Folding & Unfolding: Linkages

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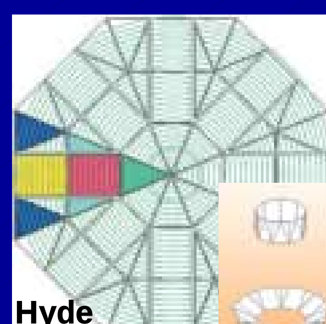
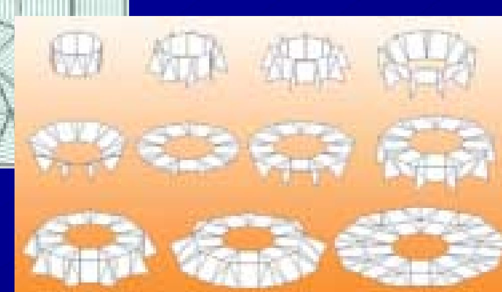
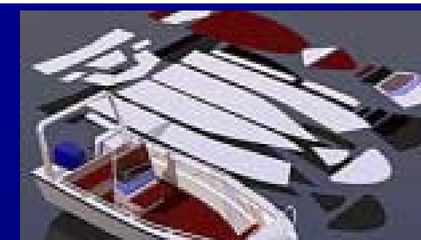
Folding and Unfolding in Science

- Linkages
  - Robotic arms
  - Proteins
- Paper
  - Airbags
  - Space deployment
- Polyhedra
  - Sheet metal



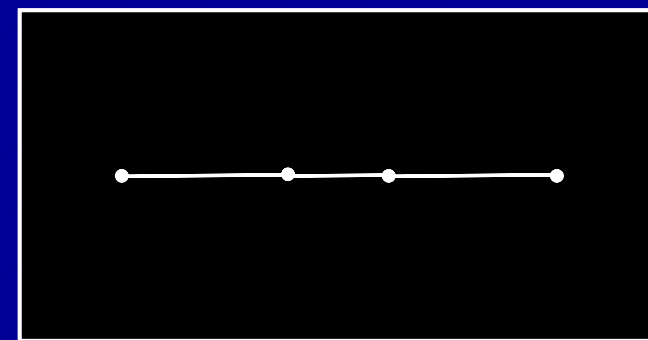
5-meter lens
(2x Hubble)



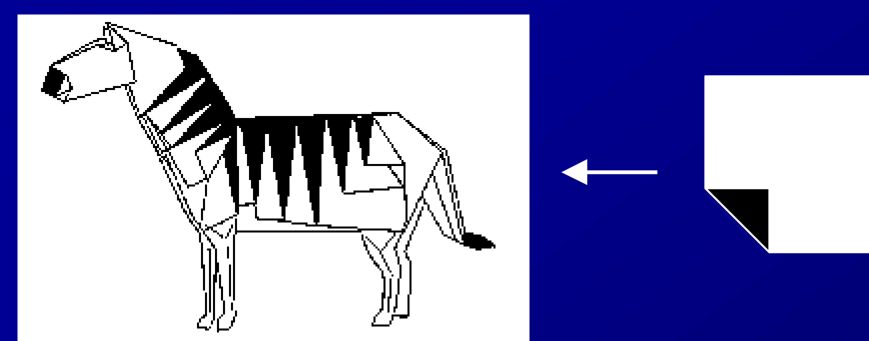


Folding and Unfolding in Computational Geometry

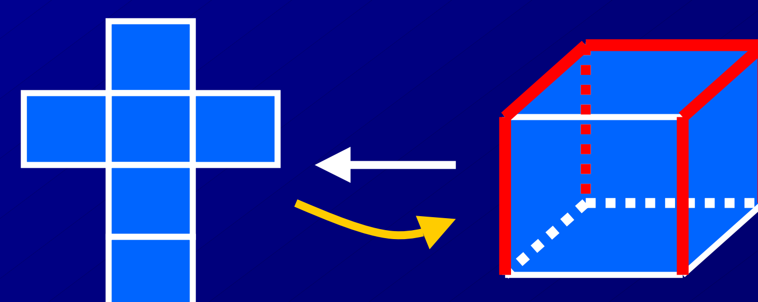
- Linkages
  - Preserve edge lengths
  - Edges cannot cross



- Paper
  - Preserve distances
  - Cannot cross itself



- Polyhedra
  - Cut the surface while keeping it connected



Folding and Unfolding Talks

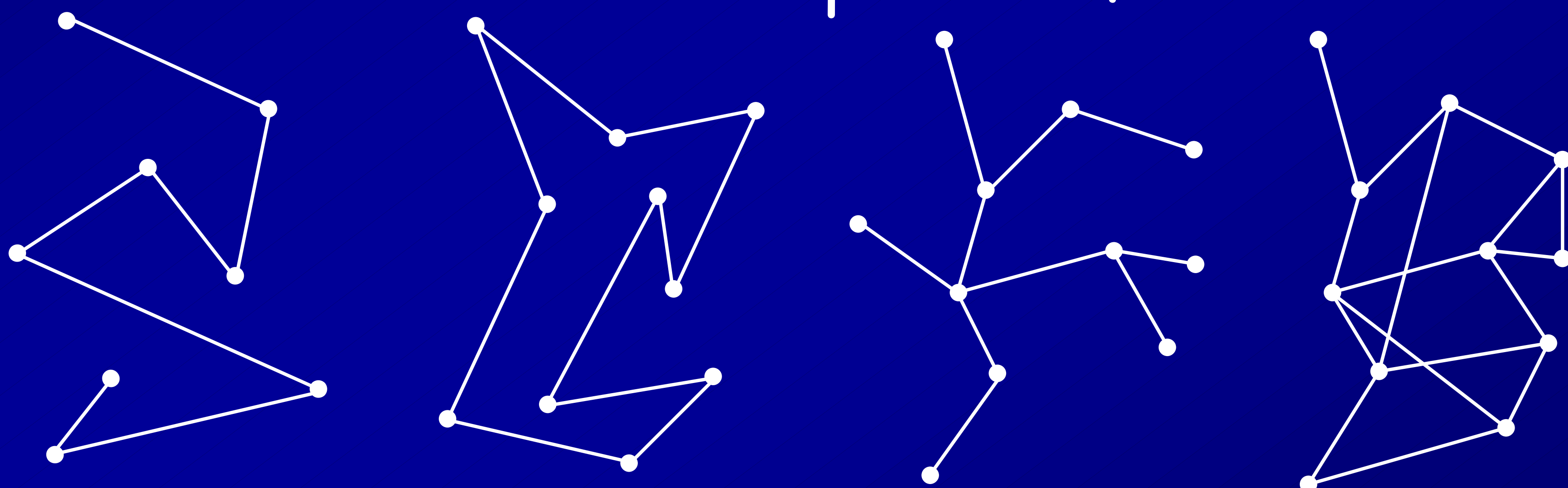
Linkage folding	**Today**	**Erik Demaine**
Paper folding	Tomorrow	Erik Demaine
Folding polygons into convex polyhedra	Friday	Joe O'Rourke
Unfolding polyhedra	Saturday	Joe O'Rourke

Outline: Linkages

- **Definitions and History**
- Rigidity
- Locked chains in 3D
- Locked trees in 2D
- No locked chains in 2D
- Algorithms
- Connections to protein folding

Linkages / Frameworks

- **Bar** / link / edge = line segment
- **Vertex** / joint = connection between endpoints of bars



Open chain / arc

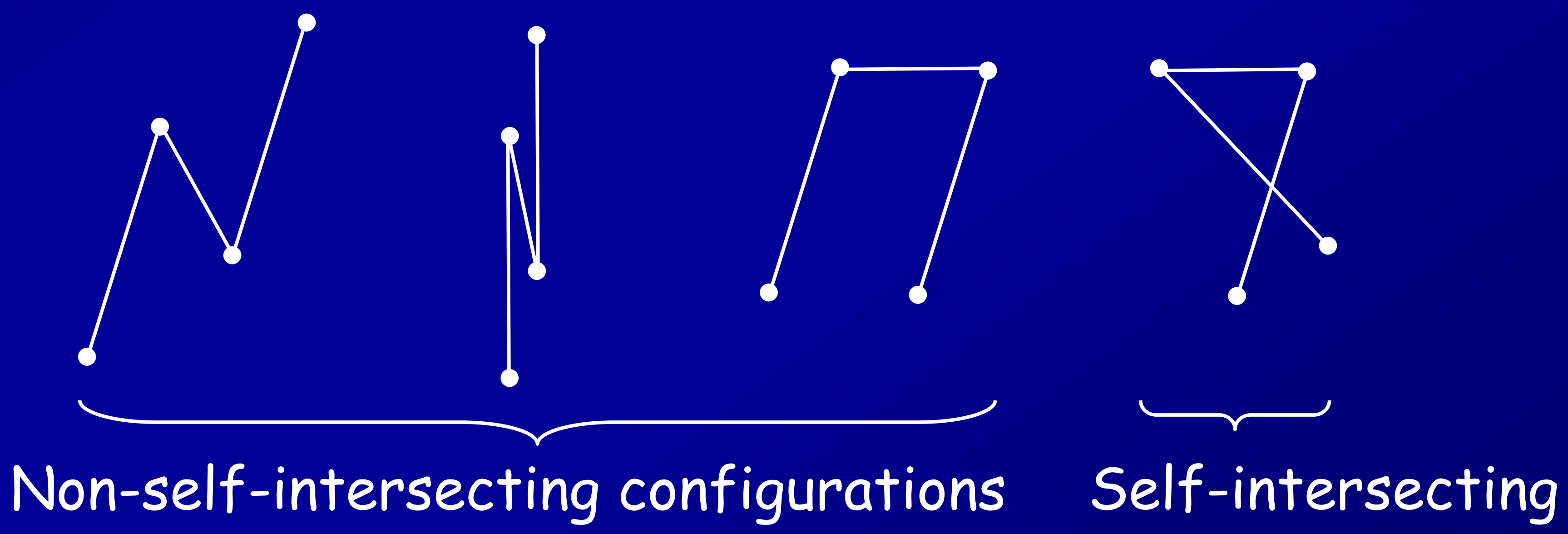
Closed chain / cycle / polygon

Tree

General

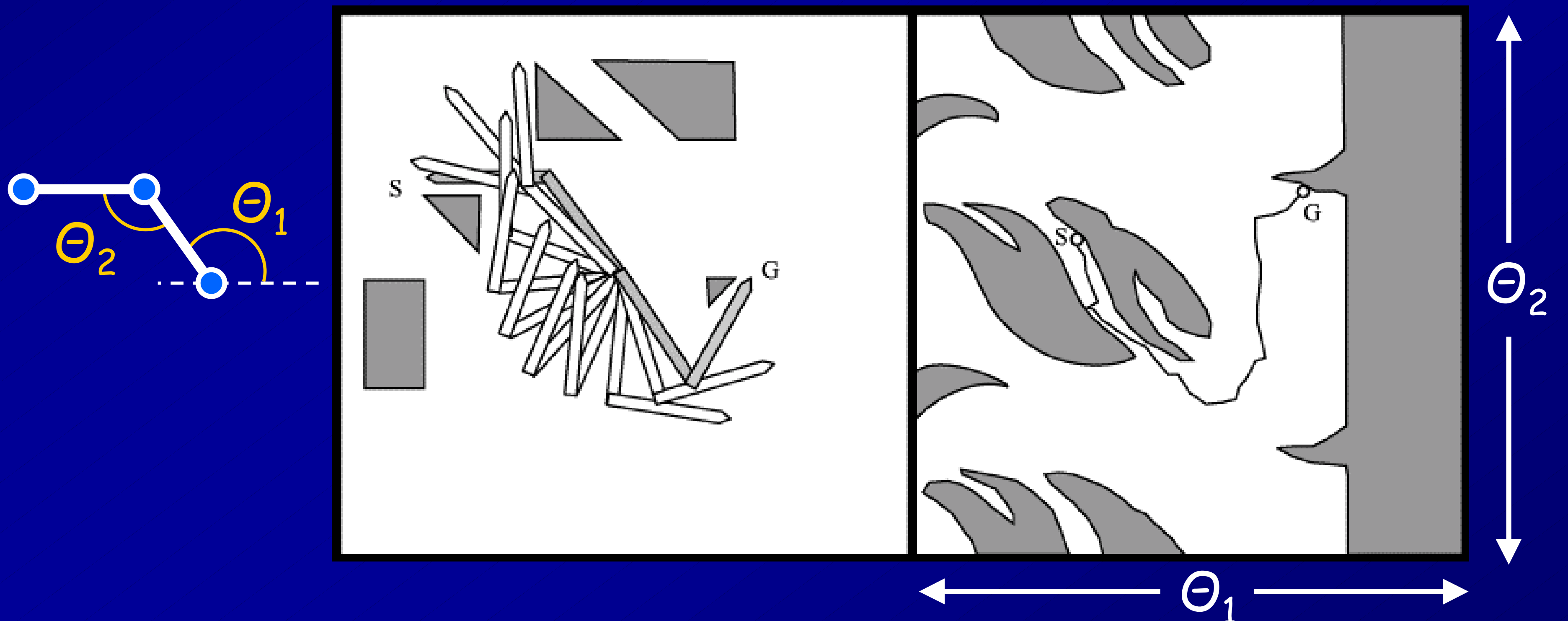
Configurations

- **Configuration** = positions of the vertices that preserves the bar lengths
- **Non-self-intersecting** = No bars cross



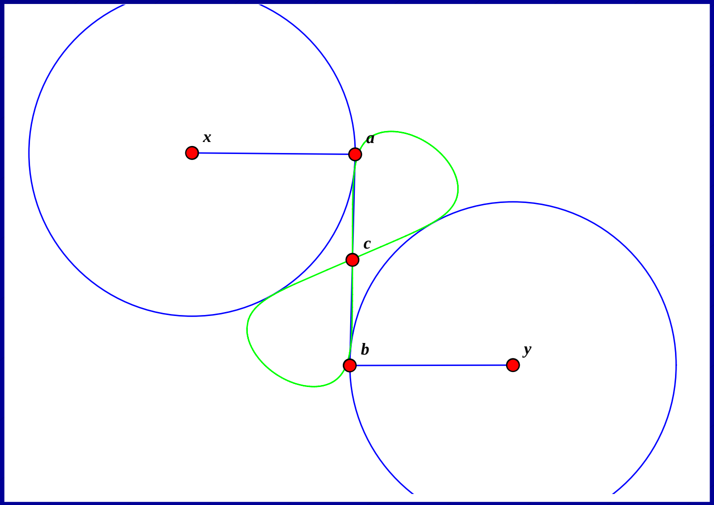
Configuration Space

- **Configuration space:** One point per config.
- **Free space:** Only non-self-intersecting configs.
- **Paths** in these spaces = **Motions** of linkage

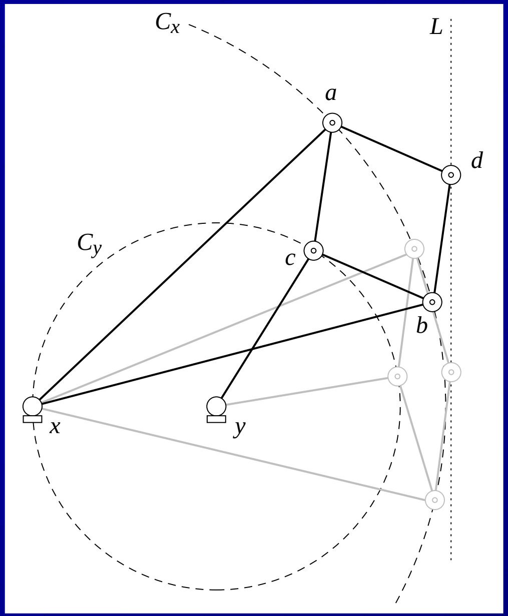


Some History

- An early quest: Converting circular motion into linear motion



Watt parallel motion (1784)



Peaucellier linkage (1864)

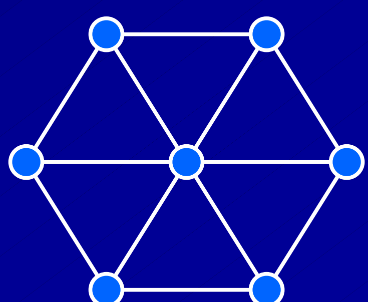
- Many more in Kempe's *How To Draw A Straight Line* (1877)

Outline: Linkages

- Definitions and History
- **Rigidity**
- Locked chains in 3D
- Locked trees in 2D
- No locked chains in 2D
- Algorithms
- Connections to protein folding

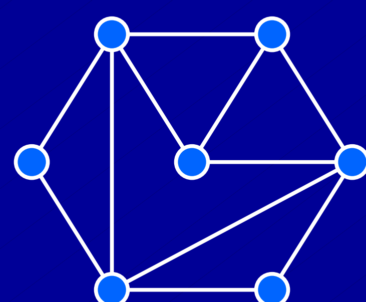
Rigidity

- Starting question: When can a config. of a linkage move *at all*? [excluding rigid motion]
- Yes ⇒ **Flexible**; No ⇒ **Rigid**



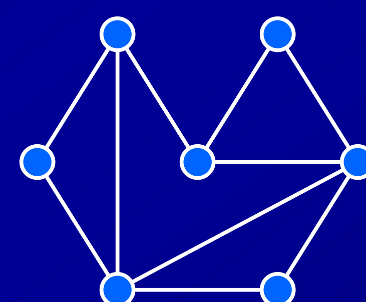
Rigid

(all triangulations)

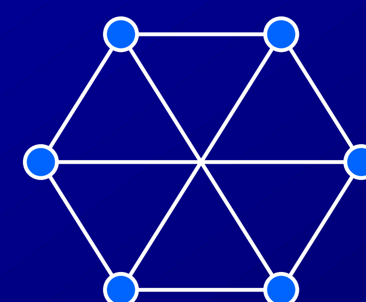


Rigid

(all "pseudo-triangulations")

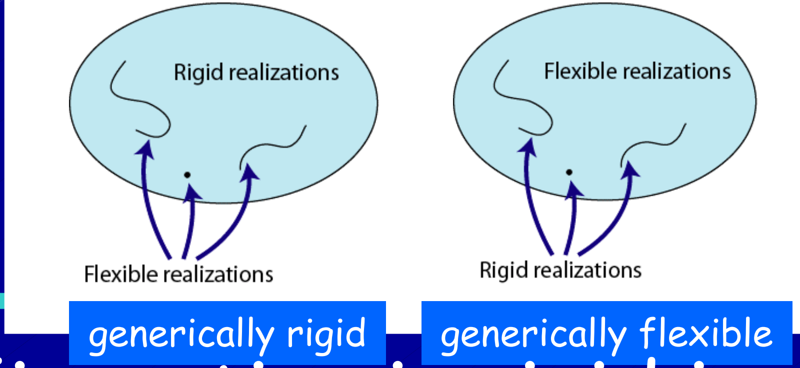


Flexible

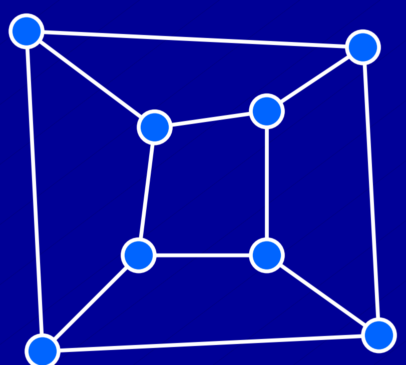


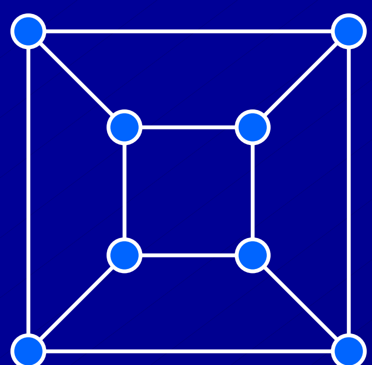
Rigid

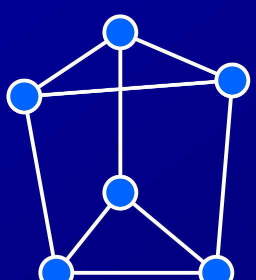
Generic Rigidity

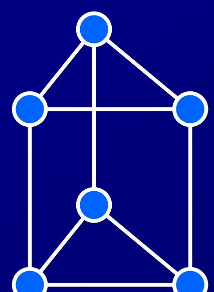


- Whether a linkage configuration is rigid is **almost always** a combinatorial property of the underlying graph structure:
  - **Generically flexible** = almost all realizations of the graph are flexible
  - **Generically rigid** = almost all realizations rigid


Generically flexible

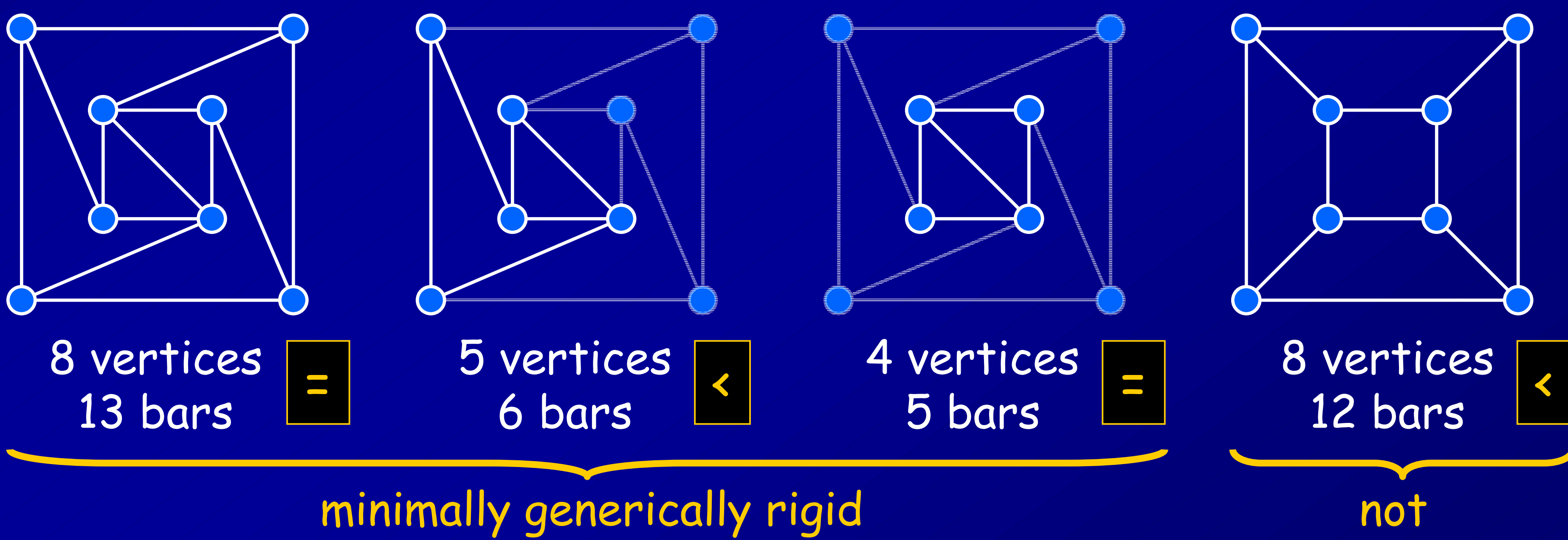

Rarely rigid


Generically rigid

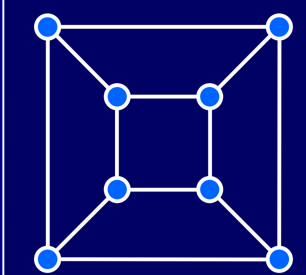

Rarely flexible

Laman's Characterization of Generic Rigidity

- **Theorem:** [Laman 1970]
  - *A graph with n joints and exactly 2n – 3 bars is generically rigid in 2D precisely if every induced subgraph on k joints has at most 2k – 3 bars*
- Such graphs are **minimally generically rigid**



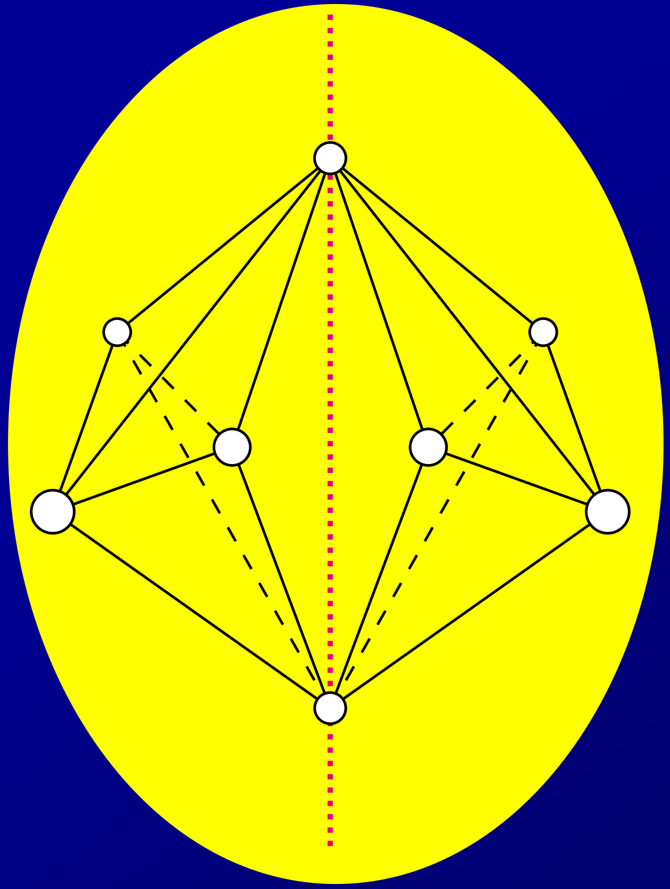
Laman's Characterization of Generic Rigidity



- **Theorem:** [Laman 1970]
  - A graph with n joints and exactly 2n – 3 bars is generically rigid in 2D precisely if every induced subgraph on k joints has at most 2k – 3 bars
  - A graph with n joints and less than 2n – 3 bars is never generically rigid in 2D
  - A graph with n joints and more than 2n – 3 bars is generically rigid in 2D precisely if it has a generically rigid subgraph with 2n – 3 bars
- Intuitively, need 2n – 3 bars to be rigid, but these bars cannot be too concentrated, else another subgraph would have too few edges

Generic Rigidity in Higher Dimensions

- **Open:** Characterize the 3D generically rigid graphs
  - Can these graphs be recognized in polynomial time?
  - Laman's theorem generalizes to a necessary condition (3n – 6)

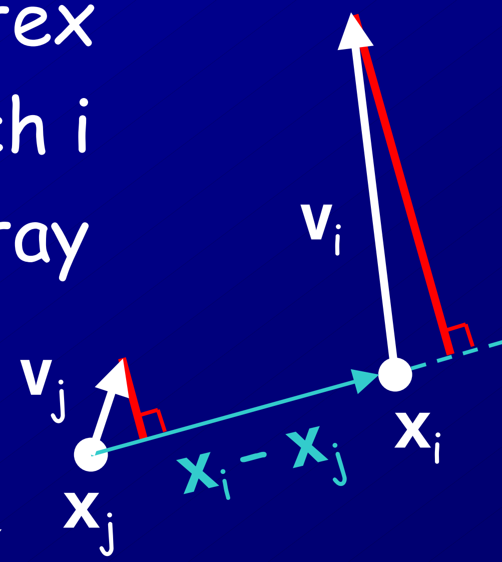


Infinitesimal Rigidity

- If a linkage is flexible, it is flexible by a smooth motion ⇒ can take first derivative
- **Infinitesimal motion** defines a motion to first order, from initial configuration **x**
  - Suppose $\mathbf{x}_i$ is the location of vertex
  - Choose **velocity vector** $\mathbf{v}_i$ for each i
  - Lengths of each bar {i, j} must stay constant to the first order:

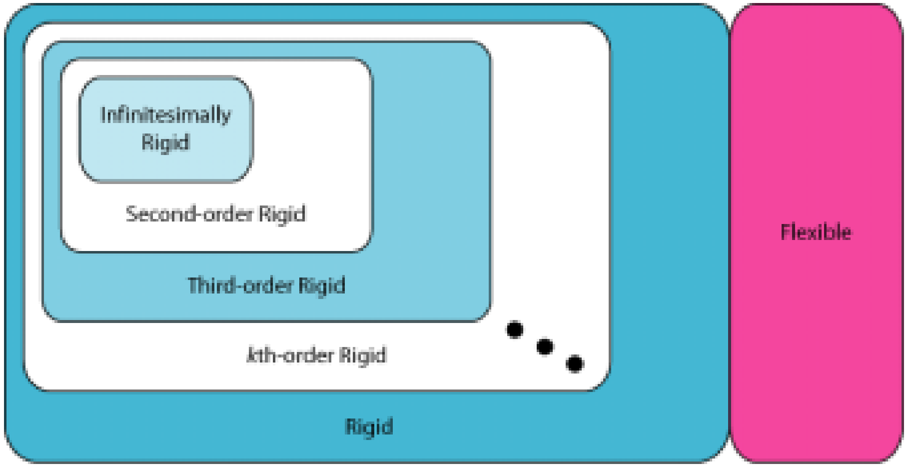
$$(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) = 0$$

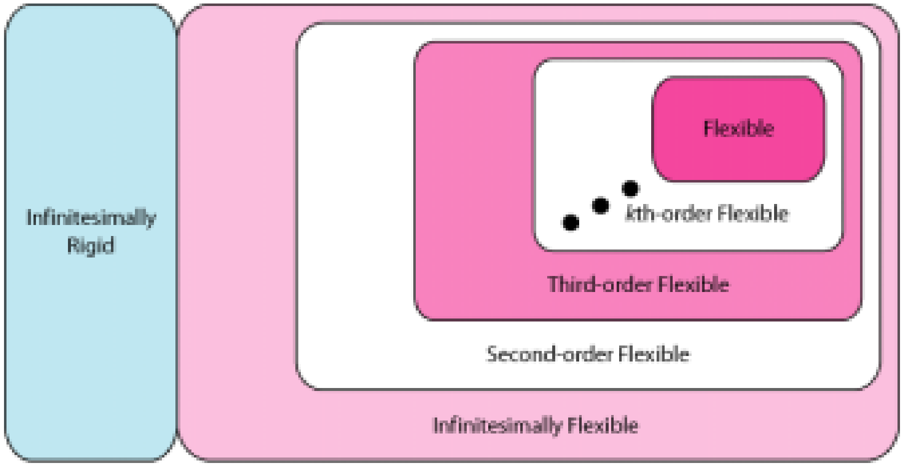
  - Constraints form **rigidity matrix**



Rigidity and Infinitesimal Rigidity

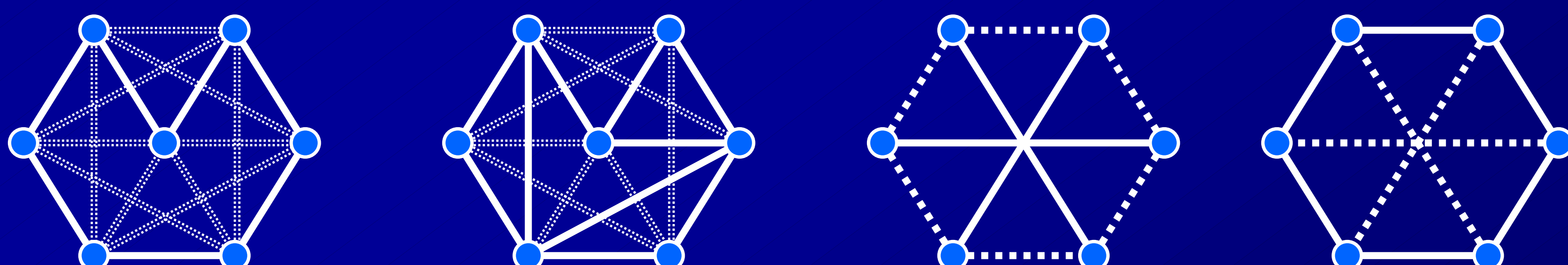
- Flexibility $\Rightarrow$ Infinitesimal flexibility
- Infinitesimal rigidity $\Rightarrow$ Rigidity
  - So infinitesimal rigidity is a stronger condition
- There is also second-order, etc. rigidity





Tensegrities

- **Tensegrity** = *generalization of linkage, where each* **edge** *can be one of*
  - **Bar** — length must stay equal
  - **Strut** — length must stay equal or **grow**
  - **Cable** — length must stay equal or **shrink**
- Plain/generic/infinitesimal rigidity similar



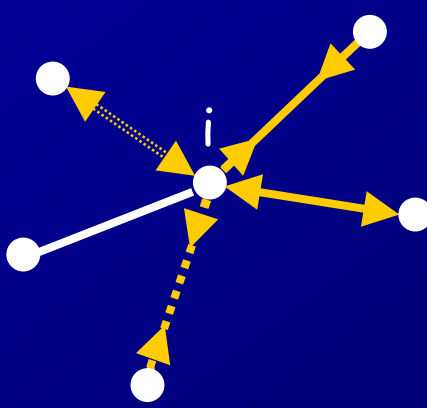
Flexible　　Flexible　　Flexible　　Rigid

Infinitesimal Flexibility is Linear Programming

- Infinitesimal flexibility can be expressed as a linear feasibility problem (special **linear program**)
- Objective: Minimize 0
- Constraints:
  - $(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) = 0$ for each bar {i, j}
  - $(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) \geq 0$ for each strut {i, j}
  - $(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j) \leq 0$ for each cable {i, j}
- $\mathbf{v}_i$ variable; $\mathbf{x}_i$ given

Dual of Infinitesimal Motions: Equilibrium Stresses [Roth & Whiteley 1981]

- Primal LP infeasible $\Rightarrow$ dual LP infeasible or unbounded
- **Equilibrium stress** = *assignment of weights* $\omega_{\{i,j\}}$ to edges {i, j} satisfying
  - $\omega_{\{i,j\}} \geq 0$ for all struts {i, j}
  - $\omega_{\{i,j\}} \leq 0$ for all cables {i, j}
  - **Equilibrium**: For each vertex i, $\sum \{ \omega_{\{i,j\}} (\mathbf{x}_i - \mathbf{x}_j) \mid$ *edge* $\{i, j\} \} = 0$



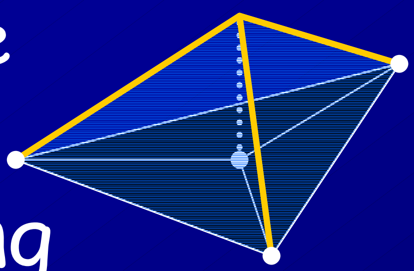
- Any infinitesimally rigid framework has an equilibrium stress that's not everywhere 0

Dual of Infinitesimal Motions: Equilibrium Stresses [Roth & Whiteley 1981]

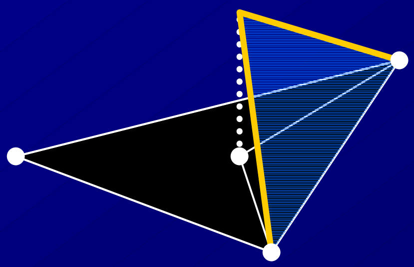
- Equilibrium stresses do not imply rigidity
- Do imply "local rigidity" where nonzero:
  - No infinitesimal motion can change the length of a strut or cable with nonzero weight in some equilibrium stress
- Tensegrity is infinitesimally rigid iff
  - There is an equilibrium stress that is nonzero on all struts and cables
  - Underlying linkage (all edges $\rightarrow$ bars) is infinitesimally rigid

Maxwell-Cremona Relation: Stresses and Liftings

- **Polyhedral lifting** = assignment of z coordinates to vertices such that faces of framework remain planar
  - Can assume z = 0 on boundary face



- **Maxwell-Cremona Theorem:** *A framework has a nonflat lifting precisely if it has a nonzero stress*
  - Valleys ↔ positive weights ω (struts and bars)
  - Mountains ↔ negative weights ω (cables and bars)

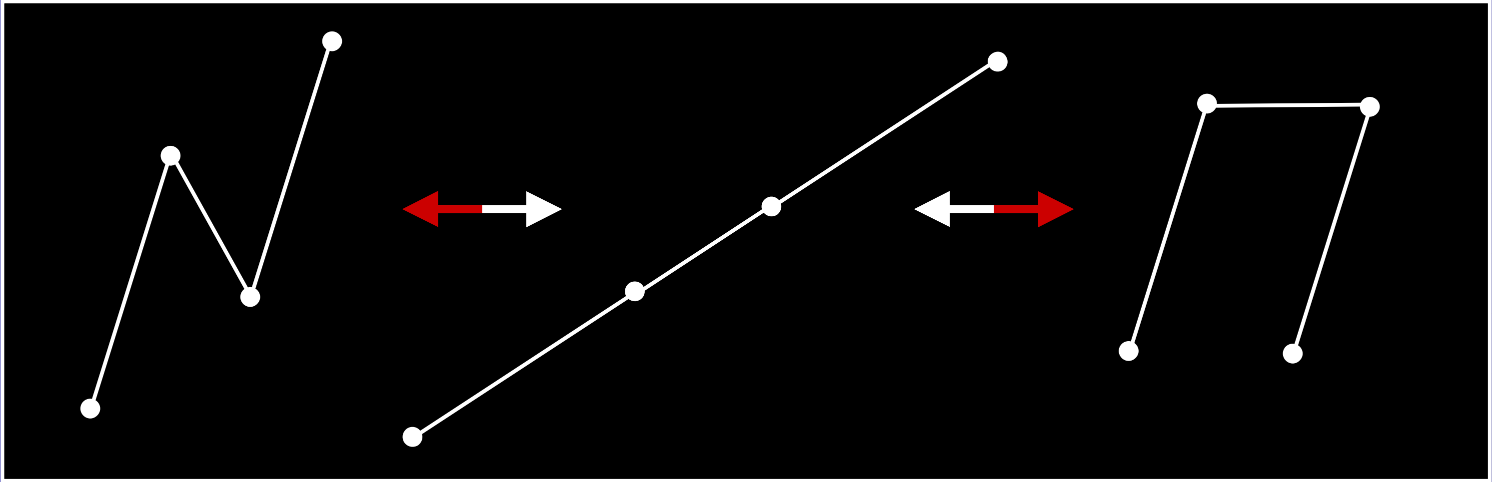


Outline: Linkages

- Definitions and History
- Rigidity
- **Locked chains in 3D**
- **Locked trees in 2D**
- **No locked chains in 2D**
- Algorithms
- Connections to protein folding

Locked Question

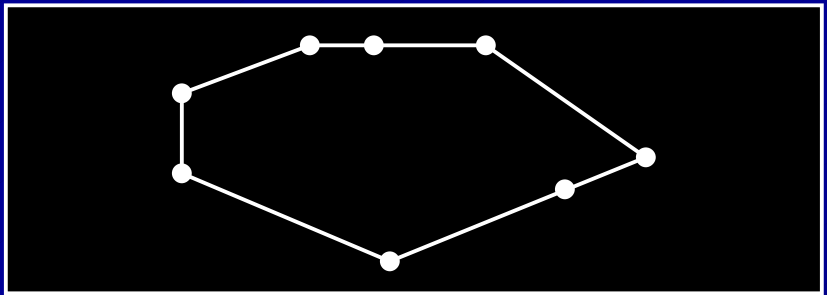
- Can a linkage be moved between any two non-self-intersecting configurations?
- Can any non-self-intersecting configuration be **unfolded**, i.e., moved to "canonical" configuration?
  - Equivalent by reversing and concatenating motions



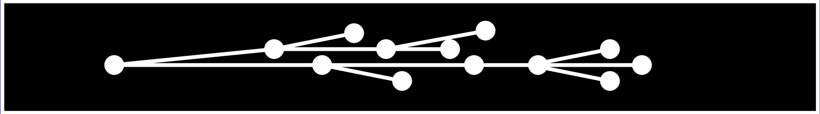
Canonical Configurations

- Arcs: Straight configuration

- Cycles: Convex configurations



- Trees: Flat configurations



What Linkages Can Lock?

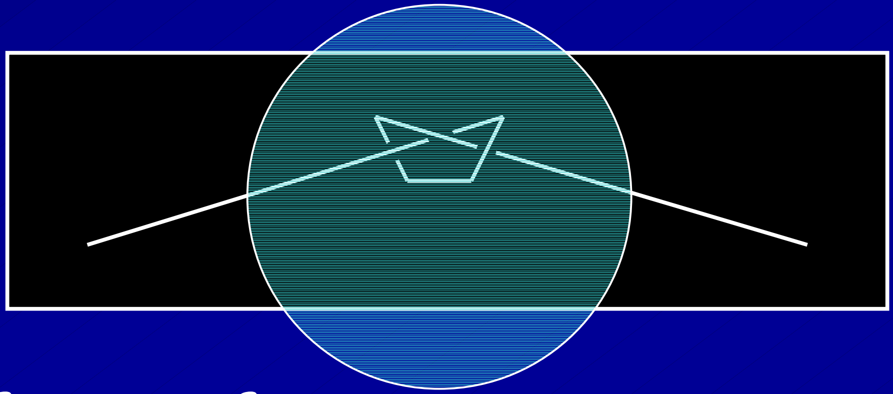
[Schanuel & Bergman, early 1970's; Grenander 1987; Lenhart & Whitesides 1991; Mitchell 1992]

- Can every arc be straightened?
- Can every cycle be convexified?
- Can every tree be flattened?

	Arcs	Cycles	Trees
2D	Yes	Yes	No
3D	No	No	No
4D & higher	Yes	Yes	Yes

Locked 3D Chains [Cantarella & Johnston 1998; Biedl, Demaine, Demaine, Lazard, Lubiw, O'Rourke, Overmars, Robbins, Streinu, Toussaint, Whitesides 1999]

- Cannot straighten some chains

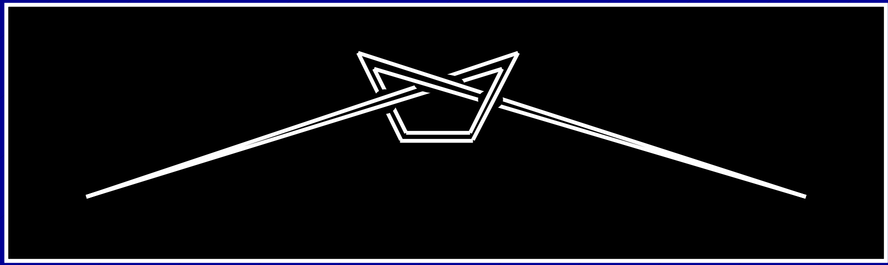


Sphere separates turns from ends

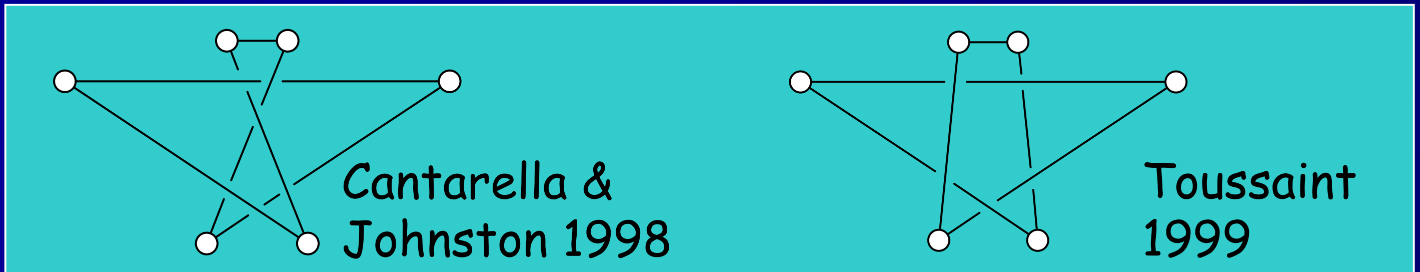
- Idea of proof:
  - Ends must be far away from the turns
  - Turns must stay relatively close to each other
  - $\Rightarrow$ Could effectively connect ends together
  - Hence, any straightening unties a trefoil knot

Locked 3D Chains [Cantarella & Johnston 1998; Biedl, Demaine, Demaine, Lazard, Lubiw, O'Rourke, Overmars, Robbins, Streinu, Toussaint, Whitesides 1999]

- Double this chain:



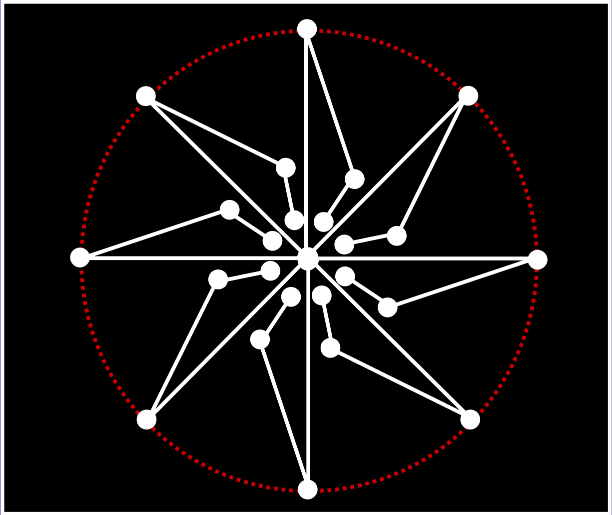
- This unknotted cycle cannot be convexified by the same argument
- Several locked **hexagons** are also known



Locked 2D Trees

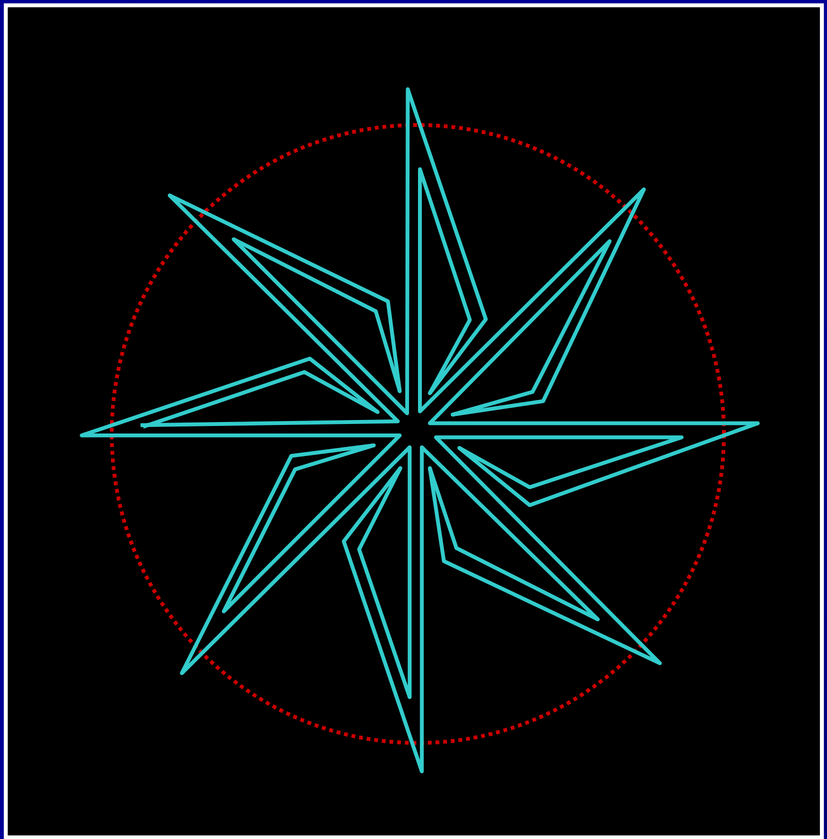
[Biedl, Demaine, Demaine, Lazard, Lubiw, O'Rourke, Robbins, Streinu, Toussaint, Whitesides 1998]

- **Theorem:** Not all trees can be flattened
  - No petal can be opened unless all others are closed significantly
  - No petal can be closed more than a little unless it has already opened



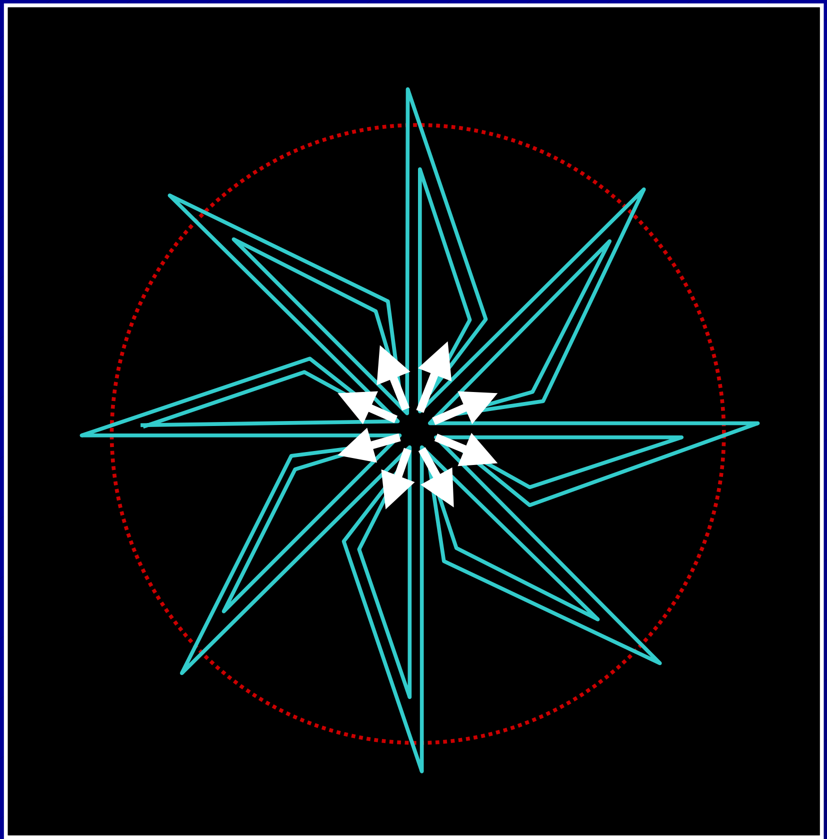
Converting the Tree into a Cycle

- Double each edge:



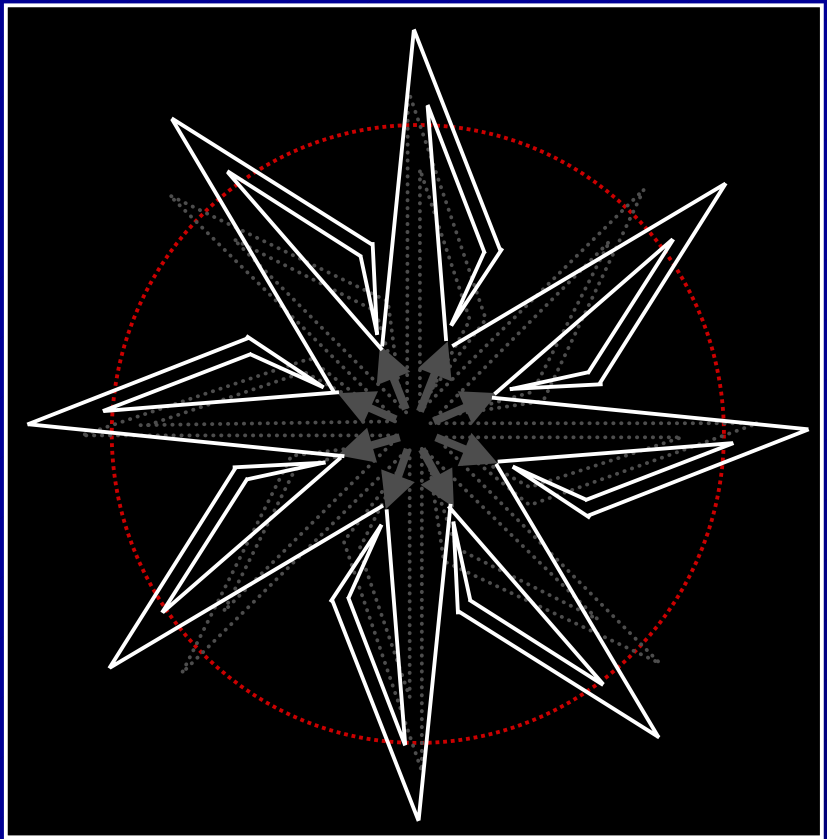
Converting the Tree into a Cycle

- But this cycle can be convexified:



Converting the Tree into a Cycle

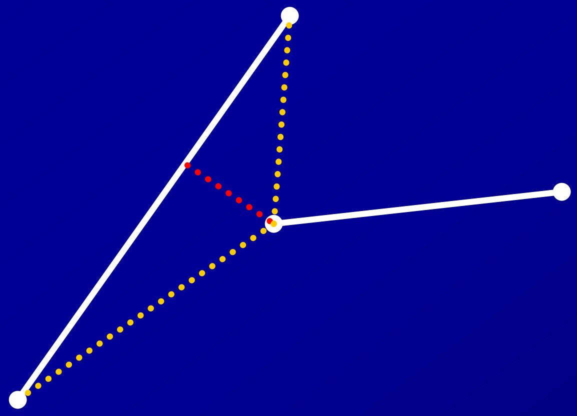
- But this cycle can be convexified:



One Key Idea for 2D Cycles: Increasing Distances

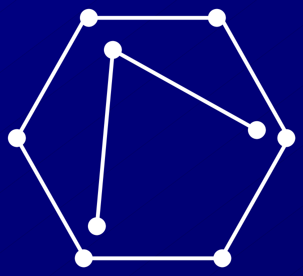
- A motion is **expansive** if no inter-vertex distances decreases

- **Lemma**: If a motion is expansive, the framework cannot cross itself



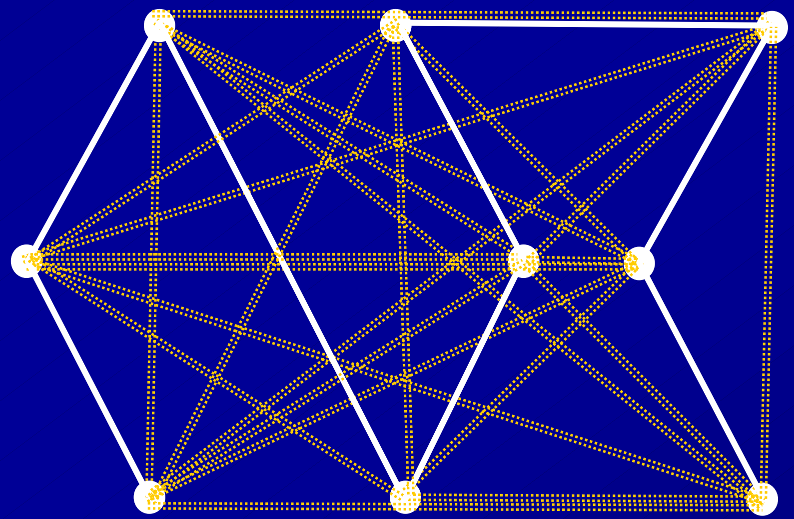
Theorem
[Connelly, Demaine, Rote 2000]

- For any family of chains and cycles, there is a motion that
  - Makes the arcs straight
  - Makes the cycles convex
  - Increases most pairwise distances (and area)
- Except: Arcs or cycles contained within a cycle might not be straightened or convexified
- Furthermore:
  Motion preserves symmetries and
  is piecewise-differentiable (smooth)



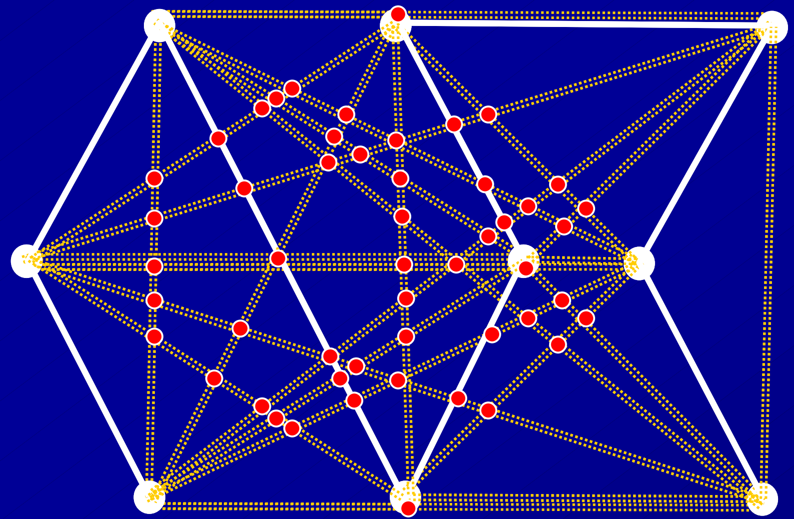
Transforming Linkage into Tensegrity

- In addition to bars of the framework, add **struts** between each pair of vertices not in a common convex cycle



Planarizing the Tensegrity

- Subdivide edges at intersection points
- Remove multiple overlapping edges
  - Replace with a bar if there is a bar
  - Replace with a strut otherwise

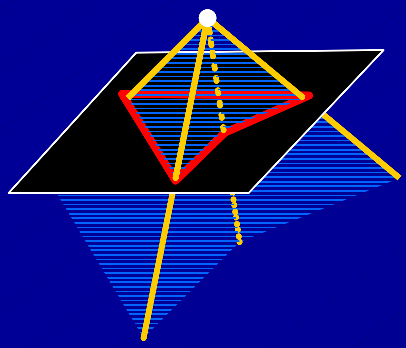


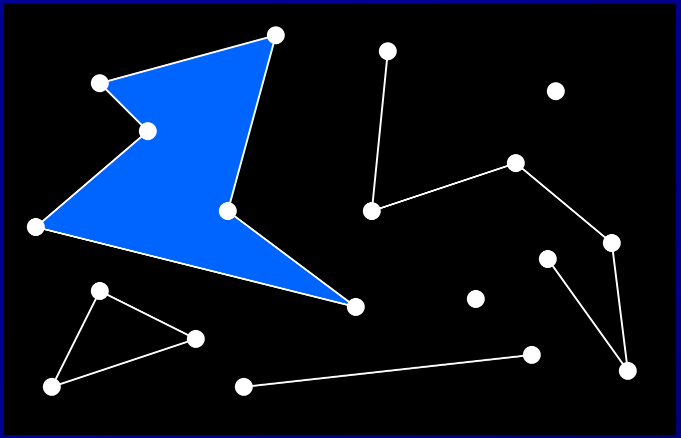
Proof of Existence of an Infinitesimal Motion

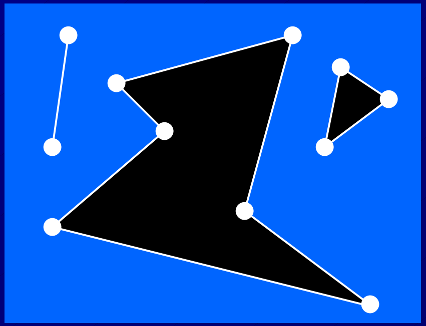
- Original framework infinitesimally flexible
  - $\Uparrow$ (duality)
- Original framework has only the zero equilibrium stress
  - $\Uparrow$ (planarization lemma)
- Planar framework has only the zero equilibrium stress
  - $\Uparrow$ (Maxwell-Cremona Theorem)
- Planar framework has only the flat polyhedral lifting

Proof of Existence of an Infinitesimal Motion

- Consider the top extreme M of some polyhedral lifting of the planar framework
  - One case: A vertex and none of its surroundings are at the top
    - Slice just below the vertex



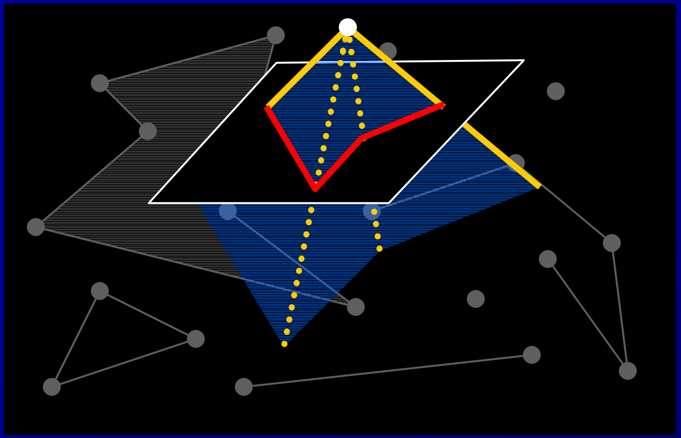


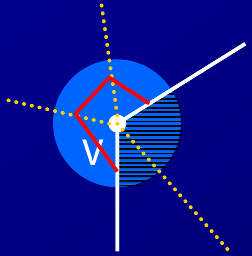


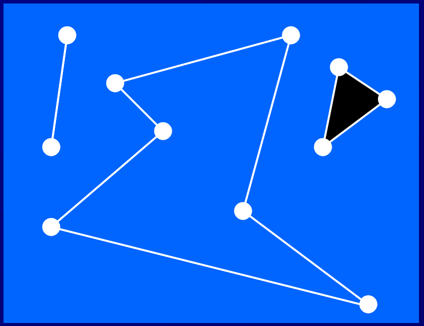
    - Red polygon has reflex vertices for valleys, convex for mountains
    - Must be at least three convex vertices

Proof of Existence of an Infinitesimal Motion

- Consider the top extreme M of some polyhedral lifting of the planar framework
  - Let v be a vertex of ∂M
  - Consider a small disk around v
  - Suppose there is a reflex portion of the disk between two consecutive bars
  - Claim this portion must be contained in M







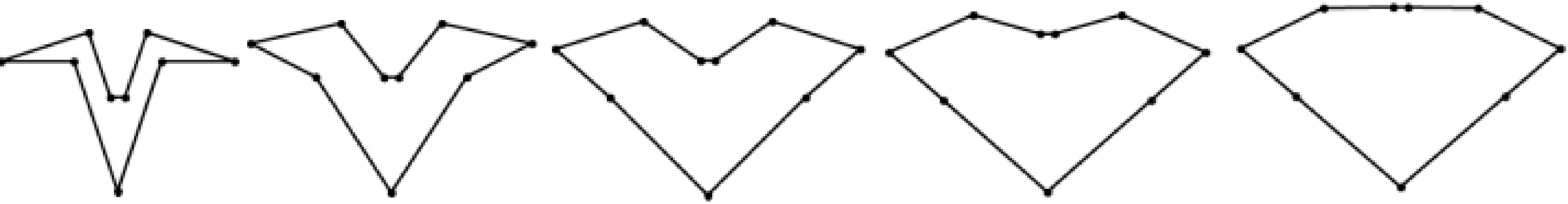
Existence of Global Motion

- Quadratic program defines a unique ordinary differential equation on an open subset of the configuration space, defined by the conditions:
  - No vertex has angle 180°
  - No vertex touches a bar
  - Some vertex is reflex
- Continuity $\Rightarrow$ There is a path to infinity or the boundary of the open set
  - Path is bounded because of bars' limited reach

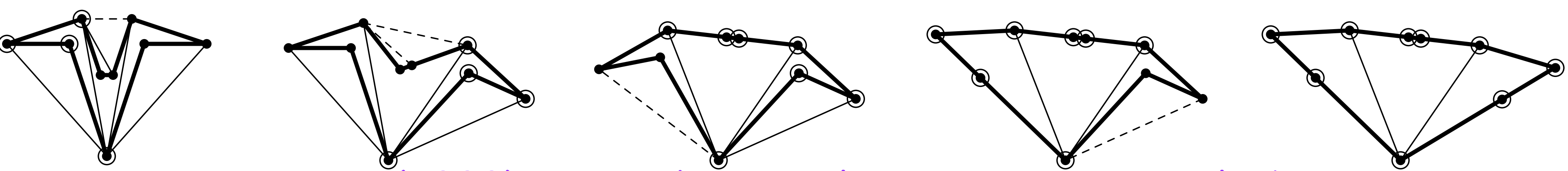
Outline: Linkages

- Definitions and History
- Rigidity
- Locked chains in 3D
- Locked trees in 2D
- No locked chains in 2D
- **Algorithms**
- Connections to protein folding

Algorithms for 2D Chains

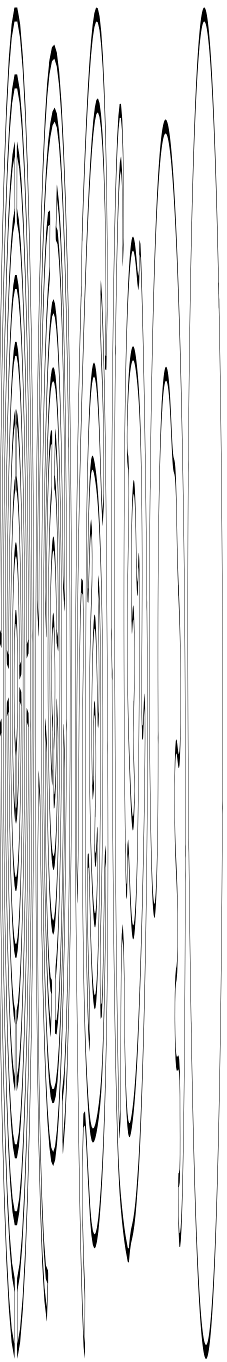


Connelly, Demaine, Rote (2000) — ODE + convex programming



Streinu (2000) — pseudotriangulations + piecewise-algebraic motions

Cantarella, Demaine, Iben, O'Brien (2003) — energy



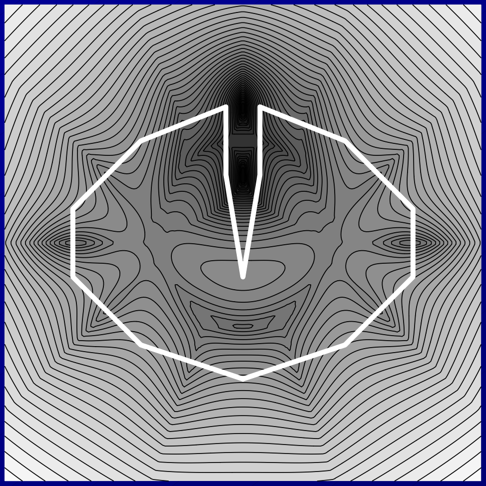
An Energy-Driven Approach to Linkage Unfolding

Jason Cantarella

Erik Demaine

Hayley Iben

James O'Brien



Outline: Linkages

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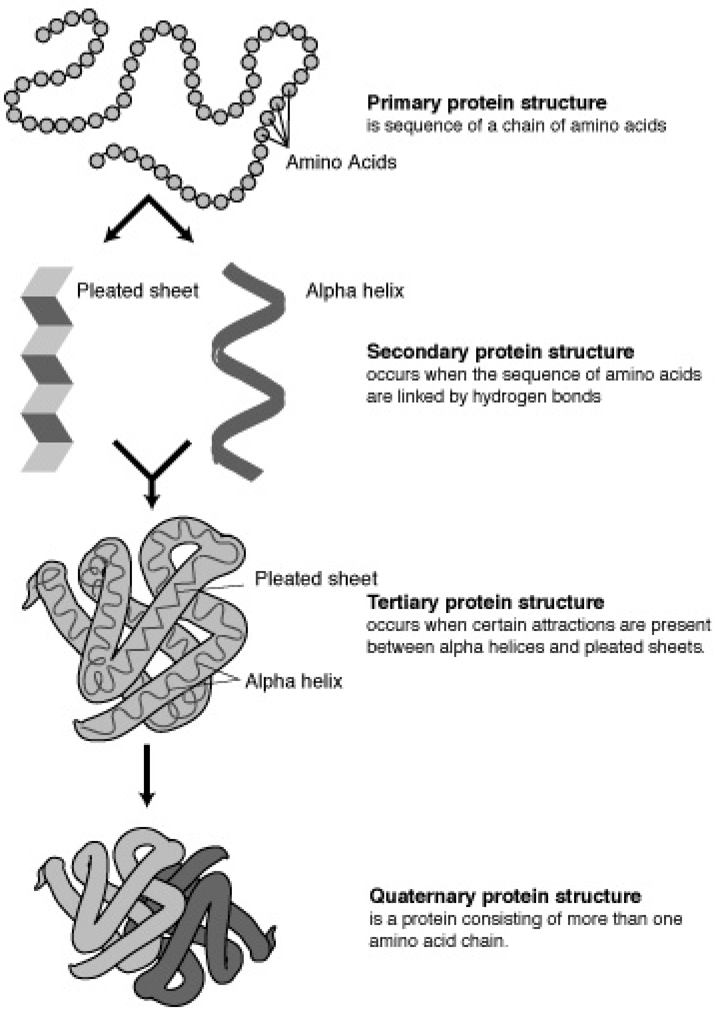
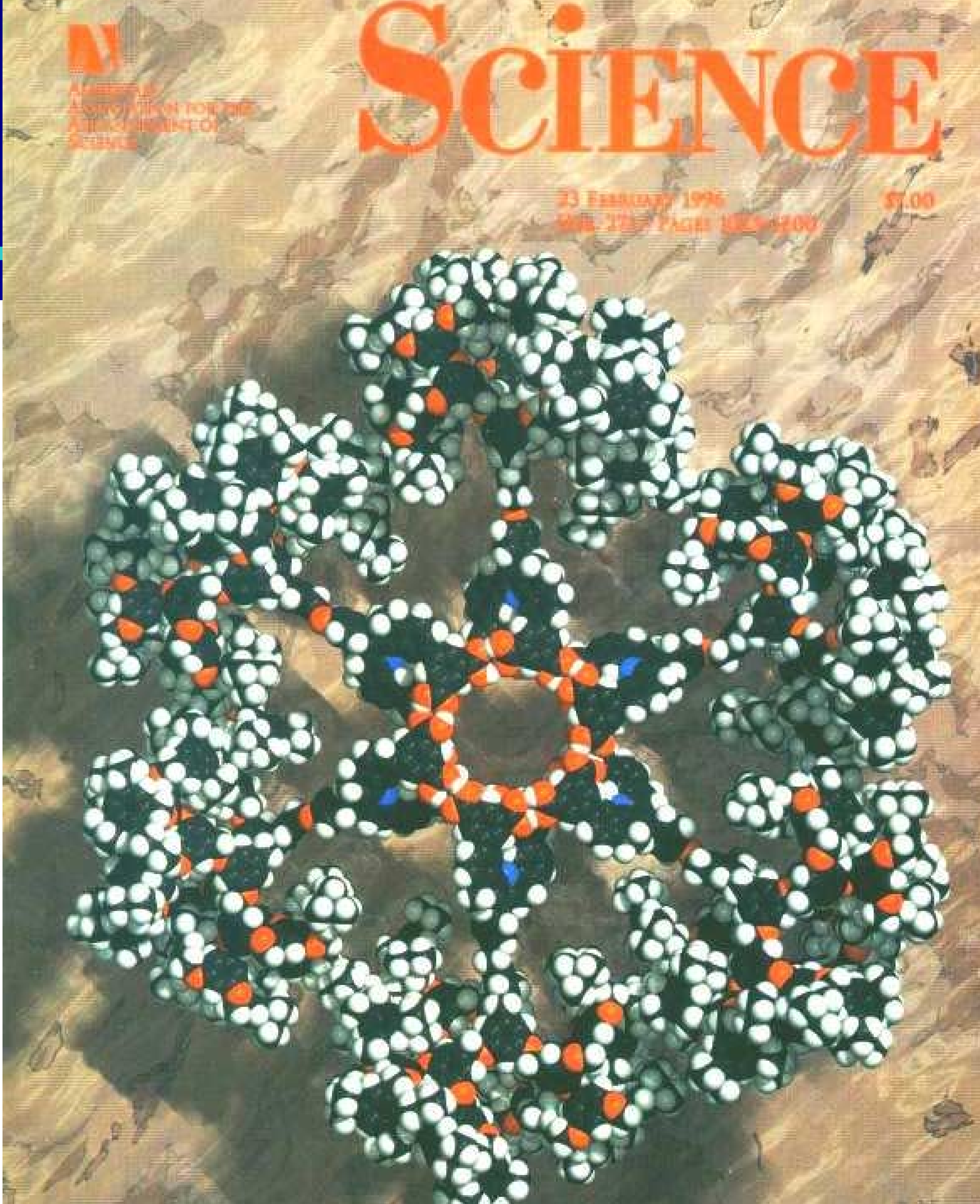
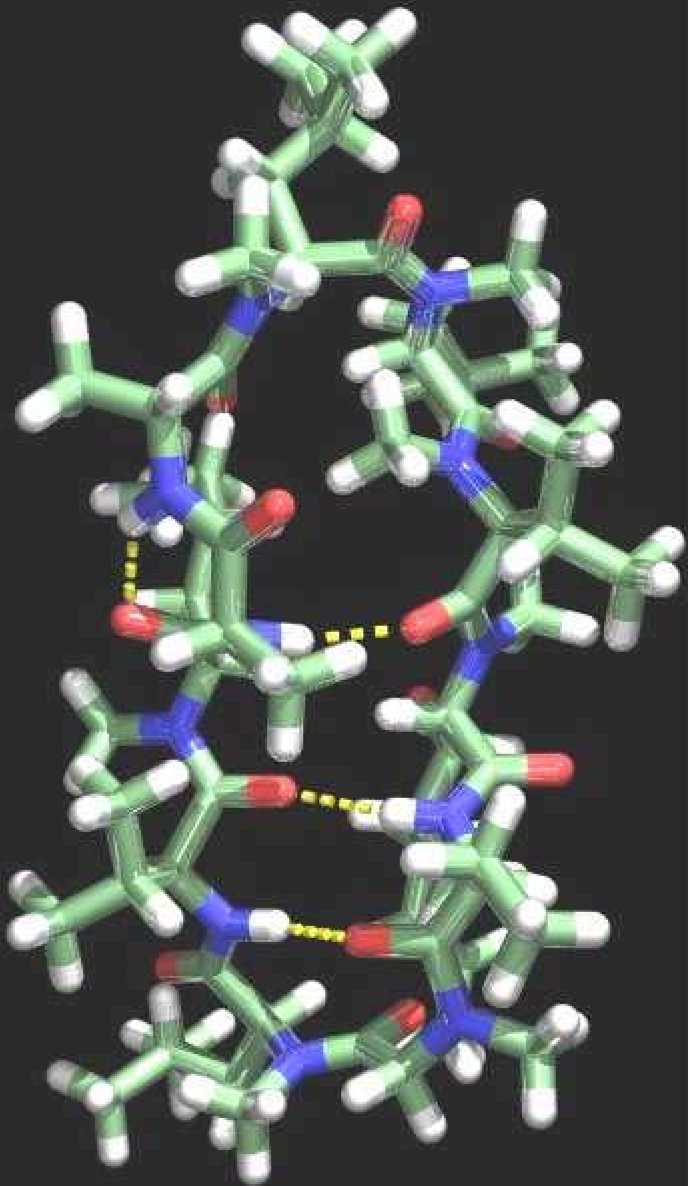
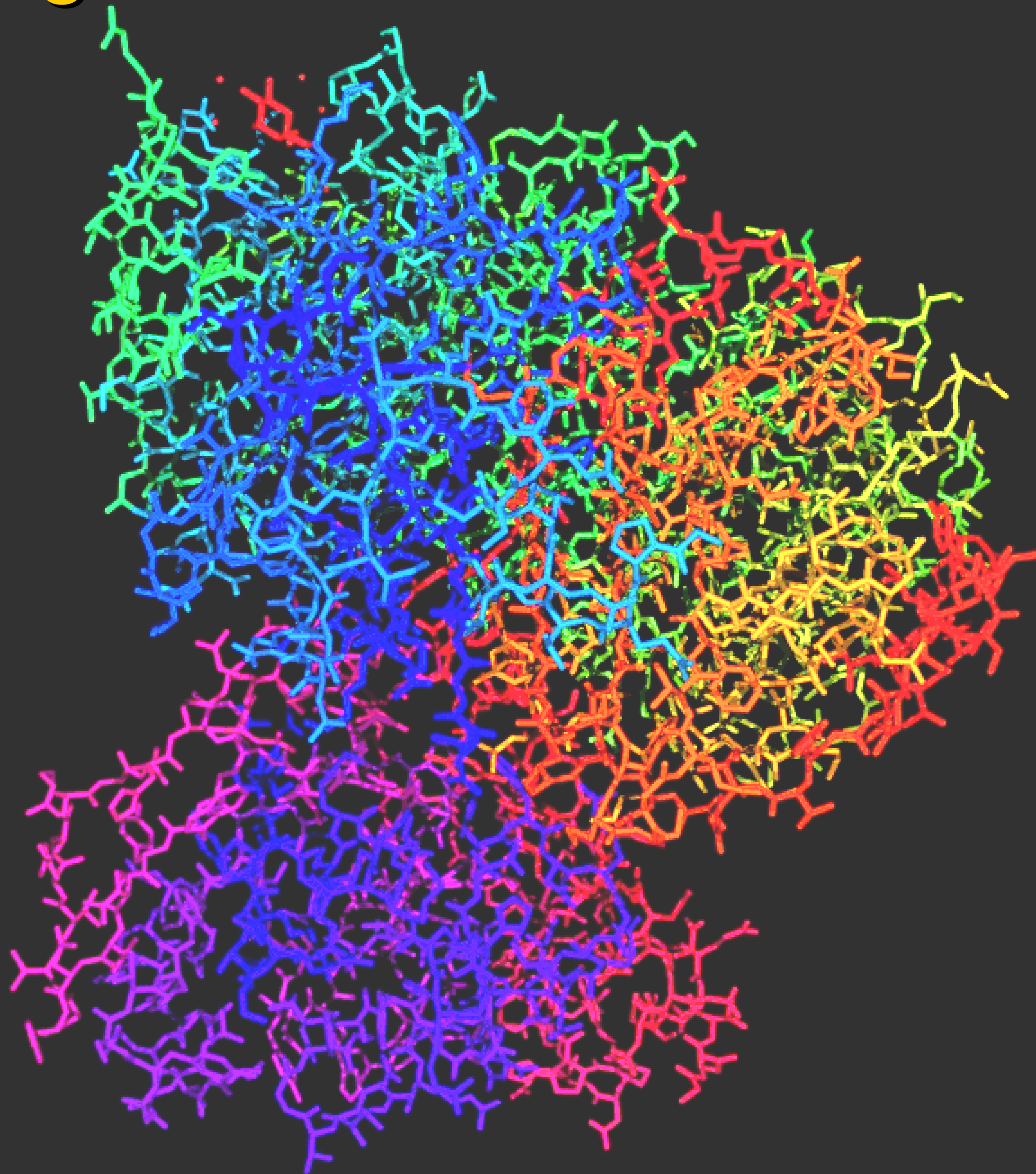
Protein Folding





Protein Folding





Motivation

- Geometry of a protein folding is an important aspect of its behavior
- Prediction of protein folding, and synthesis of proteins with desired foldings, are central problems in computational biology
  - Drug design
  - Preventing diseases (e.g., Alzheimer's, mad-cow disease, cystic fibrosis, some forms of cancer)
  - Understanding genomes

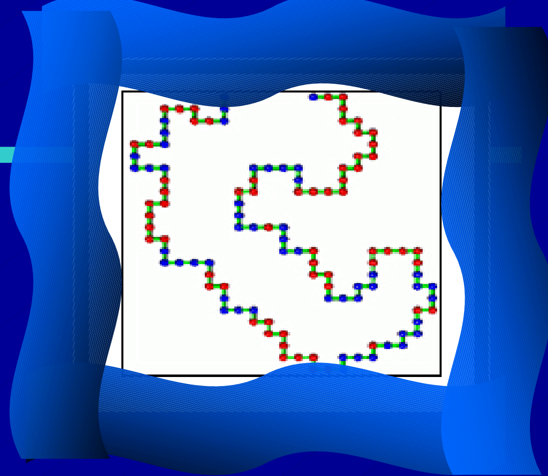
Linkage problems arising in protein folding

- Fixed-angle linkages (in 3D):
  - In addition to bar lengths, joint angles remain fixed
  - Protein is roughly a fixed-angle tree
- When are all flat states connected via motions? [Aloupis, Demaine, Dujmović, Erickson, Langerman, Meijer, O'Rourke, Overmars, Soss, Streinu, Toussaint 2002x2]
  - Nonacute chains; equal-angle acute chains
  - Not general planar graphs
- **Open:** *All chains? All trees?*

Linkage problems arising in protein folding

- Equilateral chains
  - *All bar lengths (roughly) equal*
  - Protein backbone is roughly such a chain
- **Open:** *Can all 3D equilateral chains be straightened?*
- **Open:** *Can all 3D equilateral trees be flattened?*

Hydrophobic-Hydrophilic / H-P Model [Dill 1990]



- Nodes (20 amino acids) categorized into two types:
  - Hydrophobic (H): Afraid of surrounding water
  - Hydrophilic (P): Like surrounding water
- Model: Proteins fold on 2D or 3D lattice to maximize number of **bonds** = lattice connections between nonadjacent H nodes
- NP-hard to find optimal protein folding
- **Open:** Design protein with a desired shape as (roughly) its unique optimal folding