



The Molecular Conjecture in 2D

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3-space: Generic Body and Hinge Frameworks

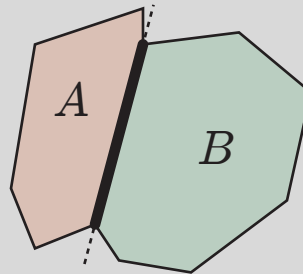
Solved

Alternate generalization to 3-space:

Two bodies, joined on linear hinge

6 degrees for each body.

Each hinge removes 5 degrees of freedom





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Graph $G = (C, H)$

C : vertices for abstract bodies,

H : for pairs which share a hinge.

Necessary count for independence becomes: $5|H| \leq 6|C| - 6$

Theorem 1 (Tay and Whiteley (84)) *Also sufficient for generic independence with hinges, with*

$$5|H| \leq 6|C| - 6$$



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Algorithms:

$$6|C| - 6 = 6(|C| - 1)$$

or

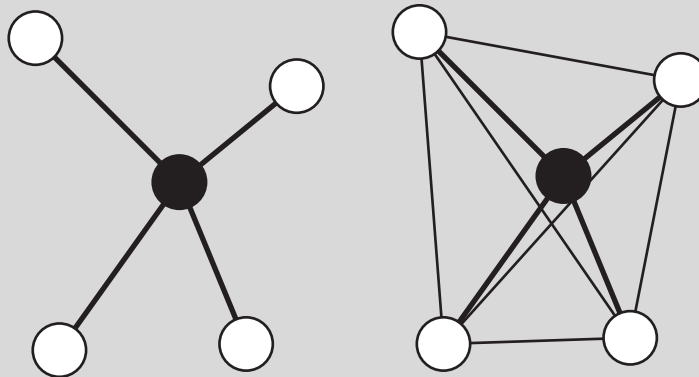
6 spanning trees if replace 'hinge edge' by five edges for multi-graph.



1. Modeling molecules

(special graphs) - can we predict rigidity?

Single atom and associated bonds



$$|V| = 5 \quad |E| = 10$$

$$|E| = 3|V| - 5 \quad \text{overbraced}$$

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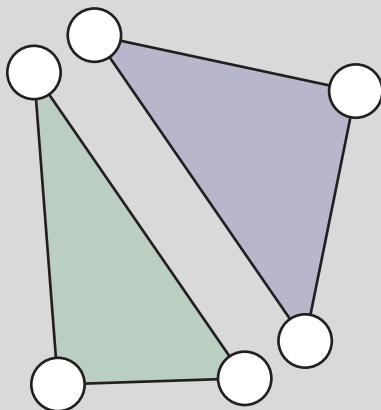
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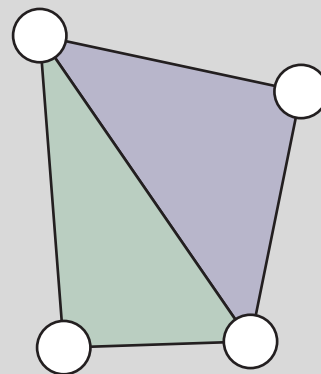


Adjacent atom clusters

Flexible



$$|C| = 2, |H| = 1, \\ |V| = 4, |E| = 5$$



$$5|H| = 6|C| - 7, \\ |E| = 3|V| - 7$$

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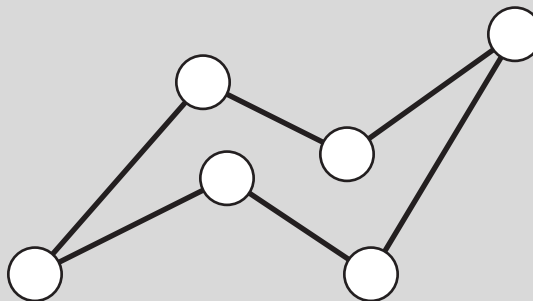
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Rings of atoms:

Ring of 6 atoms and bonds



Body and hinge: $|B| = 6$, $|H| = 6$, $5|H| = 6|B| - 6$
Just the right number to be rigid - generically.



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Graph G of atoms and covalent bonds

Body and hinge model

Atoms are bodies

bonds are hinges

count as body and hinge structure

Problem: Special geometry with hinges concurrent

Special geometry may lower rank!



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Graph G of atoms and covalent bonds
Form G^2

atoms are vertices

bonds are edges

second neighbor bond bending pairs are edges count as

$$3|V| - 6$$

priority system on bond edges.

Problem: for general graphs G the rank may be lower. (May work for G^2 ?)



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Lots of experimental evidence;

Proofs of correctness for special classes of graphs

Plausibility arguments related to other conjectures on 3-space rigidity

Sketched proof of equivalence of the two conjectures.

Conjectures embedded in implemented algorithms: FIRST on the web (Arizona State University)

Seek additional graph models for applications biochemical constraints:

Apply to other problems in biochemistry, chemistry



2. Molecular Conjecture in the Plane

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Given: Simple graph $G = (V, E)$.

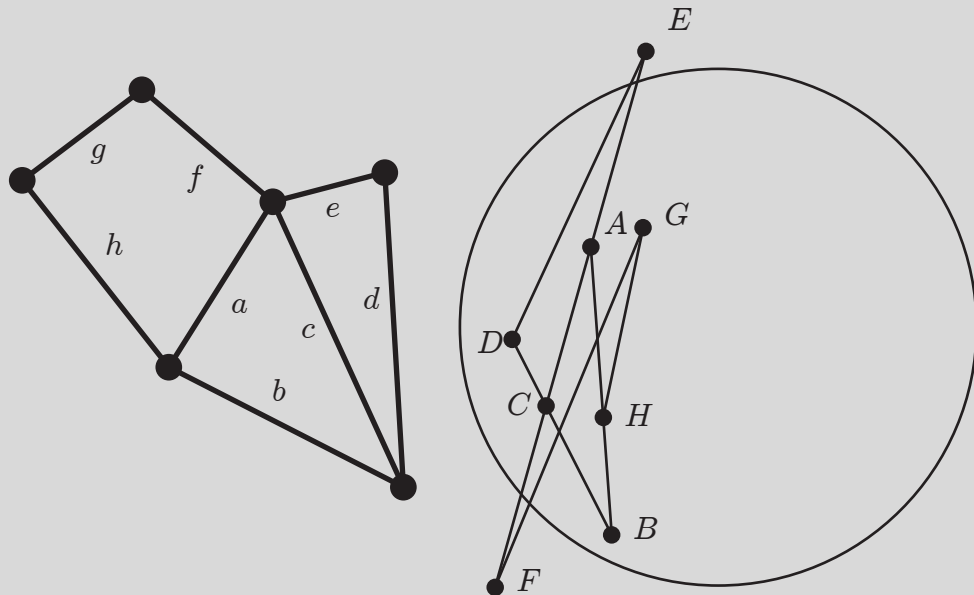
- Regard as a body and pin graph of a structure in the plane:
Vertices are bodies.
Edges denote pins.
- Note: Each pin connects just two bodies. Otherwise we would need a hypergraph.
- Realizations:
 - Amorphous bodies. Embedding specifies the location of the pins.
 - Line bodies. Embedding may specify either lines or pins.
 - Question: Does the line realization always exist?



3. Realization in the Plane.

Theorem 2 *If $G = (V, E)$ is simple, then a pin collinear structure exists.*

Take any generic embedding of the structure graph $G = (V, E)$ in \mathbb{R}^2 . Form the polar of that embedding.



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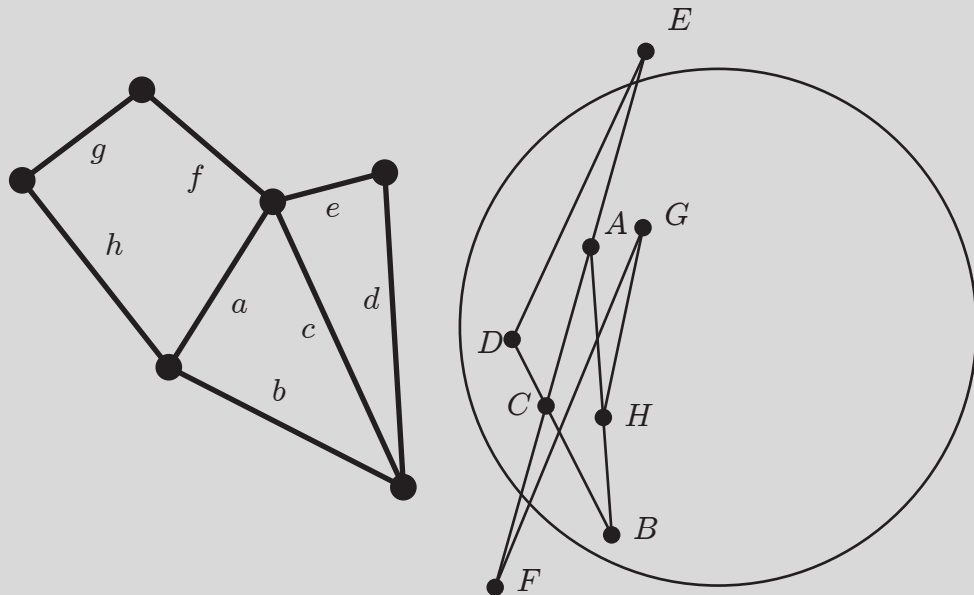


Question:

Is the polar generic as a line pin structure?

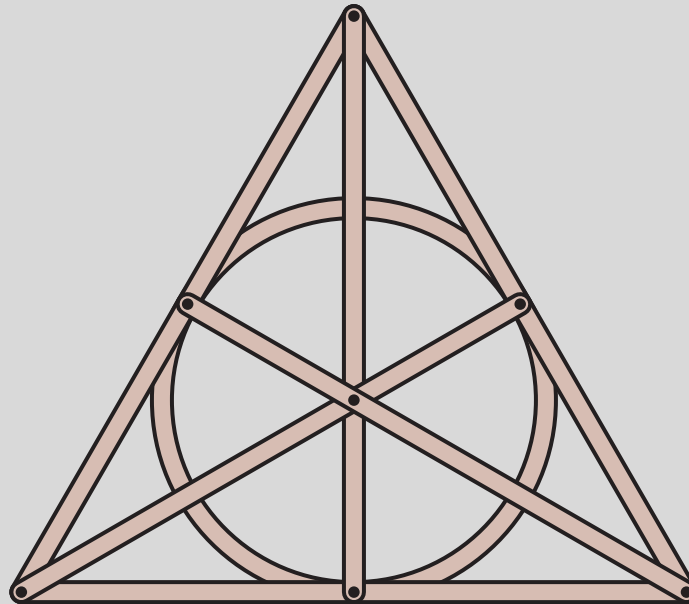
Question:

Is it generic as a body pin structure?





Note: A general pin body structure may have no pin collinear realization:



The incidence structure is a hypergraph.



EGRES TECHNICAL REPORTS TR-2006-06

Pin-collinear Body-and-Pin Frameworks and the Molecular Conjecture

Bill Jackson, Tibor Jordàn

Abstract

T-S. Tay and W. Whiteley independently characterized the multigraphs which can be realized as an infinitesimally rigid d -dimensional body-and-hinge framework. In 1984 they jointly conjectured that each graph in this family can be realized as an infinitesimally rigid framework with the additional property that the hinges incident to each body lie in a common hyperplane. This conjecture has become known as the Molecular Conjecture because of its implication for the rigidity of molecules in 3-dimensional space. Whiteley gave a partial solution for the 2-dimensional form of the conjecture in 1989 by showing that it holds for multigraphs $G = (V, E)$ in the family which have the minimum number of edges, i.e. satisfy $2|E| = 3|V| - 3$. In this paper, we give a complete solution for the 2-dimensional version of the Molecular Conjecture. Our proof relies on a new formula for the maximum rank of a pin-collinear body-and-pin realization of a multigraph as a 2-dimensional bar-and-joint framework.

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Theorem 3 *A multigraph G can be realized as an infinitesimally rigid body and hinge framework in \mathbb{R}^d if and only if $((\binom{d+1}{2} - 1)G$ has $\binom{d+1}{2}$ edge-disjoint spanning trees. (Tay and Whiteley, 1984)*



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Recent Advances in the Generic Rigidity of Structures, Tiong-Seng Tay and Walter Whiteley Structural Topology # 9, 1984
Many body and hinge structures are built under additional constraints. For example in architecture flat panels may be used in which all hinges are coplanar. In molecular chemistry, we can model molecules by rigid atoms hinged along the bond lines so that all hinges to an atom are concurrent. This is the natural projective dual for the architectural condition.

Conjecture: A multigraph is generically rigid for hinged structures in n -space iff it is generically rigid for hinged structures in n -space with all hinges of body v_i in a hyperplane H_i of the space.



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Remarks: For the plane ($n=2$ with all pins along a line), this conjecture was made in 1979 but remains unsolved. With the recent breakthrough for real structures in 3-space the problem becomes more important.

Only in 3-space does projective duality convert a hinge structure to a new hinge structure.



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Jackson-Jordan prove first:

Theorem 4 *Let $G(V, P)$ be a graph with no isolated vertices. Then the maximum rank of a pin-collinear body and pin realization of G as a bar and joint framework is $2(|V| + |P|) - 3 - \text{def}(G)$.*



A pin-collinear body and pin realization of $G(V, P)$ is the square of a subdivision of G .

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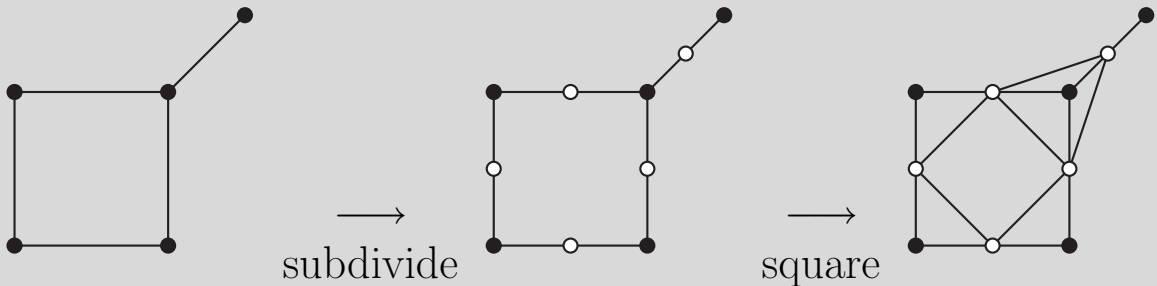
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The deficiency of $G(V, P)$ is $3V - 3 - r_2(G)$, where r_2 is the rank in the associated 2-polymatroid of G .



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2-polymatroid associated to $G(V, P)$ with a body and pin realization G^* embedded in \mathbb{R}^2 : An infinitesimal motion of G is a map $S : V \rightarrow \mathbb{R}^3$ satisfying the constraints that for all $p = uv \in P$ we have $S(u) - S(v) = \langle (x(e), -y(e), 1) \rangle$.

The set of infinitesimal motions is the nullspace of a $2|P| \times 3|V|$ matrix.



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Example: Let G be a triangle, whose edges, a, b, c are representing pins and are located at $(x_a, y_a), (x_b, y_b), (x_c, y_c)$ respectively. The vertex set represents the bodies, each body has two pins on it.

$$\begin{pmatrix} 1 & 0 & -x_a & -1 & 0 & x_a & 0 & 0 & 0 \\ 0 & 1 & y_a & 0 & -1 & -y_a & 0 & 0 & 0 \\ 1 & 0 & -x_b & 0 & 0 & 0 & -1 & 0 & x_b \\ 0 & 1 & y_b & 0 & 0 & 0 & 0 & -1 & -y_b \\ 0 & 0 & 0 & 1 & 0 & -x_c & -1 & 0 & x_c \\ 0 & 0 & 0 & 0 & 1 & y_a & 0 & -1 & -y_a \end{pmatrix}$$



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re-arrange the rows/columns:

$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & -x_a & x_a & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & -x_b & 0 & x_b \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & x_c & x_c \\ 0 & 0 & 0 & 1 & -1 & 0 & y_a & -y_a & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & y_b & 0 & -y_b \\ 0 & 0 & 0 & 0 & 1 & -1 & -y_c & y_c & 0 \end{pmatrix}$$



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Jackson and Jordan show further, that a pin-line generic body and pin collinear body and pin realization of G has maximal rank over all pin-collinear body and pin realizations of G .

The main theorem is then:

Theorem 5 *Let $G(V, P)$ be a graph with no isolated vertices. Then the maximum rank of a pin-collinear body and pin realization of G as a bar and joint framework is $2(|V| + |P|) - 3 - \text{def}(G)$.*



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Finally Jackson and Jordan show that the body-and-pin and rod-and-pin 2-polymatroids of a graph are identical. As a solution to the molecular conjecture they formulate

Theorem 6 *Let $G(V, E)$ be a multigraph. Then the following statements are equivalent:*

(a) *G has a realization as an infinitesimally rigid body and hinge framework in \mathbb{R}^2 .*

(b) *G has a realization as an infinitesimally rigid body-and-hinge framework (G, q) in \mathbb{R}^2 with each of the sets of points $\{q(e) : e \in E_G(v)\}, v \in V$, collinear.*

(c) *$2G$ contains 3 edge disjoint spanning trees.*



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In the body-and hinge frameworks so far investigated, each hinge is shared by exactly two bodies. Can one generalize from body-pin graph to body and pin incidence structure? J-J conjecture yes and point out that Whitely proved this for independent structures and made a similar conjecture in 1989.



$$\begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x - a \\ y - b \end{bmatrix} = \begin{bmatrix} a + \omega b \\ b - \omega a \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

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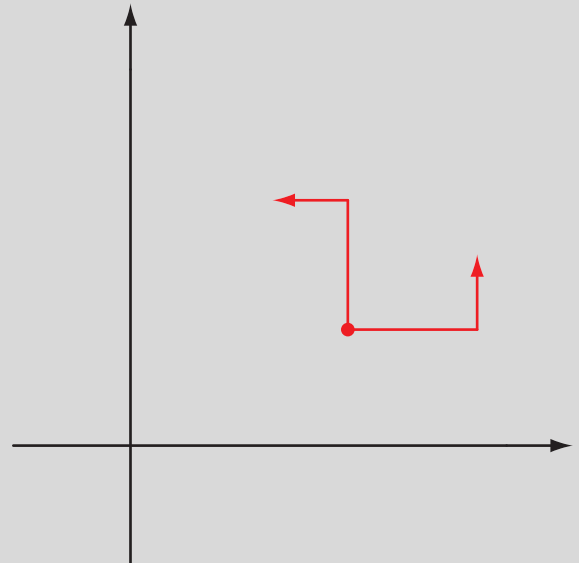
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$$\begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x - a \\ y - b \end{bmatrix} = \begin{bmatrix} a + \omega b \\ b - \omega a \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

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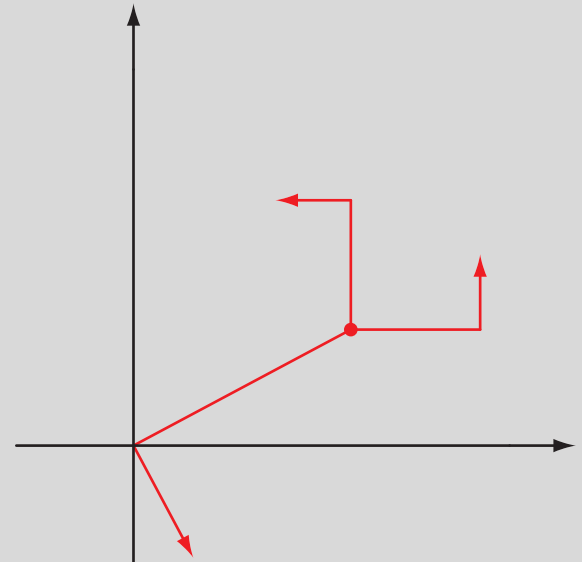
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$$\begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x - a \\ y - b \end{bmatrix} = \begin{bmatrix} a + \omega b \\ b - \omega a \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

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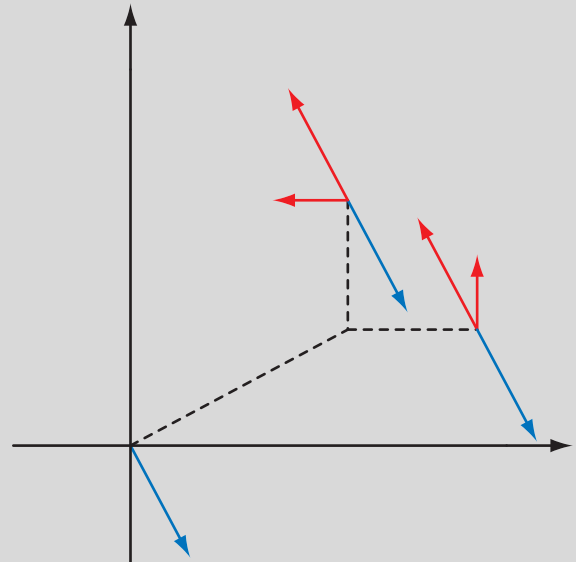
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$$\begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x - a \\ y - b \end{bmatrix} = \begin{bmatrix} a + \omega b \\ b - \omega a \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

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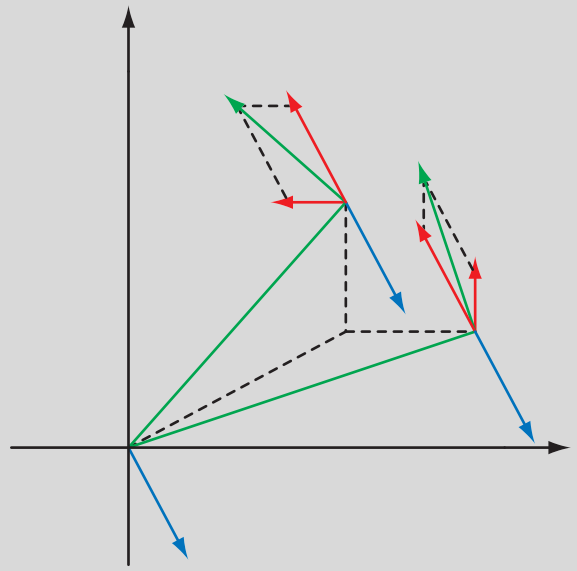
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$$\begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x - a \\ y - b \end{bmatrix} = \begin{bmatrix} a + \omega b \\ b - \omega a \end{bmatrix} + \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

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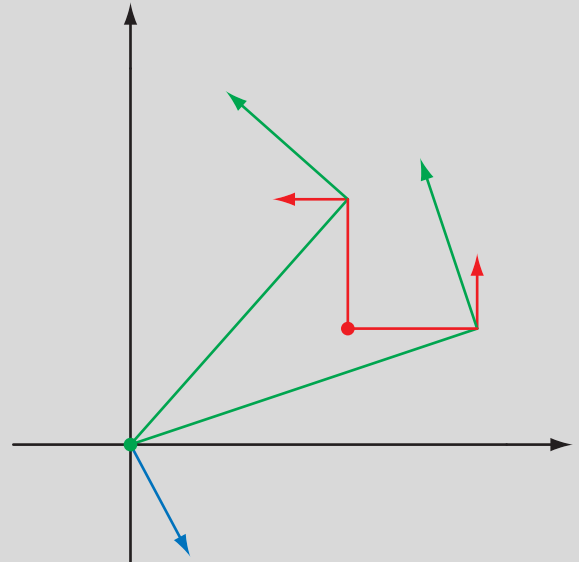
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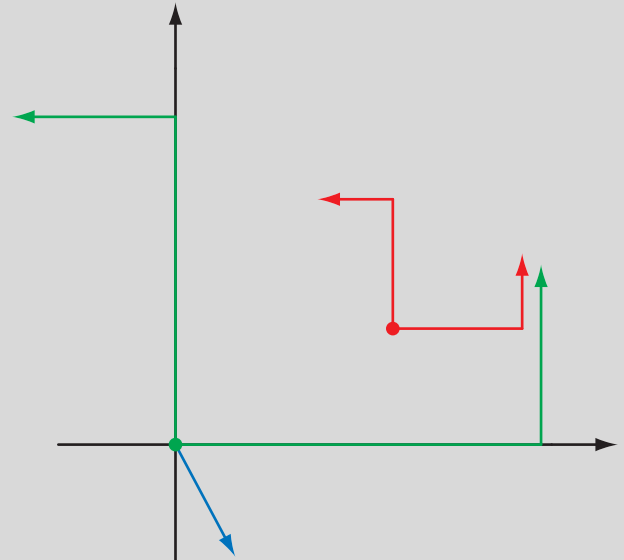
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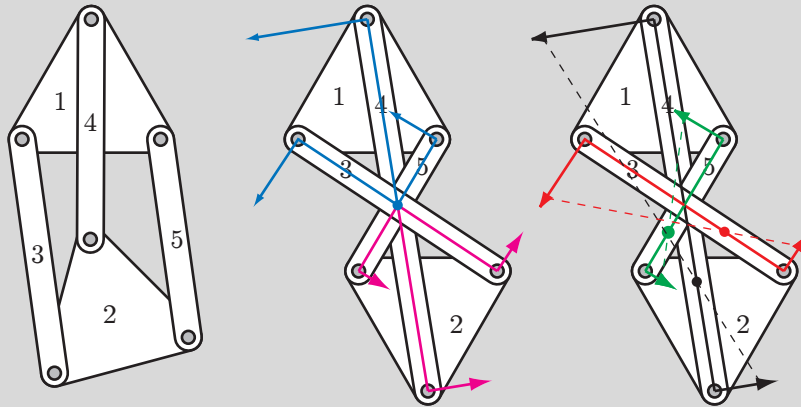
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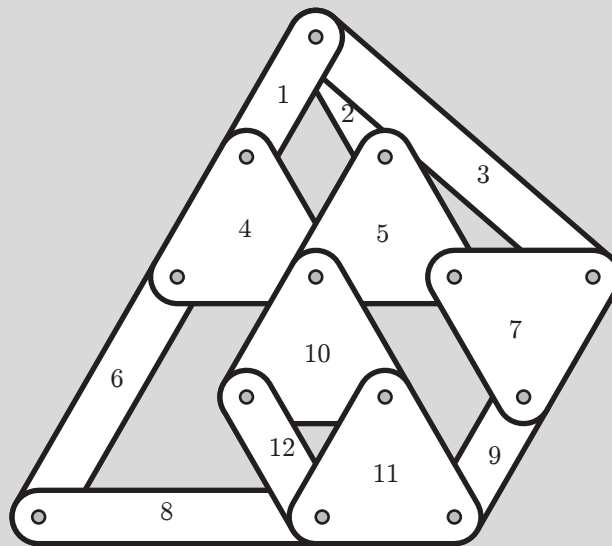
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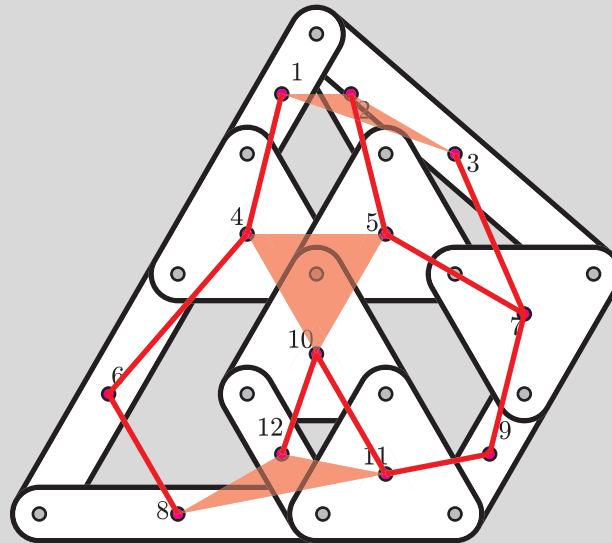
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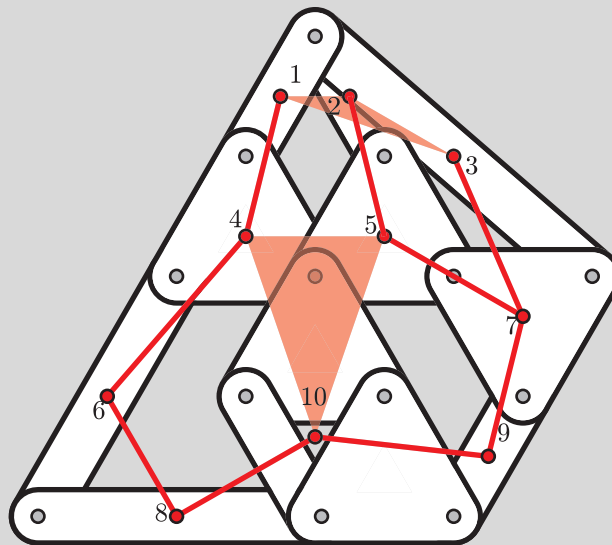
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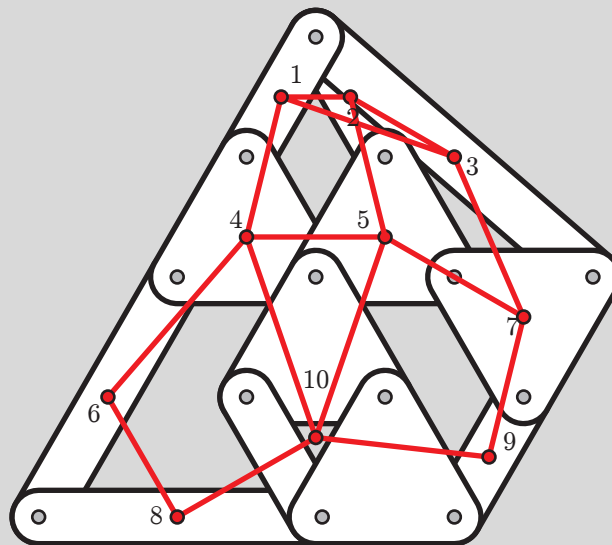
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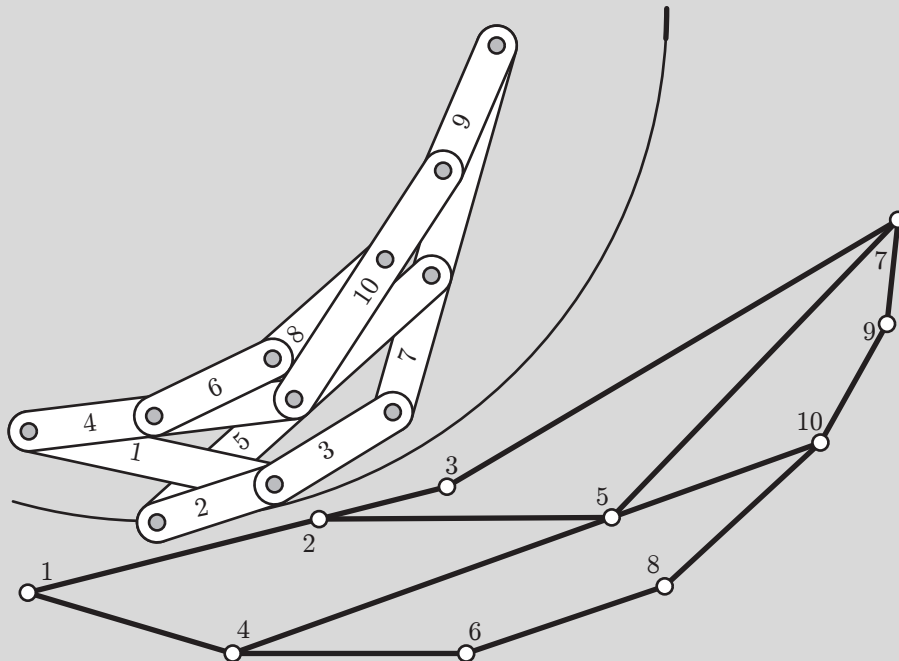
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