STABLE TRACES

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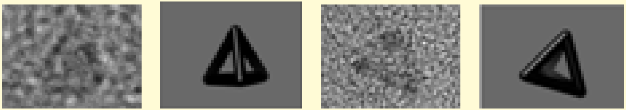
20. September 2012

Motivation

Gradišar et al. (2012) presented a novel polypeptide self-assembly strategy for nanostructure design.



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Concatenating 12 coiled-coil-forming segments in an exact order (single polypeptide chain was arranged through the 6 edges of the tetrahedron in such way that every edge was traversed exactly twice).

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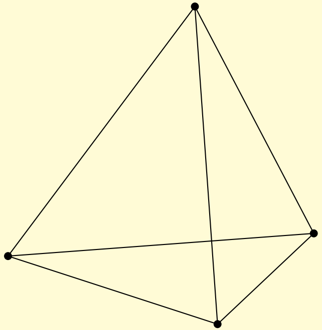

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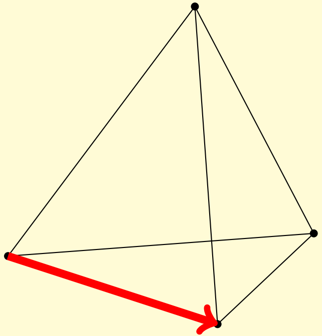

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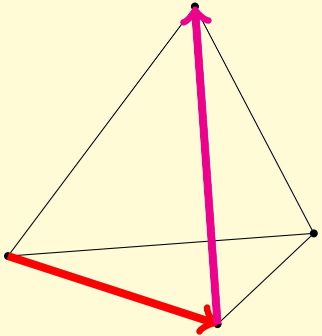

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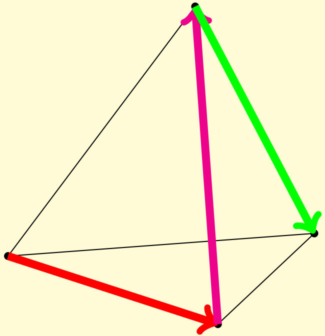

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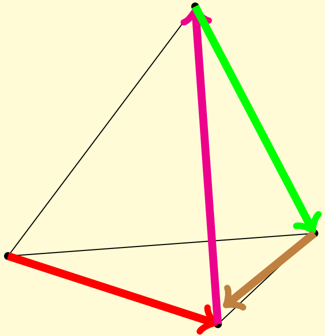

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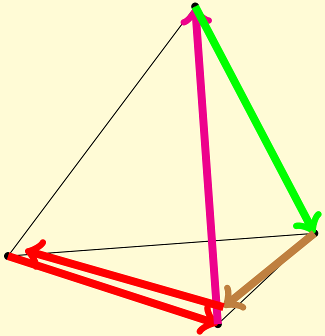

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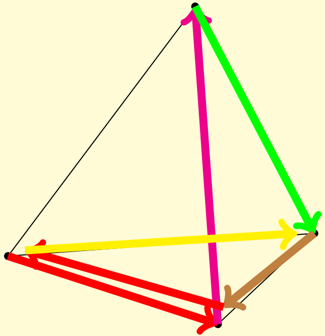

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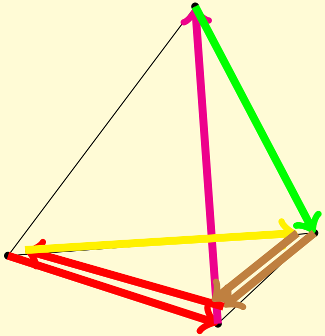

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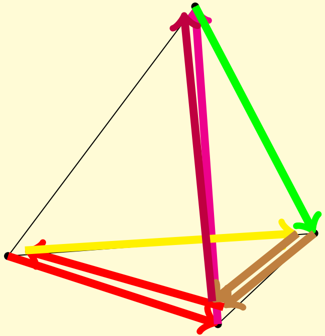

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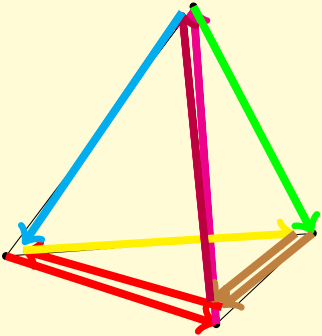

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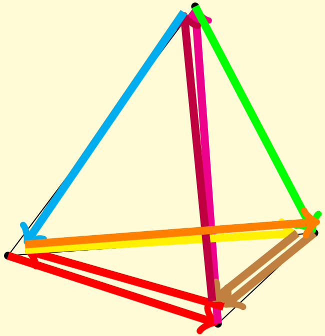

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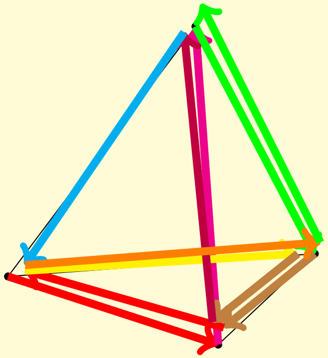

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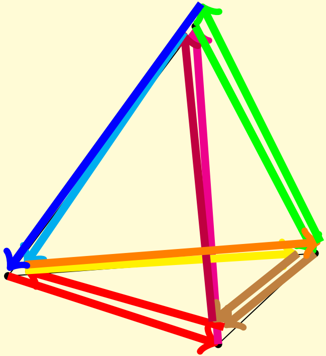

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Polyhedron P, composed from a single polymer chain, can be represented with the graph $G(P)$:

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Polyhedron P, composed from a single polymer chain, can be represented with the graph $G(P)$:

- vertices are the endpoints of segments,
- two vertices being adjacent if there is a segment connecting them,
- every edge of $G(P)$ corresponds to a coiled-coil dimer – two segments are associated with a fixed edge of $G(P)$,
- sequence of coiled-coil segments corresponds to a double trace in $G(P)$.

Double traces

Definition

A *double trace* in a graph G is a circuit which traverses every edge exactly twice.

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Theorem

Every graph G has a double trace.

Retracing

A double trace contains a *retracing* if it has an immediate succession of e by its parallel copy.

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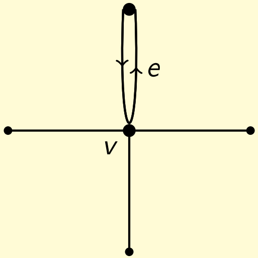

Proper traces

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Theorem (Sabidussi, 1977)

G admits a proper trace if and only if $\delta(G) \geq 2$.

Repetition

v a vertex of a G and u and w two different neighbors of v. Then double trace contains a *repetition through* v if the vertex sequence $u \to v \to w$ appears twice in any direction ($u \to v \to w$ or $w \to v \to u$).

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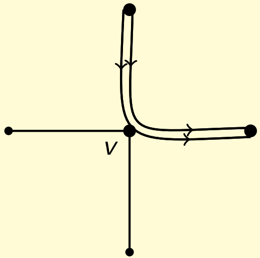

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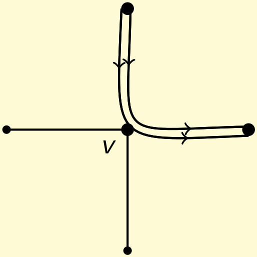

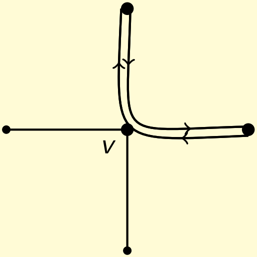

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G admits a stable trace if and only if $\delta(G) \geq 3$.

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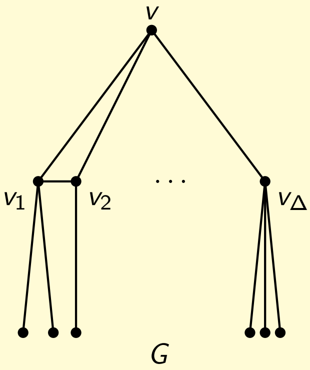

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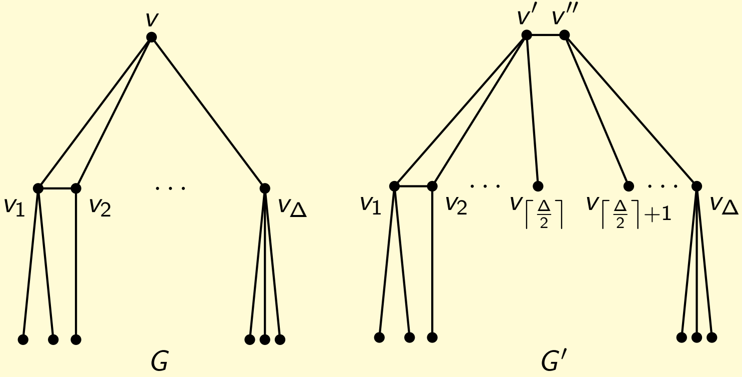

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- If G is cubic proper and stable traces are equivalent,
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- T' without $v'v''$ and $v''v'$ is stable trace in G.

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Proposition

G admits a parallel double trace (parallel proper trace) if and only if G is Eulerian.

Antiparallel double traces

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Proposition

Every graph admits an antiparallel double trace.

Theorem (Thomassen, 1990)

G admits an antiparallel proper trace if and only if $\delta(G) > 1$ and G has a spanning tree T such that each connected component of $G - E(T)$ either has an even number of edges or contains a vertex v, $d_G(v) \geq 4$.

Open problem 1

Problem

Characterize graphs that admit parallel (antiparallel) stable traces.

Numerical results

- Enumeration results for six polyhedra: the tetrahedron, 4-pyramid, 3-bipyramid, octahedron, 3-prism and 3-cube.

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  - shifting,
  - applying a permutation induced by an automorphisms of G,
  - using any combination of the previous three operations.

Numerical results

graph	PT	aPT	pPT	ST	aST	pST
tetrahedron	3	0	0	3	0	0
4-pyramid	101	5	0	82	5	0
3-bipyramid	925	24	0	470	0	0
octahedron	53372	668	1352	22246	0	275
3-prism	25	2	0	25	2	0
3-cube	40	0	0	40	0	0

Open problem 2

Problem

Analytically enumerate ((anti)parallel) proper and stable traces in graphs, in particular in polyhedra.

Thank you for your attention!