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Smooth and Polygonal Knot Energies

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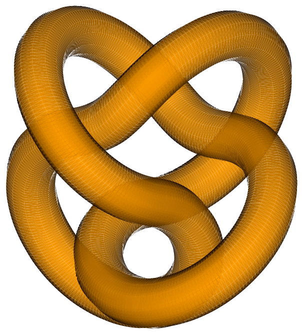
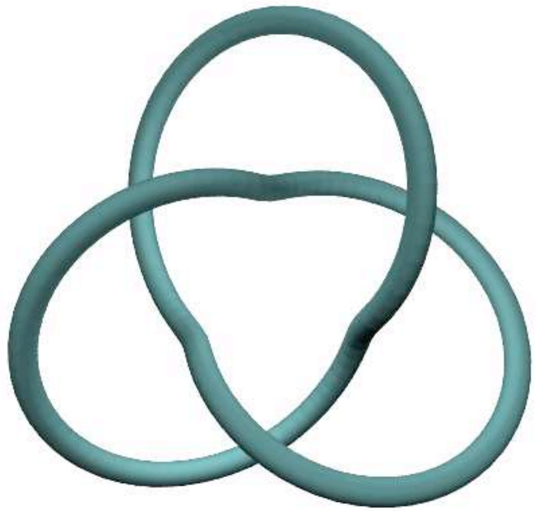
May 18, 2009



Outline

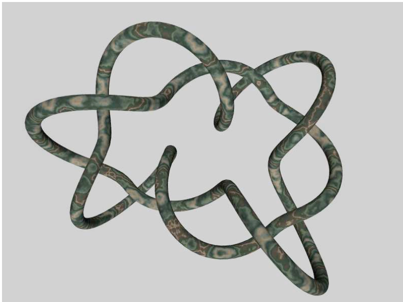
- Knot energies
- Ropelength problem – what does a fully tightened knot look like?
- Open problems



What is a Knot?

Knot: Closed one-dimensional loop in $\mathbb{R}^3$ with no self-intersections

Is a knot:



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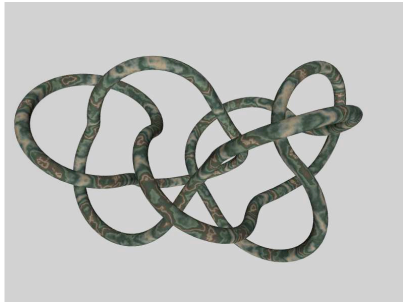
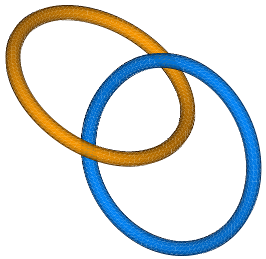
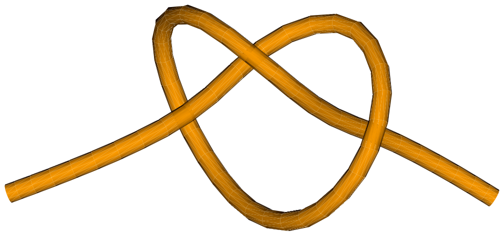


9_{24}

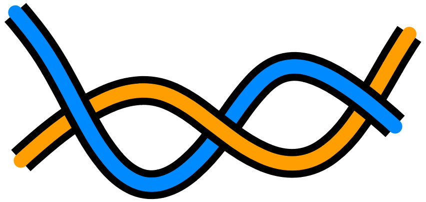
Is not a knot, but can be entangled:



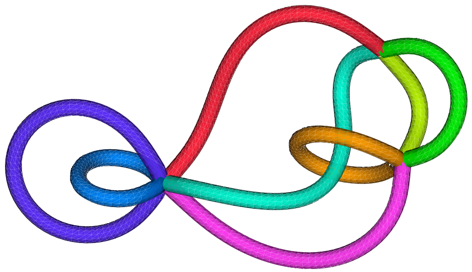
Link



Open knot



Tangle



Graph

Categories of Knots

- Smooth: Defined via a periodic function

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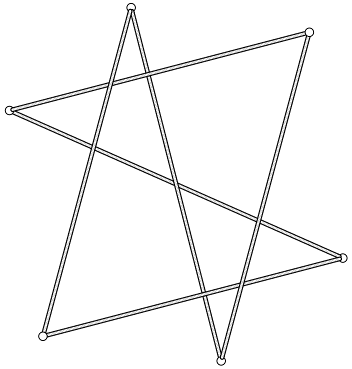
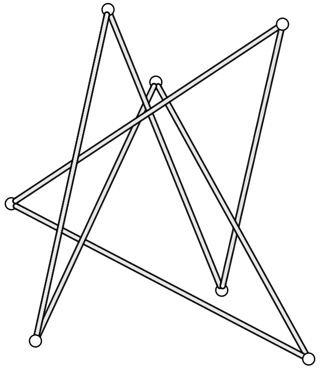
4_1

- Polygonal: Defined by a finite, ordered set of points in $\mathbb{R}^3$



6 edge 3_1

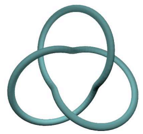


7 edge 4_1

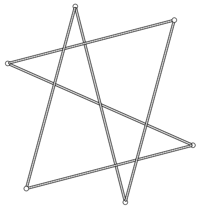
Vocabulary

unknot or trivial knot
Equivalent to a planar circle

knot type $[K]$
The set of all knots that are equivalent to K



knot conformation or configuration of $[K]$
A particular member of the knot type

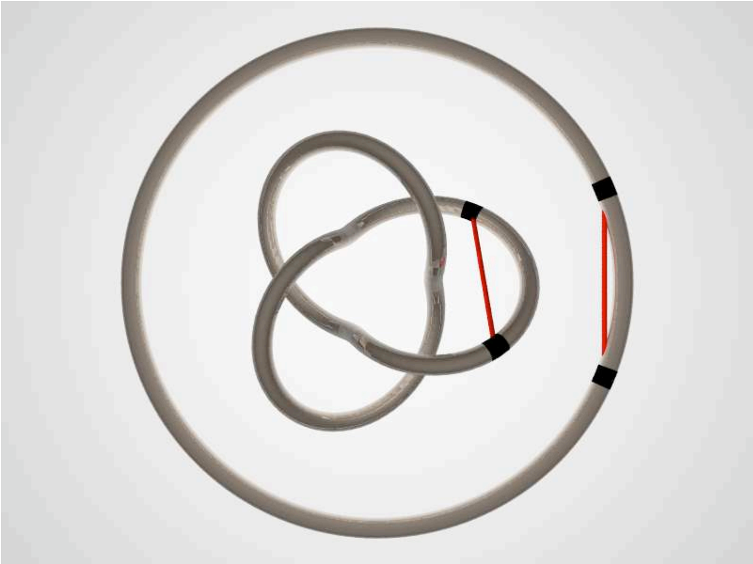


- Traditional knot theory – study properties of knot types
- Physical knot theory – study properties of the knot configurations, optimal and average

Knot Energy

Outline

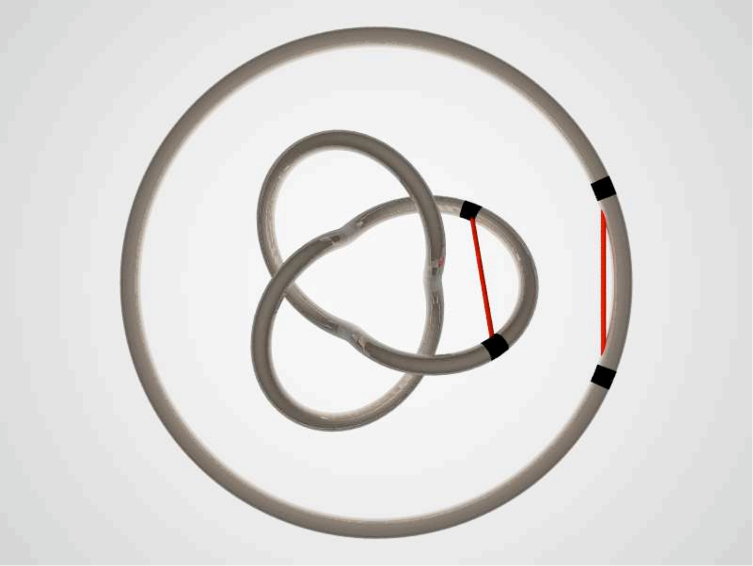
- Möbius Energy (two forms)
- Compute energy of a circle
- Movies of energy minimization
- Properties of knot energies
- Minimum Distance Energy (polygonal version)



Möbius Energy

- $x : S^1 = \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ an arclength parameterization of a knot configuration K
- E_0 (O'Hara)

$$E_0(K) = \iint_{C \times C} \frac{1}{|x(s) - x(t)|^2} - \frac{1}{|s - t|^2}$$

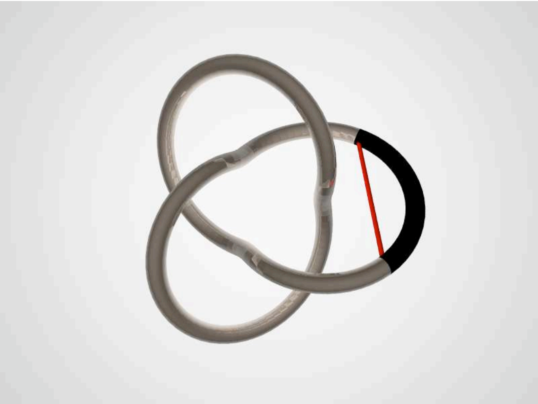


[1] O'Hara, *Topology* (1991)

Möbius Energy II

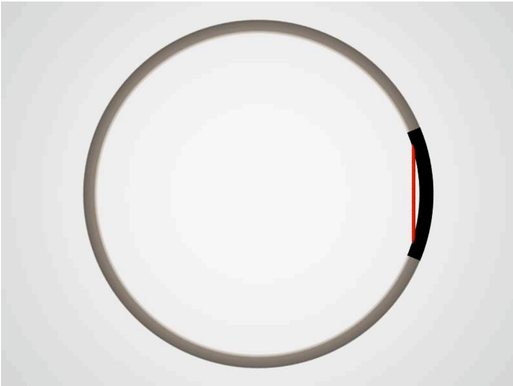
- $x : [0, L] \to \mathbb{R}^3$ an arclength parameterization of a knot configuration K
- E_4 (Freedman, He, Wang), invariant for Möbius transformations

$$E_4(K) = \iint_{[0,L]\times[0,L]} \frac{1}{|x(s) - x(t)|^2} - \frac{1}{\text{arclength}(x(s), x(t))^2}$$



[2] Freedman++, *Ann. of Math.* (1994)

Energy of a Circle



- $\gamma : [0, 2\pi R] \longrightarrow \mathbb{R}^3$
- $\gamma(t) = \langle R\cos(t/R), R\sin(t/R), 0\rangle$

$$E_4(C_R) = \int_{s=0}^{2\pi R}\int_{t=0}^{2\pi R} \frac{1}{(\gamma(t)-\gamma(s))^2} - \frac{1}{\text{arclength}^2(\gamma(t),\gamma(s))}\,dt\,ds$$

$$= 2\cdot 2\pi R\int_{\delta=0}^{\pi R} \frac{1}{4R^2\sin^2\left(\frac{\delta}{2R}\right)} - \frac{1}{\delta^2}\,d\delta$$

$$= 4\pi R\cdot\frac{1}{\pi R}$$

$$= 4$$

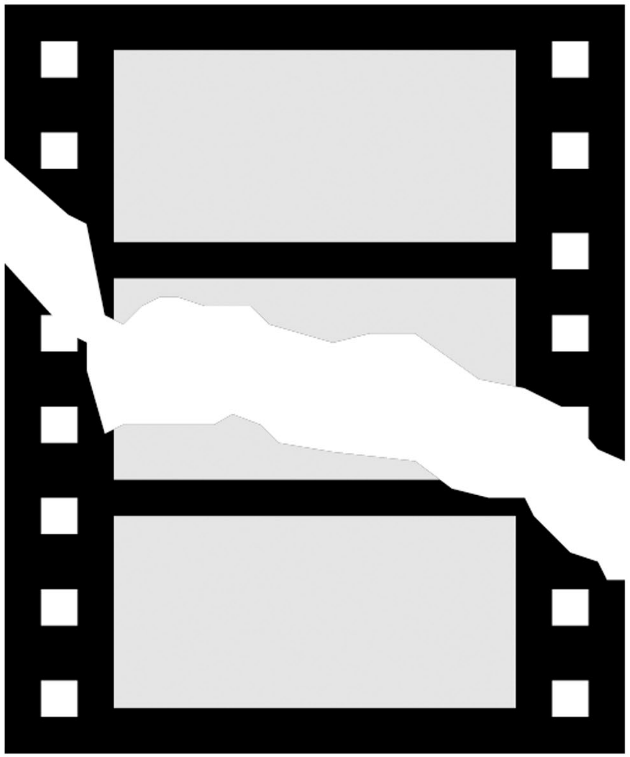
Motivation

Why?

- We would like to be able to tell the difference between knots
- Possible for unknots, bounded by $2^{100,000,000,000n}$ Reidemeister moves where n is the number of crossings in a given diagram
- Hope – flow knot types to a global minimum
- Reality – local mins, saddles, etc. cause problems
- However, energies have been pretty successful at flowing nasty unknotted configurations to the circle

[3] Hass and Lagarias, *J. Amer. Math. Soc.* (2001)

KnotPlot Movies



What is a Knot Energy?

Knot energy

A *knot energy* is a function from a space of knot configurations into $\mathbb{R}$ (usually scale-invariant).

Useful properties

- *basic* - minimum is the circle and only the circle
- *strong* - there are only finitely many knot types with energy $<$ (whatever number)
- *charge* - energy approaches ∞ upon approaching self-intersecting curves
- *tight* - compositions of a given knot type increase the energy linearly

Note - Möbius energy is not *tight* due to pull-tight phenomena

[4] Diao++, *J. Knot Theory Ramifications* (1997)

Polygonal Energy – Minimum Distance Energy

- Smooth curves have essentially an infinite amount of information
- Computers are finite
- Polygonal energies
  - Used to approximate the flow of smooth energies
  - Interesting in and of themselves (possibly more so from a physical perspective)

MD-energy

$$U_{md}(P) = \sum_{E \neq F \text{ and non-adjacent}} \sum \frac{length(E)\, length(F)}{md(E,F)^2}$$

$$E_{md}(P) = U_{md}(P) - U_{md}(\text{regular } n\text{-gon})$$

[5] Simon, *J. Knot Theory Ramifications* (1994)

Polygons vs Smooth Knots

Questions

- Do the polygonal energies "approximate" the smooth energies?
- Do the polygonal flows "approximate" the smooth flow?
- Do polygonal minima converge to smooth minima?

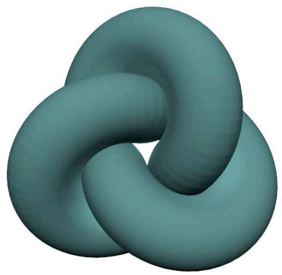
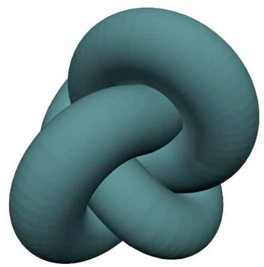
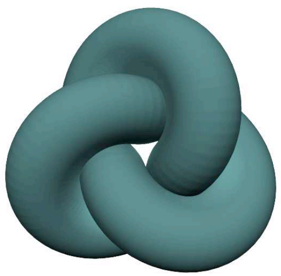
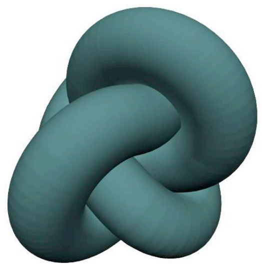
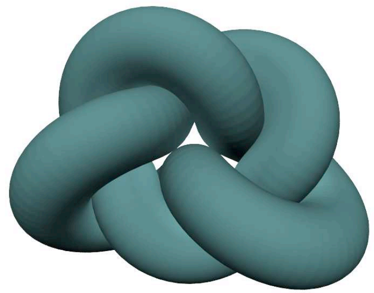
Now

We will look at the case of ropelength.

Ropelength

Outline

- Problem
- Characterization
- Applications
- What is known
- Polygonal ropelength
- Interaction between theory and simulation
- Open problems
- Offshoot projects

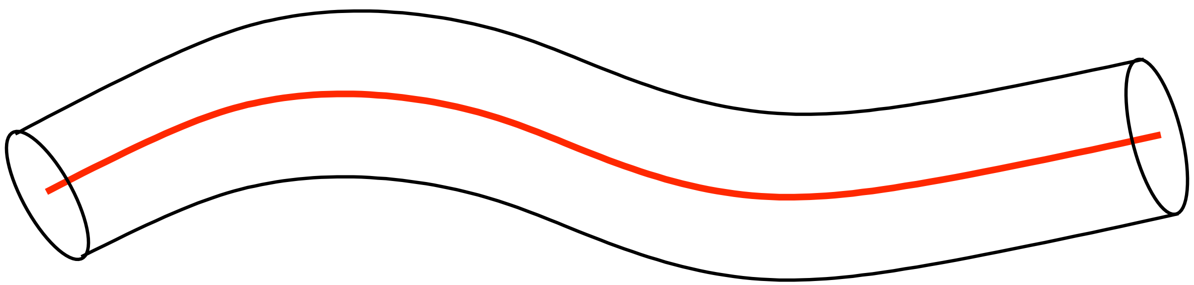
Ropelength Problem

Question: Is it possible to tie a nontrivial knot with 2 feet of 1-inch radius rope?

Goal: Find the least amount of rope needed to tie a conformation of a given knot type

Idealized rope:

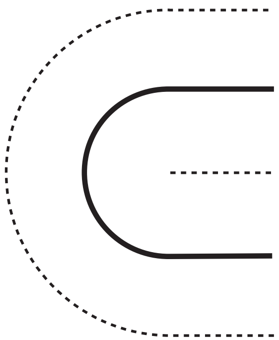
- Tube is made of circular disks perpendicular to the knot
- Thickness radius – largest non-self intersecting radius



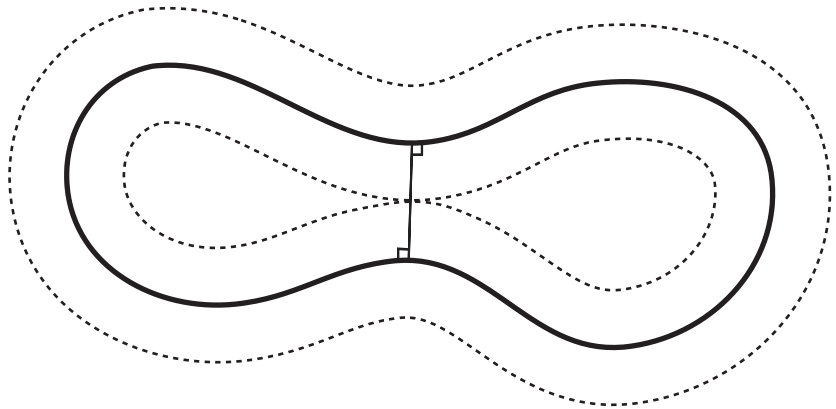
Constraints Due to Thick Tube

Imagine you have some length of rope

- Curvature constraint – knot can bend back on itself
- Distance constraint – two portions of the knot cannot be closer than twice the radius of the tube



Curvature Constraint

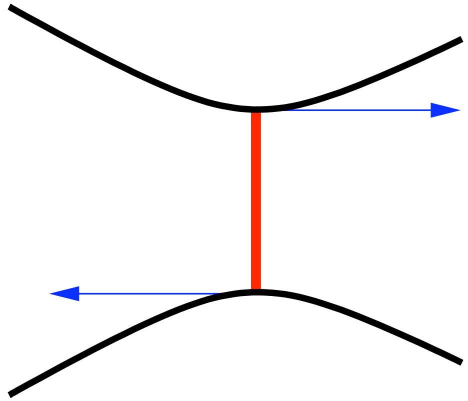


Distance Constraint

Constraints in Terms of Curve

K a smooth knot configuration, C^2 or $C^{1,1}$

- $MinRad(K)$ – minimum radius of curvature $= \frac{1}{\max \kappa}$
- $dcsd(K)$ – doubly critical self-distance, minimum distance between pairs of points looking like this



Characterizing Thickness for a Knot Configuration

Theorem: Thickest non self-intersecting tube about a knot configuration K has radius $R(K) = \min\{MinRad(K), dcsd(K)/2\}$.

Definitions

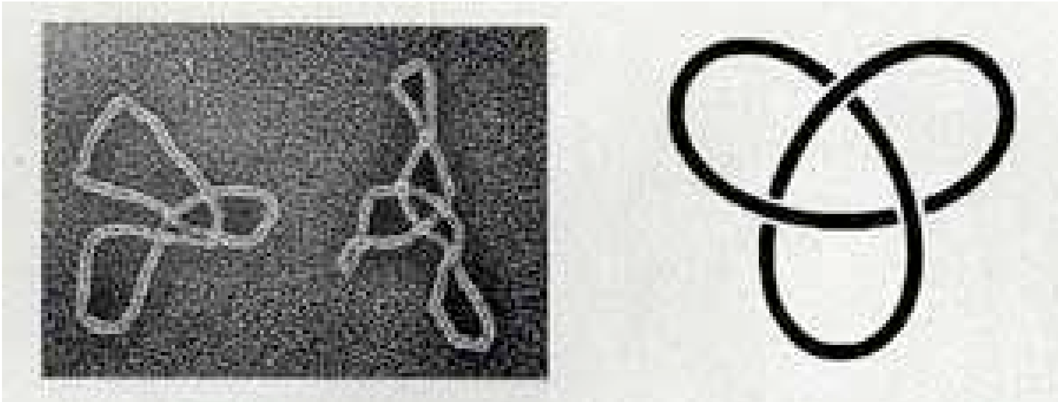
- $R(K)$ – called *thickness radius (injectivity radius)*
- $Rope(K) = Length(K)/R(K)$ – called *ropelength*
- *Ideal* or *Tight* – conformation minimizing ropelength within a knot/link type

[6] Litherland++, *Top. Appl.* (1999)

Other Versions/Definitions of Thickness

- [7] Federer, Curvature measures (1959)
- [8] Krötenheerdt++, Zur Theorie massiver Knoten (1976)
- [9] Ashton, On the theory of solid knots (translation of the above article in 2005)
- [10] Nabutovsky, Non-recursive functions, knots "with thick ropes", and self-clenching "thick" hyperspheres (1995)
- [11] Kusner++, On distortion and thickness of knots (1996)
- [12] Diao++, Knot energies by ropes (1997)
- [13] Diao++, Thicknesses of knots (1999)
- [14] Gonzalez++, Global curvature, thickness, and the ideal shapes of knots (1999)
- [15] Cantarella++, On the minimum ropelength of knots and links (2002)

Applications: DNA Topology



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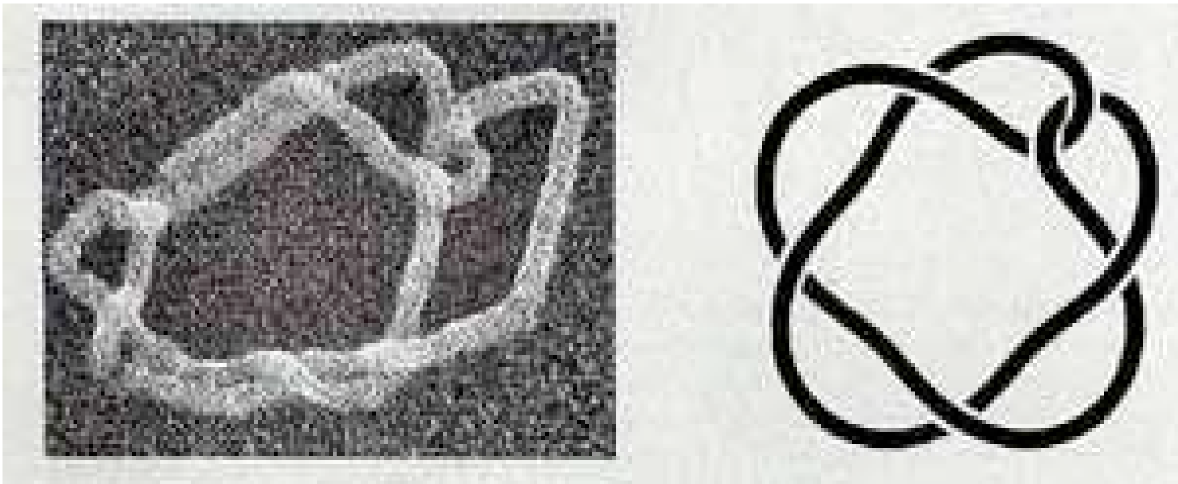

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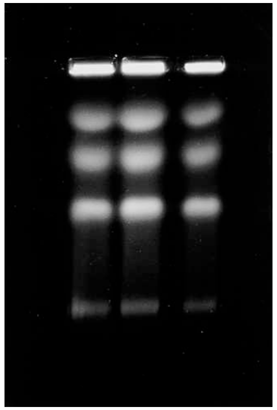
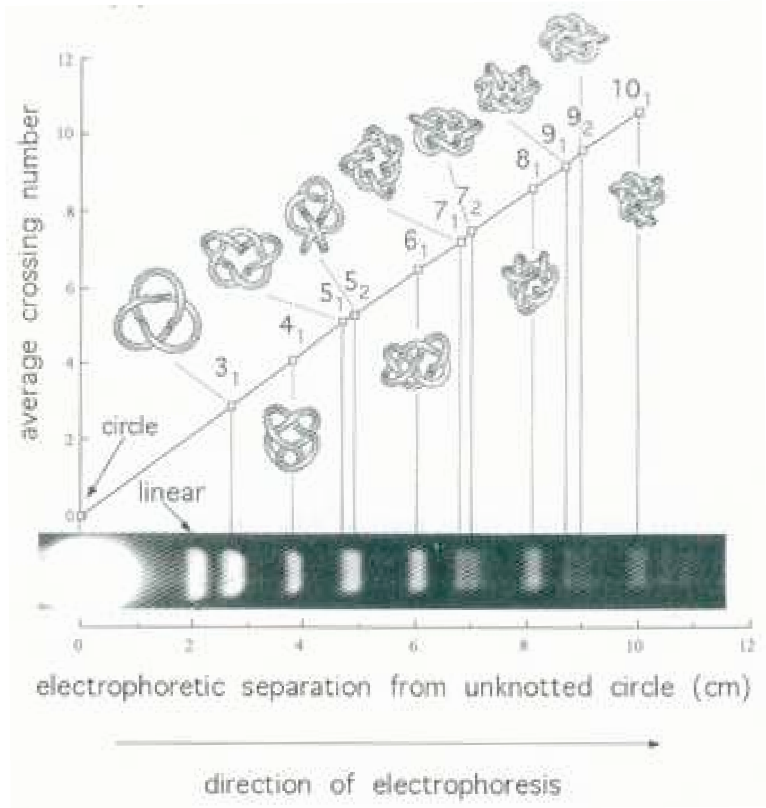
Gel Electrophoresis

- Used for court cases and such to determine identity
- Idea: DNA is cut at certain spots to get strands of different lengths
- Length determines speed through the gel
- DNA separates into bands of like lengths



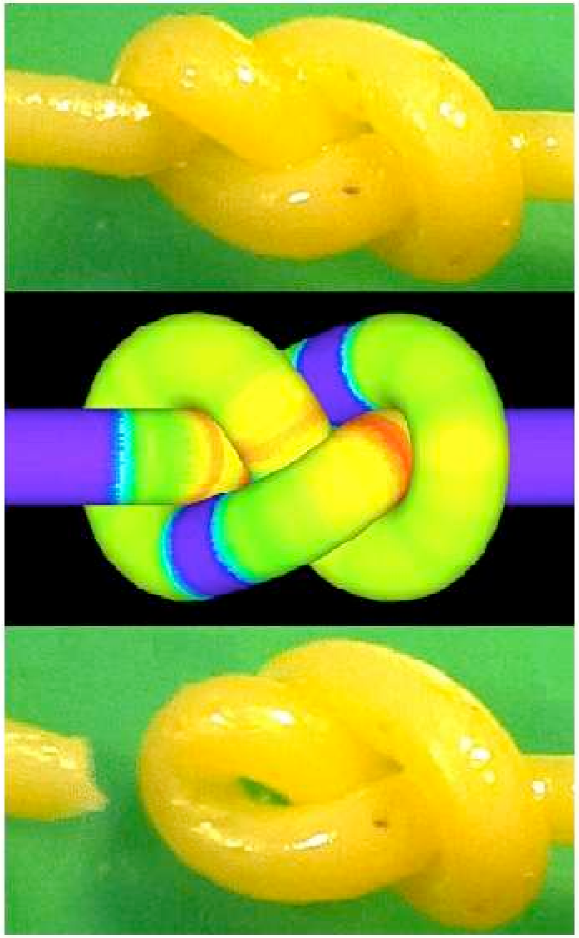
Topological Effects in Gel Electrophoresis

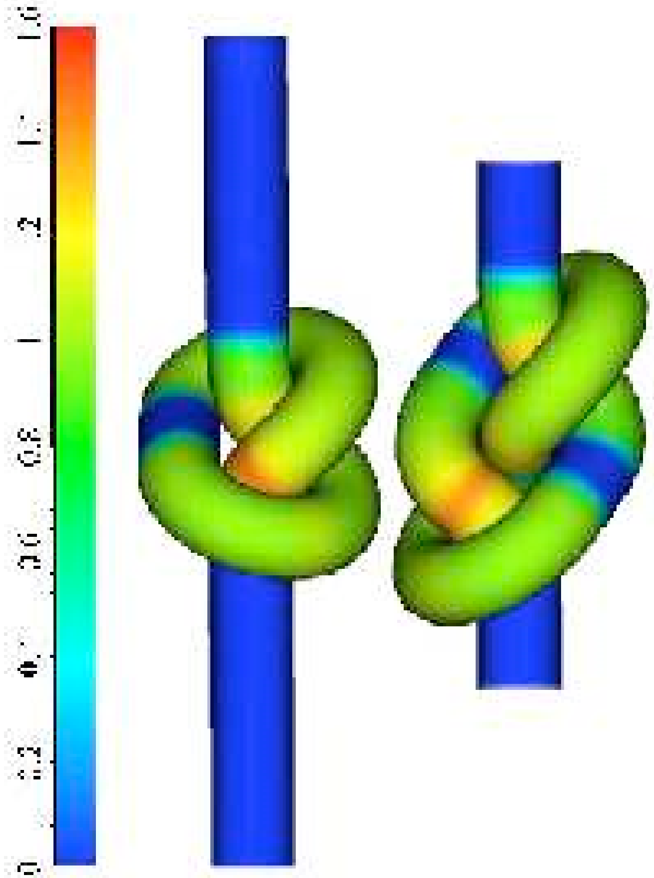
- DNA is all the same length, knot type determines the speed
- y-axis is a quantity measured on tight knots



[16] Stasiak++, *Ideal Knots* (1998)

Applications: Breaking Point



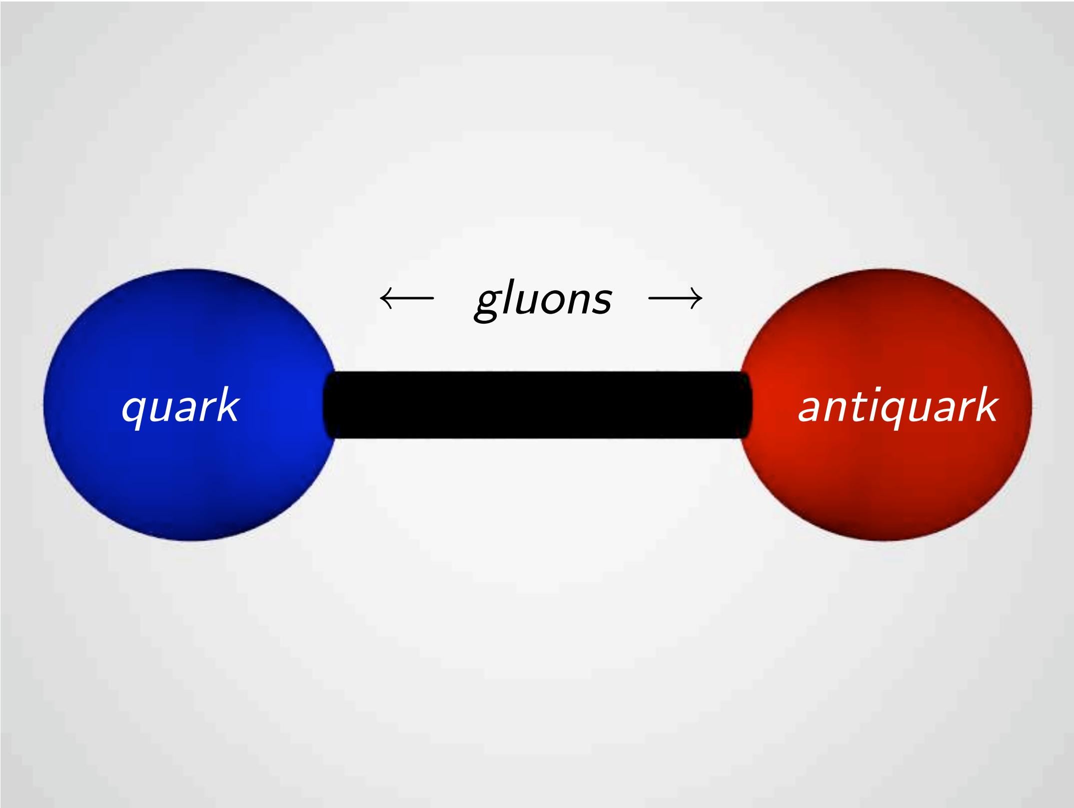


[17] Pieranski++, *New J. Phys.* (2001)

Applications: Glueballs

Warning: this is wildly out of scale, purely my vision

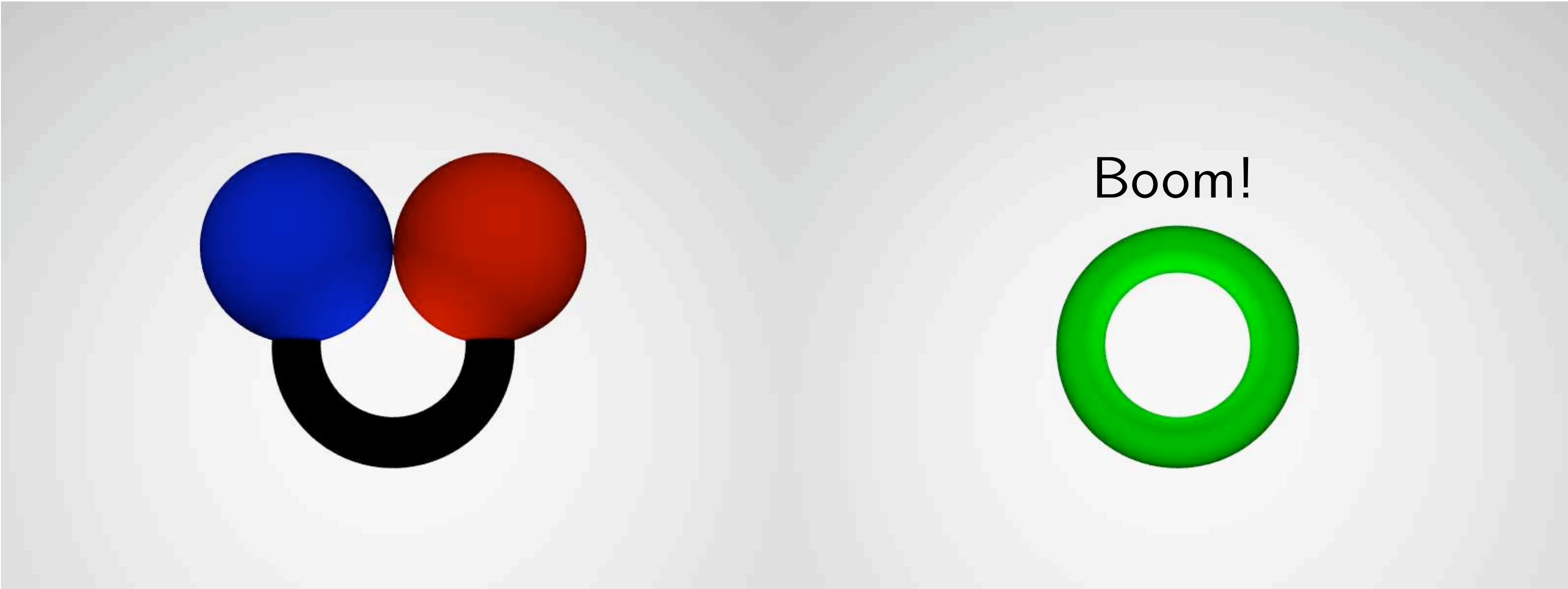
- Mesons are quark/antiquark pairs held by **strong force**
- Gluon exchange is confined to a tube



[18] Buniy++, *Phys. Lett.* (2003)

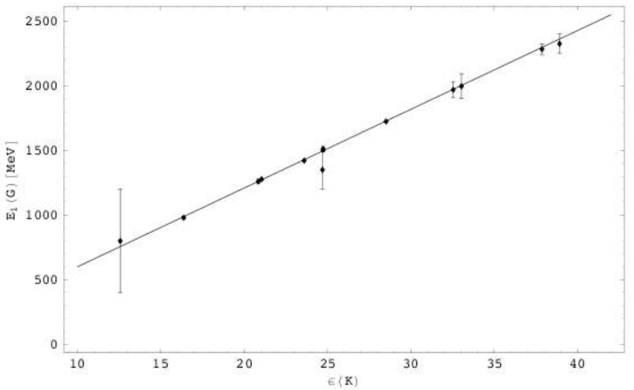
Hypothesized Creation of Glueballs

- Quarks and antiquarks self-destruct and the gluons form a loop (which can be knotted) called a *glueball*
- Glueballs exist $\approx 10^{-21}$ seconds



Glueball Model

- Hypothesis: glueballs are tight knotted and linked QCD flux tubes
- Upon creation, glueballs shrink to a tightened state
- Energy of glueballs is linearly related to the length (i.e. the length of the shortest knot/link of that type)
- Observed a linear relationship between energy and length of most simple knots and links
- Collaboration: compute table of shortest knots and links
  - Thousands of knots and links
  - Predict existence of new glueballs

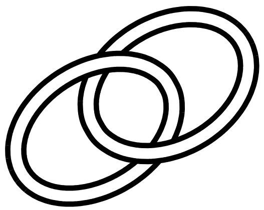


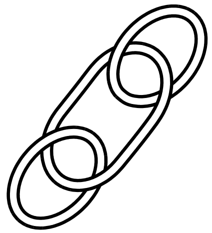
Paper in progress: Buniy, Cantarella, Kephart, Rawdon and some students

What Is Known?

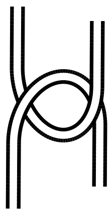
Not much!

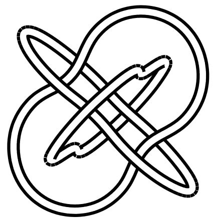
- Unknot minimized by a circle, $Rope = 2\pi$
- Links with planar unknotted components [15]





- Conjectures for tight clasp and Borromean rings



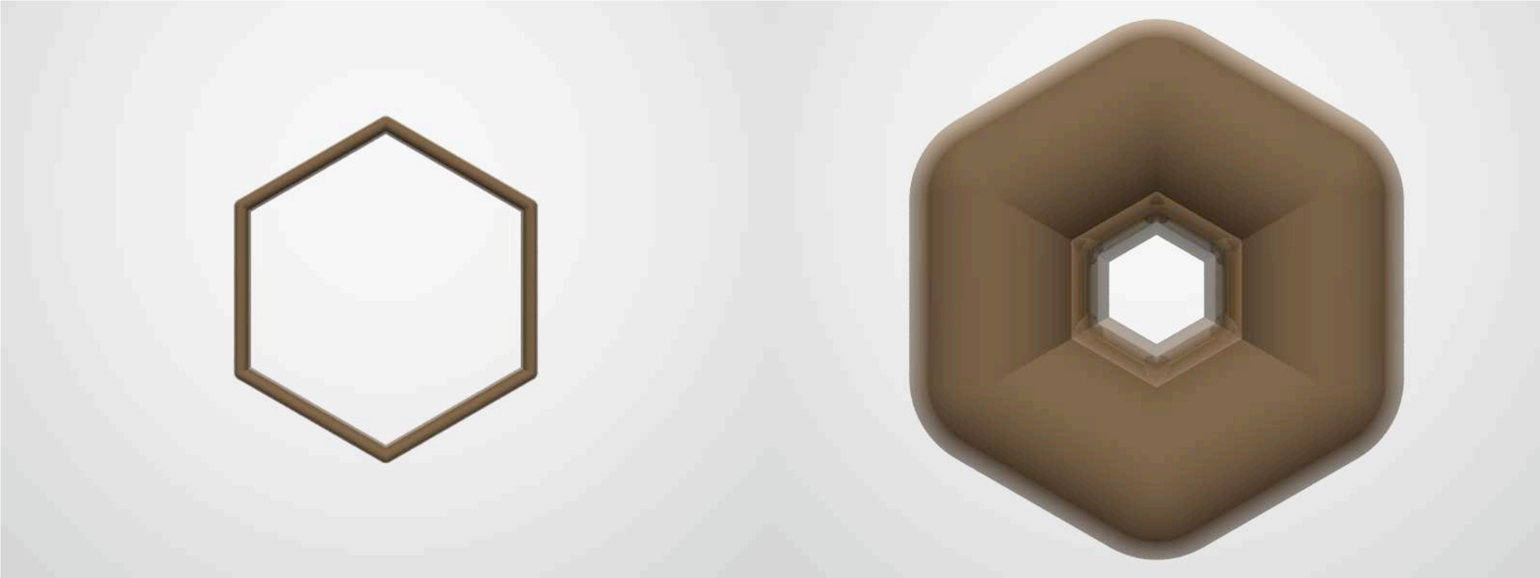


- For nontrivial knots, there are no exact results
- Goal – use polygons to get information about smooth minimizers

[19] Cantarella++, *Geom. Topol.* (2006)

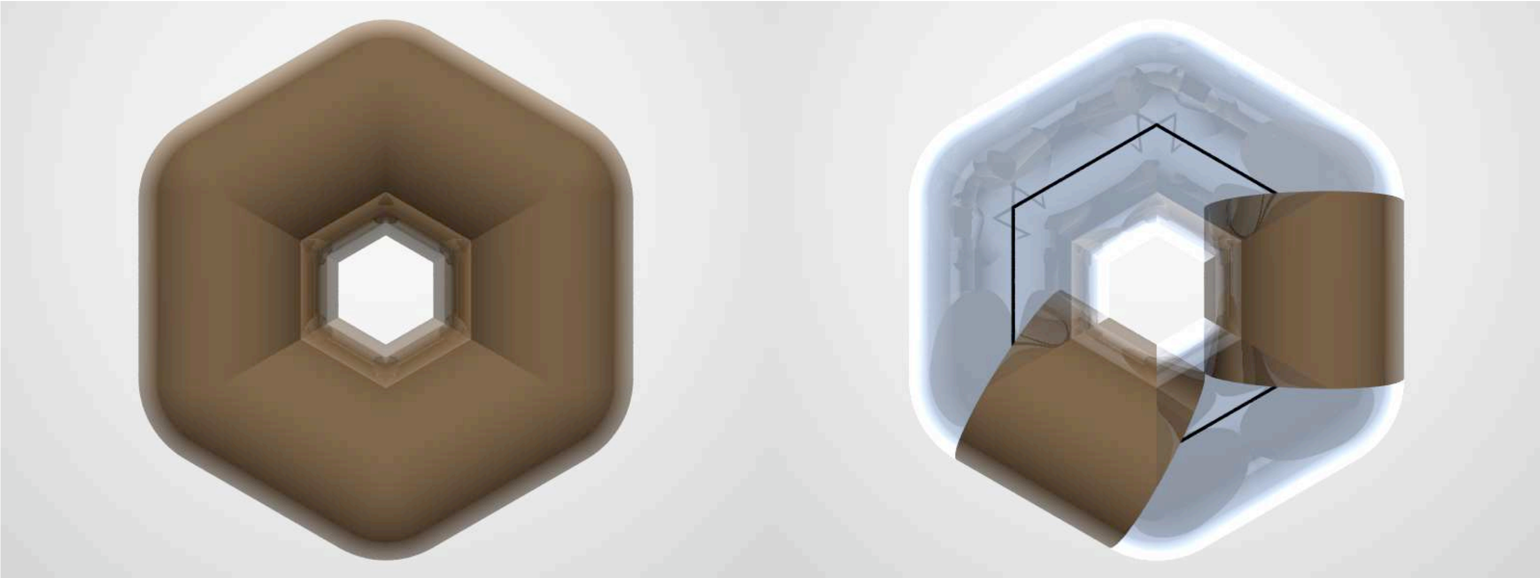
Defining Ropelength for Polygons

- First attempt, cylinders about edges $\sim$ normal disks
- Take cylinders of a given thickness about the edges
- Thickness radius $=$ max radius with empty non-adjacent cylinder intersections



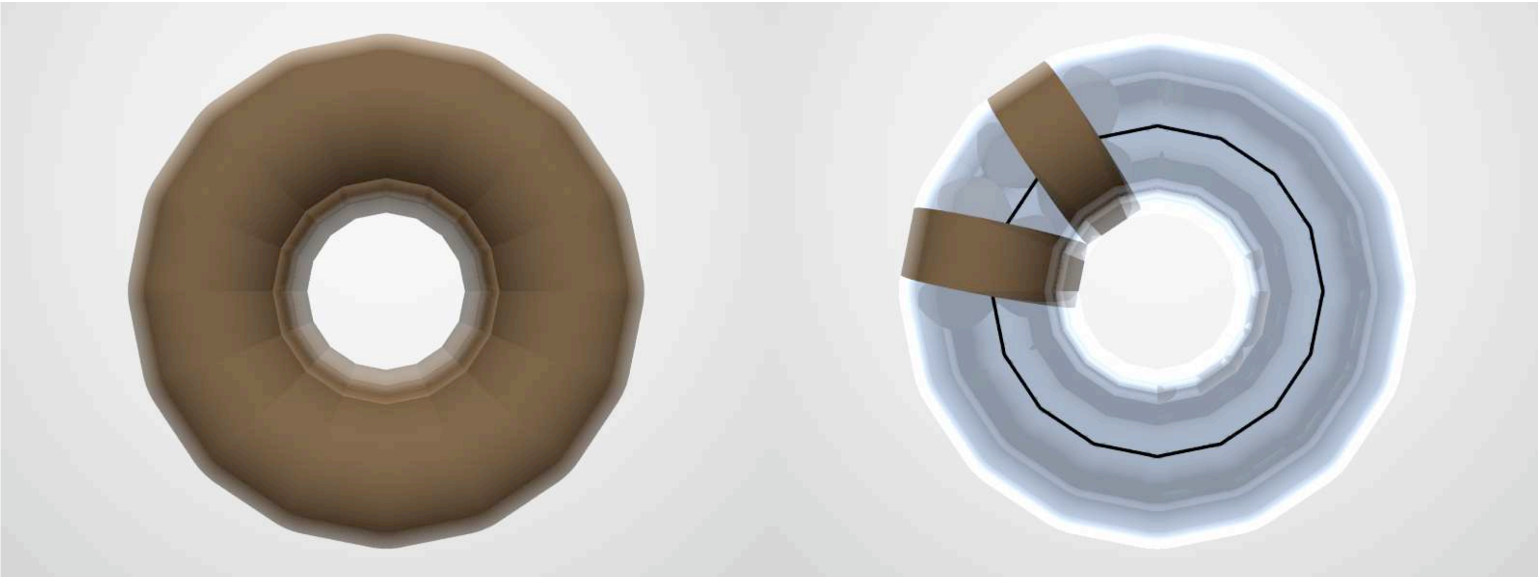
Problems?

Regular 6-gon



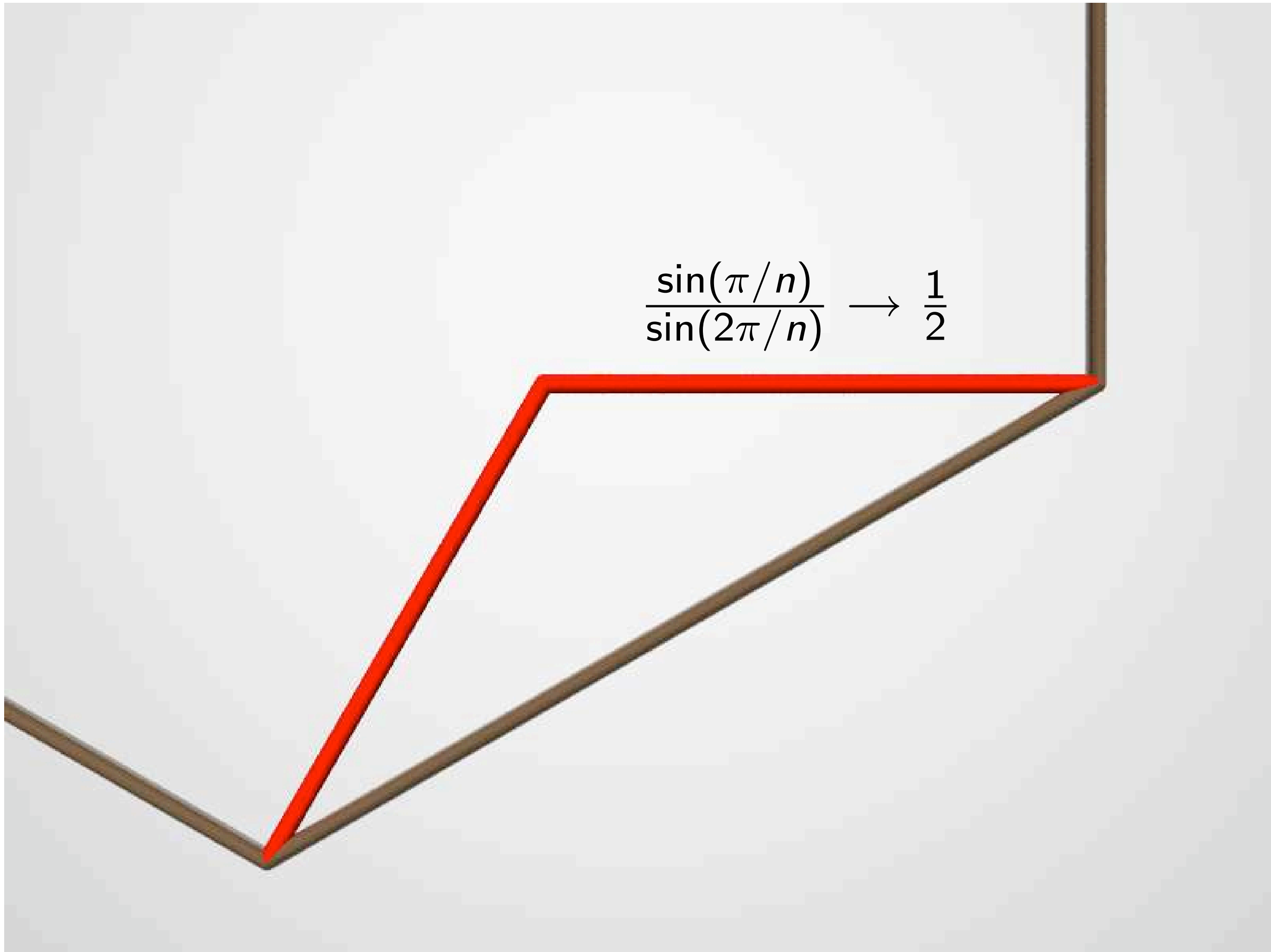
- Cylinders intersect “short” of the radius
- Question: Does this go away when *edges* $\to \infty$?

Regular 16-gon



- Answer: This problem does not appear to go away when *edges* $\to \infty$?

Cylinder Thickness of Polygons Inscribed in Unit Circle



$$\frac{\sin(\pi/n)}{\sin(2\pi/n)} \longrightarrow \frac{1}{2}$$

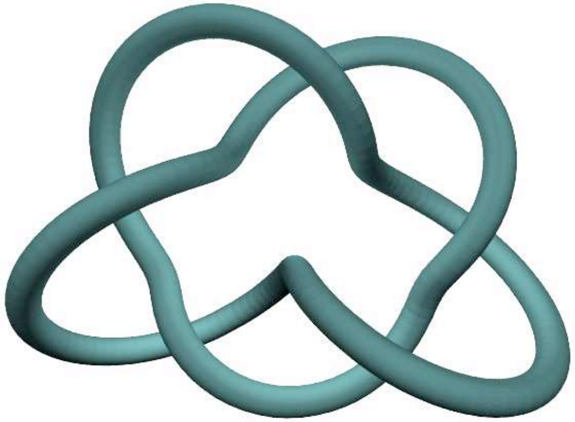
How to Define Polygonal Ropelength

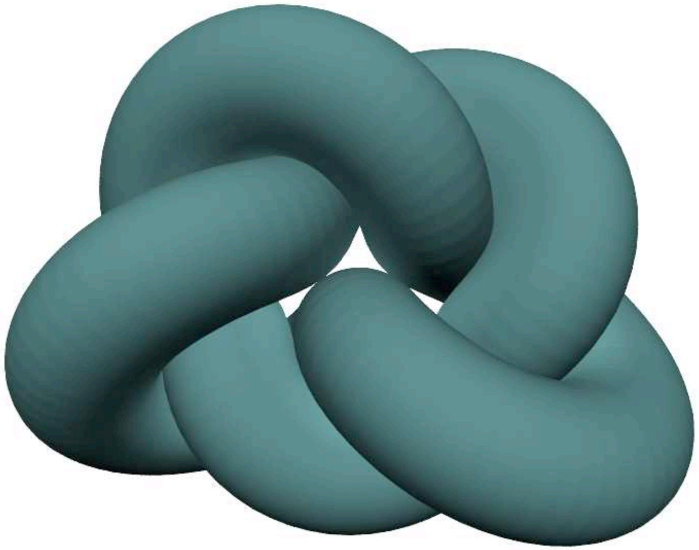
Thickness Characterization

Theorem: Thickest non self-intersecting tube about K has radius $R(K) = \min\{MinRad(K), dcsd(K)/2\}$.

Question

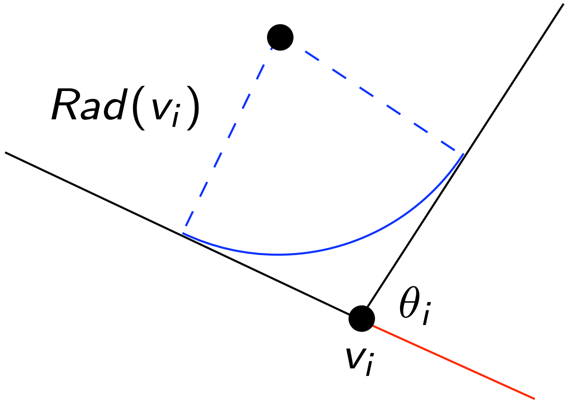
Can we define *MinRad* and *dcsd* for polygons?



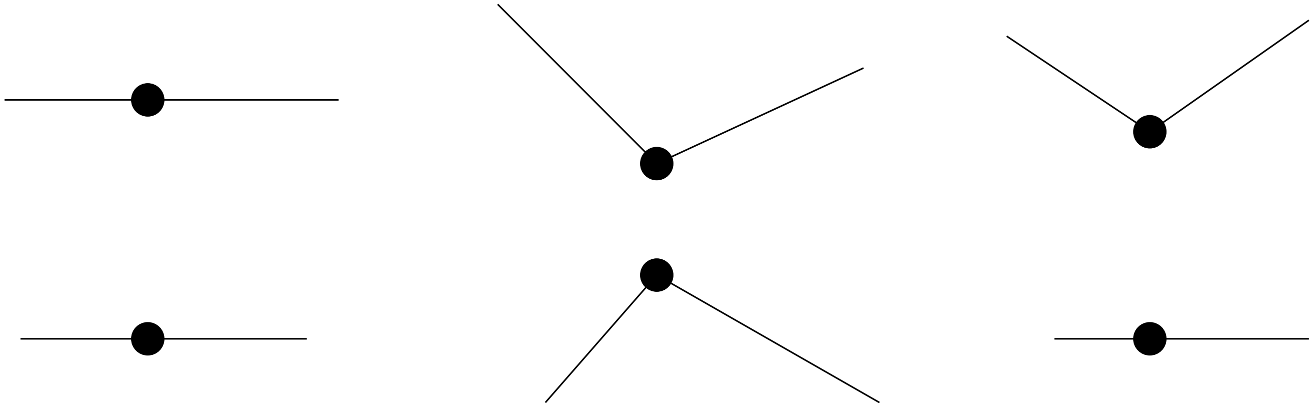


Polygonal Ropelength

- $MinRad(P) = \min Rad(v_i) = \min \frac{length(edge)}{2\tan(\theta_i/2)}$

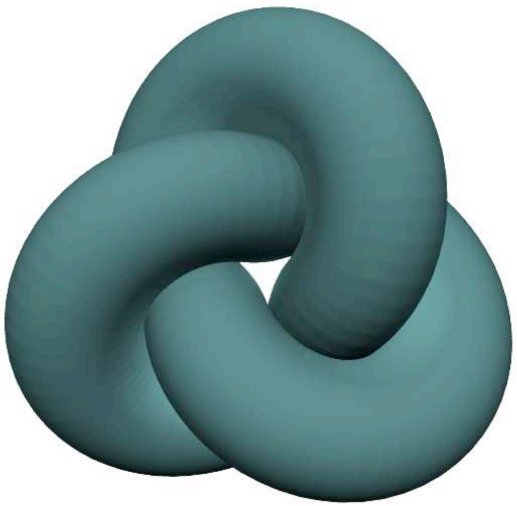


- $dcsd(P)$ = minimum distance over pairs like this

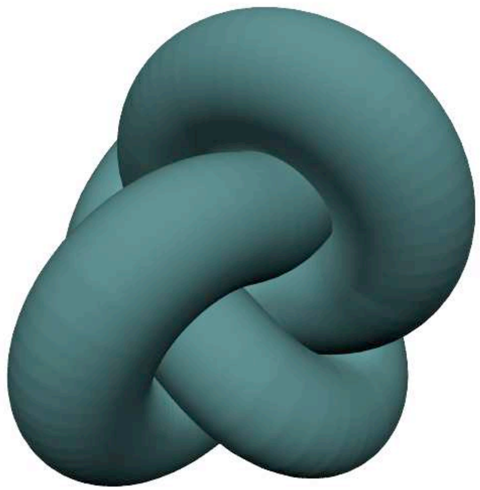


More Polygonal Ropelength

- $R(P) = \min\{MinRad(P), dcsd(P)/2\}$ (*thickness radius*)
- $Rope(P) = Length(P)/R(P)$ (*ropelength*)



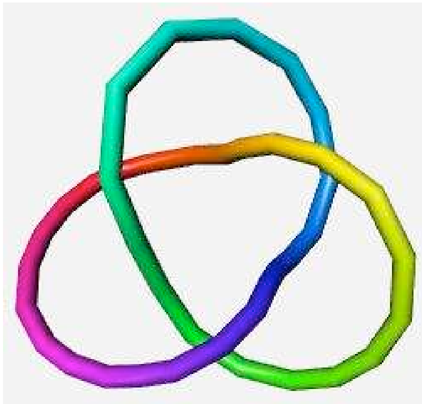
3_1



4_1

Trying to Find Ropelength Minima

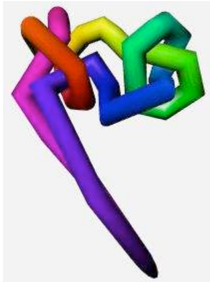
- Vertex perturbations
  - Descent: shake and check
  - Simulated annealing: temperature and energy difference determine the extent to which you take “bad” steps

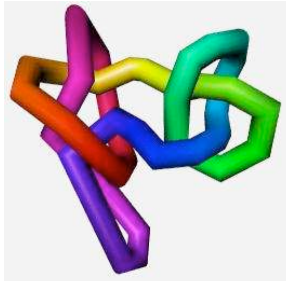
- Problem – need coordinated movement, especially with links
  - `ridgerunner`: Ashton, Cantarella, Piatek, Rawdon

Simulated Annealing

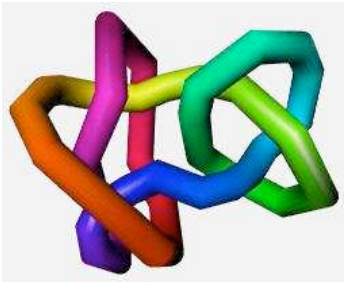
300.85



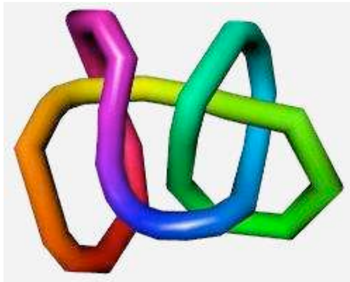
127.80



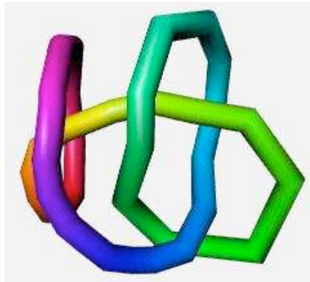
93.08



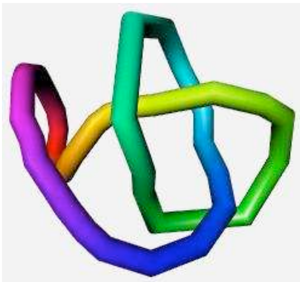
76.25



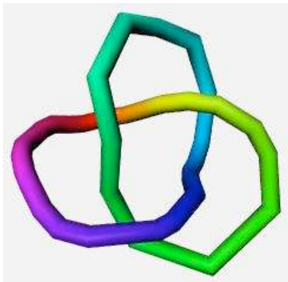
59.73



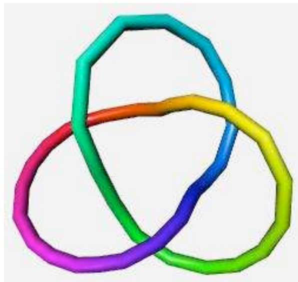
48.56



44.39



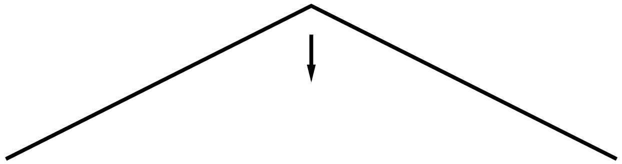
35.71



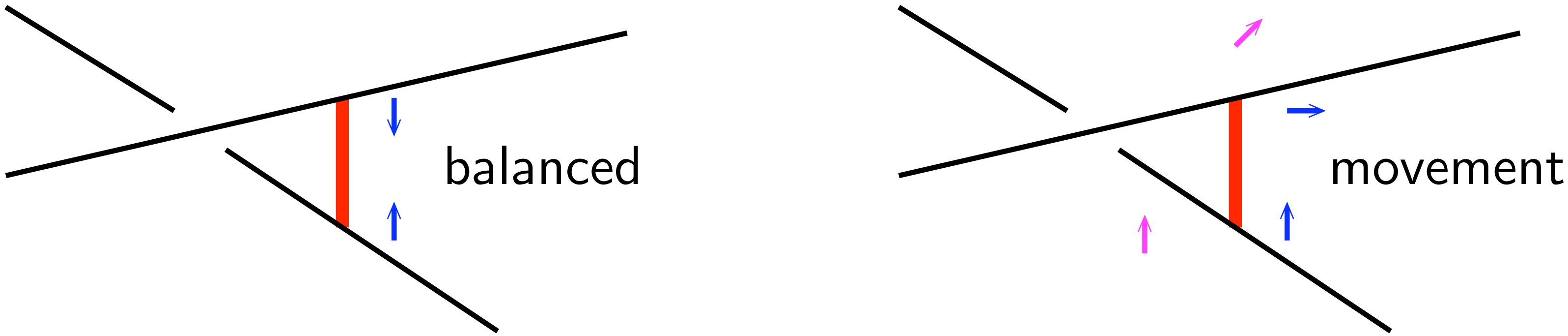
33.60

ridgerunner

- Tightening algorithm based on constrained length minimization
- Construct a length minimizing gradient



- Place a strut between close pairs (tensegrity theory)



- Turns into a big linear algebra problem (`tsnnls`)
- Resolves forces due to balancing

Ashton++, Knot tightening by constrained gradient descent, *in preparation*.

Approximation Theorem

Theorem: If *polygons* $\longrightarrow$ *smooth* then
ropelength(*polygons*) $\longrightarrow$ *ropelength*(*smooth*).

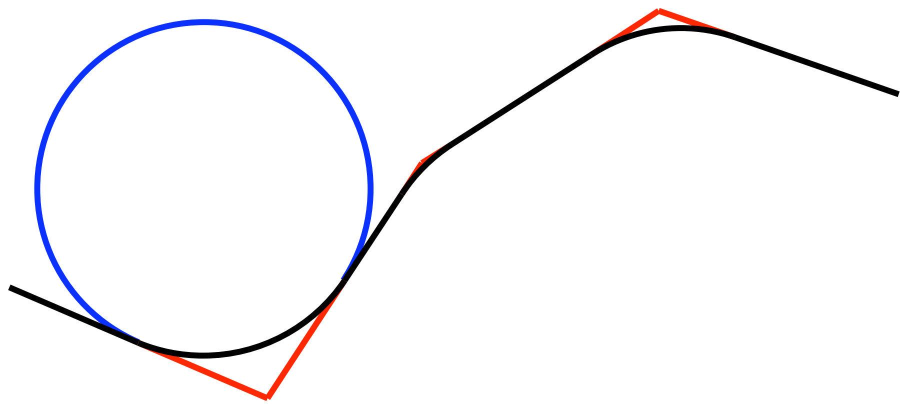
- The first $\longrightarrow$ is a bit loaded
- Result: polygonal ropelength approximates smooth ropelength

[20] Rawdon, *J. Knot Theory Ramifications* (2000)

Polygons Tell Us About Smooth Curves

Anti-Approximation Theorem

Theorem: There is a smooth curve inscribed in a polygon so that $\textit{ropelength}(\textit{smooth}) \leq \textit{ropelength}(\textit{polygon}) + \textit{error}$.

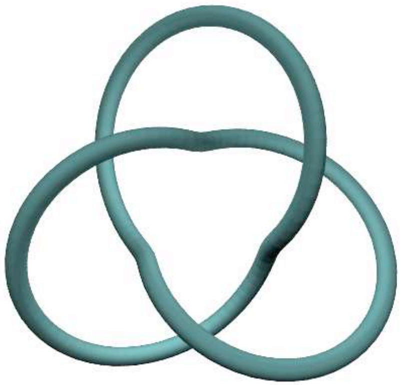


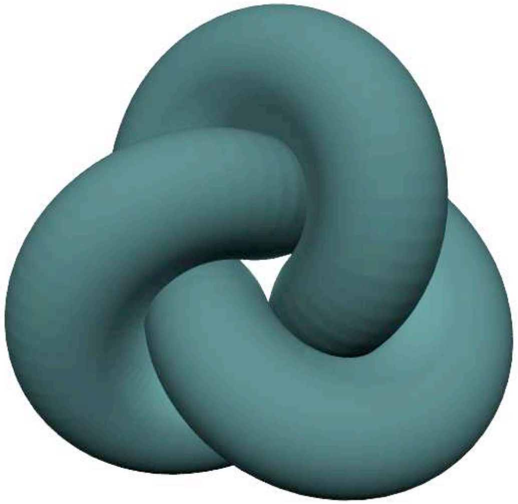
- This allows us to find upper bounds for the minimum ropelength from ropelength minimized polygons

[21] Rawdon, *Experiment. Math.* (2003)

Ropelength Upper Bounds for Trefoil

- 34.18 (Pieranski++ 2001 [22])
- 32.77 (Rawdon 2003 [21])
- 32.74446 (Carlen, Laurie, Maddocks, Smutny 2005 [23])
- 32.74391 (Baranska, Pieranski, Rawdon 2005 [24])
- 32.74339 (Baranska, Pieranski, Przybyl, Rawdon 2005 [25])
- 32.74317 (Baranska, Pieranski, Przybyl 2008 [26])





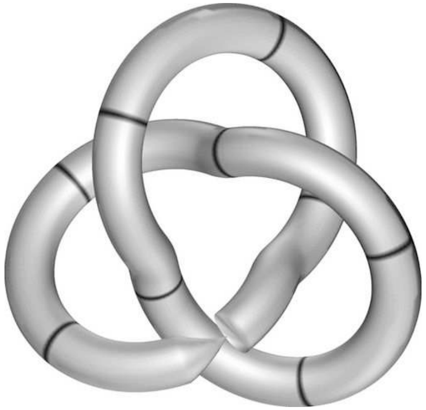
http://george.math.stthomas.edu/rawdon/data.php

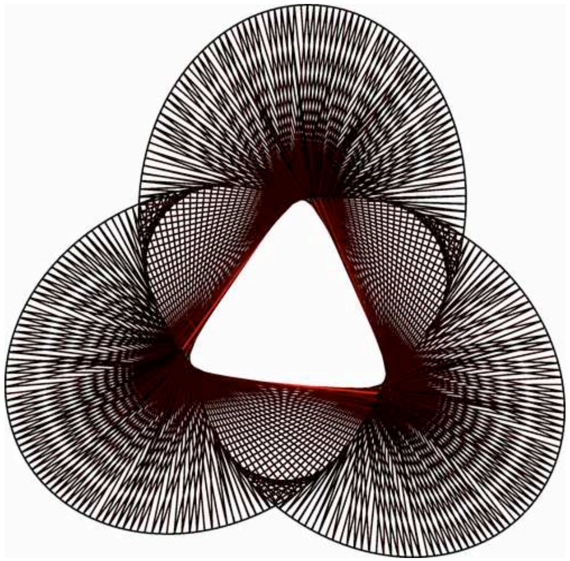
Ropelength Lower Bounds

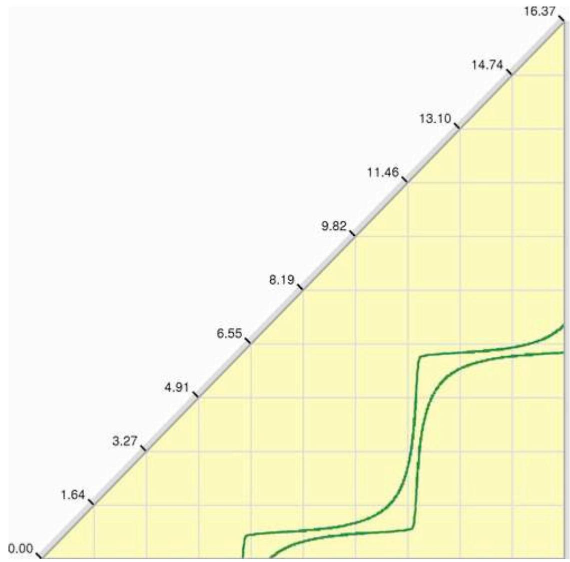
- $4\pi \approx 12.57$ (Fenchel [27] 1929, Milnor [28] 1950)
- $5\pi \approx 15.71$ (Litherland, Simon, Durumeric, Rawdon 1999 [6])
- $4\pi + 2\pi\sqrt{2} \approx 21.45$ (Cantarella, Kusner, Sullivan 2001 [15])
- > 24 (Diao 2003 [29])
- 31.32 (Denne, Diao, Sullivan 2006 [30])

So $31.32 < \mathit{Rope}(\text{trefoil}) < 32.74317$

The ridgerunner Trefoil







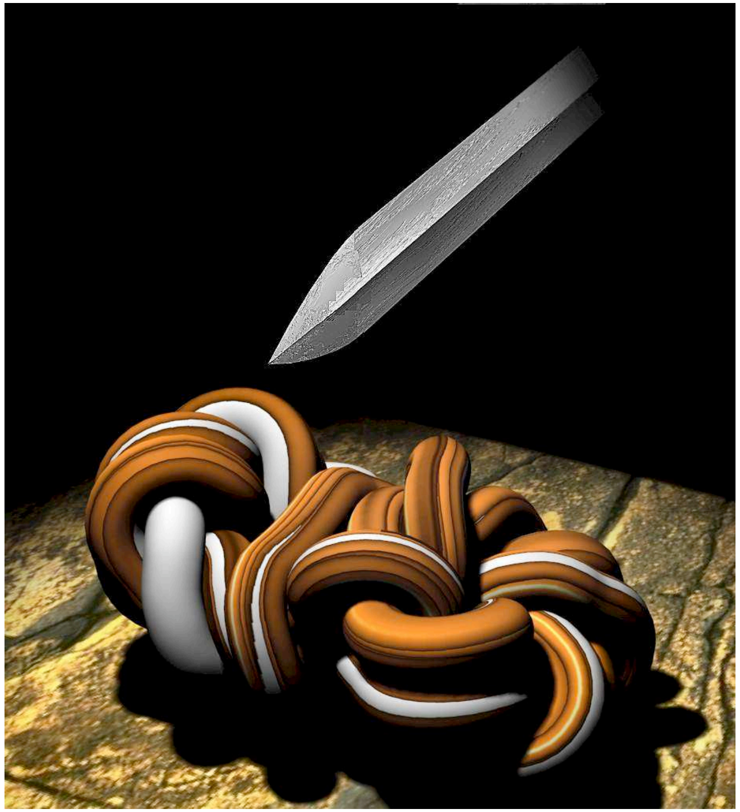
[31] Ashton++, Self-contact sets for 50 tightly knotted and linked tubes (2005)

http://www.cs.washington.edu/homes/piatek/contact_table/webTable.html

Open Problems

Gordian Unknot

- Prove that there exists a local min of the unknot.

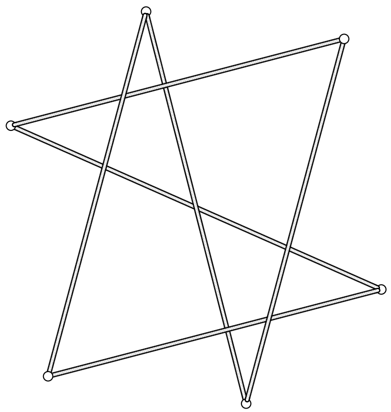


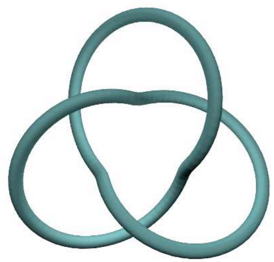
[32] Pieranski++, Gordian unknots (2001)

Open Problems 2

Tight knots

- Find a 6 edge equilateral trefoil of critical (minimal) ropelength and prove that it is critical (minimal).
- Find a 6 edge trefoil of critical (minimal) ropelength and prove that it is critical (minimal).
- Parametrize a non-planar non-trivial ropelength critical (minimizing) smooth knot (possibly with the help of polygonal computations).

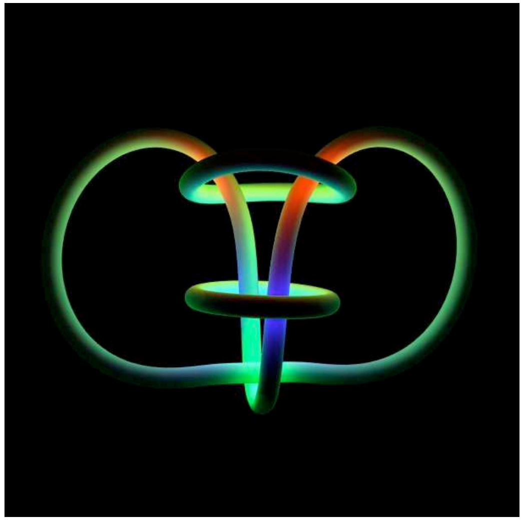


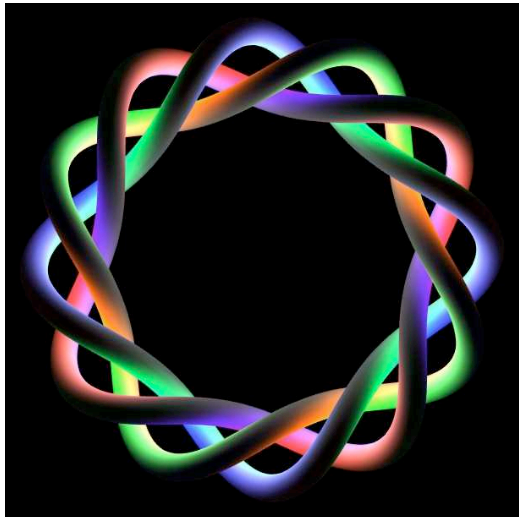


Open Problems 3

Symmetric Energy

- Idea: point is a heat source projecting most strongly in the normal plane and dissipating to 0 in the tangent directions
- Möbius Energy subtracts the infinity, Symmetric Energy multiplies it to 0





$$r = \frac{x - y}{|x - y|}$$

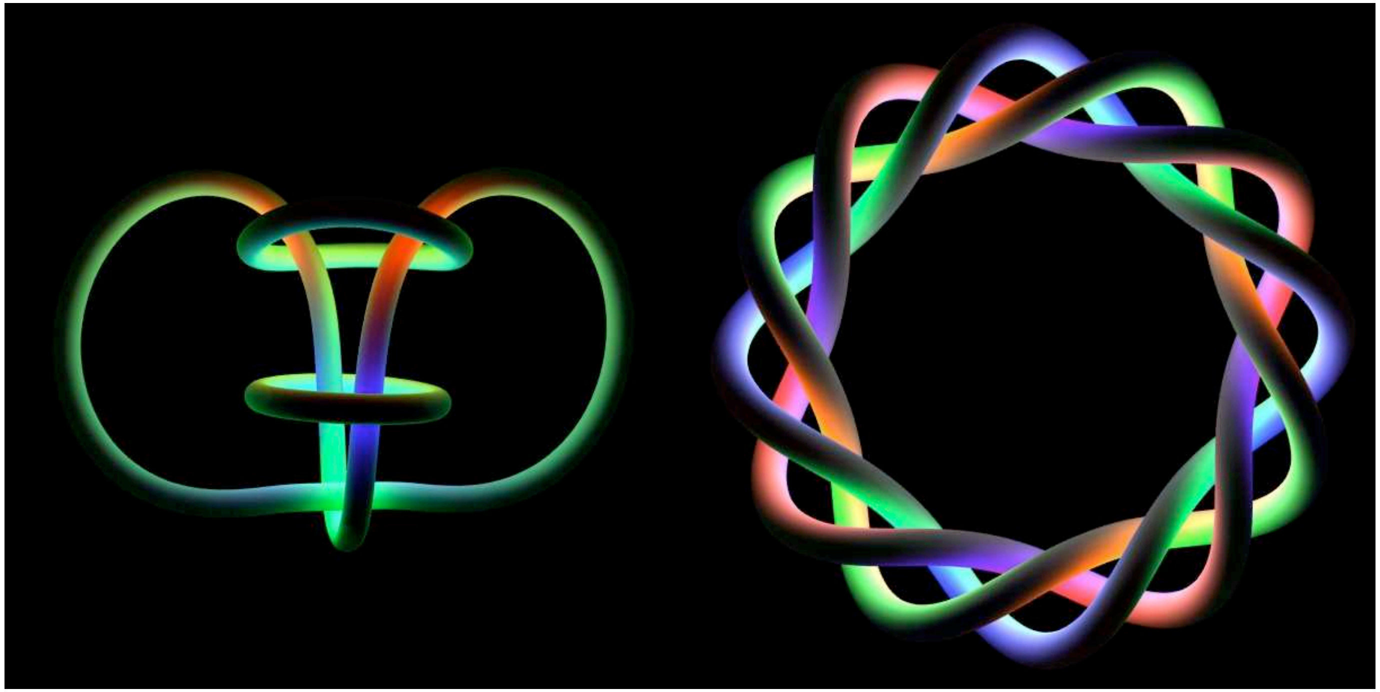
$$E_S(K) = \int\int \frac{|d\mathbf{x} \times r|\,|d\mathbf{y} \times r|}{|x - y|^2}$$

[33] Buck and Simon, *Lectures at KNOTS '96* (1997)

Symmetric Energy Open Problems

Problems

- Polygonal symmetric energy is relatively unexplored (KnotPlot)
- Approximation theorem
- Anti-approximation theorem



Open Problems 4

Möbius Energy

- Approximation theorem [34]
- Anti-approximation theorem [35]

Open Problem

Prove that *MD*-Energy minimizing polygons converge to a Möbius energy minimum.

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