Closed Random Walks and Symplectic Geometry

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Geometry–Topology Seminar
University of Pennsylvania
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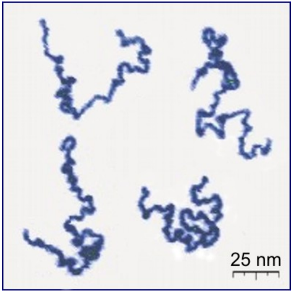
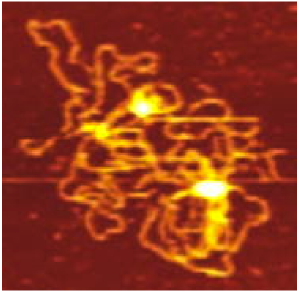
Physics Question

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, n-step random walks? More generally, how should we (numerically) integrate over the space of closed random walks?

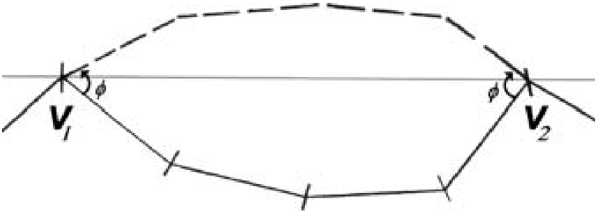


Illustration of crankshaft algorithm of Vologoskii et. al.
Benham/Mielke

Exploit the symplectic geometry of polygon space to find good sampling algorithms for closed random walks, to compute expected values, and to establish a framework for proving theorems.

Let $\mathrm{Arm}(n; \vec{1})$ be the moduli space of random walks in $\mathbb{R}^3$ consisting of n unit-length steps up to translation.

Then $\mathrm{Arm}(n; \vec{1}) \cong S^2(1) \times \ldots \times S^2(1)$.

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This space is easy to sample uniformly: choose $\vec{w}_1, \ldots, \vec{w}_n$ independently from a spherically-symmetric distribution on $\mathbb{R}^3$ and let

$$\vec{e}_i = \frac{\vec{w}_i}{\|\vec{w}_i\|}.$$

Theorem (Archimedes)

Let $f : S^2 \to \mathbb{R}$ be given by $(x, y, z) \mapsto z$. Then the pushforward of the standard measure on the sphere to the interval is 2π times Lebesgue measure.

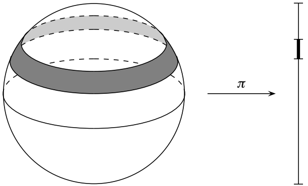

Illustration by Kuperberg.

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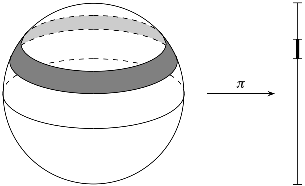

Illustration by Kuperberg.

Therefore, we can sample uniformly on (a full-measure subset of) S^2 by choosing a z-coordinate uniformly from $[-1, 1]$ and a θ-coordinate uniformly from S^1.

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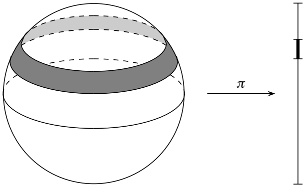


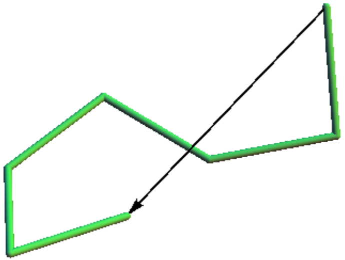
Illustration by Kuperberg.

Thus, we can sample uniformly on (a full-measure subset of) $\mathrm{Arm}(n; \vec{1})$ by choosing $(z_1, \ldots, z_n)$ uniformly from the cube $[-1, 1]^n$ and $(\theta_1, \ldots, \theta_n)$ uniformly from the n-torus T^n.

Theorem (Rayleigh, 1919)

The length ℓ of the end-to-end vector of an n-step random walk has the probability density function

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



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Therefore, the expected end-to-end distance of an n-step random walk is

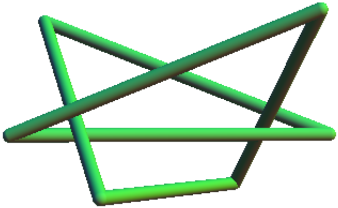
$$E(\ell; \mathrm{Arm}(n; \vec{1})) = \int_0^n \ell \phi_n(\ell) \, \mathrm{d}\ell$$

$E(\ell; \mathrm{Arm}(n; \vec{1}))$ for small n

n	$E(\ell; \mathrm{Arm}(n; \vec{1}))$	Decimal	$\sqrt{\frac{8n}{3\pi}}$
2	$\frac{4}{3}$	1.33333	1.30294
3	$\frac{13}{8}$	1.625	1.59577
4	$\frac{28}{15}$	1.86667	1.84264
5	$\frac{1199}{576}$	2.0816	2.06013
6	$\frac{239}{105}$	2.27619	2.25676
7	$\frac{113{,}149}{46{,}080}$	2.45549	2.43758
8	$\frac{1487}{567}$	2.62257	2.60588
9	$\frac{14{,}345{,}663}{5{,}160{,}960}$	2.77965	2.76395
10	$\frac{292{,}223}{99{,}792}$	2.92832	2.91346

Let $\mathrm{Pol}(n;\vec{1}) \subset \mathrm{Arm}(n;\vec{1})$ be the codimension-3 submanifold of closed random walks; i.e., those walks which satisfy

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



Individual edges are no longer independent!

A symplectic manifold (M^{2n}, ω) is a smooth $2n$-dimensional manifold M with a closed, non-degenerate 2-form ω called the *symplectic form*. The nth power of this form ω^n is a volume form on M^{2n}.

The circle *acts by symplectomorphisms* on M^{2n} if the action preserves ω. A circle action generates a vector field X on M^{2n}. We can contract the vector field X with ω to generate a one-form:

$$\iota_X\omega(\vec{v}) = \omega(X, \vec{v})$$

If $\iota_X\omega$ is exact, the map is called *Hamiltonian* and it is dH for some smooth function H on M^{2n}. The function H is called the *momentum* associated to the action, or the *moment map*.

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 (inverse images of points).

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 the symplectic (or 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 ***Lebesgue measure*** *on the polytope.*

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 $[-1, 1]$, and S^2 is a toric symplectic manifold.

Theorem (Archimedes, Duistermaat–Heckman)

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

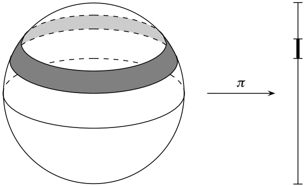


Illustration by Kuperberg.

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

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

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

Proposition

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

Therefore, we can integrate over M with respect to the symplectic measure by integrating over $P \times T^n$ and we can sample M by sampling P and T^n independently and uniformly. For example, we can sample S^2 uniformly by choosing z and θ independently and uniformly.

- Toric symplectic manifold $\rightarrow$

An Extended Example: Equilateral Arm Space

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$$\alpha(z_i, \theta_i) = (\sqrt{1 - z_i^2} \cos\theta_i, \sqrt{1 - z_i^2} \sin\theta_i, z_i).$$

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Theorem (Marsden–Weinstein, Meyer)

If $\vec{v} \in \mathfrak{g}^*$ is a regular value of μ and if G acts freely and properly on $\mu^{-1}(\vec{v})$, then the quotient

$$\mu^{-1}(\vec{v})/G =: M//_{\vec{v}}G$$

inherits a natural symplectic structure from M. This quotient is called the ***symplectic reduction*** *of M by G at $\vec{v}$.*

The SO(3) Action on Random Walks

The diagonal action of SO(3) on $\mathrm{Arm}(n; \vec{1}) = \prod S^2$ is Hamiltonian, with moment map $\mu : \prod S^2 \to \mathfrak{so}(3)^* = \mathbb{R}^3$ given by

$$\vec{e}_1, \dots, \vec{e}_n \mapsto \vec{e}_1 + \dots + \vec{e}_n.$$

Therefore, $\mathrm{Pol}(n; \vec{1}) = \mu^{-1}(\vec{0})$.

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Definition

Let $\widehat{\mathrm{Pol}}(n; \vec{1}) = \mathrm{Pol}(n; \vec{1}) / \mathrm{SO}(3)$ be the moduli space of closed equilateral random walks up to translation **and rotation.**

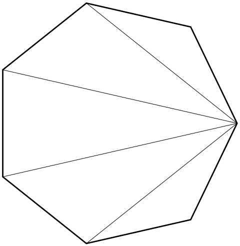
Toric Symplectic Structure on Closed Random Walks

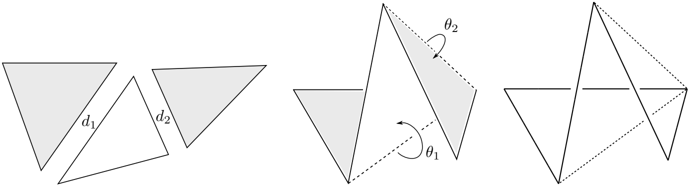
Theorem (Kapovich–Millson 1996, Hitchin 1987, Howard-Manon-Millson 2011)

If we let $\widehat{\mathrm{Pol}}(n; \vec{1})$ be the space of closed equilateral random walks up to translation and rotation, then given an abstract triangulation T of the n-gon:

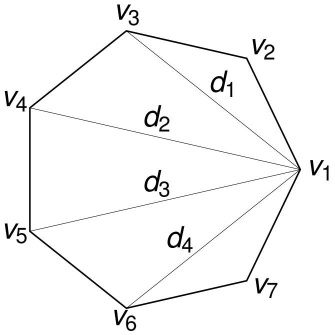
- *symplectic structure* $\rightarrow$ $\widehat{\mathrm{Pol}}(n; \vec{1})$ *is the* $(2n - 6)$*-dimensional symplectic reduction of* $\prod_{i=1}^{n} S^2$ *by the (Hamiltonian) diagonal* $SO(3)$ *action.*
- *torus action* $\rightarrow$ *fold polygon around* $n - 3$ *chords in* T
- *moment map* μ $\rightarrow$ *lengths of* $n - 3$ *chords in* T
- *moment polytope* P $\rightarrow$ *determined by triangle inequalities*
- *action-angle coordinates* α $\rightarrow$ *build triangles and embed with given dihedrals*

Triangulations and the Action-Angle Parametrization





We call this the “fan” triangulation:

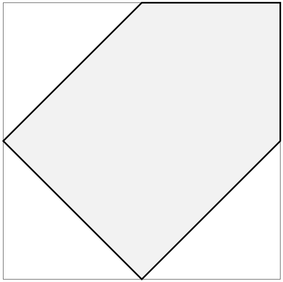


The corresponding moment polytope is given by the inequalities:

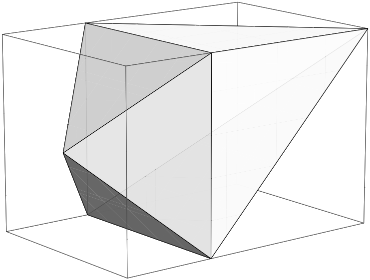
$$0 \leq d_1 \leq 2 \qquad \begin{matrix} 1 \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq 1 \end{matrix} \qquad 0 \leq d_{n-3} \leq 2$$

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

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



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



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

Theorem (with Cantarella)

The expected length of a chord skipping k edges in an n-edge closed equilateral random walk is the $(k-1)$*st coordinate of the center of mass of the moment polytope for* $\mathrm{Pol}(n; \vec{1})$.

$n\backslash k$	2	3	4	5	6	7	8
4	1						
5	$\frac{17}{15}$	$\frac{17}{15}$					
6	$\frac{14}{12}$	$\frac{15}{12}$	$\frac{14}{12}$				
7	$\frac{461}{385}$	$\frac{506}{385}$	$\frac{506}{385}$	$\frac{461}{385}$			
8	$\frac{1,168}{960}$	$\frac{1,307}{960}$	$\frac{1,344}{960}$	$\frac{1,307}{960}$	$\frac{1,168}{960}$		
9	$\frac{112,121}{91,035}$	$\frac{127,059}{91,035}$	$\frac{133,337}{91,035}$	$\frac{133,337}{91,035}$	$\frac{127,059}{91,035}$	$\frac{112,121}{91,035}$	
10	$\frac{97,456}{78,400}$	$\frac{111,499}{78,400}$	$\frac{118,608}{78,400}$	$\frac{120,985}{78,400}$	$\frac{118,608}{78,400}$	$\frac{111,499}{78,400}$	$\frac{97,456}{78,400}$

Expected Squared Chord Lengths and Radii of Gyration

Theorem (with Cantarella and Deguchi; Zirbel–Millett)

The expected squared length of a chord skipping k edges in an n-edge closed equilateral random walk is

$$E(\mathrm{Chord}(k,n)^2) = \frac{k(n-k)}{n-1}.$$

Theorem (with Cantarella)

At least $3/4$ *of the space* $\widehat{\mathrm{Pol}}(6; \vec{1})$ *of equilateral hexagons consists of unknots.*

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Proof.

Consider the triangulation of the hexagon given by joining vertices 1, 3, and 5 by diagonals and its corresponding action-angle coordinates $\alpha : \mathcal{P} \times T^3 \to \widehat{\mathrm{Pol}}(6; \vec{1})$. Using a result of Calvo, the dihedral angles $\theta_1, \theta_2, \theta_3$ of a hexagonal trefoil must all be either between 0 and π or between π and 2π. Therefore, the fraction of knots is no bigger than

$$\frac{\mathrm{Vol}([0,\pi]^3) + \mathrm{Vol}([\pi, 2\pi]^3)}{\mathrm{Vol}(T^3)} = \frac{2\pi^3}{8\pi^3} = \frac{1}{4}$$

$\square$

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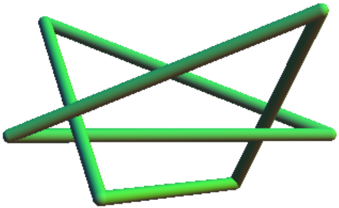

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$\square$

Markov Chain on Toric Symplectic Manifold

We can sample any toric symplectic manifold (such as $\widehat{\mathrm{Pol}}(n;\vec{1})$) using a Markov chain in action-angle coordinates:

TORIC-SYMPLECTIC-MCMC($\vec{p},\vec{\theta},\beta$)

prob $=$ UNIFORM-RANDOM-VARIATE$(0,1)$
if *prob* $< \beta$
then $\triangleright$ Get point in P using hit-and-run.
$\vec{v} =$ RANDOM-RN-DIRECTION(n)
$(t_0,t_1) =$ FIND-INTERSECTION-ENDPOINTS($P,\vec{p},\vec{v}$)
$t =$ UNIFORM-RANDOM-VARIATE(t_0,t_1)
$\vec{p} = \vec{p} + t\vec{v}$
else $\triangleright$ Get point in T^n uniformly.
for *ind* $= 1$ **to** n
do $\theta_{ind} =$ UNIFORM-RANDOM-VARIATE$(0,2\pi)$
return $(\vec{p},\vec{\theta})$

We can then convert a point $(p,\vec{\theta}) \in P \times T^n$ to a point in M^{2n} using the map α.

Convergence of TSMCMC(β)

Proposition (with Cantarella)

TORIC-SYMPLECTIC-MCMC(β) *converges uniformly geometrically to the symplectic measure on* M^{2n}.

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Proposition (with Cantarella)

Suppose that M^{2n} *is a toric symplectic manifold with moment polytope* P *and action-angle coordinates* $\alpha \colon P \times T^n \to M^{2n}$*. Further, let* $\mathcal{P}^m(\vec{p}, \vec{\theta}, \cdot)$ *be the m-step transition probability of the Markov chain given by* TORIC-SYMPLECTIC-MCMC(β) *and let* ν *be the symplectic measure on* M^{2n}*.*
There are constants $R < \infty$ *and* $\rho < 1$ *so that for any* $(\vec{p}, \vec{\theta}) \in \operatorname{int}(P) \times T^n$*,*

$$\left| \alpha_\star \mathcal{P}^m(\vec{p}, \vec{\theta}, \cdot) - \nu \right|_{\text{TV}} < R\rho^m.$$

Error Analysis for Integration with TSMCMC(β)

Suppose f is a function $M^{2n} \to \mathbb{R}$. If a run R of the TSMCMC(β) algorithm produces $((\vec{p}_0, \vec{\theta}_0), (\vec{p}_1, \vec{\theta}_1), \ldots)$, let

$$\mathrm{SMean}(f; R, m) := \frac{1}{m} \sum_{k=1}^{m} f(\alpha(\vec{p}_k, \vec{\theta}_k))$$

be the sample average of the values of f over the first m steps of R.

Proposition (with Cantarella)

If f is square-integrable, there exists a real number $\sigma(f)$ so that

$$\sqrt{m}\,(\mathrm{SMean}(f; R, m) - E(f)) \xrightarrow{w} \mathcal{N}(0, \sigma(f)^2),$$

where $\mathcal{N}(0, \sigma(f)^2)$ is the Gaussian distribution with mean 0 and standard deviation $\sigma(f)$, the superscript w denotes weak convergence, and $E(f)$ is the expectation of f.

Given a length-m run R of TSMCMC and a square integrable function $f\colon\ M \to \mathbb{R}$, we can compute SMean$(f; R, m)$ and the **Geyer IPS Estimator** $\bar{\sigma}_m(f)$ for the true standard deviation $\sigma(f)$.

Then a 95% confidence interval for the true expectation of f is given by

$$E(f) \in \mathrm{SMean}(f; R, m) \pm 1.96\bar{\sigma}_m(f)/\sqrt{m}.$$

Proposition (with Cantarella)

Expected total curvature of an equilateral 64-gon is 101.72777*.*

Total Curvature for Equilateral 64-gons
10-minute runs of PTSMCMC(0.5,δ), 3 to 7 million steps

δ	Sample Mean	IPS Error	Actual
0.	101.736	0.184489	0.00822679
0.1	101.724	0.0150058	0.00377321
0.2	101.725	0.0123642	0.00277321
0.3	101.725	0.00894214	0.00277321
0.4	101.732	0.00733317	0.00422679
0.5	101.724	0.00639885	0.00377321
0.6	101.722	0.00568469	0.00577321
0.7	101.727	0.00529789	0.00077321
0.8	101.731	0.00543157	0.00322679
0.9	101.728	0.00440235	0.00022679

Definition

A polygon $p \in \operatorname{Pol}(n; \vec{1})$ 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.

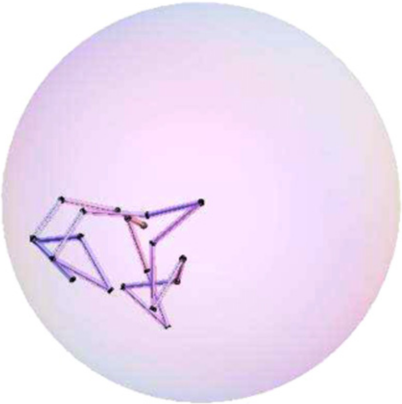


Illustration by Diao et al.

Proposition (with Cantarella)

Polygons in $\mathrm{Pol}(n; \vec{1})$ *in rooted spherical confinement in a sphere of radius* R *are a toric symplectic manifold with moment polytope determined by the fan triangulation inequalities*

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

together with the additional linear inequalities

$$d_i \leq R.$$

These polytopes are simply subpolytopes of the fan triangulation polytopes. Many other confinement models are possible!

Expected Total Curvature of Tightly-Confined Equilateral 50- and 90-gons

R	50-gons	90-gons
1.1	103.1120 ± 0.0093	185.701 ± 0.028
1.2	100.1900 ± 0.0089	180.261 ± 0.028
1.3	97.8369 ± 0.0088	175.947 ± 0.028
1.4	95.8891 ± 0.0090	172.346 ± 0.027
1.5	94.1979 ± 0.0091	169.271 ± 0.028
1.6	92.7501 ± 0.0094	166.660 ± 0.029
∞	79.74197470	142.5630093

Unconfined 100-gons

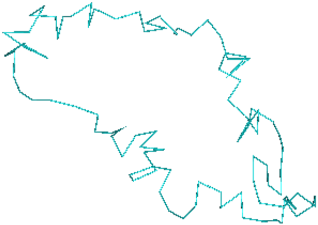
Unconfined 100-gons

Unconfined 100-gons

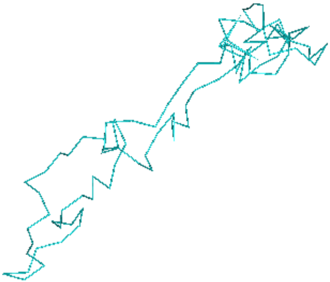
Unconfined 100-gons

50-confined 100-gons

50-confined 100-gons



50-confined 100-gons

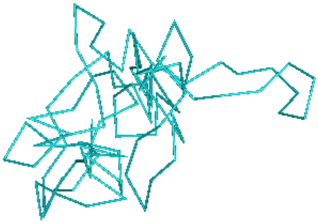


20-confined 100-gons

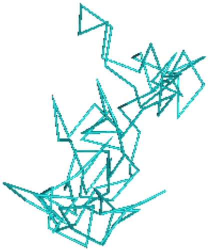
20-confined 100-gons

20-confined 100-gons

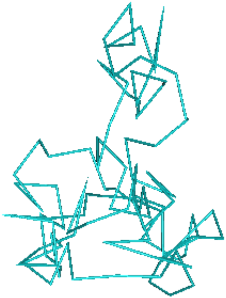
10-confined 100-gons



10-confined 100-gons

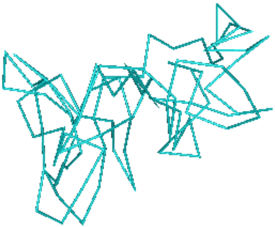


10-confined 100-gons



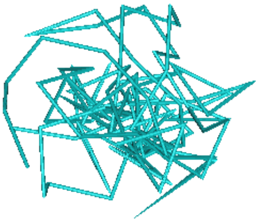
5-confined 100-gons

5-confined 100-gons

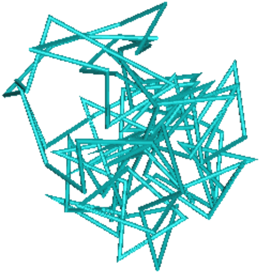


5-confined 100-gons

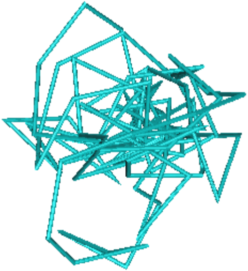
2-confined 100-gons



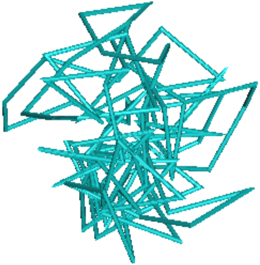
2-confined 100-gons

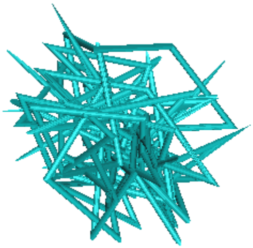


2-confined 100-gons

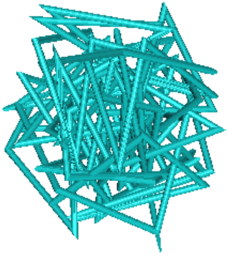


2-confined 100-gons

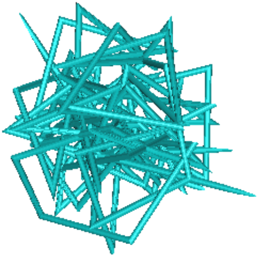


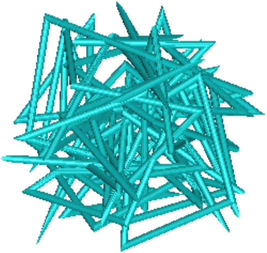


1.1-confined 100-gons



1.1-confined 100-gons





Thank you for listening!

- *Probability Theory of Random Polygons from the Quaternionic Viewpoint*
  Jason Cantarella, Tetsuo Deguchi, and Clayton Shonkwiler
  arXiv:1206.3161
  Communications on Pure and Applied Mathematics
  (2013), doi:10.1002/cpa.21480.

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

- *The symplectic geometry of closed equilateral random walks in 3-space*
  Jason Cantarella and Clayton Shonkwiler
  arXiv:1310.5924.