The Symplectic Geometry of Polygon Space

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University of Georgia

Workshop on Geometric Knot Theory
Oberwolfach
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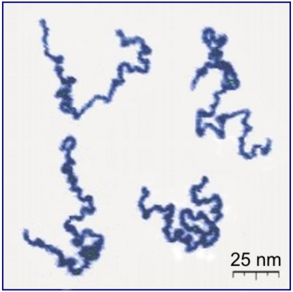
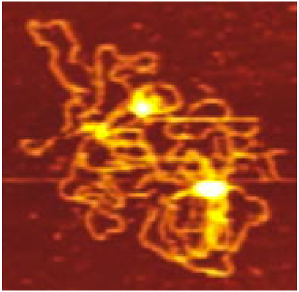
Physics Question

What is the average shape of a polymer in solution?





Protonated P2VP
Roiter/Minko
Clarkson University

Plasmid DNA
Alonso-Sarduy, Dietler Lab
EPF Lausanne

Physics Question

What is the average shape of a polymer in solution?

Physics Answer

> *Modern polymer physics is based on the analogy between a polymer chain and a random walk.*
> *—Alexander Grosberg, NYU.*

Math Question

How can we construct random samples drawn from the space of closed space n-gons? More generally, how should we (numerically) integrate over the space of closed polygons?

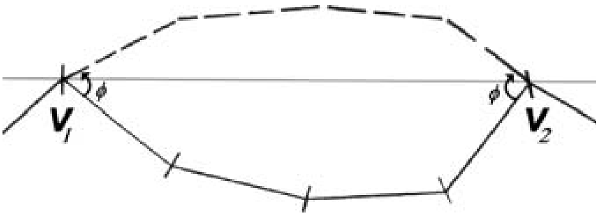


Illustration of crankshaft algorithm of Vologoskii et. al.
Benham/Mielke

Goal

Exploit the (symplectic) geometric structure of polygon space to find good sampling algorithms for random polygons, to compute expected values, and to establish a framework for proving theorems.

Let $\widetilde{\mathrm{Pol}(n;\vec{r})}$ be the moduli space of closed polygons in $\mathbb{R}^3$ with edgelengths given by the vector $\vec{r} = (r_1, \ldots, r_n)$ up to translation.

Proposition

$\widetilde{\mathrm{Pol}(n;\vec{r})}$ is the codimension-three submanifold of $\widetilde{\mathrm{Arm}(n,\vec{r})} = \prod_{i=1}^{n} S^2(r_i)$ determined by the linear equation

$$\sum_{i=1}^{n} \vec{e}_i = \vec{0}$$

where $\vec{e}_i$ is the ith edge of the polygon.

The geometry of this space seems difficult to get our hands on.

Theorem (Kapovich–Millson, 1996)

$\mathrm{Pol}(n; \vec{r})$ is the symplectic reduction of $\prod_{i=1}^{n} S^2(r_i)$ by the (Hamiltonian) diagonal $SO(3)$ action.

In particular, $\mathrm{Pol}(n; \vec{r})$ is a $(2n-6)$-dimensional symplectic manifold.

Moreover, the Liouville measure induced by the symplectic structure agrees with standard measure.

Symplectic Geometry Review

Recall that a symplectic manifold (M^{2n}, ω) consists of an even-dimensional manifold together with a closed 2-form ω such that $\omega^n \neq 0$. A *symplectomorphism* is a diffeomorphism which preserves the symplectic form.

A torus T^k which acts by symplectomorphisms on M so that the action is Hamiltonian induces a *moment map* $\mu : M \to \mathbb{R}^k$ where the action preserves the fibers.

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Theorem (Atiyah, Guillemin–Sternberg, 1982)

The image of μ is a convex polytope in $\mathbb{R}^k$ called the moment polytope.

Theorem (Duistermaat–Heckman, 1982)

The pushforward of Liouville measure to the moment polytope is piecewise polynomial. If $k = n$ the manifold is called a toric symplectic manifold and the pushforward measure is a constant multiple of Lebesgue measure.

Let (M, ω) be the 2-sphere with the standard area form. Let $T^1 = S^1$ act by rotation around the z-axis. Then the moment polytope is the interval $[-1, 1]$.

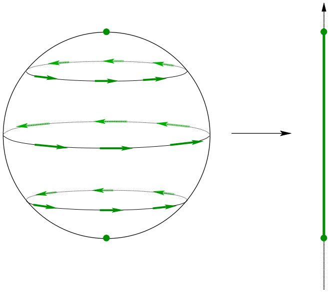

Illustration by Holm.

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Theorem (Archimedes, Duistermaat–Heckman)

The pushforward of the standard measure on the sphere to the interval is 2π times Lebesgue measure.

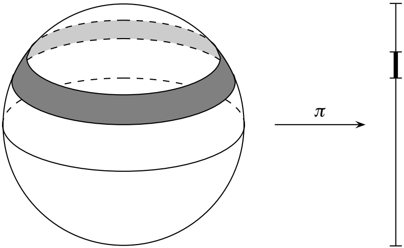

Illustration by Kuperberg.

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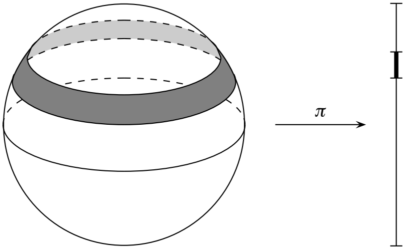

Illustration by Kuperberg.

We can sample uniformly on S^2 by choosing z and θ coordinates independently and uniformly.

A Sampling Algorithm for Toric Symplectic Manifolds

More generally, if M^{2n} is a toric symplectic manifold with moment polytope $P \subset \mathbb{R}^n$, then the inverse image of each point in P is an n-torus. This yields

$$\alpha : P \times T^n \to M$$

which parametrizes a full-measure subset of M by so-called "action-angle coordinates".

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Proposition

The map $\alpha : P \times T^n \to M$ is measure-preserving.

Therefore, we can sample M with respect to Liouville measure by sampling P and T^n independently and uniformly.

A Toric Structure on the Space of Arms

The torus T^n acts on $\widetilde{\mathrm{Arm}(n; \vec{r})} = \prod_{i=1}^n S^2(r_i)$, the space of open polygons in space up to translation, by spinning each factor around the z-axis. This action is Hamiltonian, with moment polytope the hypercube

$$\prod_{i=1}^{n} [-r_i, r_i]$$

which records the z-coordinate z_i of each edge $\vec{e}_i$.

Proposition (with Cantarella)

Let $p \in \mathrm{Arm}(n; \vec{r})$. Then the length $\ell \in [0, \sum r_i]$ of the failure-to-close vector $\vec{e}_1 + \ldots + \vec{e}_n$ has pdf

$$\phi(\ell) = -2\ell f_n'(\ell),$$

where

$$f_n(x) = \frac{1}{\prod_{i=1}^n 2r_i} \frac{1}{\sqrt{n}} \mathrm{SA}(x, r_1, \ldots, r_n)$$

is the pdf of the sum of uniform random variates $z_1 + \ldots + z_n$. Here $\mathrm{SA}(x, r_1, \ldots, r_n)$ is the volume of the slice of the hypercube $\Pi_{i=1}^n [-r_i, r_i]$ by the plane $\sum_{i=1}^n x_i = x$.

End-to-End pdf

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Corollary (Pólya, 1912)

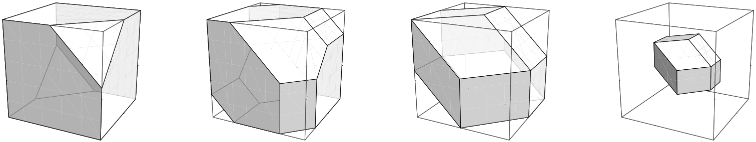
$$\phi(\ell) = \frac{2\ell}{\pi} \int_0^\infty y \sin \ell y \operatorname{sinc}^n y \, \mathrm{d}y$$

Proposition (with Cantarella)

A polygon $p \in \mathrm{Arm}(n; \vec{1})$ is confined to a slab of width h if and only if the vector $\vec{z} = (z_1, \ldots, z_n)$ of action variables lies in the parallelotope determined by the inequalities

$$-1 \leq \langle \vec{z}, \vec{x}_i \rangle \leq 1, \quad -h \leq \langle \vec{z}, \vec{w}_{ij} \rangle \leq h$$

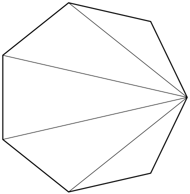
where $\vec{w}_{ij} = \sum_{k=1}^{j} \vec{e}_k$. Hence, such arms can be uniformly sampled using the sampling algorithm for toric manifolds.



$h = 2$ $\quad$ $h = \frac{3}{2}$ $\quad$ $h = 1$ $\quad$ $h = \frac{1}{2}$

Theorem (Kapovich and Millson, 1996)

Any triangulation T of the standard n-gon yields a Hamiltonian action of T^{n-3} on $\mathrm{Pol}(n;\vec{r})$ where the angle θ_i acts by folding the polygon around the ith diagonal of the triangulation.



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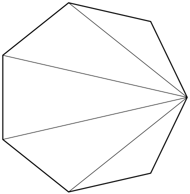
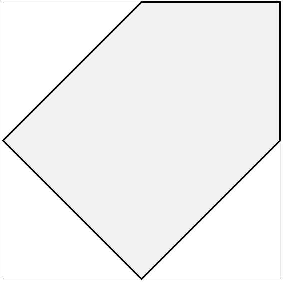


The moment map $\mu : \mathrm{Pol}(n;\vec{r}) \to \mathbb{R}^{n-3}$ records the lengths d_i of the diagonals of the triangulation.

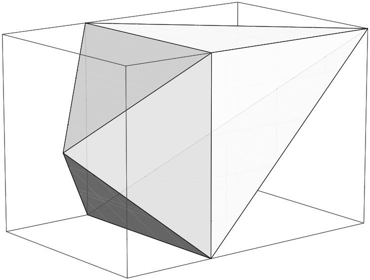
The portion of $\mathrm{Pol}(n;\vec{r})$ in the inverse image of the interior of the moment polytope is an (open) toric symplectic manifold.

The moment polytope corresponding to a fan triangulation is determined by the “fan triangulation inequalities”

$$0 \leq d_1 \leq r_1 + r_2 \qquad \begin{array}{c} r_{i+2} \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq r_{i+2} \end{array} \qquad 0 \leq d_{n-3} \leq r_n + r_{n-1}$$



Moment polytope for $\mathrm{Pol}(5; \vec{1})$



Moment polytope for $\mathrm{Pol}(6; \vec{1})$

Theorem (Takakura, 2001, Khoi, 2005)

The fan triangulation polytope for $\mathrm{Pol}(n; \vec{r})$ *has volume*

$$\frac{-1}{2(n-3)!} \sum_{I} (-1)^{n-|I|} \left(\sum_{i \in I} r_i - \sum_{j \notin I} r_j \right)^{n-3},$$

where the outer sum is over all multindices $I = (i_1, \ldots, i_p)$ *for* $p \leq n$ *so that the term in parentheses is positive.*

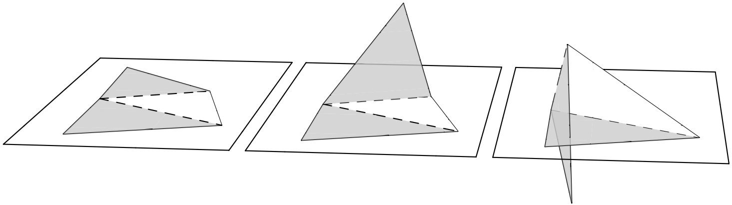
Corollary

The fan triangulation polytope for $\mathrm{Pol}(n; \vec{1})$ *has volume*

$$\frac{-1}{2(n-3)!} \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n}{k} (n-2k)^{n-3}.$$

Proposition (with Cantarella)

Polygons in $\mathrm{Pol}(n;\vec{r})$ *are sampled according to the standard measure if and only if the diagonal lengths* $(d_1,\ldots,d_{n-3})$ *are uniformly sampled from the moment polytope and the dihedral angles are sampled independently and uniformly in* $[0,2\pi)$.



Polygons in the fiber over $(d_1,d_2)=(1.15,0.75)$ in the moment polytope. The middle and right pentagons correspond to bending angles $(0,2.2)$ and $(2.15,2.2)$, respectively.

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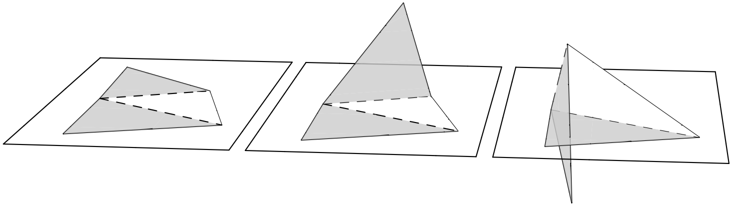


Note: This gives criteria for evaluating the quality of polygon sampling algorithms!

Definition

A polygon $p \in \mathrm{Pol}(n; \vec{r})$ is in *rooted spherical confinement* of radius r if each diagonal length $d_i \leq r$. Such a polygon is contained in a sphere of radius r centered at the first vertex.

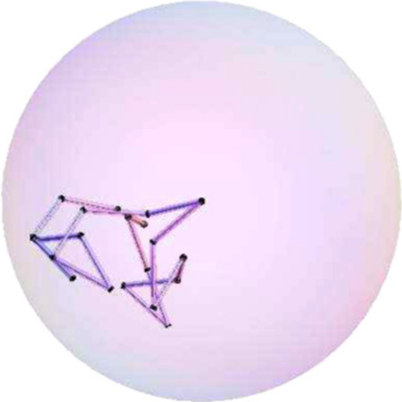


Illustration by Diao et al.

Proposition (with Cantarella)

Polygons in $\mathrm{Pol}(n; \vec{r})$ *are sampled according to the standard measure on rooted sphere-confined polygons in a sphere of radius r if and only if the diagonal lengths* $(d_1, \ldots, d_{n-3})$ *are uniformly sampled from the polytope determined by both the fan triangulation inequalities*

$$0 \leq d_1 \leq r_1 + r_2 \qquad \begin{array}{c} r_{i+2} \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq r_{i+2} \end{array} \qquad 0 \leq d_{n-3} \leq r_n + r_{n-1}$$

and the additional linear inequalities

$$d_i \leq r$$

and the dihedral angles ***around those diagonals*** *are sampled independently and uniformly in* $[0, 2\pi)$.

Definition

Let $\mathrm{ChordLength}(k, n; \vec{r})$ be the length of the chord skipping the first k edges in a polygon sampled according to the standard measure on $\mathrm{Pol}(n; \vec{r})$.

Proposition (with Cantarella and Deguchi, Millett and Zirbel, 2012)

The second moment of the random variable $\mathrm{ChordLength}(k, n; \vec{1})$ *is* $\frac{k(n-k)}{n-1}$. *This implies the expected squared radius of gyration of an equilateral n-gon is* $\frac{n+1}{12}$.

Proposition (with Cantarella)

The pth moment of $\mathrm{ChordLength}(k, n; \vec{1})$ *is given by the* $(k-1)$*st coordinate of the pth center of mass of the equilateral fan polytope.*

Expected Value of ChordLength$(k, n; \vec{1})$ for various values of n and k computed using `polymake`

n	k: 2	3	4	5	6	7	8
4	1						
5	$\frac{17}{15}$	$\frac{17}{15}$					
6	$\frac{7}{6}$	$\frac{5}{4}$	$\frac{7}{6}$				
7	$\frac{461}{385}$	$\frac{46}{35}$	$\frac{46}{35}$	$\frac{461}{385}$			
8	$\frac{73}{60}$	$\frac{1{,}307}{960}$	$\frac{7}{5}$	$\frac{1{,}307}{960}$	$\frac{73}{60}$		
9	$\frac{112{,}121}{91{,}035}$	$\frac{42{,}353}{30345}$	$\frac{133{,}337}{91{,}035}$	$\frac{133{,}337}{91{,}035}$	$\frac{42{,}353}{30{,}345}$	$\frac{112{,}121}{91{,}035}$	
10	$\frac{6{,}091}{4{,}900}$	$\frac{111{,}499}{78{,}400}$	$\frac{1{,}059}{700}$	$\frac{24{,}197}{15{,}680}$	$\frac{1{,}059}{700}$	$\frac{111{,}499}{78{,}400}$	$\frac{6{,}091}{4{,}900}$

Hit-and-Run Sampling for Convex Polytopes

Suppose $P \subset \mathbb{R}^n$ is a convex polytope given as the intersection of a collection of linear inequalities. The hit-and-run algorithm for sampling P is the following:

- Given $\vec{p}_i \in P$, choose a random line ℓ through $\vec{p}_i$.
- Sample $\ell \cap P$ uniformly to find $\vec{p}_{i+1}$.
- Iterate.

Proposition (Lovász, 1999)

After appropriate preprocessing, hit-and-run produces an approximately uniformly distributed sample point on an arbitrary convex polytope in time $O^*(n^3)$. The constant depends on the square of the ratio of the inradius and circumradius.

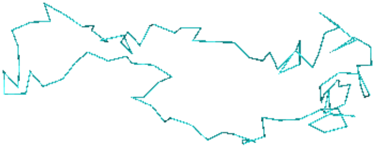
A Moment Polytope Sampling Algorithm

To sample fixed edgelength (confined or not) n-gons, we can

- Generate points in the $(n-3)$-dimensional moment polytope using hit-and-run.
- Pair each such point with $n-3$ independent uniform dihedral angles and construct the associated polygon.

Optimizations are probably possible. For example, permuting edges between steps of hit-and-run seems to speed things up a lot.

Unconfined 100-gons



Unconfined 100-gons

Unconfined 100-gons

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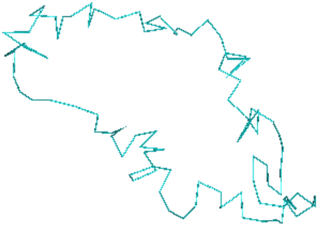
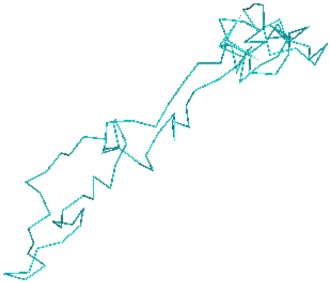
50-confined 100-gons

50-confined 100-gons



50-confined 100-gons

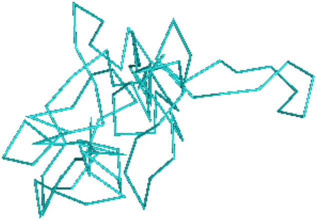


20-confined 100-gons

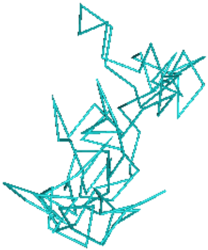
20-confined 100-gons

20-confined 100-gons

10-confined 100-gons



10-confined 100-gons



10-confined 100-gons

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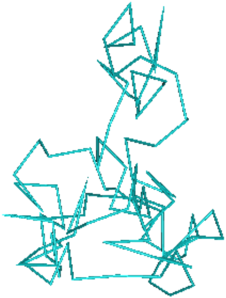

5-confined 100-gons

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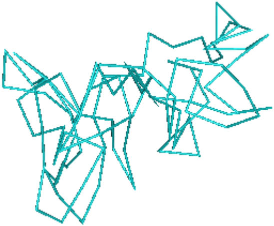

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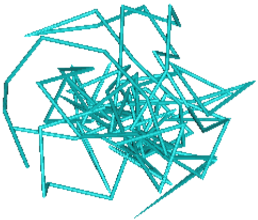
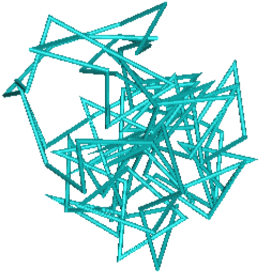
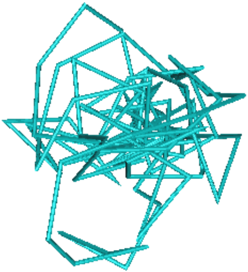


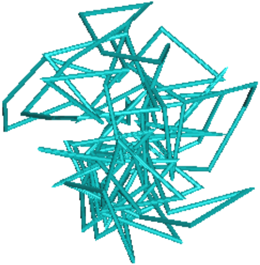
2-confined 100-gons



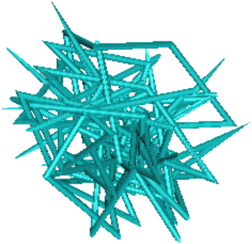
2-confined 100-gons



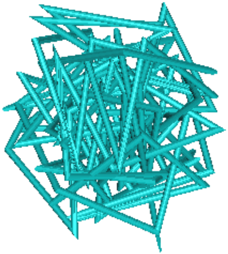
2-confined 100-gons

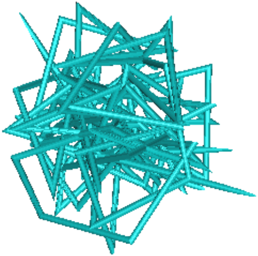


1.1-confined 100-gons

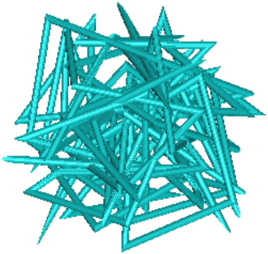


1.1-confined 100-gons





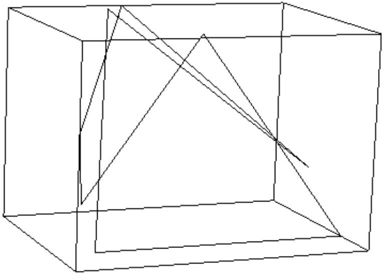
1.1-confined 100-gons



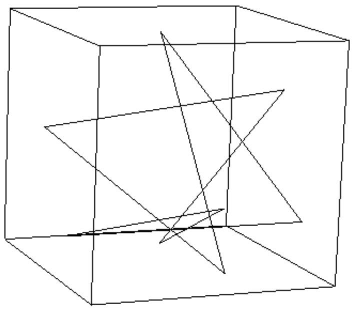
Questions

- Can we find bounds on the volume of the space of slab-confined arms? Does this give bounds on the energy required to confine a polymer?
- Can we find bounds on the volume of the space of confined closed polygons? Can such bounds be used to bound the probability of rare knots?
- Is there a combinatorial description of the fan triangulation polytope? This would give a direct sampling algorithm for fixed edgelength polygons.
- Can we compute expected values of the sedimentation coefficient or of other quantities related to moments of chordlengths?

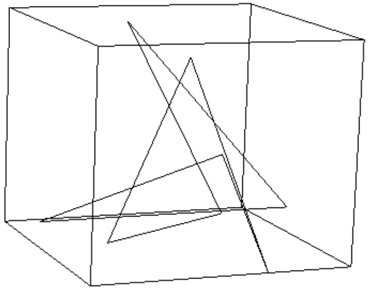
Equilateral 8-edge 5_2



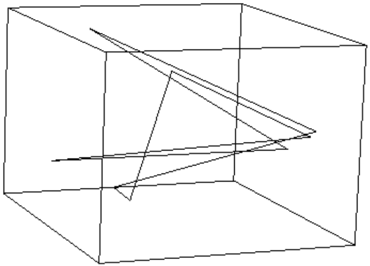
Equilateral 8-edge 5_2



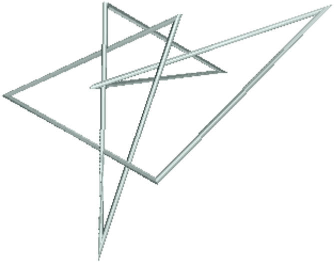
Equilateral 8-edge 5_2



Equilateral 8-edge 5_2



Equilateral 8-edge 6_2



Questions

- Can we find bounds on the volume of the space of slab-confined arms? Does this give bounds on the energy required to confine a polymer?
- Can we find bounds on the volume of the space of confined closed polygons? Can such bounds be used to bound the probability of rare knots?
- Is there a combinatorial description of the fan triangulation polytope? This would give a direct sampling algorithm for fixed edgelength polygons.
- Can we compute expected values of the sedimentation coefficient or of other quantities related to moments of chordlengths?

Thank you!

Thank you for inviting me!

References

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  arXiv:1206.3161
  To appear in *Communications on Pure and Applied Mathematics*.

- *The Expected Total Curvature of Random Polygons*
  Jason Cantarella, Alexander Y. Grosberg, Robert Kusner, and Clayton Shonkwiler
  arXiv:1210.6537.

- *Symplectic Methods for Random Equilateral Polygons and the Moment Polytope Sampling Algorithm*
  Jason Cantarella and Clayton Shonkwiler
  In preparation.