Counts for predicting symmetric motions in frameworks with applications to protein flexibility

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October 18, 2011

Joint work with Adnan Sljoka (York U.) and Walter Whiteley (York U.)

Outline

1. Part I: Symmetric counts for detecting flexibility in frameworks
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    - Symmetric Maxwell counts from the orbit rigidity matrix
    - Examples
    - Further results and extensions
2. Part II: Applications to protein flexibility
    - Symmetry in molecules
    - Generic rigidity of molecular frameworks
    - Added flexibility due to $\mathcal{C}_2$ symmetry: counts and algorithms
    - Added flexibility due to $\mathcal{D}_2$ and $\mathcal{D}_3$ symmetry
    - Conclusions

Part I

Symmetric counts for detecting flexibility in frameworks

Rigidity

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$$f_G(p_1, \dots, p_n) = \big(\dots, \|p_i - p_j\|^2, \dots\big),$$

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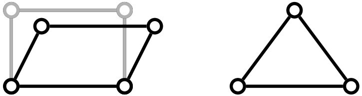

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Infinitesimal rigidity

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- (G,p) is called infinitesimally flexible in $\mathbb{R}^d$ if there exists a non-trivial infinitesimal motion. Otherwise, (G,p) is called infinitesimally rigid.

Rigidity vs. infinitesimal rigidity

- **Thm.** A framework (G, p) in $\mathbb{R}^d$ with $|V(G)| \geq d$ is infinitesimally rigid if and only if $\mathrm{rank}\big(\mathbf{R}(G, p)\big) = d|V(G)| - \binom{d+1}{2}$.

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- **Thm. (Maxwell, 1864)** If a graph G is generically d-rigid, then

$$|E(G)| \geq d|V(G)| - \binom{d+1}{2}.$$

Symmetry in frameworks

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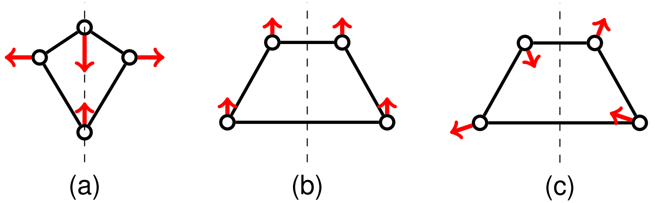

Figure: (a), (b) $\mathcal{C}_s$-symmetric infinitesimal motions; (c) a non-symmetric infinitesimal motion.

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- The orbit matrix is of size $|\mathscr{O}_e| \times \sum_{i=1}^{k} c_i$, where $c_i = \dim \bigcap_{x \in S : x(p_i) = p_i} F_x$ and $F_x = \{a \in \mathbb{R}^d : x(a) = a\}$.

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- The row corresponding to an edge $\{i, x(j)\}$ is of the form

$$\begin{array}{ccccc} & i & & j & \\ \big(0 \dots 0 & (p_i - x(p_j))\mathbf{M}_i & 0 \dots 0 & (p_j - x^{-1}(p_i))\mathbf{M}_j & 0 \dots 0 \big) \end{array}$$

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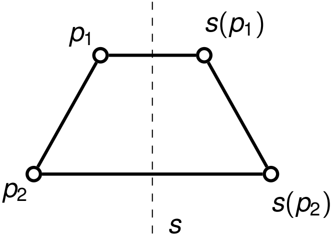
$$\begin{array}{ccccc} & i & & & \\ \big(0 \dots 0 & (2p_i - y(p_i) - y^{-1}(p_i))\mathbf{M}_i & 0 \dots 0 & 0 & 0 \dots 0 \big) \end{array}$$

Examples of orbit rigidity matrices



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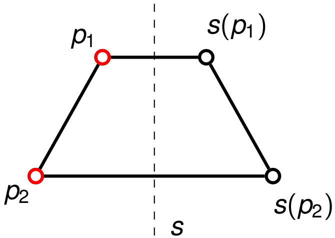

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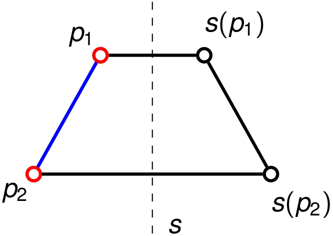

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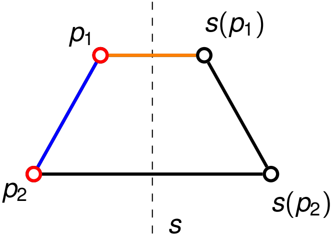

$$\begin{bmatrix} (p_1 - p_2) & (p_2 - p_1) \\ 2(p_1 - s(p_1)) & 0 \quad 0 \\ & \end{bmatrix}$$

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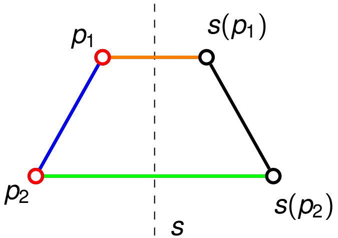

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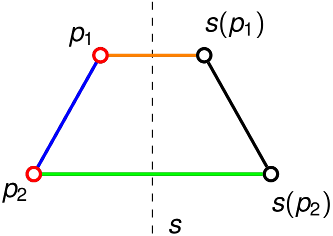

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3×4 matrix

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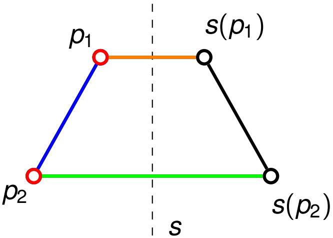

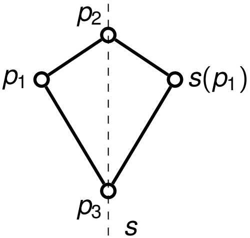

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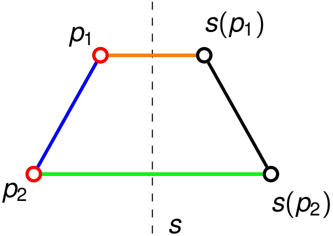

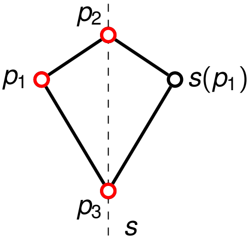

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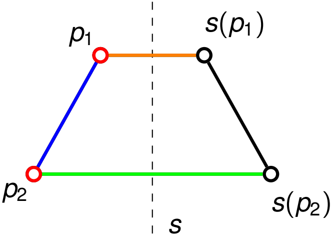

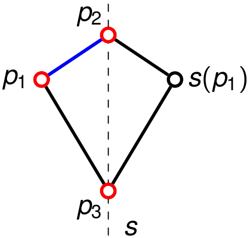

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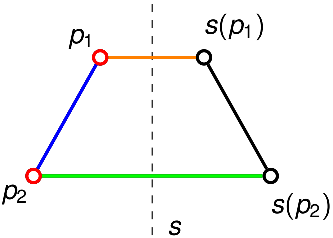

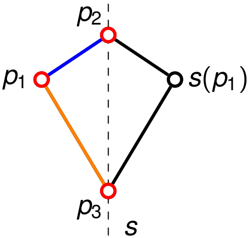

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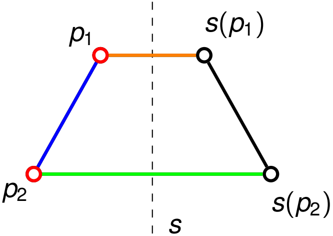

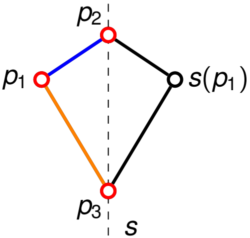

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Properties of the orbit rigidity matrix $\mathbf{O}(G, p, S)$

- **Thm. (S. and Whiteley, 2010)** Let (G, p) be a framework with symmetry group S. Then

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- **Thm. (S., 2009)** If p is S-regular and (G, p) has an S-symmetric infinitesimal flex, then there also exists a finite flex of (G, p) which preserves the symmetry of (G, p) throughout the path.

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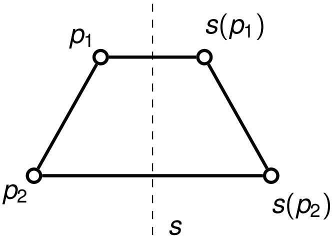
- **Rem.** It can be tricky to find m.

Example 1: quadrilaterals with mirror symmetry



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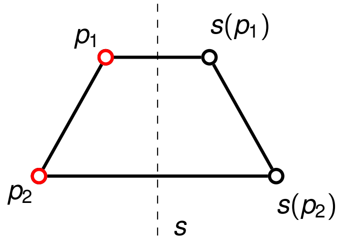

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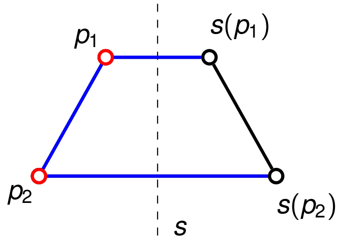

$c = 2 \cdot 2 = 4$

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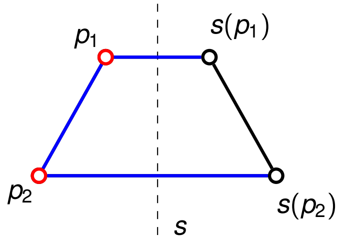

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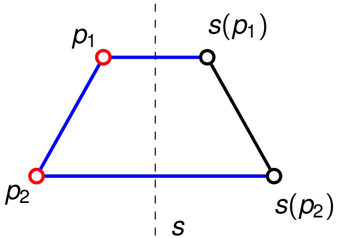

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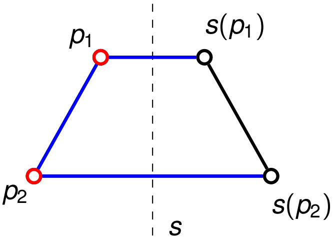

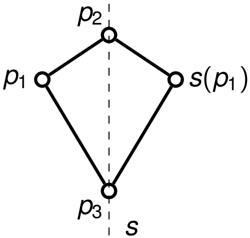

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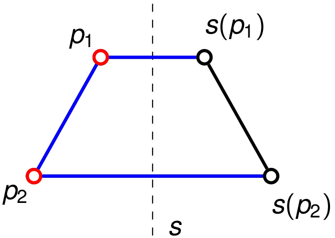

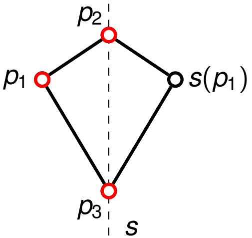

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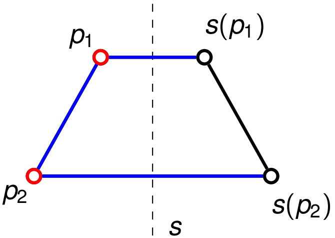

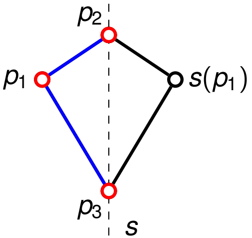

$c = 2 \cdot 2 = 4$

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$c = 2 + 2 \cdot 1 = 4$

$r = 2$

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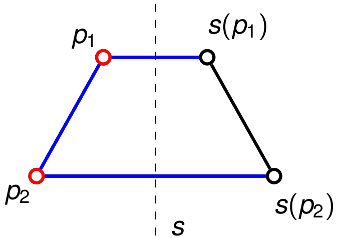

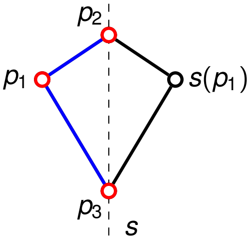

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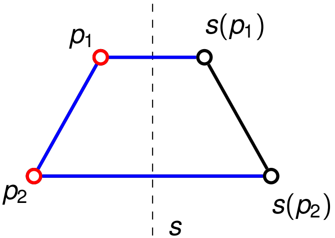

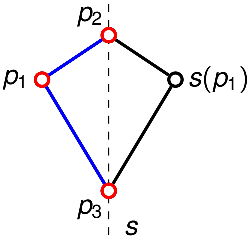

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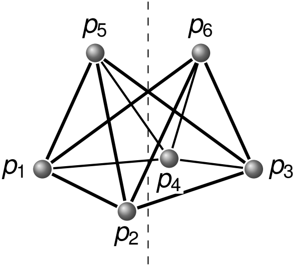
$$r = 3 \qquad r = 2$$

$$m = 1 \qquad m = 1$$

$$r = 3 = c - m \qquad r = 2 < 3 = c - m$$

Example 2: the Bricard octahedra



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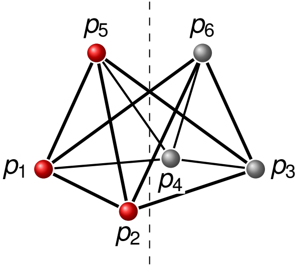

$c = 3 \cdot 3 = 9$

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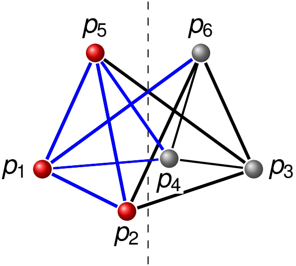

$$c = 3 \cdot 3 = 9$$
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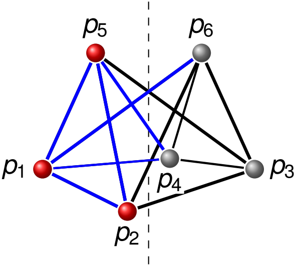

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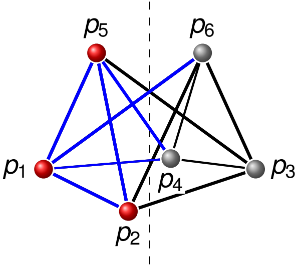

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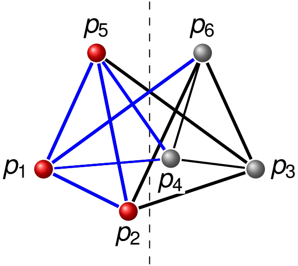

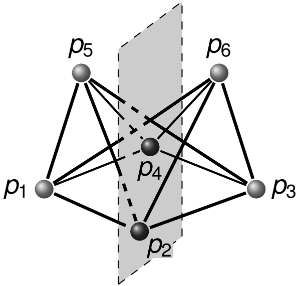

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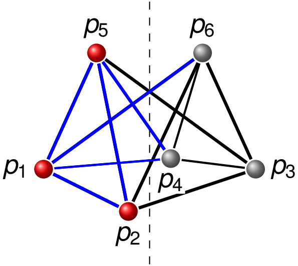

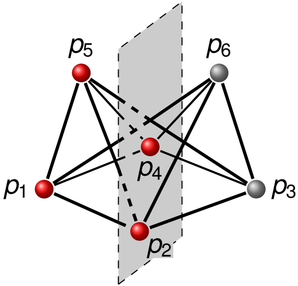

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$c = 2 \cdot 3 + 2 \cdot 2 = 10$

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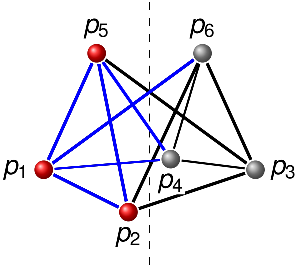

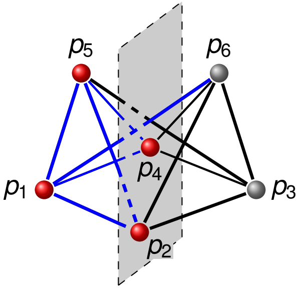

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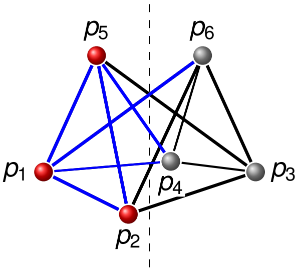

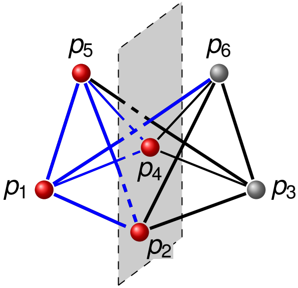

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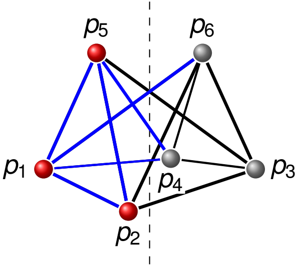

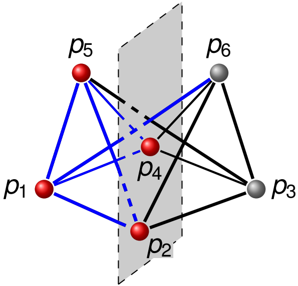

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$r = 6$

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$r = 6 < 7 = c - m$

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A general result for $\mathcal{C}_2$

Thm. Let G be a graph with $|E(G)| = 3|V(G)| - 6$ and let $\mathcal{C}_2 = \{Id, C_2\}$ be the half-turn symmetry group in 3-space.

If $j_{C_2} = b_{C_2} = 0$ (i.e., no vertices and no edges fixed by C_2), then $\mathcal{C}_2$-regular realizations of G have a symmetry-preserving finite flex.

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Thus, $r < c - m$. $\square$

Further results and extensions

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  Symmetric infinitesimal flexes and finite flexes (at *S*-regular points) can be transferred from frameworks in $\mathbb{E}^d$ to coned frameworks in $\mathbb{E}^{d+1}$ and to frameworks in $\mathbb{S}^d$, $\mathbb{H}^d$, and $\mathbb{M}^d$ (using symmetric coning).
  [S. and Whiteley: Coning, symmetry and spherical frameworks, arXiv:1108.2174, 2011]

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- Combined orbit matrices for periodic frameworks with additional symmetries allow detection of finite flexes which preserve the entire crystallographic group.
  In particular: Inversion symmetry in 3-space gives 4 degrees of freedom in a generically minimally rigid graph on the flexible torus!
  [Ross, S., and Whiteley: Finite motions from periodic frameworks with added symmetry, IJSS 48, 1711-1729, 2011]

Part II

Applications to protein flexibility

Symmetry in molecules

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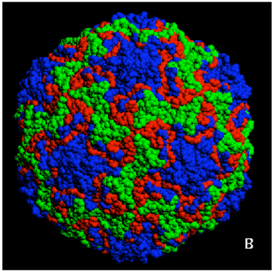
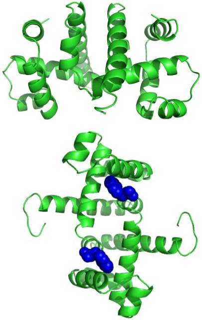
- The well developed theory of generic rigidity of frameworks allows for basic predictions of flexibility of molecules
- Observation: molecules often exhibit rotational symmetries:

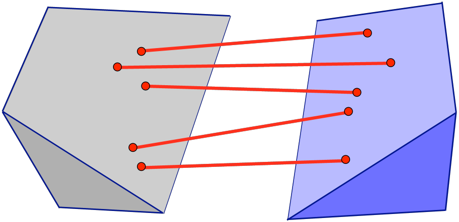




Protein	Number of subunits	Point symmetry: Crystallographic symbol	Point symmetry: Schönflies symbol
Alcohol dehydrogenase (234)	2	2	C_2
Immunoglobulin (294)	4	2	C_2
s-Malate dehydrogenase (233)	2	2	C_2
Superoxide dismutase (286)	2	2	C_2
Triose phosphate isomerase (305)	2	2	C_2
Phosphorylase (236)	2	2	C_2
Alkaline phosphatase (317)	2	2	C_2
6-Phosphogluconate dehydrogenase (318)	2	2	C_2
Wheat germ agglutinin (316)	2	2	C_2
Glucose phosphate isomerase (313)	2	2	C_2
Tyr–tRNA-synthetase (221)	2	2	C_2
Glutathione reductase (124)	2	2	C_2
Aldolase (306)	3	3	C_3
Bacteriochlorophyll protein (303)	3	3	C_3
Glucagon (278)	(3)	3	C_3
TMV-protein disc (218)	17	17	C_{17}
Concanavalin A (281, 282)	4	222	D_2
Glyceraldehyde-3-phosphate dehydrogenase (230, 231)	4	222	D_2
Lactate dehydrogenase (232)	4	222	D_2
Prealbumin (206)	4	222	D_2
Pyruvate kinase (80)	4	222	D_2
Phosphoglycerate mutase (307)	4	222	D_2
Hemoglobin (human) (274)	2 + 2	Pseudo 222	Pseudo D_2
Insulin (259)	6	32	D_3
Aspartate transcarbamoylase (319)	6 + 6	32	D_3
Hemerythrin (217)	8	422	D_4
Apoferritin (320)	24	432	O
Coat of tomato bushy stunt virus (263)	180	532	Y

Body-bar frameworks

- Molecular flexibility can be studied via the theory of rigid body-bar frameworks in 3-space



A body-bar framework in 3D

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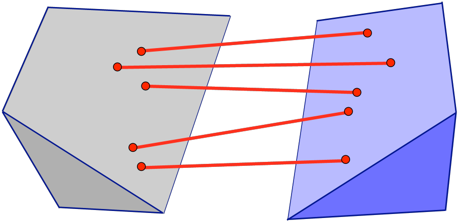

A body-bar framework in 3D

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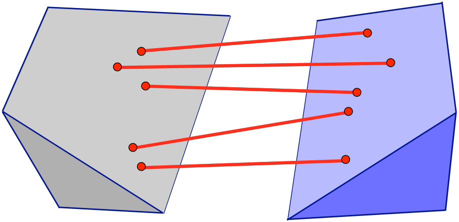

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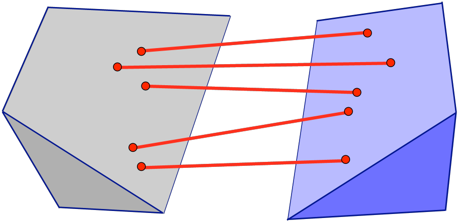

A body-bar framework in 3D

- A body-bar framework consists of ‘rigid bodies’ in the given dimension, attached by bars with rotatable vertex attachments
- The underlying combinatorial structure is a multi-graph
- A body-bar framework can be modeled as a bar-joint framework by replacing each body with an isostatic bar-joint framework

Necessary and sufficient conditions for rigidity

- **Theorem (Tay, 1980):** A body-bar framework in 3D with a multi-graph $G = (B, E)$ is infinitesimally rigid (and rigid) for generic selections of the lines of the bars if and only if there is a subset of bars E^* such that:

  (i) $|E^*| = 6|B| - 6$;

  (ii) $|E'| \leq 6|B'| - 6$ for all subgraphs induced by subsets E' of E^*.

Necessary and sufficient conditions for rigidity

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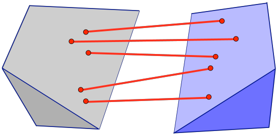
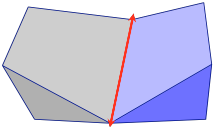
- Algorithmically, Tay's counts lead to a greedy algorithm called the pebble game, which has a running time of $O(|B||E|)$.

Application: Flexibility of molecular frameworks

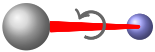
- Tay's counts (and the corresponding pebble game algorithms) also characterize generically rigid body-hinge frameworks (Tay, Whiteley, 1985) and even generically rigid molecular frameworks (Katoh, Tanigawa, 2010).



Body-bar framework



Body-hinge framework



Molecular framework

Example

Cyclohexane:

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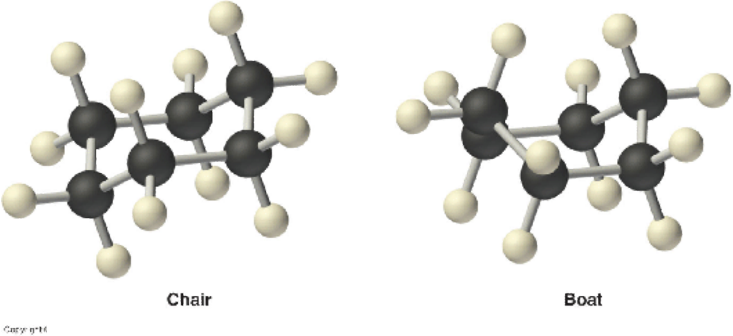
Conclusion: Cyclohexane is generically rigid (in fact, isostatic).

Symmetry can lead to added flexibility

Two basic conformations of cyclohexane:



Three-fold symmetry
Rigid

Half-turn symmetry
Flexible

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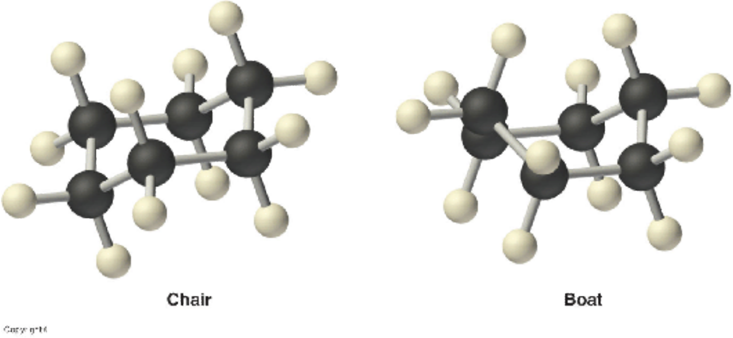

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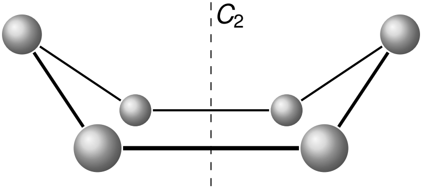
We can detect this via our symmetric Maxwell counts (under the assumption that the 'Symmetric Molecular Conjecture' holds)!

Symmetric counts for the 'boat'

Cyclohexane (boat conformation - $\mathcal{C}_2$ symmetry)



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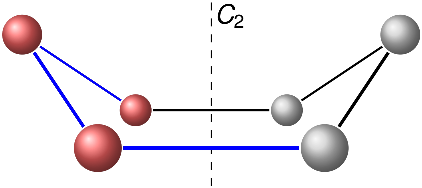

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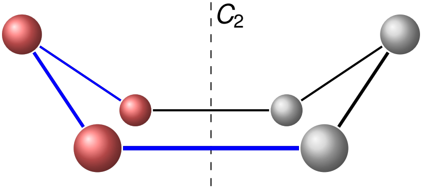

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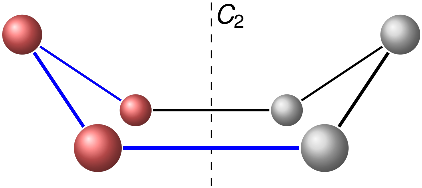

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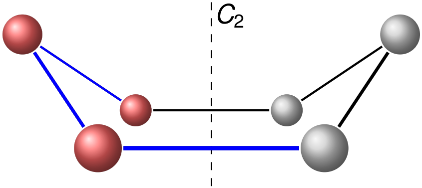

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Conclusion: There exists a symmetry-preserving finite motion!

Symmetric Tay's theorem for the group $\mathcal{C}_2$

- **Theorem:** A body-bar framework in 3D (with multi-graph $G = (B, E)$) which has $\mathcal{C}_2$ symmetry, has no body and no bar 'fixed' by the half-turn, and is generic modulo the $\mathcal{C}_2$ symmetry, has only trivial symmetry-preserving motions only if there is a subset of bars E_0^* such that:

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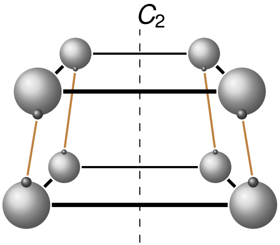
Another example

Two 4-fold molecular rings sharing a 2-fold axis, connected by 4 bars



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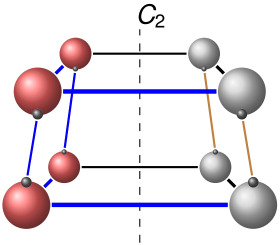

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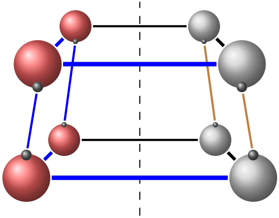

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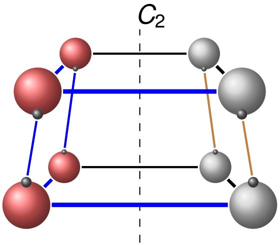

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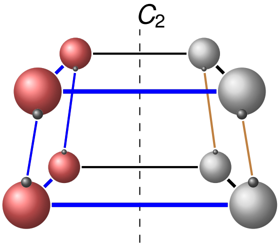

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Conclusion: We detect a finite motion which is not detected by the symmetric counts. To test for rigidity we need both of the criteria!

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Algorithm: Given a body-bar multi-graph $G = (B, E)$ with $\mathcal{C}_2$ symmetry (e.g., a dimer), apply the following sequence of steps:

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Further remarks on the flexibility of dimers with $\mathcal{C}_2$ symmetry

- We might anticipate that a dimer pair which is initially predicted to be flexible, moves along the path and stabilizes with an additional hydrogen bond. This would lead to a redundantly rigid structure (which is conjectured to be a 'stable' molecule), because

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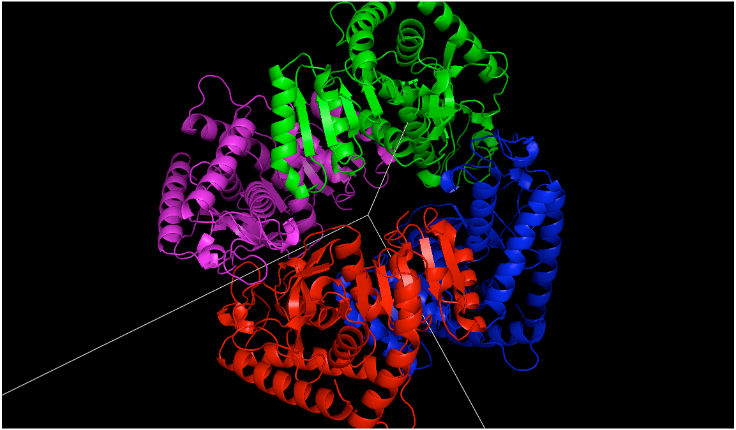
The symmetry group $\mathcal{D}_2$



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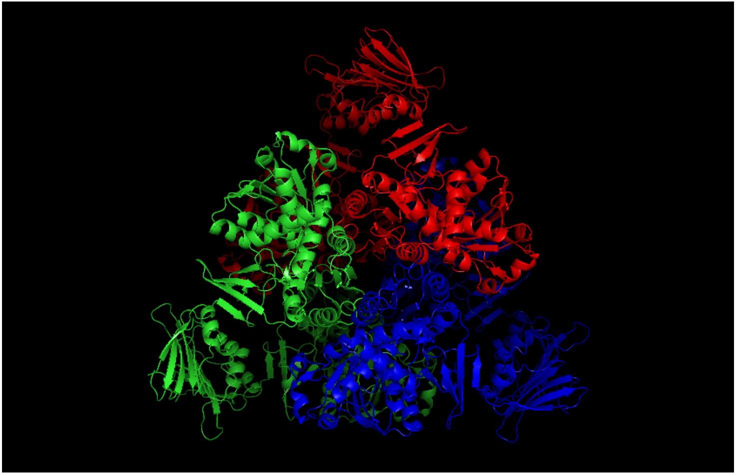

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- The symmetric pebble game for $\mathcal{D}_3$ is analogous to the one for $\mathcal{D}_2$.

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Further work

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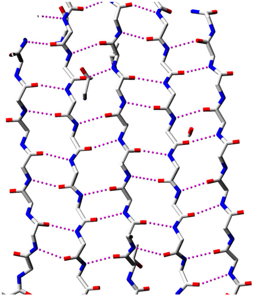

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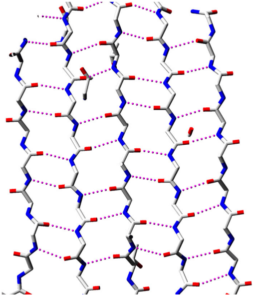
- Orbit matrices for other (non-trivial) irreducible representations
- How can we detect flexes in structure which possess multiple symmetric components (such as β-sheets e.g.)?



- How do we detect motions in finite repetitive structures?

Thanks!

Questions?

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