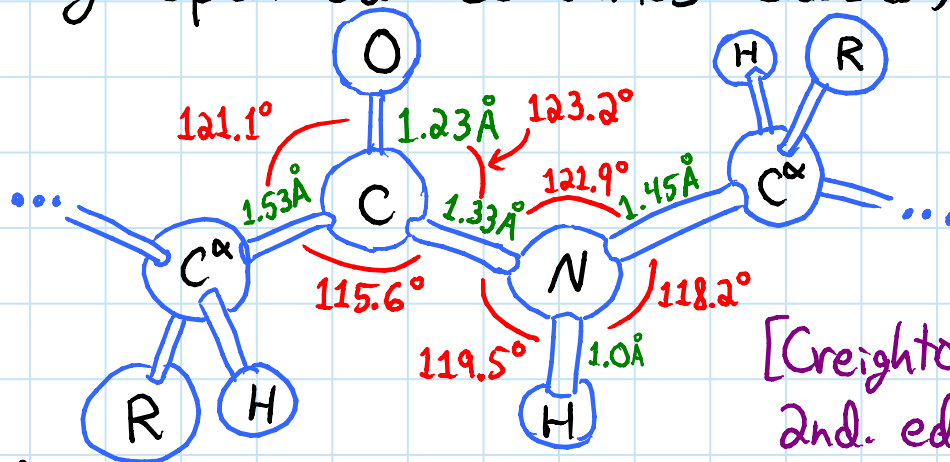


Fixed-angle linkages: fix angles between incident bars

- 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:

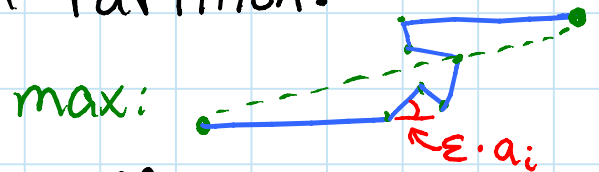


Major problems in fixed-angle linkages (esp. chains)

- 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:

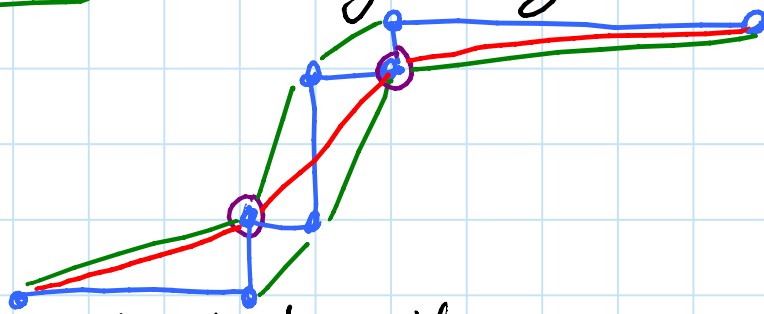


- OPEN: pseudopoly. alg. for flat min/max. span?
- OPEN: complexity of 3D min/max span?

3D max span: structural characterization & poly. time for orthogonal (90°)

[Benbernou & O'Rourke 2006/2010; Borcea & Streinu 2010]

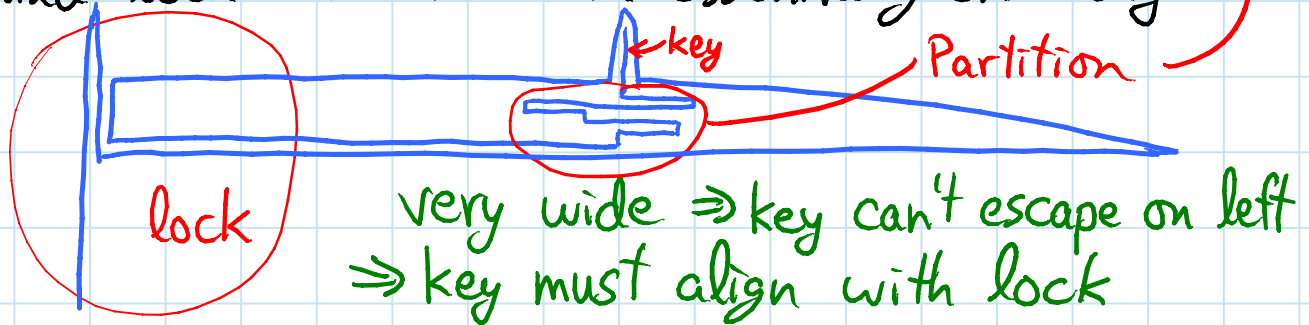
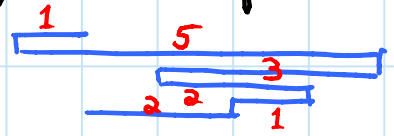
- triangulate into body & hinge assembly:



- 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]

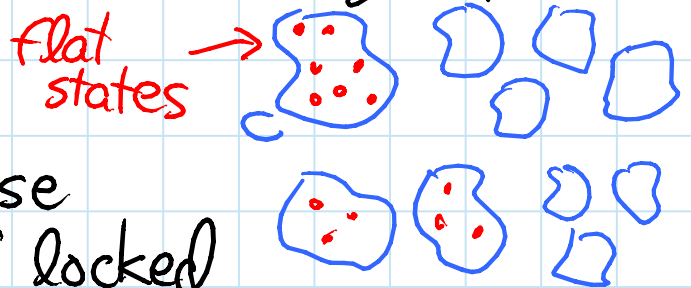
- reduction from Partition: divide n integers into 2 equal sums
- horizontal bars for integers
- vertical bars in between, length $< \frac{1}{n}$
- \Rightarrow can flip horizontal bars left & right
- build lock that folds in essentially one way:



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
 - \Rightarrow 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: [Aloupis et al. 2002 & 2002]

open chain

- nonacute angles
- equal acute angles
- [- angles strictly between 60° & 90° & unit edge lengths
- has a monotone state
- angles strictly between 60° & 150° & unit edge lengths [Aloupis & Meijer 2006]
- using 180° edge spins
- orthogonal & using 180° edge spins

OPEN
connected
connected
connected
connected
connected
disconnected
connected

set of open chains, pinned at one end

- orthogonal
- orthogonal & partially rigid
some edges can't spin

connected
disconnected

closed chain

- nonacute
- orthogonal
- orthogonal & unit edge lengths

OPEN
OPEN
OPEN
connected

tree

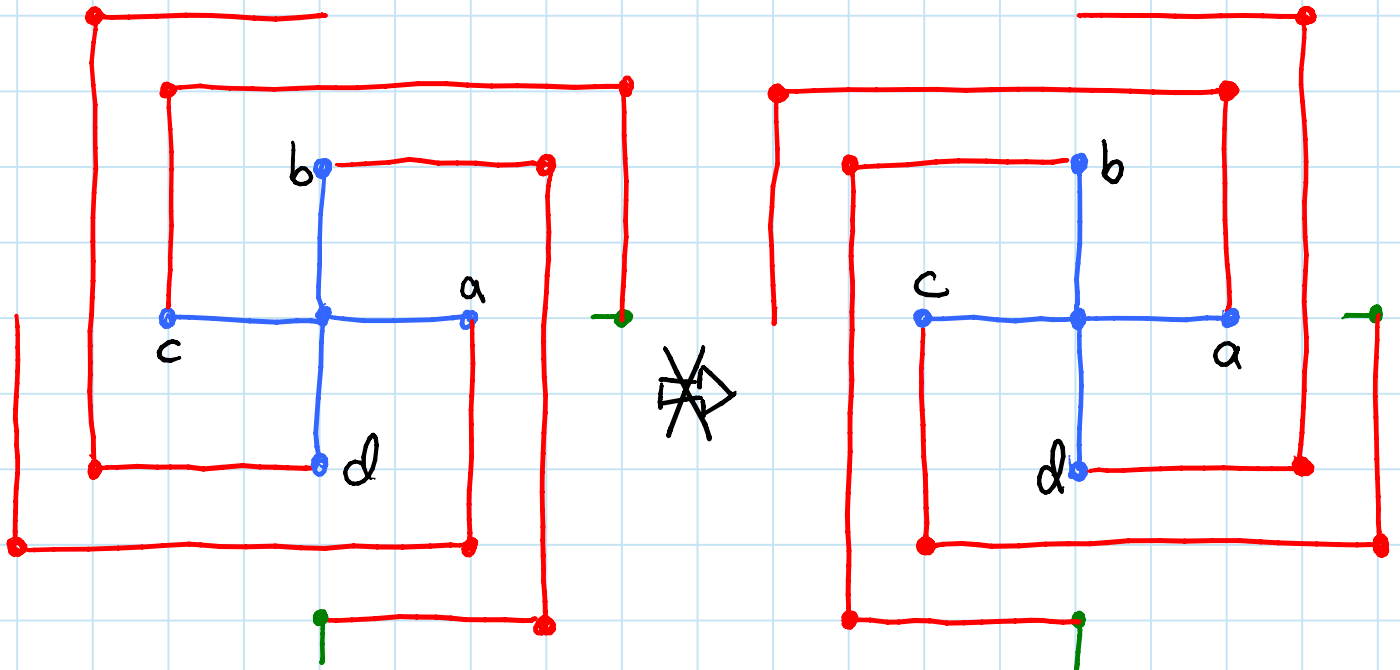
- orthogonal
- orthogonal & partially rigid

OPEN
OPEN
disconnected

graph - orthogonal

disconnected

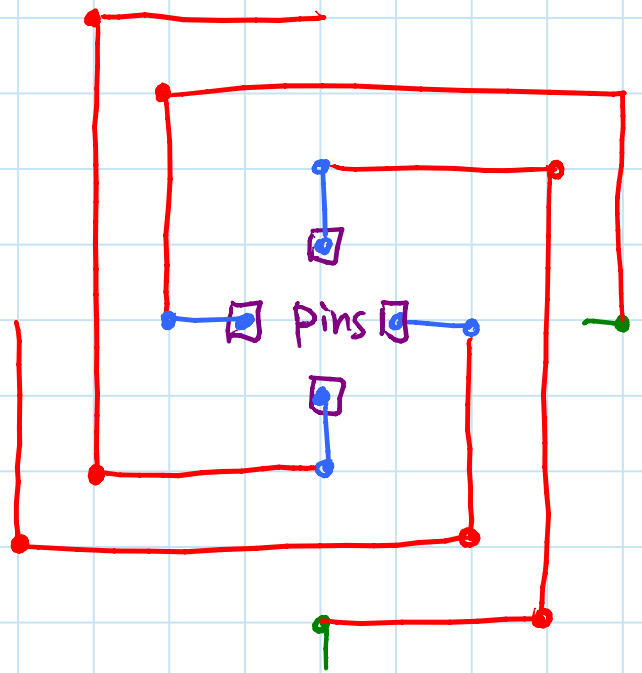
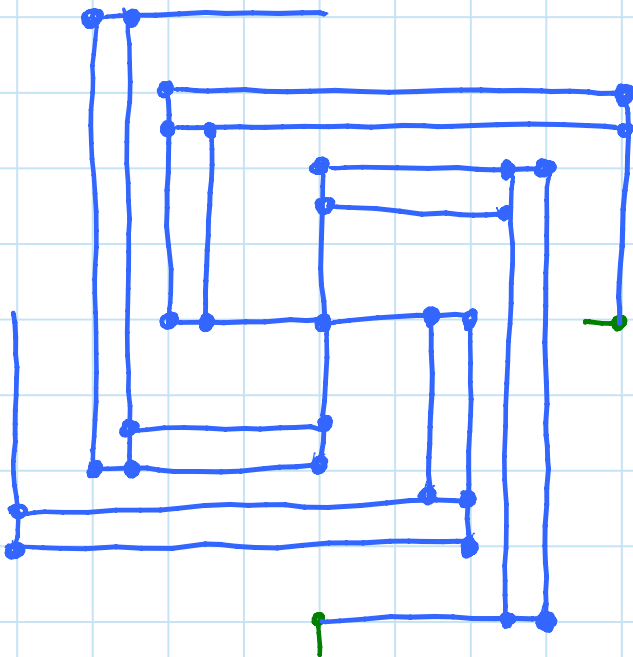
Flat-state disconnected partially rigid tree:



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

Variations:

① four pinned chains, partially rigid

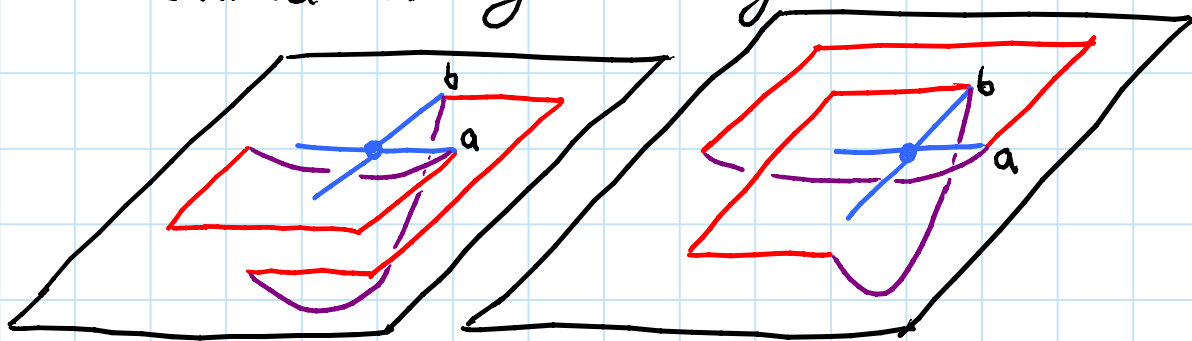


② orthogonal graph

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 \rightarrow end of a branch
 - connect deeper rope b \rightarrow 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 \square

OPEN: flexible tree? orthogonal tree?

Orthogonal open chains are flat-state connected:

- canonical form: staircase (trans config. from L16)
(alternate $\pm 90^\circ$ turns)



- lift a flat state into canonical form:

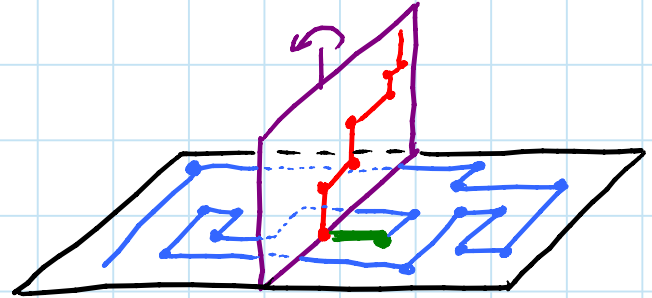
⊗ induction hypothesis:

- half of chain

- remains in plane

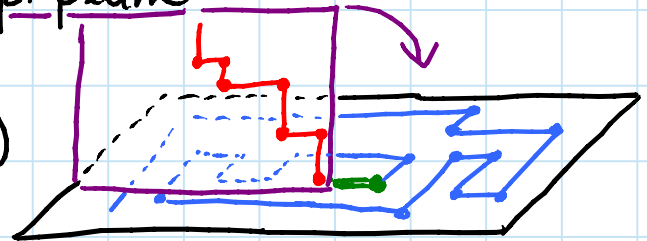
- half of chain in

- canonical form in perp. plane

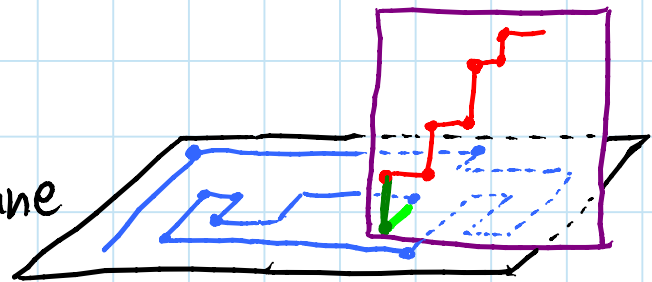


① rotate canonical half
(and its containing plane)

so that next edge
makes a larger staircase



② rotate larger staircase
(around following edge)
to lift into staircase plane



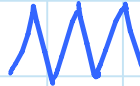
③ repeat

- FedEx via canonical form

Nonacute open chains: similar


- canonical state = z-monotone (\Rightarrow never hit $z=0$)

Equal acute chains: similar

- canonical state = zig-zag  (\Rightarrow 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:

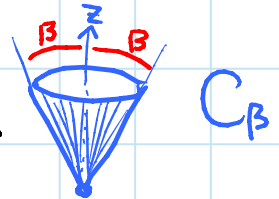
[Demaine, Langerman, O'Rourke 2003/6]

Ribosome = "machine" built from proteins & RNA translating messenger RNA into proteins



β -producible chain = simple geometric model of chains & configurations resulting from ribosome

- cone C_β of half-angle β
- 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



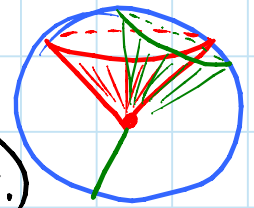
(somewhat local model though ~ really long protein might reach around ribosome)

$(\leq \alpha)$ -chain = chain of max. turn angle $\leq \alpha$

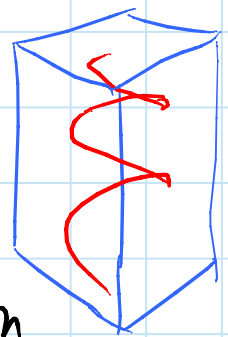
- β -producible $\Rightarrow \alpha/2 \leq \beta \leq 180^\circ - \alpha/2$
- we'll assume $\alpha = \beta$

Canonical configuration for $(\leq \alpha)$ -chains:

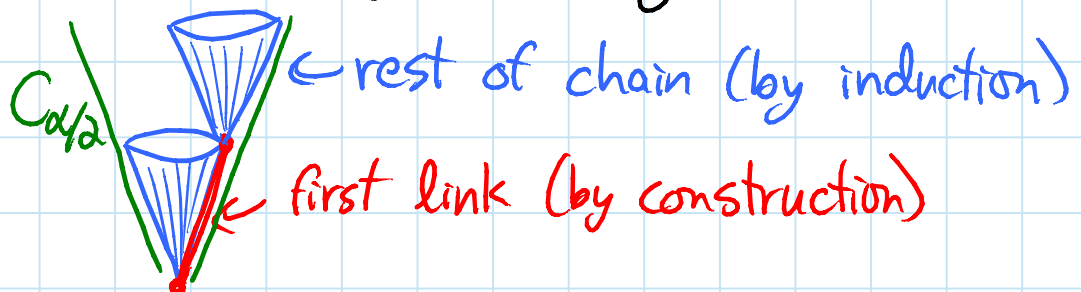
- put v_0 at origin $(0, 0, 0)$
- put v_{i+1} on cone $C_{\alpha/2}$ centered at v_i
- v_1 chosen to maximize x coordinate
- v_{i+1} chosen to get correct turn angle at v_i :
 - view on sphere centered at v_i & radius $\alpha/2$
 - $C_{\alpha/2}$ intersects along circle around north pole
 - turn-angle cone intersects along tilted circle of radius τ_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 α -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 $C_{\beta(\geq \alpha)}$ 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?

- α -canonical configuration is β -producible for $\alpha/2 \leq \beta \leq 180^\circ - \alpha/2$ (full range)
 - keep canonical configuration in complementary cone B_β
 - \Rightarrow produces "rigidly" (no spinning required)
 - $(\leq \alpha)$ -chain $(\geq \alpha)$ -producible
 - $\Rightarrow \beta$ -producible for $\alpha/2 \leq \beta \leq 180^\circ - \alpha/2$
 - β -produce α -canonical configuration
 - reverse canonicalization procedure far away from production cone C_β
 - flat states of $(\leq \alpha)$ -chains are β -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 flatterable \Leftrightarrow it is β -producible

