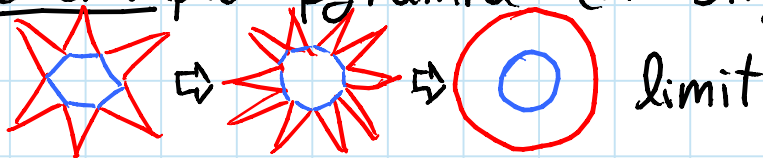
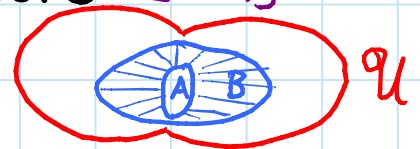


# Unfolding smooth prisms: [Benbernou, Cahn, O'Rourke 2004]

- convex hull of two parallel smooth convex shapes
- keep bottom  $B$ , unroll side ribs, place top  $A$  (how?)
- simple example: pyramid ( $A$  = single point)



- surface area not preserved (unlike regular unfolding)
- like source unfolding of sphere [L14]



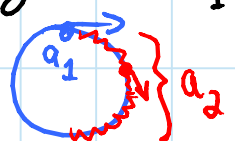
## ① Flat polyhedron & $A \subseteq B$

- parameterize ribs as  $(a(t), b(t))$ ,  $0 \leq t < 1$
- convexity of  $A$  &  $B \Rightarrow$  tangents  $\dot{a}(t)$ ,  $\dot{b}(t)$  turn right as  $t$  increases (clockwise param.)
- also, tangents  $\dot{a}(t)$  &  $\dot{b}(t)$  are parallel (discrete analog: faces of prismatoid are trapezoids)
- unfolded  $A$ :  $u(t) = a(t)$  reflected thru  $\dot{b}(t)$

Lemma: unfolded ribs don't intersect

Proof: consider  $(b_1, u_1)$  vs.  $(b_2, u_2)$ . [ $x_i = x(t_i)$ ]

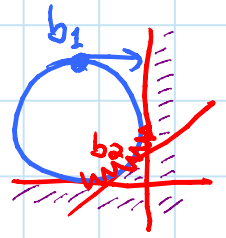
- assume by rotation that  $\dot{a}_1$  is horizontal
- assume by reflection that  $a_2$  is right of  $a_1$  (- ditto for  $b_1$  &  $b_2$ )



# Unfolding smooth prisms: (cont'd)

Case (a):  $a_2$  in bottom-right quarter

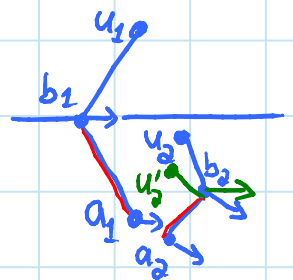
- $(b_2, u_2)$  is on outside of tangent  $b_2$
- $A \leq B \Rightarrow a_2$  is left of red region
- $b_1$  horizontal  $\Rightarrow u_2$  is left of red region
- $\Rightarrow (b_1, u_1)$  not in outside region



Case (b):  $a_2$  in top-right quarter

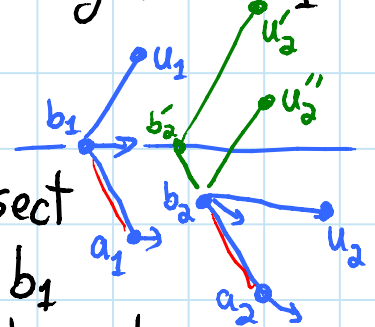
Subcase (i): rib  $(a_i, b_i)$  slopes have opposite signs

- $a_1$  is left of  $a_2$
- $\Rightarrow u_1$  (straight above  $a_1$ ) is left of reflection  $u'_2$  of  $a_2$  thru horizontal thru  $b_2$
- rotating horizontal to true  $b_2$  rotates  $u_2$  clockwise  $\Rightarrow$  away from  $u_1$



Subcase (ii): same signs

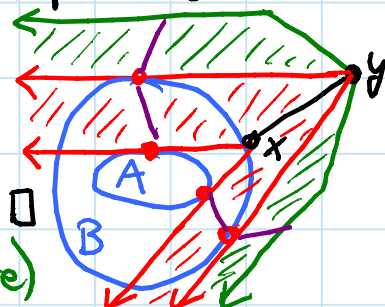
- $(a_1, b_1)$  &  $(a_2, b_2)$  don't intersect
- $\Rightarrow$  horizontal reflections thru  $b_1$   $(b_1, u_1)$  &  $(b'_2, u'_2)$  don't intersect
- $\Rightarrow (b_1, u_1)$  doesn't intersect reflection  $(b_2, u''_2)$  of  $(a_2, b_2)$  thru horiz. line thru  $b_2$
- translate rightward & shrink length
- rotate clockwise to true  $b_2$  as before  $\square$



# Unfolding smooth prisms: (cont'd)

Simpler proof of rib lemma: [NEW - Matt Ince]

- extend  $\vec{a}_1, \vec{a}_2$  till intersection point  $x$
- extend  $\vec{b}_1, \vec{b}_2$  till intersection point  $y$
- $xy$  divides red wedge into two regions, one per rib
- reflections disjoint by convexity  $\square$   
(positive curvature)



Mutual tangency: if top attaches at  $a(t)$ ,  
locally avoid overlap

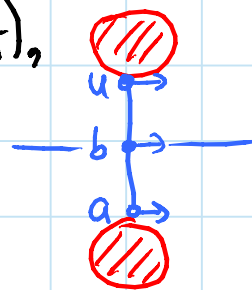
$\Leftrightarrow \vec{a}(t)$  is parallel to  $\vec{u}(t)$

- maximize  $|\vec{a}(t) - \vec{u}(t)|$

$\Rightarrow$  mutual tangency

&  $\vec{u}(t)$  on convex hull of  $U$

$\Rightarrow$  global nonoverlap



② Flat polyhedron,  $A \& B$  arbitrary

- argue  $\max |\vec{a}(t) - \vec{b}(t)|$  still mutual tangency

③ Nonflat polyhedron

- show "easier": rounded out more
- more algebra

OPEN: edge unfolding of polyhedral prisms?

## Flexible polyhedra: (rigid faces & hinged edges)

### Convex polyhedra are rigid:

- Cauchy's Rigidity Theorem  $\Rightarrow$  any motion must make polyhedron nonconvex
- can't happen immediately (if no flat edges)
- in fact, convex polyhedra are (second-order) rigid with finitely many creases (flat edges) [Connelly 1980]

### Square-bottom paper bag: contrasting example

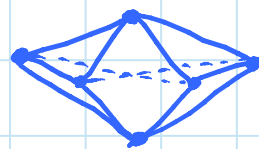
(convex, with boundary) [Balkcom, Demaine, Demaine 2004]

- rigid with usual creases
- flattenable with additional creases

Generic/almost all triangulated polyhedra are infinitesimally rigid [Gluck 1986; Euler 1766 conjecture]

### Flexible nonconvex polyhedra exist nonetheless:

- Bricard "octahedron" [~1900]
- self-intersecting (more of linkage)
- Connelly polyhedron [1978]
- modification to avoid self-intersection
- 30 faces, 50 edges, 22 vertices
- Steffen's polyhedron [Klaus Steffen]
- simplification with 14 triangles, 9 vertices
- need  $\geq 9$  vertices  $\Rightarrow$  optimal



## Flexible polyhedra: (cont'd)

Bellows Theorem: [Connelly, Sabitov, Walz 1997]

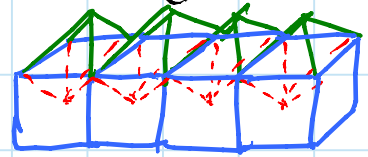
volume remains constant during any flex of a nonconvex polyhedron

Volume polynomials: [Sabitov 1996; Astrelin & Sabitov 1999]

volume of a polyhedron is a root of a polynomial  $p(x)$  determined by just combinatorial structure & face geometries  
 $\Rightarrow$  constant during continuous motion (finite set)

— degree must be exponential:

— each house can pop in or out




— degree  $\leq 2^{\#edges}$  [Fedorchuk & Pak 2004]

— true even for generalized (self-intersecting) polyhedra: volume = sum of signed volumes of tetrahedra from (any) point

# Protein folding: some biochemistry background

## DNA (Deoxyribonucleic Acid)

- genetic information in every cell & many viruses
- essentially a string over alphabet  $\{A, C, G, T\}$   
Adenine  $\leftrightarrow$  Cytosine  $\leftrightarrow$  Guanine  $\leftrightarrow$  Thymine
- geometrically, two complementary strings woven together in double helix   
[Watson & Crick 1953]

## RNA (Ribonucleic Acid)

- similar but (usually) one strand &  $T \rightarrow U$  (Uracil)
- short-term "DNA" for transfer out of cell

## Protein: fundamental building block of life

- form enzymes, cytoskeleton, antibodies, etc.
- essentially chain of amino acids (20 kinds)
- translated from (portions of) RNA/DNA by genetic code: by triples of acids
  - AUG & GUG: "start" } codes [Nirenberg, Mathaei, & Leder by 1965]
  - UAG, UGA, UAA: "stop" }
  - AUG  $\rightarrow$  Methionine (also) } uniques
  - UGG  $\rightarrow$  Tryptophan
  - CGU, CGC, CGA, CGG, AGA, AGG  $\rightarrow$  Arginine } most popular
  - UUA, UUG, CUU, CUC, CUA, CUG  $\rightarrow$  Leucine }
  - UCU, UCC, UCA, UCG, AGU, AGC  $\rightarrow$  Serine }
  - ...



Protein folding: proteins fold into 3D structure

- quickly (milliseconds to seconds)
- fairly consistently ... but how?
- influenced by ribosome & chaperones

Motivation: geometry strongly influences function

- protein misfolding correlated with several diseases: mad cow, Alzheimer's, cystic fibrosis, cancer
- synthetic protein design (drug design)

Two aspects:

① mechanics: linkages, geometry, algorithms

- how might protein fold
- "relatively tractable"

② energetics: modeling, simulation, optimization

- problems less clearly specified
- thermodynamics hypothesis: protein globally minimizes free-energy function
  - which energy function?
  - really global? simplest models NP-hard