Stable Self-Assembled Polyhedra

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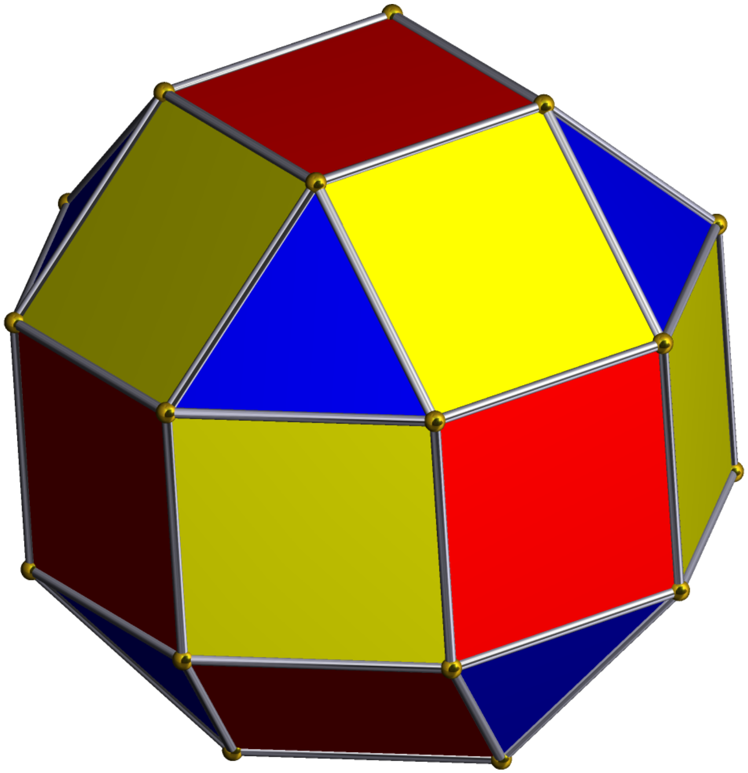
The Model

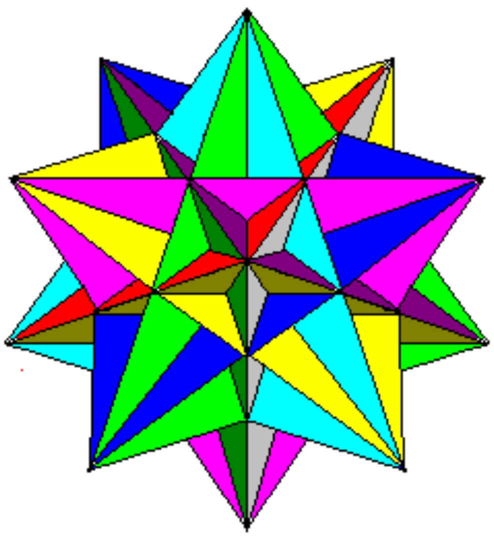
- 3. Stable
- 2. Self-assembled
- 1. Polyhedron

Polyhedron

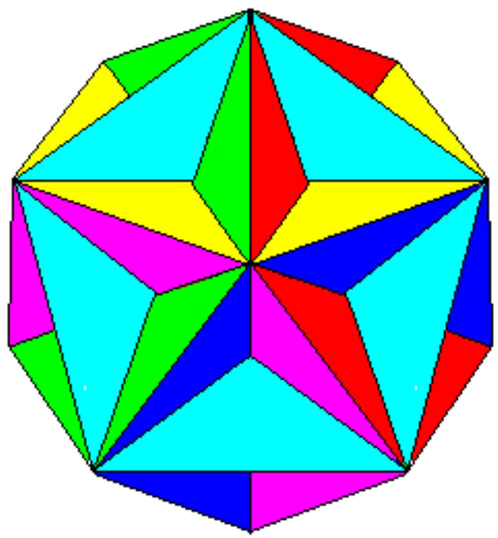


- Most people agree on the definition of a convex polyhedron.
- Polyhedron – convex
- Faces – convex

Polyhedron



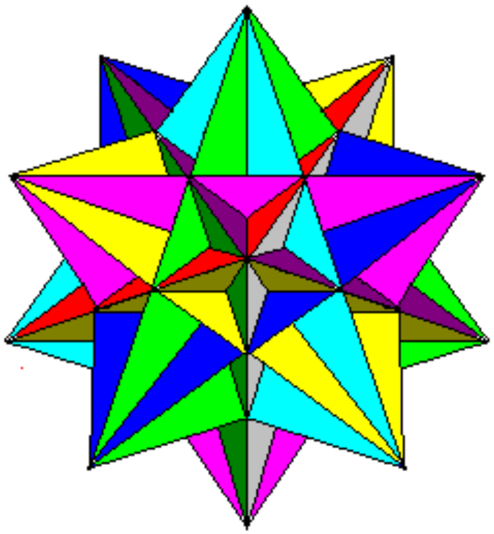
Great Icosahedron

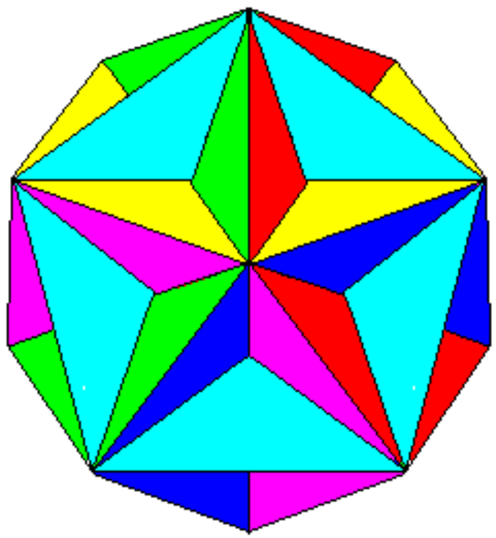


Great Dodecahedron

- Most people agree on the definition of a convex polyhedron.
- However, throughout the history the notion of polyhedron has been constantly generalized and refined.

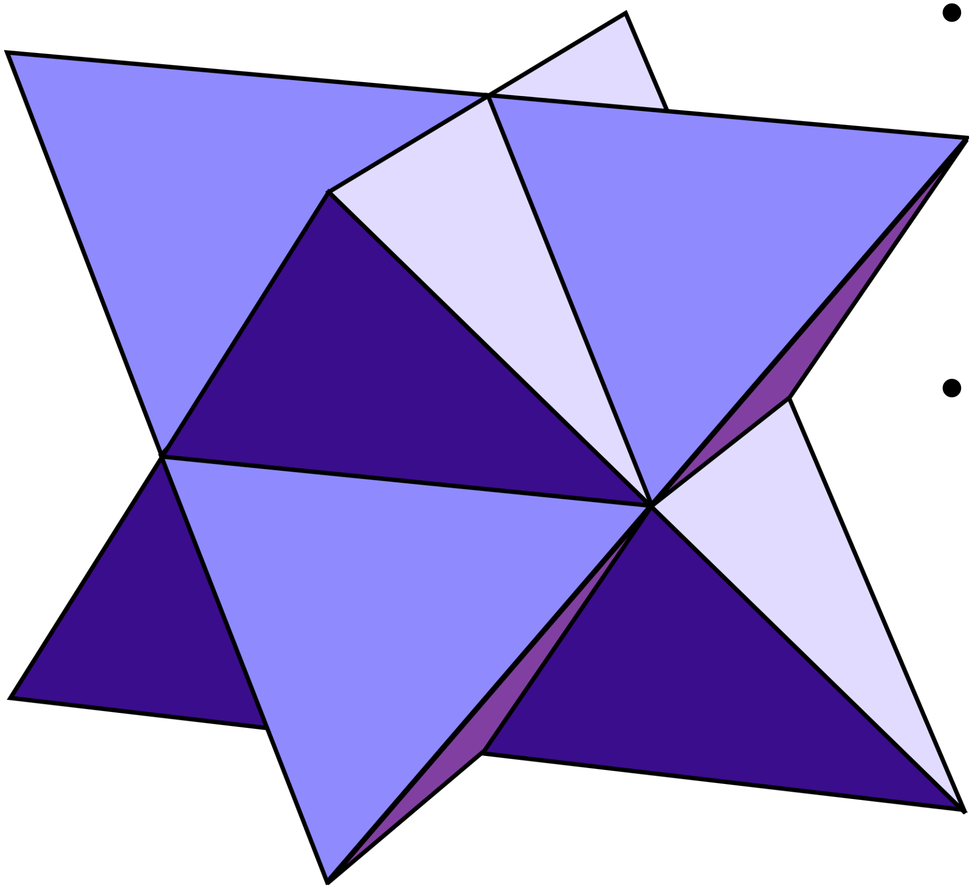
Polyhedron


Great Icosahedron


Great Dodecahedron

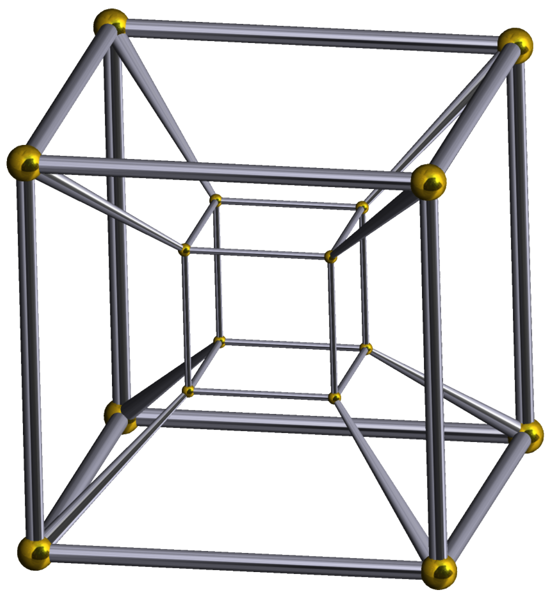
- Here faces are convex but the polyhedron itself is not convex.

Polyhedron



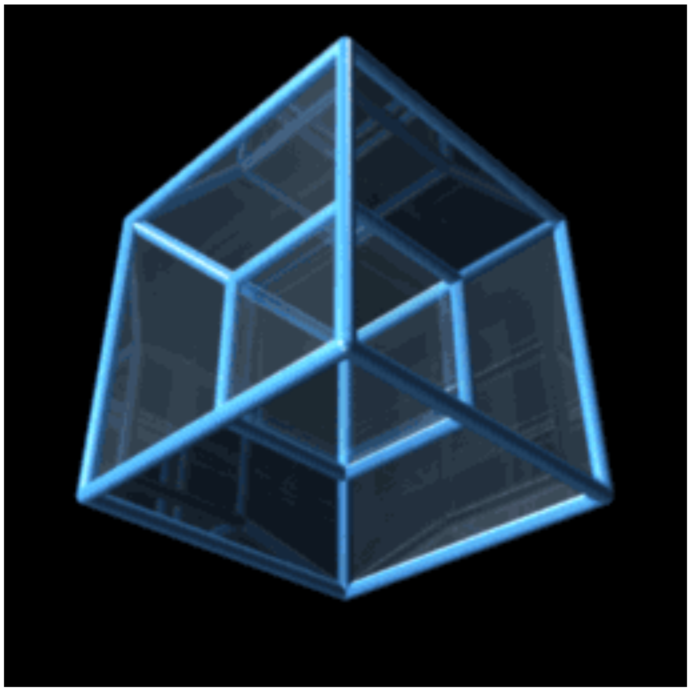
- **Stella octangula** (named by J. Kepler 1611) is not a polyhedron.
- Is it a composite.

Polytope



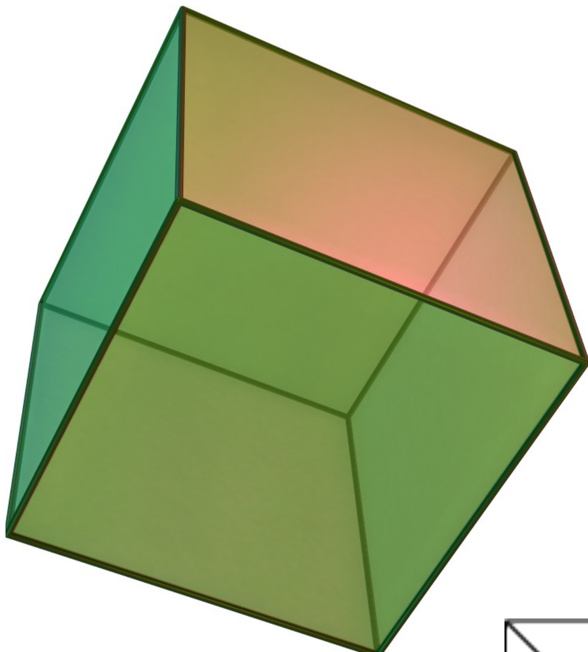
- **Polytope** is a generalization of a polyhedron in higher ranks (dimensions).
- Vertices, Edges, Faces, Facets.

Polytope

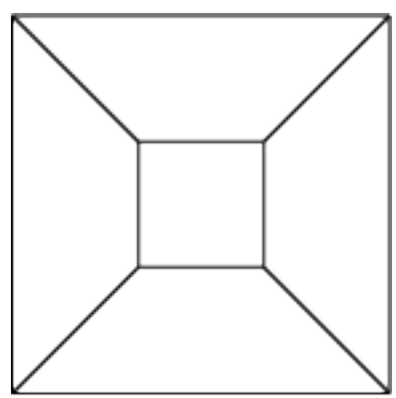


- **Polytope** is a generalization of a polyhedron in higher ranks (dimensions).
- Vertices, Edges, Faces, Facets.
- Polyhedron – convex
- Faces – convex
- Faces – planar
- Faces - skew

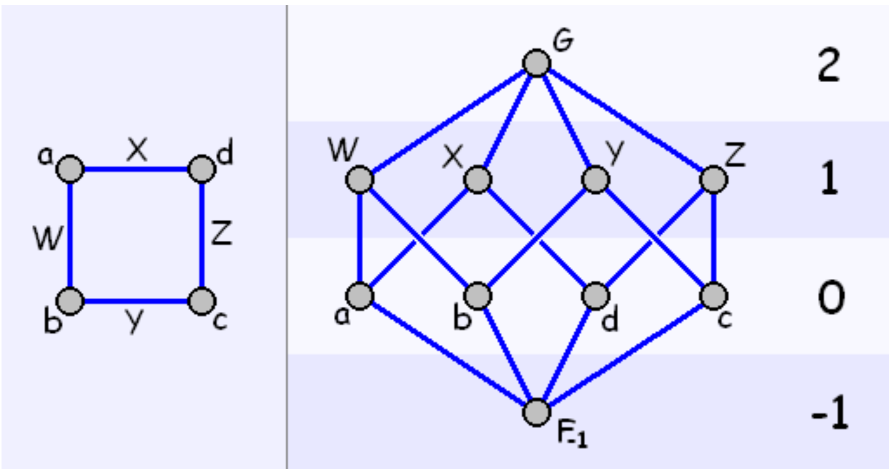
Polyhedron -> Skeleton



- Each polyhedron P gives rise to its **skeleton**, a graph G composed of vertices and edges of P.
- For our purposes the idea of skeleton suffices.



Most general: Abstract Polytope

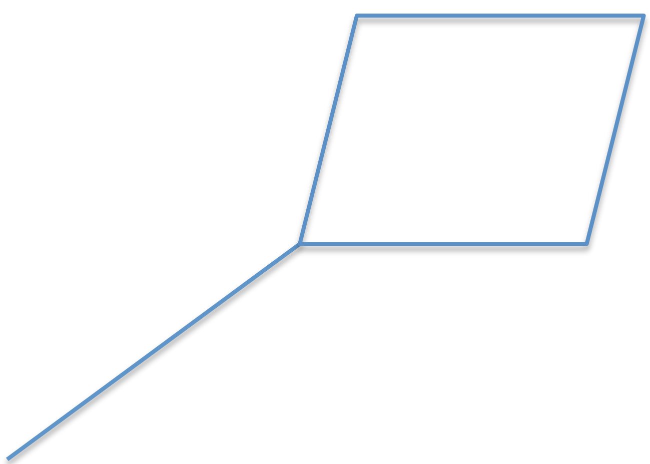


- Abstract polytopes were defined.
- Abstract Faces.
- Ranked Poset with 0 and 1
- Diamond condition
- Strong connectivity

Polyhedron in our work

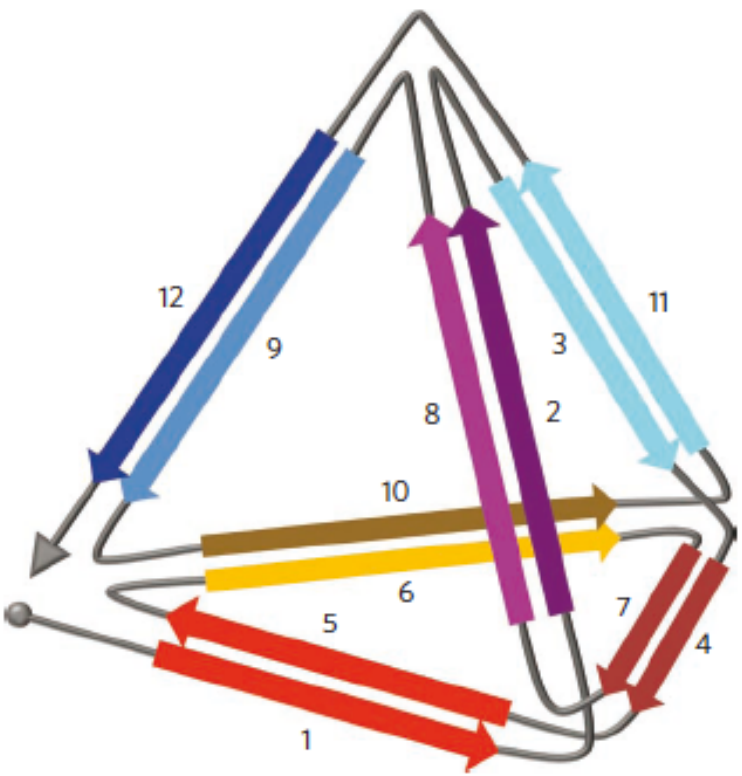
- We understand the term *Polyhedron* in a very general sense.
- On the one hand it is much more general and abstract than the usual use of this term.
- On the other hand several geometric and physical properties make certain substructures (e.g. loops) less favorable or even forbidden.

Polyhedron



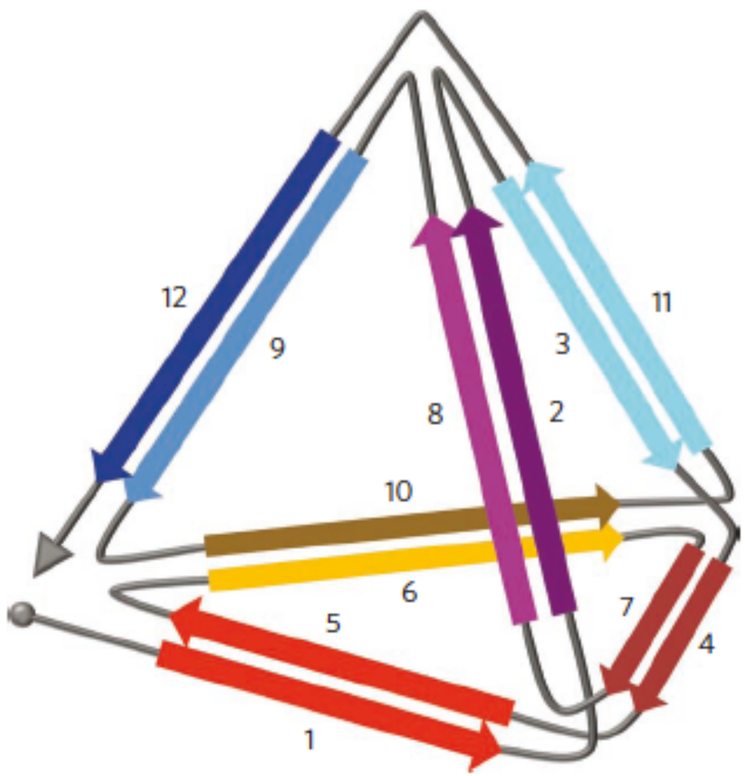
- Our polyhedron is just a connected geometric graph in ordinary space.
- It may be a skeleton of an ordinary polyhedron.
- However, it my also be just a polygon, such as triangle.
- Usually, only simple graphs are allowed.
- All edge lengths are nearly equal length.

Self-assembly by dimers (double trace)



- Ingredients:
  - Directed paths
  - Directed cycles
- Directed edges (segments) are labeled (colored).
- We assume "orthogonality" of pairs of segments that may **glue** together.
  - Only orthogonal pairs of segments (dimers) may **glue** together.
  - Each orthogonal pair is either **paralle**l or **anti-parallel**.
  - An orthogonal pair may be either a **homo-dimer** or **hetero-dimer**.

Self-assembly



- Up till now we have considered only single strand polyhdral self-assembly by dimers.
- Currenly we are looking at more general situation:
  - More than one path/ cycle) allowed.
  - Some edges may be covered only once.

Stability

Synthesis

- Given collection of ingredients, determine structures S that they form.
- Such a structure is called stable

Analysis

- For a given structure S, determine all possible gluing of ingredients that may self-assemble into S (in a stable way.)

Stability

Synthesis

- One collection of ingredients
- Several polyhedra
- All stable.

Analysis

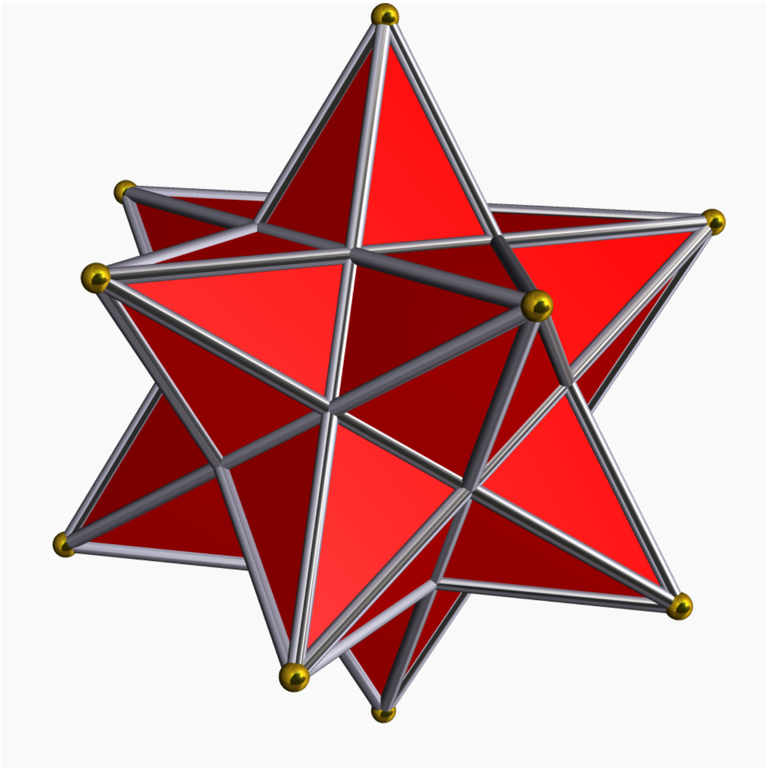
- One polyhedron
- Several solutions
- Some may be unstable.

What is stability?

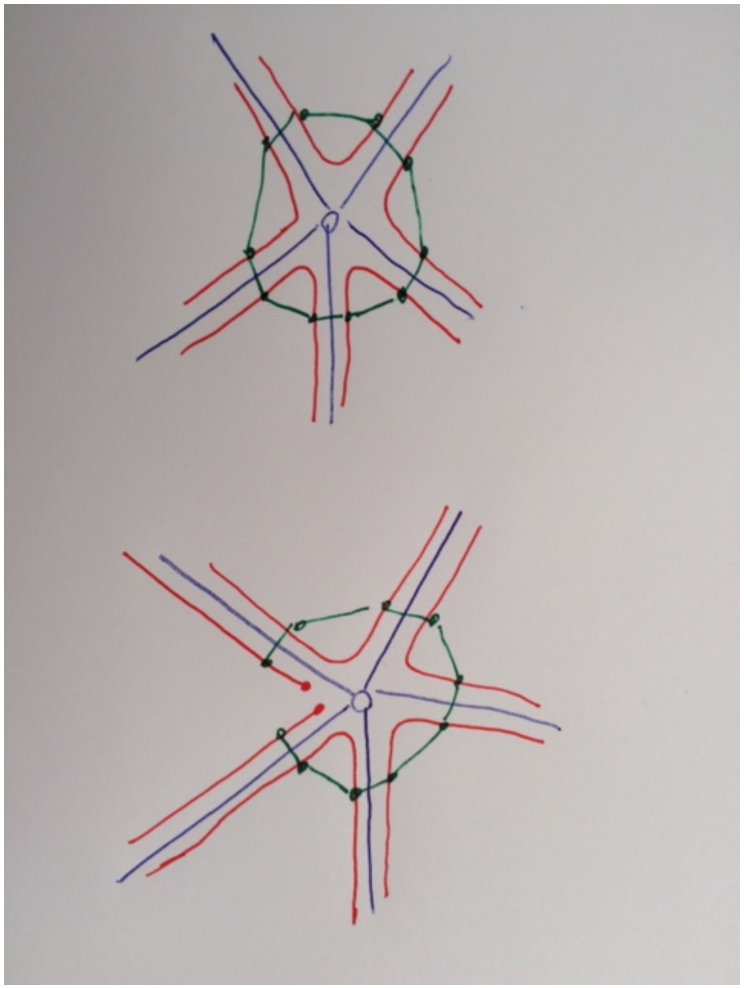
- The best way to describe stability is *vertex-figure*.

Vertex-figure

- In polytope theory the vertex-figure of a rank r polytope is a rank (r-1) polytope formed by faces incident with a give vertex.
- For polyhedra, the vertex figure must be a polygon.



Vertex-figure

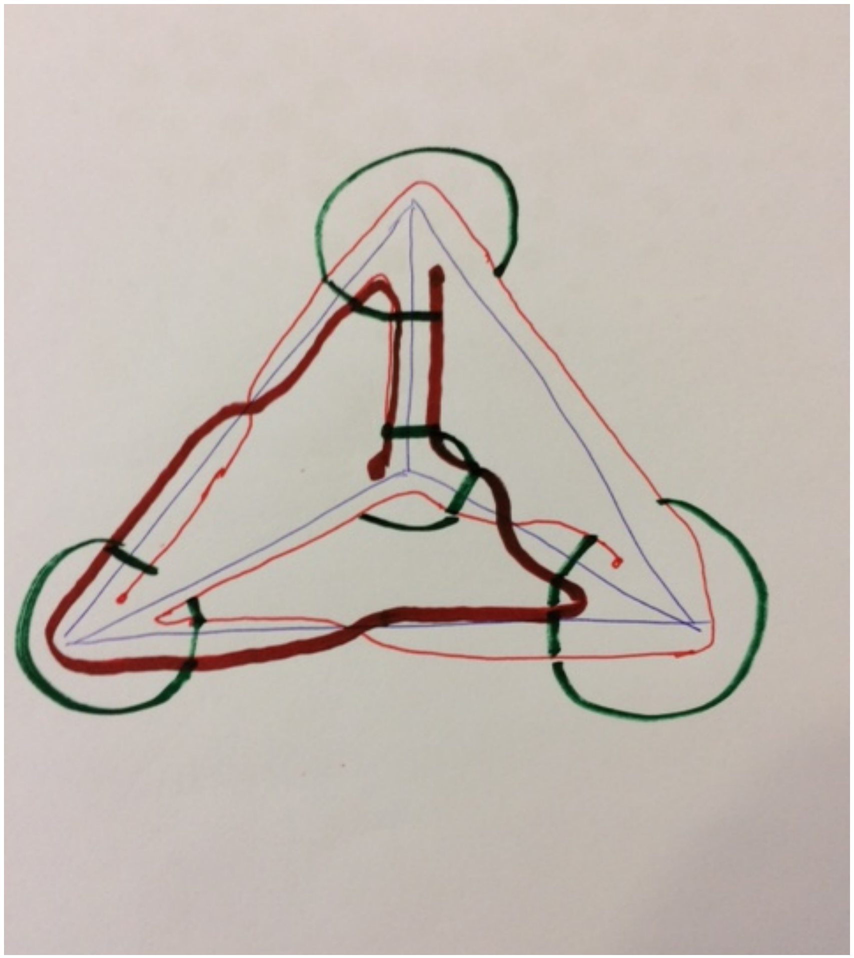


- Let v be a vertex, hit a some point by some path or cycle X along an edge e by some segment s.
- The triple (v,e,s) is a vertex of the vertex-figure graph.
- Two triples (v,e,s) and (v,e',s') are adjacent if and only if either e = e' or s and s' are adjacent (= consecutive) along X.

Stability via vertex-figures

- A polyhedron P properly covered by paths and cycles is **stable** if and only if for each of its vertices, the corresponding vertex-figure is connected graph.
- **Theorem**. Every self-assembled polyhedron is stable.

Vertex-figure



- Using the same notion of vertex figure we may define **stable** polyhedra even in case when we have more than one strand and some edges are covered only once.

Thank you!

- http://www.8ecm.si/ (July, 2020, maybe a minisymposium or satllite conference?)
- http://amc-journal.eu/index.php/amc/article/view/1269/1039 Slovenian Discrete and Applied Mathematics Society
- http://amc-journal.eu/index.php/amc/article/view/1273/1041 (ADAM - a new journal)
- http://2017.bioorigami.eu/ (Bioorigami 2017, Ljubljana, June 21-23)