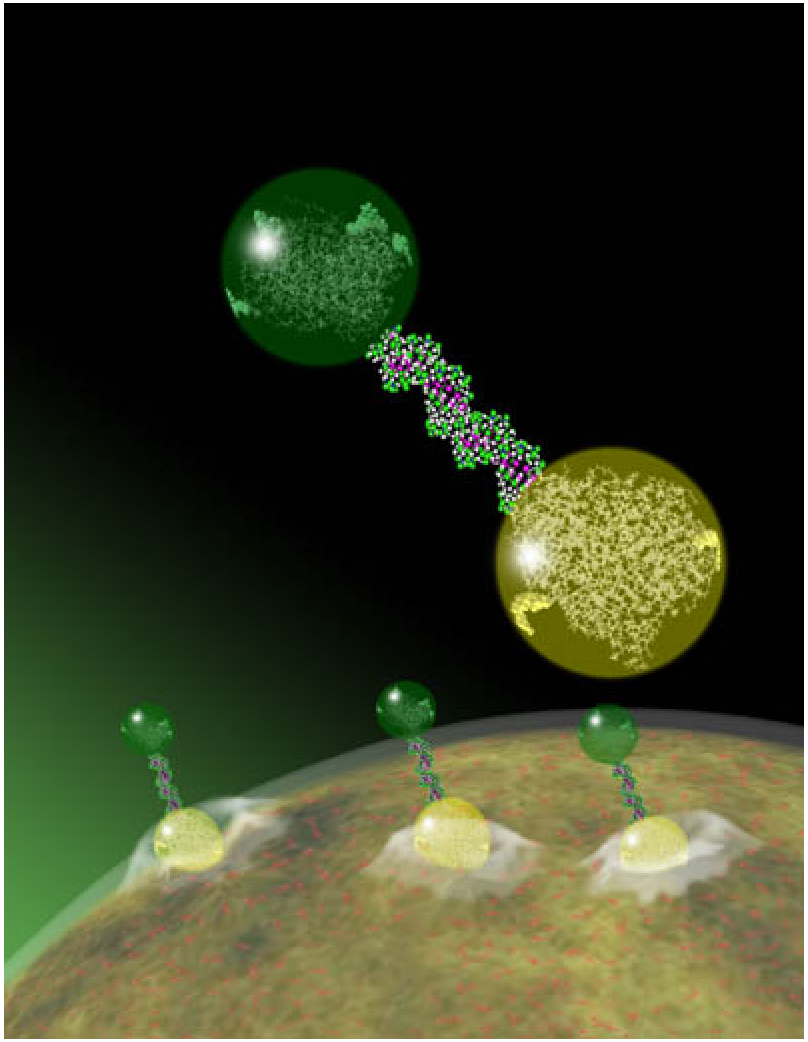




Potential Applications

- Biomolecular computing
- Targeted drug delivery
- Nanoelectronics

[1]



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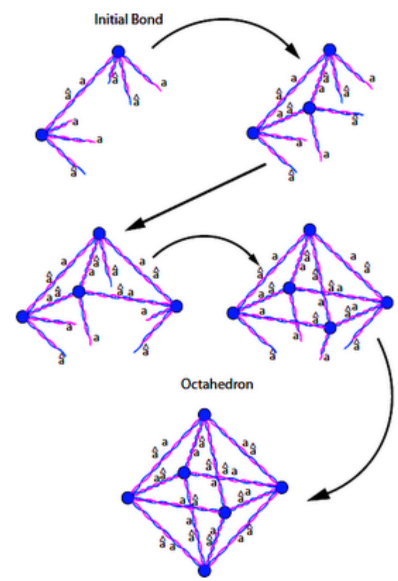
New work in nanotechnology holds promise for a diverse range of applications including biomolecular computing, drug delivery and biosensors (see [Adl94, CS91, LL07, See07]). DNA is an ideal material for building nanostructures because Watson-Crick complementarity allows for self-assembly of molecules, with single of strands of DNA bonding to complementary strands to form larger molecules.



Several different graphs have been constructed from self-assembling DNA molecules, including cubes [CS91], truncated octahedra [ZS94], rigid octahedra [SQJ04], and tetrahedra, dodecahedra, and buckyballs [H+08]. A 3D crystalline lattice has also been constructed [Z+09]. Recent origami methods have resulted in DNA folding into 2D images and designs (see [Rot06,HLS09]), and these methods are adaptable to 3D structures [DDS09].

We are particularly interested in questions related to optimal design strategies for a number of different self-assembly techniques. For example: What is the minimum number of branched junction molecule types needed to create a particular polytope? What is the best way to thread a target polytope or lattice to create the target molecule using a DNA origami technique?

Works Cited

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