## Nucleation-free 3D rigidity and Convex Cayley configuration space

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## Nucleation-free 3D rigidity

#### Meera Sitharam Jialong Cheng and Ileana Streinu

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1 Implied non-edges and nucleation

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- 2 The construction
- 3 Proofs

## Implied non-edges

### • A <u>non-edge</u> of G = (V, E) is a pair $(u, v) \notin E$ .

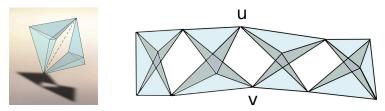
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## Implied non-edges

- A <u>non-edge</u> of G = (V, E) is a pair  $(u, v) \notin E$ .
- A non-edge is said to be implied if there exists an independent subgraph G' of G such that  $G' \cup (u, v)$  is dependent. I.e., generic frameworks G'(p) and  $G' \cup (u, v)(p)$  both have the same rank.

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- <u>Independence</u> = independence in the 3D rigidity matroid.
- Rank = rank of the 3D rigidity matroid.

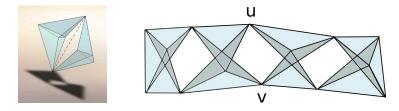


**Nucleation property.** A graph G has the <u>nucleation property</u> if it contains a non-trivial rigid induced subgraph, i.e., a <u>rigid nucleus</u>. Trivial means a complete graph on 4 or fewer vertices.

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Nucleation-free 3D rigidity

## Two natural questions in 3D

Question 1 Nucleation-free Graphs with implied non-edges: Do all graphs with implied non-edges have the nucleation property?

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- Question 1 Nucleation-free Graphs with implied non-edges: Do all graphs with implied non-edges have the nucleation property?
- <u>Question 2</u>: Nucleation-free, rigidity circuits Does every rigidity circuit automatically have the nucleation property?

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## Answering the two questions in the negative

In order to answer Question 1, we construct an infinite family of flexible 3D graphs which have no proper rigid nuclei besides trivial ones (triangles), yet have implied edges.

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#### Our main result

## Answering the two questions in the negative

- In order to answer <u>Question 1</u>, we construct an infinite family of flexible 3D graphs which have no proper rigid nuclei besides trivial ones (triangles), yet have implied edges.
- We also settle <u>Question 2</u> in the negative by giving a family of arbitrarily large examples that follow directly from the examples constructed for <u>Question 1</u>.

## The construction: a ring of k roofs

A <u>roof</u> is a graph obtained from K<sub>5</sub>, the complete graph of five vertices, by deleting two non-adjacent edges.

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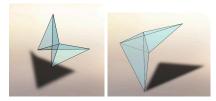
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- A <u>roof</u> is a graph obtained from K<sub>5</sub>, the complete graph of five vertices, by deleting two non-adjacent edges.
- A roof together with (either) one of its two non-edges forms a banana.

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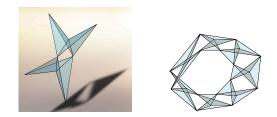
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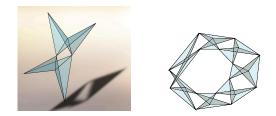
## Ring graph

A <u>ring graph</u>  $\mathscr{R}_k$  of  $k \ge 7$  roofs is constructed as follows. Two roofs are connected along a non-edge. We refer to these two non-edges within each roof as <u>hinges</u>. Such a chain of seven or more roofs is closed back into a ring.



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This example graph appears often in the literature.

## Main theorem

#### Theorem

In a ring of roofs, the hinge non-edges are implied.

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The ring  $\mathscr{R}_k$  of k roofs is independent.

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#### Lemma

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We will construct a specific framework  $\mathscr{R}_k(p)$  that is independent, thus the generic frameworks must also be independent.

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If we add any (or all) hinge edge(s) into  $\mathcal{R}_k$ , the rank does not change.

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This follows immediately from either one of two existing theorems.

## Option 1

#### Theorem (Tay and White and Whiteley)

If  $\forall i \leq k$ , the *i*<sup>th</sup> banana  $B_i(p_i)$  is rigid, then the bar framework  $\mathscr{B}_k(p)$  is equivalent to a body-hinge framework and is guaranteed to have at least k - 6 independent infinitesimal motions.

#### Observation

If  $\mathscr{R}_k(p)$  is generic, then for all *i*, the rigidity matrix given by the banana framework  $B_i(p_i)$  is independent, which in this case implies rigidity. Here  $p_i$  is the restriction of *p* to the vertices in the *i*<sup>th</sup> roof  $R_i$ .

## Option 2

A <u>cover</u> of a graph G = (V, E) is a collection  $\mathcal{X}$  of pairwise incomparable subsets of V, each of size at least two, such that  $\bigcup_{X \in \mathcal{X}} E(X) = E$ . A cover  $\mathcal{X} = \{X_1, X_2, \dots, X_n\}$  of G is 2-thin if  $|X_i \cap X_j| \le 2$  for all  $1 \le i < j \le n$ .

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#### Observation

If  $\mathcal{X} = \{X_1, X_2, \dots, X_m\}$  is a 2-thin cover of graph G = (V, E)and subgraph  $(V, H(\mathcal{X}))$  is independent, then in 3D, the rank of the rigidity matrix of a generic framework G(p), denoted as rank(G), satisfies the following

$$rank(G) \leq \sum_{X_i \in \mathcal{X}} rank(G_1[X_i]) - \sum_{(u,v) \in H(\mathcal{X})} (d(u,v) - 1), \quad (1)$$

where  $G_1 = G \cup H(\mathcal{X})$ .

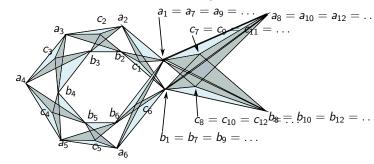
## Proof of independence of ring

■ We will show a specific framework *ℛ<sub>k</sub>(p)* is independent, thus the generic frameworks must also be independent.

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## Proof of independence of ring

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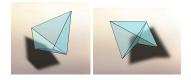
The repeated roofs have some symmetries that are utilized in the proof.

## Proof of independence of ring

- Use induction: two base cases, according to the parity of number of roofs.
- Induction step is proved by contradiction and inspection of the rigidity matrix of  $\mathscr{R}_{k+2}(p)$  and of  $\mathscr{R}_k(p)$ : after adding 2 new roofs to the current ring, if the new ring does not have full row rank, then the original one does not have full row rank either.
- The the  $k^{th}$  roof is identical to the  $k + 2^{nd}$  roof. This is true for both even and odd k's and hence the induction step is the same.

Nucleation-free 3D rigidity

## A special generic framework



#### Lemma

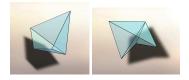
The hinge non-edges are implied, for all rings  $\mathscr{R}_k(p)$  of k-1, pointed pseudo-triangular roofs and one convex roof.

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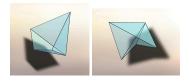


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The hinge non-edges are implied, for all rings  $\Re_k(p)$  of k-1, pointed pseudo-triangular roofs and one convex roof.

This uses previous results by Connelly, Streinu and Whiteley about expansion/contraction properties of convex polygons, the infinitesimal properties of single-vertex origamis and pointed pseudo-triangulations.

## A special generic framework



#### Lemma

The hinge non-edges are implied, for all rings  $\Re_k(p)$  of k-1, pointed pseudo-triangular roofs and one convex roof.

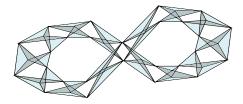
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#### Lemma

There are generic frameworks  $\mathscr{R}_k(p)$  as in the previous Lemma.

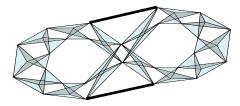
## Nucleation-free dependent graph

## Question 1 Do all graphs with implied non-edges have the nucleation property?



## Nucleation-free non-rigid dense graph

Question 2 If a graph G = (V, E) with at least 3|V| - 6 edges is non-rigid, i.e, dependent, then does it automatically have the nucleation property?

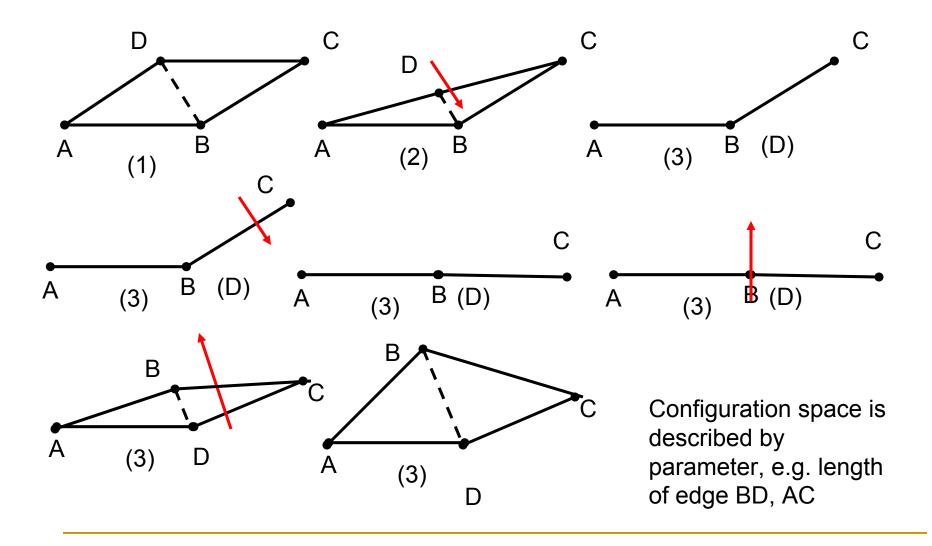


Graphs with Convex Cayley Configuration Spaces

> Meera Sitharam Heping Gao Jialong Cheng

- Useful representation of configuration spaces of flexible linkages (machines, molecules) – important problems, many applications, little progress
- Obstacles to progress so far
  - (a). Good formalization of "useful representation of configuration space"
  - (b). Which linkages have such a representation
- Novel feature of our results relate combinatorial properties of underlying graph (forbidden minors and other graph properties) with:
  - geometric properties (convexity) of configuration space and topological properties (connectedness, number of connected components) of configuration space
  - algebraic complexity of configuration space
- Applications to molecular biology and chemistry

# Representation of Configuration Space



## Outline

- Definition and notation
- Cayley configuration space
- 2D connected/convex configuration space
- 3D connected configuration space
- Arbitrary dimensions
- Application: Helix packing configurations

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#### Definition and notation

- Cayley configuration space
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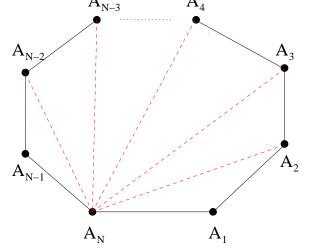
## Notation

- Graph: G=(V,E)
- non-edge : f in E (the complement of E)
- non-edge set : F, subset of E
- linkage: (G, d<sub>E</sub>)
- realization of (G, d<sub>E</sub>) in δ-dimensions: a realization or coordinate values of all vertices in δ-dimension preserving distance constraints

#### Definition: Cayley configuration space

 Definition: given linkage (G, d<sub>E</sub>) non-edge set F, the Cayley configuration space on F is

 $Φ_F^{\delta}$  (G, d<sub>E</sub>):={d<sub>F</sub> | (G U F, d<sub>E</sub> U d<sub>F</sub>) has a solution in δ-dimension } Short: "configuration space of (G,d<sub>E</sub>) on F"



non-edges: dashed line

The projection on the non-edges is described by triangle inequalites

#### Schoenberg's Theorem (1935):

Given an  $n \times n$  matrix  $\Delta = (d_{ij})_{n \times n}$ , there exists a Euclidean realization in  $\mathbb{R}^{\delta}$ , i.e., a set of points  $p_1, p_2, \ldots, p_n \in \mathbb{R}^{\delta}$  s.t.  $\forall i, j, ||p_i - p_j||^2 = \delta_{ij}$  if and only if matrix  $\Delta$  is negative semidefinite of rank  $\delta$ .

- Negative semidefinite matrices form a convex cone.
- The rank- $\delta$  stratum of this cone may not be convex.
- A linkage (G, d<sub>E</sub>) is a partially filled distance matrix: this is a section consisting of all possible negative semidefinite completions (of rank δ).
- (δ-dimensional )Cayley configuration space, Φ<sub>F</sub>(Δ(G, d<sub>E</sub>), of the linkage (G, d<sub>E</sub>) on non-edge set F is the projection of this section (completions) onto F.

**Question:** For which graphs  $G \cup F$  is this projection "nice" for all  $d_E$ ?

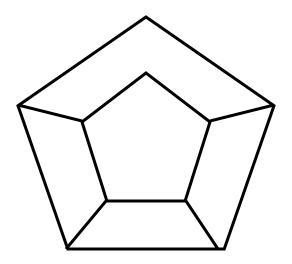
#### Easier to deal with $\delta$ -Projection on d<sup>2</sup>

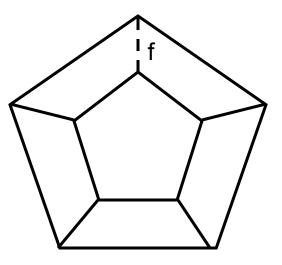
 Definition: given distance constraint system (G, d<sub>E</sub>) and non-edge set F, the squared-distance configuration space of (G, d<sub>E</sub>) on F is

 $(\Phi_F^{\delta})^2 = (G, d_E) := \{ d_F^2 \mid (G \cup F, d_E \cup d_F) \text{ has a solution in } \delta \text{-dimension } \}$ 

#### Configuration Space Description

Definition: constraint system (G, d<sub>E</sub>) has connected configuration space description (CCS) in δ dimension if there exists a non-edge set F such that the Cayley space on F is connected. We say (G, d<sub>E</sub>) has a CCS on F.





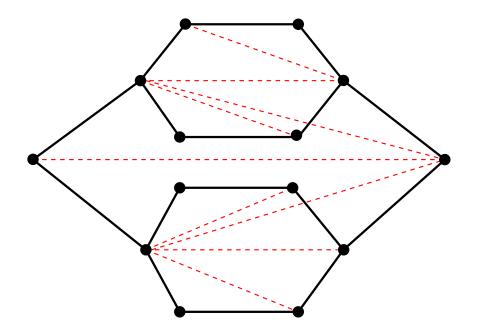
No CCS in 2D

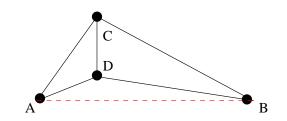
Has CCS on f in 3D

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- Arbitrary dimensions
- Application: Helix packing configurations

## 2D Connected Configuration Space: Examples



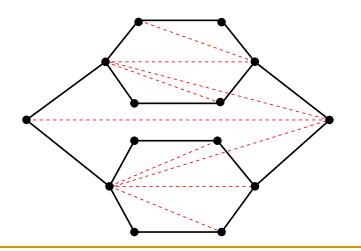


Projection on the non-edges is convex, connected, and polytope

Projection on the non-edges is not connected

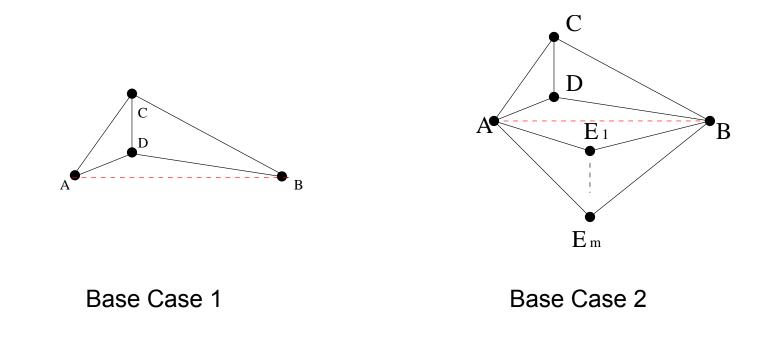
Simple & Complete Configuration Space in 2D

 Theorem : There exists connected & convex configuration description in 2D if and only if all the non-rigid 2-sum components are partial 2-trees.



#### 2D Connected configuration space: Theorem

 Lemma : Given a graph G=(V,E) and non-edge f, G can be reduced to base case 1 and base case 2 only by edge shrinking if and only if there exists one 2-Sum component of G U f which contains f and is not a partial 2-Tree.



## Proof

Proof needs graph reduction technique different from minor: keep the non-edge.

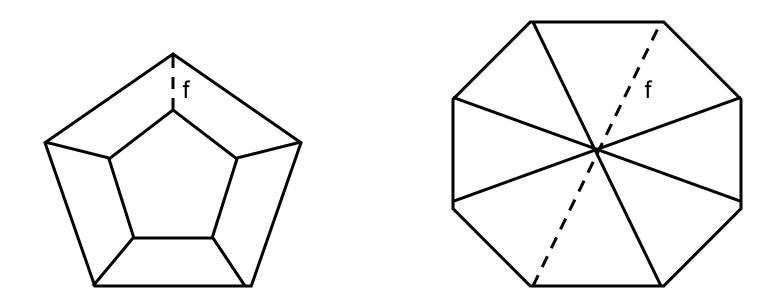
#### 2D Connected configuration space: Theorem

- Theorem : Given graph G and non-edge f=AB, if G has 2D CCS on f (single interval) if and only all 2-Sum components of G U AB containing both A and B are partial 2-trees.
- Theorem : Given a graph G=(V,E) and nonedge set F, G has 2D CCS on F if and only if all 2-Sum components containing any subset of F are partial 2-trees.

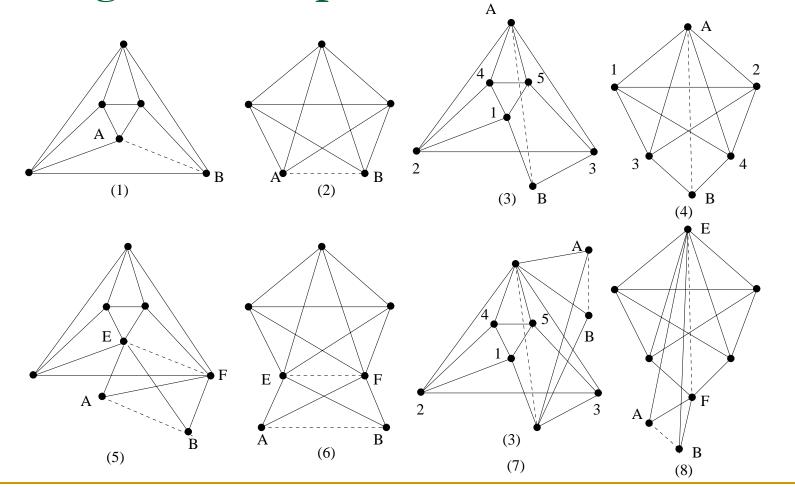
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### 3D Connected Configuration Space

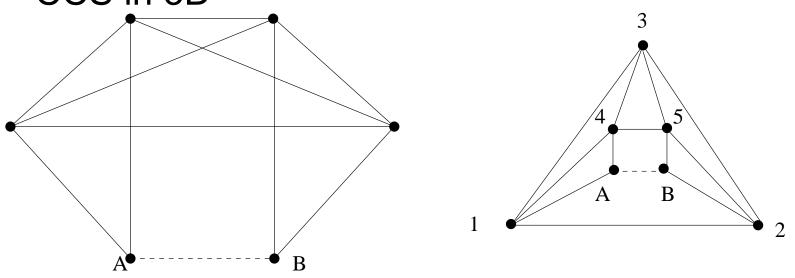


Examples without 3D Connected Configuration Space



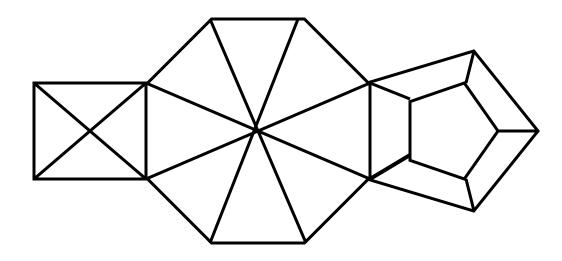
Examples with 3D Connected Configuration Space

- Case 1: G U f has universally inherent CCS in 3D
- Case 2: G U f doesn't have universally inherent CCS in 3D



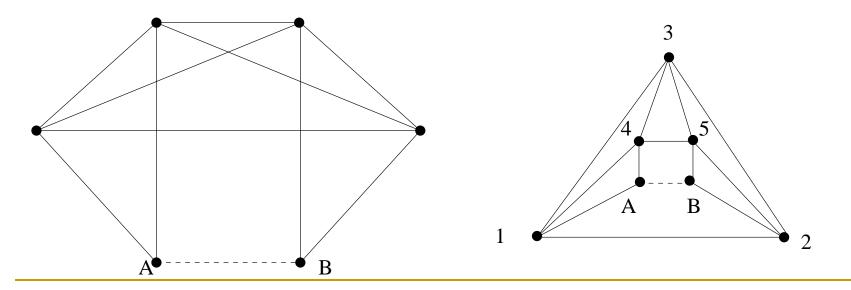
Theorem on Maximal 3-realizable Graphs

 Theorem : if a graph G is maximal 3realizable, for any non-edge f, G doesn't have 3D connected configuration space on f.

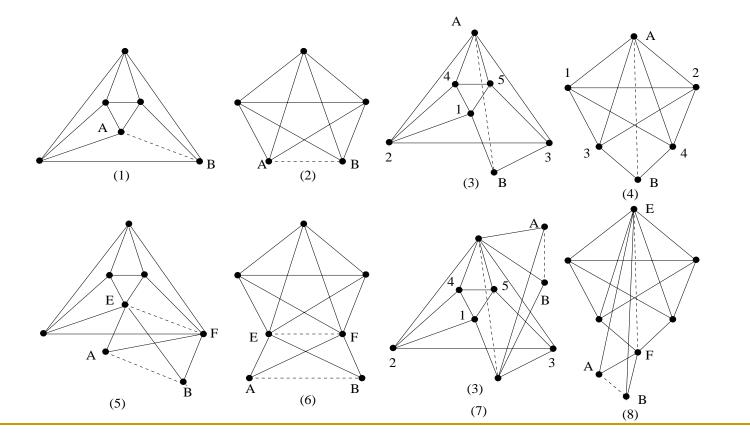


# 3D Connected Configuration Space : Conjectures

 Conjecture 1: Given partial 3-tree G and virtual edge AB, if A and B must be shrunk together in order to get a K<sub>5</sub> or K<sub>222</sub> minor, then G has 3D connected configuration space on f.



**Conjecture 2**: given graph G and non-edge AB, G doesn't have 3D connected configuration space on f if and only if G can be reduced to one of the eight cases by edge shrinking while preserving AB as non-edge



# Outline

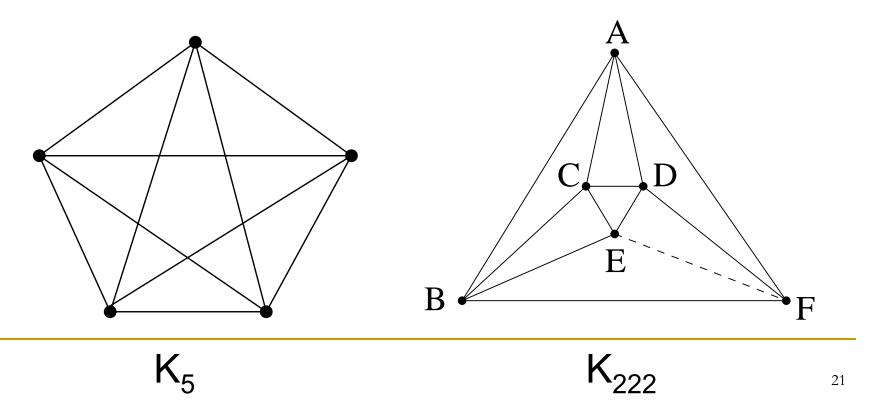
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Universally Inherent CCS

We obtain strong results in arbitrary dimension for more restrictive class of graphs

 Definition: H has an *universally inherent* CCS in δ-dimension if for every partition of H as G U F where G has a CCS on F. Universally Inherent CCS : Examples

- K<sub>5</sub> and K<sub>222</sub> doesn't have universally inherent CCS in 3D.
- Any proper subgraph of K<sub>5</sub> or K<sub>222</sub> has universally inherent CCS in 3D.



#### Universally Inherent CCS: Results

- Definition: a graph G is δ-realizable if, for any d<sub>E</sub>, (G, d<sub>E</sub>) has a solution in some dimension implies that (G, d<sub>E</sub>) has a solution in δ-Dimension [Belk & Connelly].
- Theorem 1: A graph G is δ-realizable iff G has universally inherent CCS in δ-dimension. In fact, G has a universally inherent convex squared-distance configuration space in δdimension.

Previous results on  $\delta$ -realizability

 Previous Theorem: a graph G is 2-realizable if and only if G has no K<sub>4</sub> minor; a graph G is 3-realizable if and only if it has no K<sub>5</sub> or K<sub>222</sub> minor [Belk, Connelly].

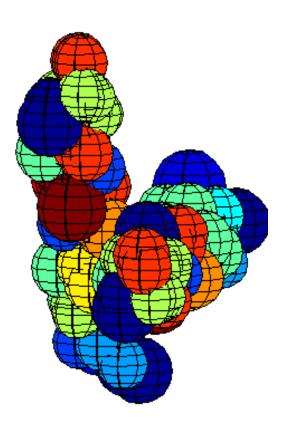
#### Graph Characterization for Universally Inherent CCS

**Theorem** : a graph G has universally inherent CCS in 2D if and only if it has no  $K_4$  minor; in 3D if and only if it has no  $K_5$  or  $K_{222}$  minor.

## Outline

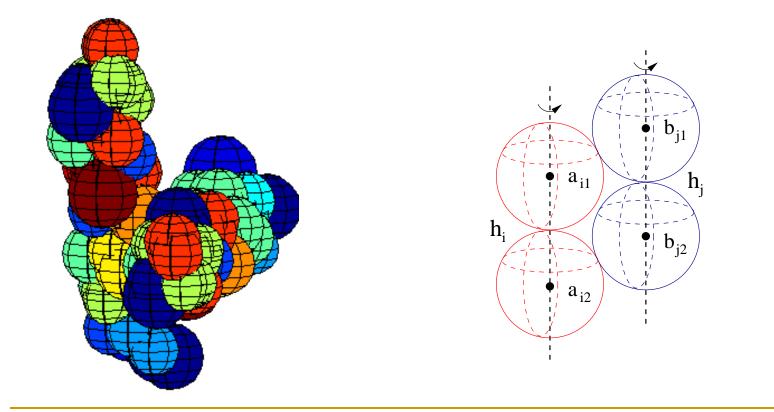
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#### Helix Packing: Problem

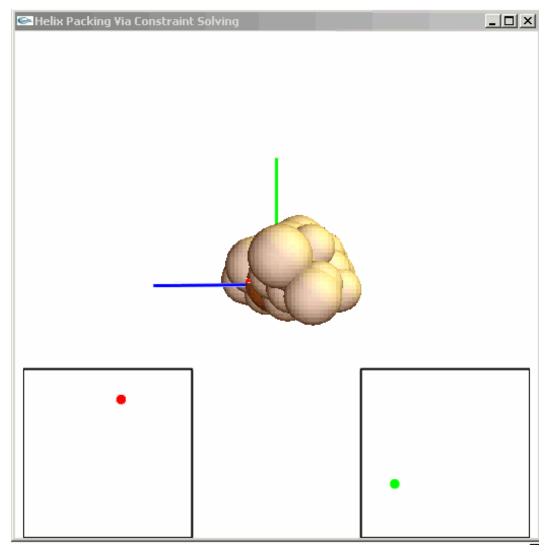


- Simulate and sample the configuration space of helices
- Focused on two helices in the current stage
- Helix is modeled as a collection of rigid balls; collision should be avoided between two balls from two different helices
- "Critical" configurations should be captured

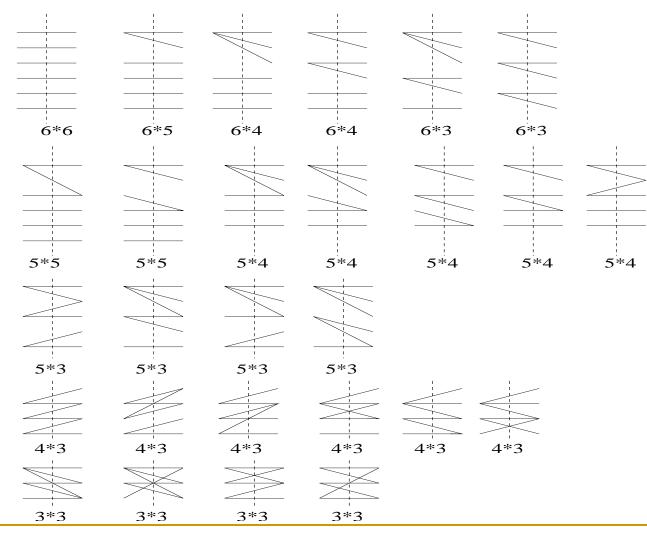
#### Helix Packing: Bi-Incidence



#### **Bi-Incidence**



Helix Packing: Graphs for Which Configuration Space is Sought for all possible edge subgraphs



#### Thanks!