Fixed-angle linkages: fix angles between incident bars
- roughly the mechanics of a protein (ignore energy/actuation until next lecture)
- in fact, roughly fixed-angle tree
- protein backbone is roughly fixed-angle chain (usually open but sometimes closed)

[Creighton: PROTEINS, 2nd. ed., p. 5]

- usually focus on backbone, ignoring amino-acid "side chains" ~ reasonable approximation
- basic move: edge spin / local dihedral motion:

Major problems in fixed-angle linkages (esp. chains)
1. Span = max/min distance between endpoints
2. Flattening = motion to flat state
3. Flat-state connectivity = motions between flat states
4. (un)locked = motion between any two states
Span of chain configuration = distance between endpoints
- distribution of span over configuration space heavily studied in e.g. polymer physics [≥20 papers]
- weakly NP-hard to find flat state with min or max span (among flat states) [Soss 2001]
- easy reductions from Partition:
  \[ \min: \quad 1 \quad 5 \quad 2 \quad \max: \quad \epsilon \cdot a_i \]

- OPEN: pseudopoly. alg. for flat min/max. span?
- OPEN: complexity of 3D min/max span?

3D max span: structural characterization & poly. time for orthogonal (90°)
  [Benbernou & O'Rourke 2006/2010; Borcea & Streinu 2010]
  - triangulate into body & hinge assembly:
    - geodesic shortest path = max span length
    - each part stays planar & zigzag (this part gets hard for nonorthogonal)
    - twist connections to align path edges
Flattening: weakly NP-hard [Soss & Toussaint 2000]
- reduction from Partition: divide n integers into 2 equal sums
- horizontal bars for integers
- vertical bars in between, length < \frac{1}{n}
- can flip horizontal bars left & right
- build lock that folds in essentially one way:

![Diagram of lock and partition]

very wide \Rightarrow key can't escape on left
\Rightarrow key must align with lock

**OPEN**: pseudopolynomial-time algorithm?

Flat-state connectivity: [Aloupis et al. 2002 & 2002]
- connected if there's a motion between any two non-self-intersecting flat configurations
- weaker form of connected config. space
- flat states are "canonical" for C
- disconnected otherwise
- stronger notion of locked

- fixed-angle chain might have no flat states (even NP-hard to know which) but proteins do, and seems important
Summary of results:  

open chain  
- nonacute angles  
- equal acute angles  
- angles strictly between $60^\circ$ & $90^\circ$ & unit edge lengths  
- has a monotone state  
- angles strictly between $60^\circ$ & $150^\circ$ & unit edge lengths  
- using $180^\circ$ edge spins  
- orthogonal & using $180^\circ$ edge spins  

[Aloupis et al. 2002 & 2002]  

set of open chains, pinned at one end  
- orthogonal  
- orthogonal & partially rigid  

[Aloupis & Meijer 2006]  

closed chain  
- nonacute  
- orthogonal  
- orthogonal & unit edge lengths  

[OPEN]  

tree  
- orthogonal  
- orthogonal & partially rigid  

[OPEN]  

graph  - orthogonal  

[OPEN]  

connected  
connected  
connected  
connected  
connected  
disconnected  
connected  
connected  
connected  
disconnected  
disconnected  

some edges can't spin
Flat-state disconnected partially rigid tree:

- inner edges flexible; rest rigid
- pins to remove reflectional symmetry

Variations:
1. four pinned chains, partially rigid
2. orthogonal graph
Flat-state disconnected partially rigid tree: (cont'd)

**Claim:** these two flat states are disconnected

**Proof:**
- View plane abcd as stationary
- Four branches & two sides of plane
  \[\Rightarrow \geq 2\] branches must flip through same side
- Opposite branches (ac or bd) can't share:
  - Geometric argument
  - Links parallel to axis of rotation hit exactly
  - Can shrink a & b edges for proper collision
- Adjacent branches (say, ab) can't share:
  - Topological argument
  - Connect shallow rope \(a \to \text{end of a branch}\)
  - Connect deeper rope \(b \to \text{end of b branch}\)
  - Unlinked in left config.
  - Linked in right config

- Ropes stay as-is during motion above plane
  \[\Rightarrow a \& b\] branches intersect

**Open:** flexible tree? orthogonal tree?
Orthogonal open chains are flat-state connected:
- canonical form: staircase (trans config. from L 16)
  (alternate ±90° turns)

- lift a flat state into canonical form:
  0) induction hypothesis:
  - half of chain remains in plane
  - half of chain in canonical form in perp. plane
  1) rotate canonical half (and its containing plane) so that next edge makes a larger staircase
  2) rotate larger staircase (around following edge) to lift into staircase plane
  3) repeat
  - FedEx via canonical form

Nonacute open chains: similar
- canonical state = z-monotone (⇒ never hit z=0)

Equal acute chains: similar
- canonical state = zig-zag (⇒ lifting harder)

OPEN: general chains?
Locked proteins:
- locked universal-joint chains are locked fixed-angle too
- even simpler, 4-link “crossed-legs”:
  [Langerman 2002]
- existence of locked chains suggests config. space is hard to navigate ~ yet nature does it well
- Conjecture: additional constraints in nature prevent existence of locked chains
  - bond lengths all roughly equal (1-1.53Å)
  - bond angles all obtuse & roughly equal (115.6-123.2°)
- OPEN: is there a locked fixed-angle chain that’s equilateral, equiangular, & obtuse
  - crossed legs satisfies all but obtuse
  - subdivided knitting needles all but equi-ang.
- proteins also produced sequentially by ribosome:
Producible protein (fixed-angle) chains:

Ribosome = “machine” built from proteins & RNA translating messenger RNA into proteins

“creation”

\[ \text{narrow tunnel} \sim \text{protein} \sim \text{straight} \sim \text{conjectured amino acid attaches} \]

\( \beta \)-producible chain = simple geometric model of chains & configurations resulting from ribosome
- cone \( C_\beta \) of half-angle \( \beta \)
- chain produced in cone, link by link
- latest link passes through cone apex
- when latest vertex \( v_i \) reaches cone apex, next link \( (v_i, v_{i+1}) \) is instantly created in cone & \( v_i \) can never re-enter cone

Reality: \( \beta = 90^\circ \) (halfspace) is the closest model (somewhat local model though ~ really long protein might reach around ribosome)

\( (\leq \alpha) \)-chain = chain of max. turn angle \( \leq \alpha \)
- \( \beta \)-producible \( \Rightarrow \alpha/2 \leq \beta \leq 180^\circ - \alpha/2 \)
- we'll assume \( \alpha = \beta \)
Canonical configuration for \((\leq \alpha)\)-chains:
- put \(v_0\) at origin \((0,0,0)\)
- put \(v_{i+1}\) on cone \(C_{\alpha/2}\) centered at \(v_i\)
- \(v_1\) chosen to maximize \(\alpha\) coordinate
- \(v_{i+1}\) chosen to get correct turn angle at \(v_i\):
  - view on sphere centered at \(v_i\) & radius \(\alpha/2\)
  - \(C_{\alpha/2}\) intersects along circle around north pole
  - turn-angle cone intersects along tilted circle of radius \(\tau_i\)
- intersections overlap (at 1 or 2 pts.) because center of turn-angle circle is on \(C_{\alpha/2}\) circle & \(\tau_i \leq \alpha\)
- take counterclockwise-most intersection for \(v_{i+1}\) relative to origin
- kind of spiral
- similar to nature's \(\alpha\)-helix
- contained in \(C_{\alpha/2}\) cone: by induction
- in fact, strictly inside cone \(C_{\alpha/2}\) except for first link because \((v_0,v_1)\) & \((v_1,v_2)\) not parallel
Canonicalizing \((\geq \alpha)\)-producible \((\leq \alpha)\)-chains:

- **Main idea:** Play production movie backwards
  \(\Rightarrow\) as links enter the cone, they disappear
- maintain these links in canonical configuration,
  translated to start at last existing vertex \(v_i\) &
  rotated to make cone as vertical as possible
  while satisfying turn angle at \(v_i\)
- viewed on sphere centered at \(v_i\):
  put canonical cone axis
  \(2\tau_i\) up from previous edge direction
  toward north pole (maxing out at north pole)
  \(\Rightarrow\) canonical configuration is in \(C\beta(2\alpha)\)
  because \((v_{i-1}, v_i)\) is too (by production)
- if \((v_{i-1}, v_i)\) is vertical, then
  orientation of first link is not determined
- choices for smaller & larger times may differ
- freeze movie & continuously spin \((v_{i-1}, v_i)\)
  to switch from previous choice to next
- when \(v_i\) reaches cone apex, need to extend
  canonical configuration & maintain invariant
- spin \((v_{i-1}, v_i)\) to make \((v_i, v_{i+1})\) as vertical
  as possible \(\Rightarrow\) new canon. config. rotation
- spin \((v_i, v_{i+1})\) to bring \((v_i, v_{i+1})\) into
  canonical configuration
- note: already canonical \(\Rightarrow\) rigid\(\square\)
What is producible?

- $\alpha$-canonical configuration is $\beta$-producible for $\alpha/2 \leq \beta \leq 180^\circ - \alpha/2$ (full range)
- keep canonical configuration in complementary cone $B_\beta$
- produces “rigidly” (no spinning required)

- $(\leq \alpha)$-chain $(\geq \alpha)$-producible
  $\Rightarrow$ $\beta$-producible for $\alpha/2 \leq \beta \leq 180^\circ - \alpha/2$
- $\beta$-produce $\alpha$-canonical configuration
- reverse canonicalization procedure far away from production cone $C_\beta$
- flat states of $(\leq \alpha)$-chains are $\beta$-producible for $\alpha \leq \beta \leq 90^\circ$

- imagine moving cone instead of chain
- create next link in vertical plane
- slide up to plane of flat configuration with cone just touching plane
- repeat

$\Rightarrow$ flat-state connected
- canonicalize both, combine motions
$\Rightarrow$ for $(\leq \alpha)$-chains & $\alpha \leq \beta \leq 90^\circ$,
configuration is flattenable $\Rightarrow$ it is $\beta$-producible