Topology with Biological Applications

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Geometry and Shape Analysis in Biological Sciences
IMS, NUS, Singapore
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Berlin opportunities

Berlin Mathematical School

- International graduate school
- Courses in English at three universities
- www.math-berlin.de

Geometric energies for surfaces

- Symmetric quadratic function of principal curvatures

$$E := \iint \left(a + bK + c(H - H_0)^2\right) dA$$

- Gauß–Bonnet says $\iint K =$ const.
  thus irrelevant for variational problems
- If symmetric and fixed area

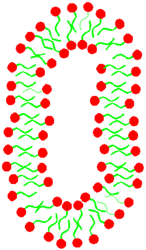
$$W := \frac{1}{4\pi} \iint H^2 \, dA$$

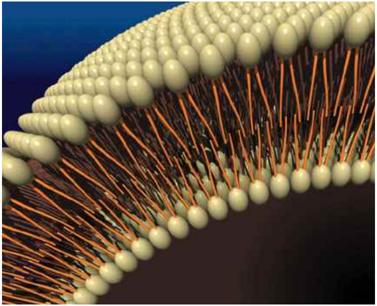
elastic bending energy for surfaces

- Scale-invariant, even Möbius-invariant

Lipid bilayer membranes

- Lipid vesicles as models of cell membranes
- Hydrophobic tails hidden by hydrophilic heads
- Fluid surface of lipid (surfactant) molecules: free to shear



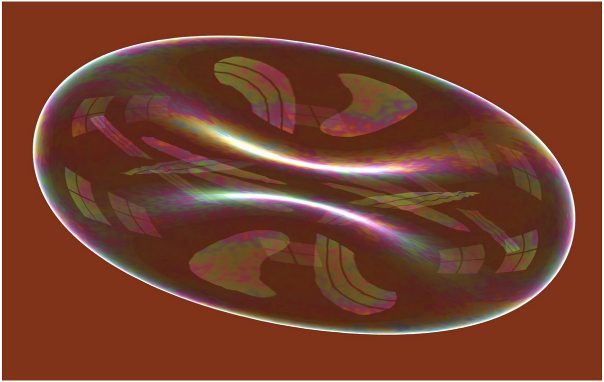


Images from NASA Ames and Vrije Univ. Amsterdam

- Minimize W (or perhaps $\iint (H - H_0)^2$ if sides differ)

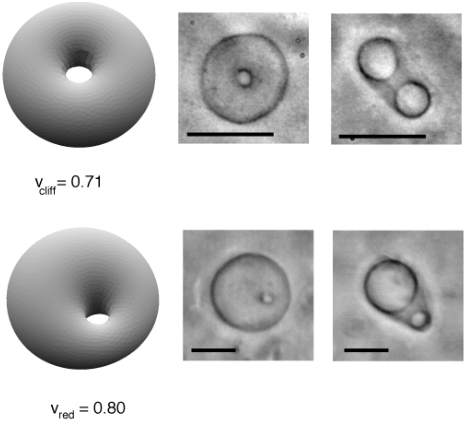
Physical constraints

- Fixed volume enclosed
- Fixed surface area
- Fixed $\Delta A = \iint H \, dA$



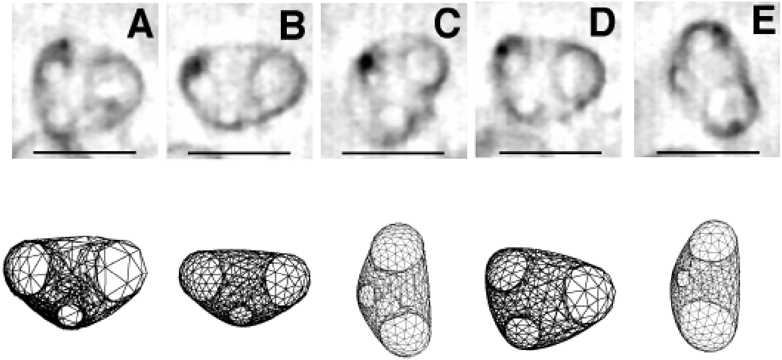
Toroidal vesicles

- Studied by Xavier Michalet (now UCLA)
- Agree with W-minimizing simulations



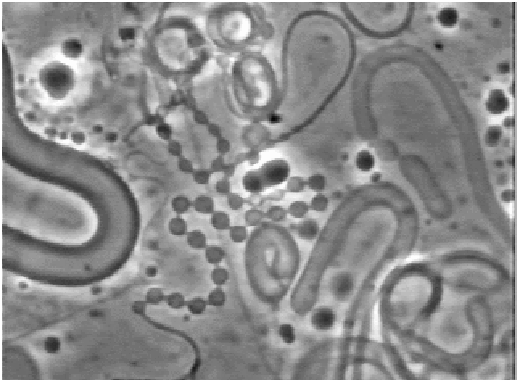
Higher-genus vesicles

- Again studied by Michalet
- Demonstrate Möbius invariance



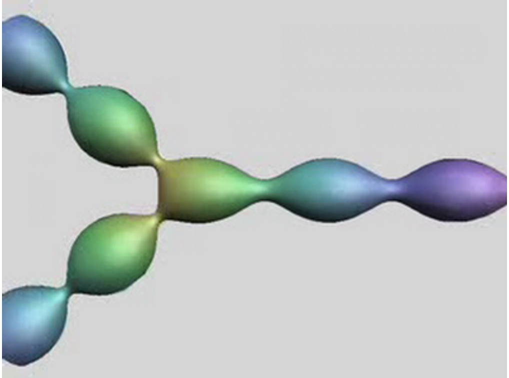
Lipid membranes as tubes

- Work with Sahraoui Chaïeb (now KAUST)
- Pearling by changing H_0 or ΔA

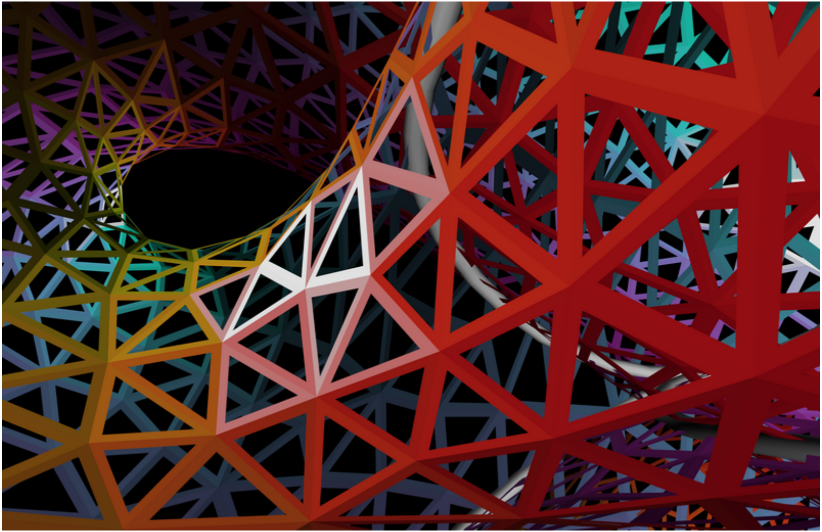


CMC trinoid pump

- 3-parameter family of 3-ended CMC surfaces



Minimax Sphere Eversion

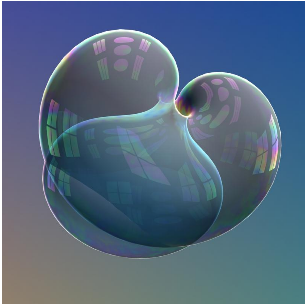


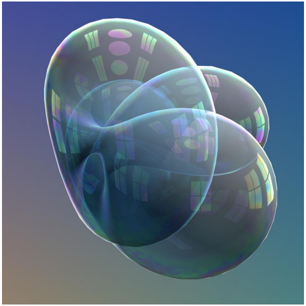
Sphere eversion

- Turn a sphere inside out
- Mathematical rules
  Not too hard (embedded)
  Not too easy (hole or crease)
- Possible [Smale 1959]
  But no explicit eversion for many years
  [Phillips 1966]
- Must have quadruple point [BanMax 1981]
  Simplest sequence of events [Morin 1992]
- Usually work from half-way model
  Suffices to simplify this to round sphere

Minimax eversion

- Energy $\geq k$ for surface with k-tuple point
- Spheres critical for W known [Bryant]
  Lowest saddle at $W = 4$
- Use this as halfway model for eversion [Kusner]





Geometric Knot Theory

Geometric properties of knotted space curve

determined by knot type or implied by knottedness
(e.g. Fáry/Milnor: $TC > 2\pi \mathrm{br} \geq 4\pi$)

Optimal shape for a given knot

usually by minimizing geometric energy

Ropelength

Definition

- *Thickness* of space curve = 2 *reach*
  $=$ diameter of largest embedded normal tube
- *Ropelength* $=$ length / thickness

Positive thickness implies $C^{1,1}$

Definition

- *Gehring thickness* = minimum distance between components

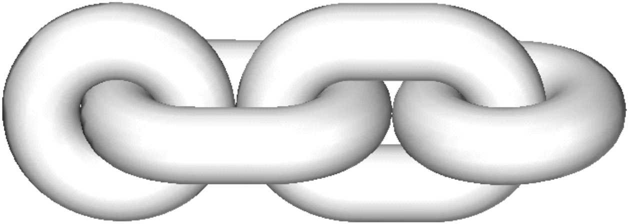
works with Milnor's *link homotopy*

Ropelength

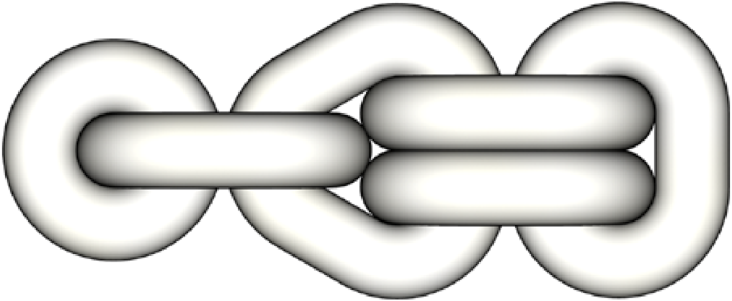
Inventiones **150** (2002) pp 257–286, `arXiv:math.GT/0103224`
with Jason Cantarella, Rob Kusner

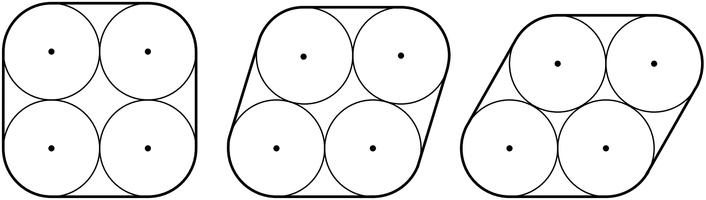
Results

- Minimizers exist for any link type
- Some known from sharp lower bounds
- Simple chain $=$ connect sum of Hopf links
  Middle components stadium curves: not C^2



Minimizers





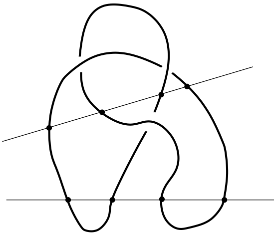
Lower bounds

Geom. & Topol. **10** (2006) pp 1–26,
`arXiv:math.DG/0408026`
with Elizabeth Denne and Yuanan Diao

Theorem

K *knotted* $\implies$ *ropelength* ≥ 15.66 *(within 5% for trefoil)*

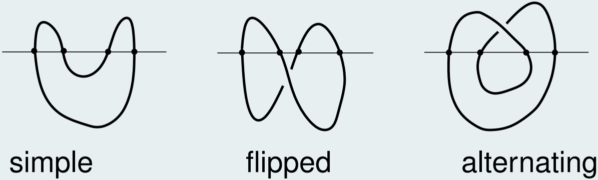
Proof uses *essential alternating quadrisecants*:



Quadrisecant

- Line intersecting a curve four times
- Every knot has one (Pannwitz – 1933 Berlin)

Three order types



Theorem (Denne thesis)

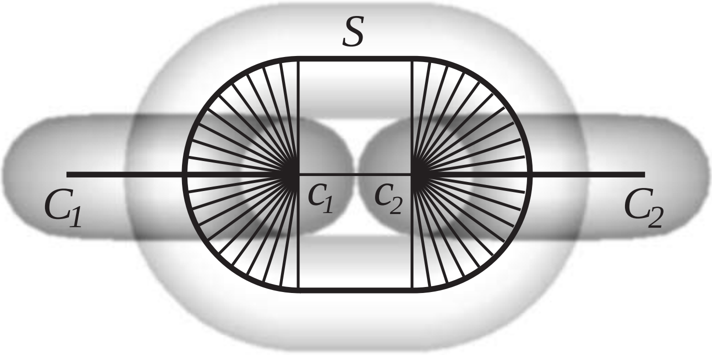
Every knot has an essential alternating quadrisecant

(Essential means no disk in $\mathbb{R}^3 \setminus K$ spans secant plus arc of K.)

Criticality

Balance Criterion: tension vs. contact force

Characterizes ropelength-critical links by force balance



Criticality papers

Gehring case – no curvature bound

Geom. & Topol. **10** (2006) pp 2055–2115,

`arXiv:math.DG/0402212`

with Jason Cantarella, Joe Fu, Rob Kusner, Nancy Wrinkle

Ropelength case – with curvature bound

Geom. & Topol. **18** (2014) pp 1973–2043,

`arXiv:1102.3234`

with Cantarella, Fu, Kusner

Kuhn–Tucker

Minimization problem

Given $f, g_i \colon \mathbb{R}^n \to \mathbb{R}$, $(i = 1, \ldots, m)$, minimize $f(p)$ s.t. $g_i(p) \geq 0$.

Definition

p is a *constrained critical point* for minimizing f if for any tangent vector v at p with $\langle \nabla f, v \rangle < 0$ we have $\langle \nabla g_i, v \rangle < 0$ for some *active* g_i.

p is *balanced* if $\nabla f =$ nonnegative combination of active ∇g_i.

Theorem (Modified Kuhn–Tucker)

p is constrained-critical $\iff$ balanced.

Only involves derivatives of f and g_i at p (linear functions).
Linear algebra $\sim$ Farkas alternative

Infinite dimensions

Strategy: combine Clark's theorem on derivatives of min-functions with our version of K–T that applies to:
X vector space (of variations), Y compact space (of active constraints), $C(Y) = \{$continuous functions$\}$, $C^*(Y) = \{$Radon measures$\}$.

Theorem (CFKSW'06)

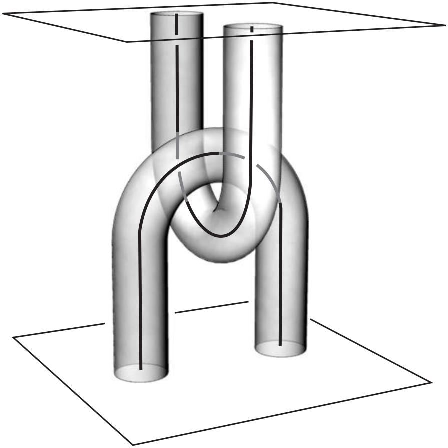
For any linear $f\colon X \to \mathbb{R}$ and $g\colon X \to C(Y)$, t.f.a.e.:

- *Balanced: $\exists$ nonneg. Radon meas. μ on Y s.t. $f(\xi) = \int_Y g(\xi)\,d\mu$.*
- *Strongly critical: $\exists \varepsilon > 0$ s.t.*

$$f(\xi) = -1 \implies \exists y\ (g\xi)y \leq -\varepsilon.$$

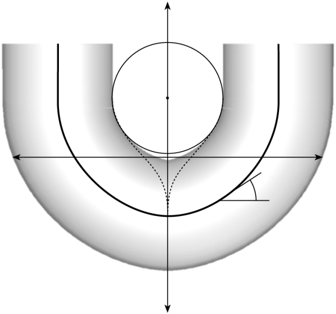
The clasp

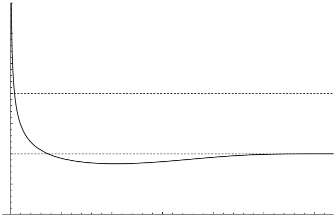
- Clasp: one rope attached to ceiling, one to floor
- Again with semicircles?



The Gehring clasp

- Gehring clasp has unbounded curvature (is $C^{1,2/3}$ and $W^{2,3-\varepsilon}$)
- Half a percent shorter than naive clasp





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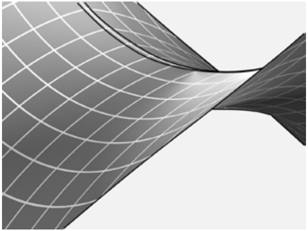
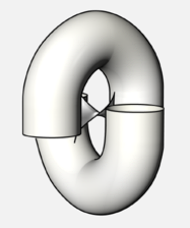
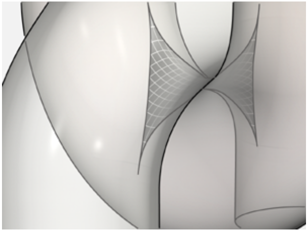


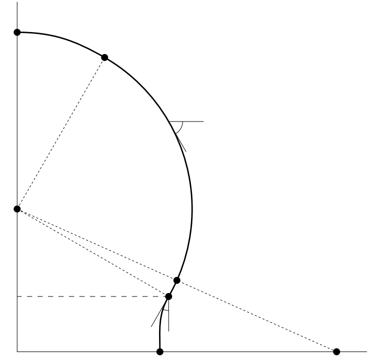


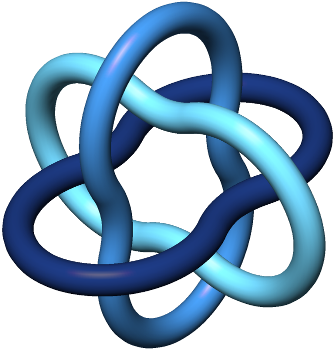


Example Tight Link

Critical Borromean rings – IMU logo

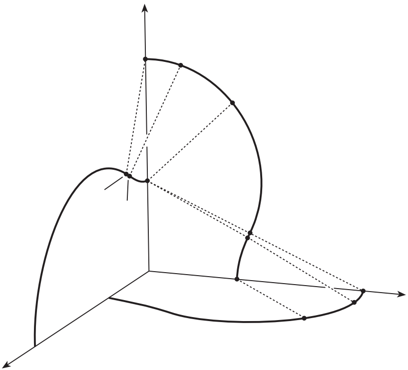
- maximal (pyritohedral) symmetry, each component planar
- piecewise smooth (42 pieces in total)
- some described by elliptic integrals

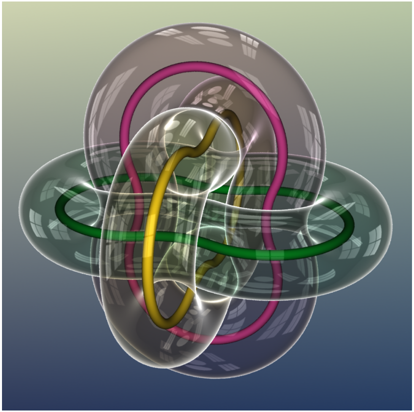




Borromean Rings

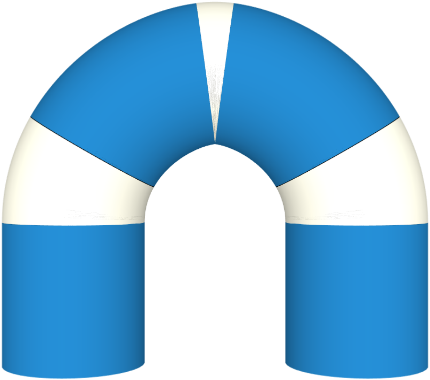
- Uses clasp arcs and circles; 0.08% shorter than circular
- Curvature < 2 everywhere $\implies$ also ropelength-critical

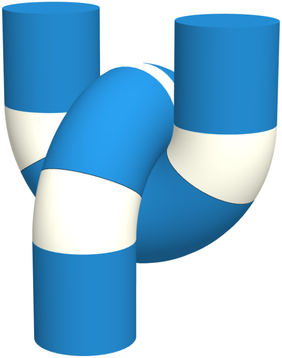




The tight clasp

- Tight clasp slightly longer
- Kink (arc of max curvature) at tip





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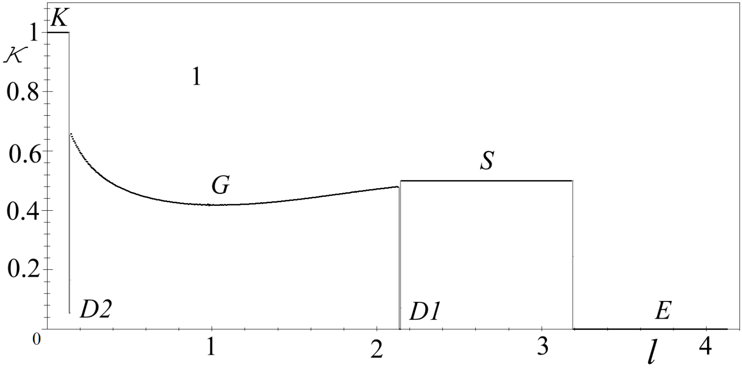
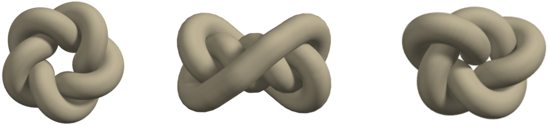


Other ways to find critical points

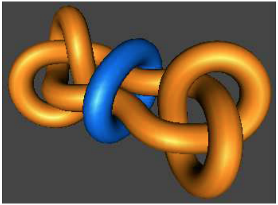
Symmetric criticality for tight knots

Cantarella, Ellis, Fu, Mastin: JKTR, 2014



Gordian split link

Coward, Hass: Pacific J, 2015



Biological applications

Knotted DNA

- Great source of motivation for geometric knot theory
- Are tight shapes correlated with ensemble average shapes?

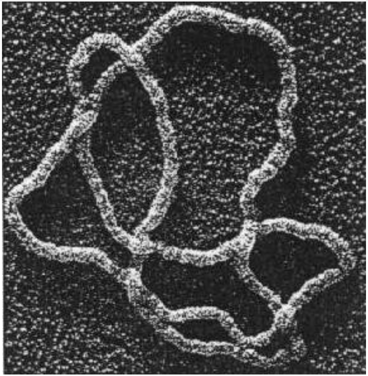


Image from Andrzej Stasiak, EPFL

Periodic links

Links in 3-torus

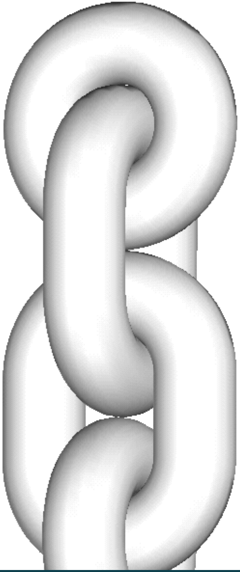
- Closed and infinite components when lifted to $\mathbb{R}^3$
- Not enumerated yet
- Can extend ropelength criticality theory
- Work with Myf Evans ++

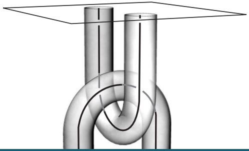
Periodic links

Singly periodic case

- Links in solid torus $\mathbb{S}^1 \times D^2$
- Diagrams in annulus
- Enumeration of small knots
  extended to links by Franziska Schlösser
- Stress/strain relationship as we vary periodicity

Singly periodic links





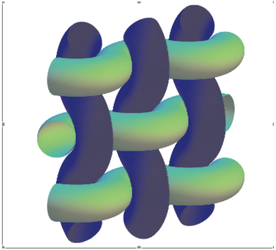
Rainbow loom bands

"Brunnian link making device and kit"

Doubly periodic links

Links in thickened torus $T^2 \times I$

Links in thickened surfaces
equivalent to Kaufmann's virtual knots



Triply periodic links

Chiral rod packing Π^+ becomes close to helical

Periodic entangled structures

Entanglement at mesoscale

- Important in physics of soft materials
- Can lead to exotic macroscopic properties
- Like negative Poisson ratio

Periodic entangled structures

Keratin filaments in skin cells under expansion (Evans)