Closed Random Walks and Symplectic Geometry

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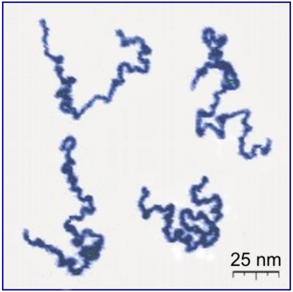
Georgia Southern Colloquium
November 22, 2013

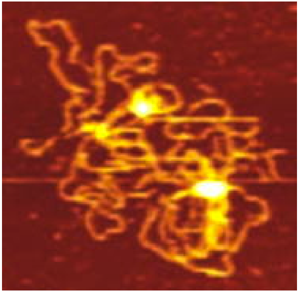
Random Polygons (and Polymer Physics)

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

Random Polygons (and Polymer Physics)

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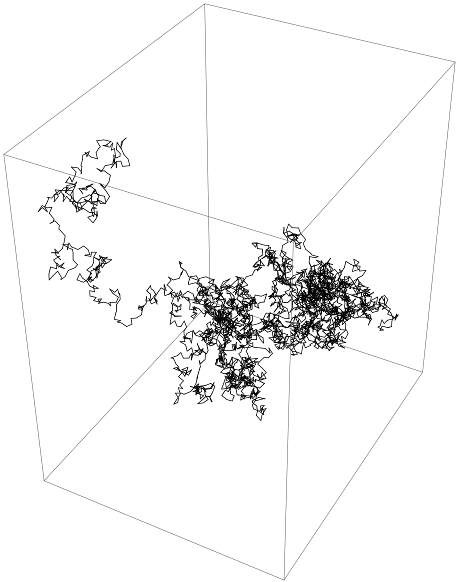
Physics Answer

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

Open Equilateral Random Polygon with 3,500 edges



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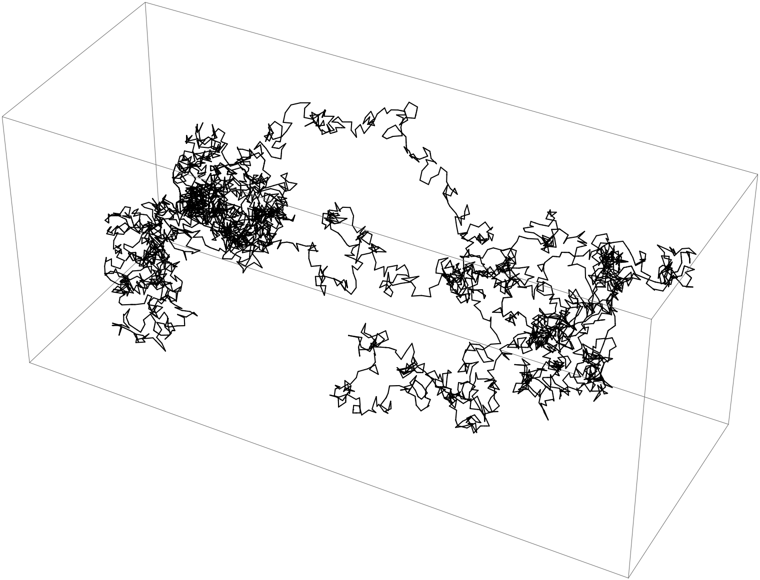

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Classical Problems

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  - What if the edge lengths vary? (Loop closures)
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Point of Talk

New sampling algorithms backed by deep and robust mathematical framework. Guaranteed to converge, relatively easy to code.

(Incomplete?) History of Sampling Algorithms

- Markov Chain Algorithms
  - crankshaft (Vologoskii 1979, Klenin 1988)
  - polygonal fold (Millett 1994)
- Direct Sampling Algorithms
  - triangle method (Moore 2004)
  - generalized hedgehog method (Varela 2009)
  - sinc integral method (Moore 2005, Diao 2011)

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- Direct Sampling Algorithms
  - triangle method (Moore et al. 2004)
    - samples a subset of closed polygons
  - generalized hedgehog method (Varela et al. 2009)
    - unproved whether this is correct pdf
  - sinc integral method (Moore et al. 2005, Diao et al. 2011)
    - requires sampling from complicated 1-d polynomial pdfs

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

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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.

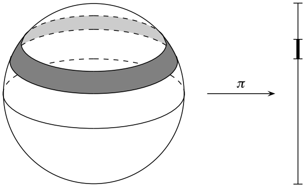

Illustration by Kuperberg.

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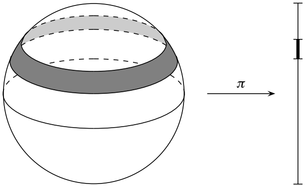

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Therefore, we can sample uniformly on (a full-measure subset of) S^2 by choosing a z-coordinate uniformly from $[-1, 1]$ and a θ-coordinate uniformly from S^1.

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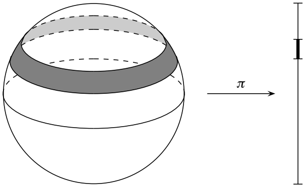


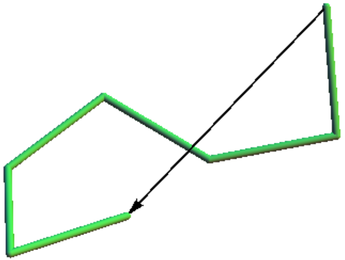
Illustration by Kuperberg.

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

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



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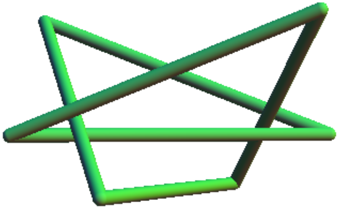
Therefore, the expected end-to-end distance of an *n*-step random walk is

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

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)

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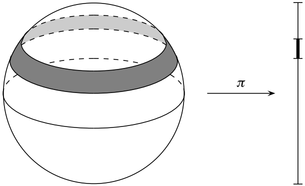

Illustration by Kuperberg.

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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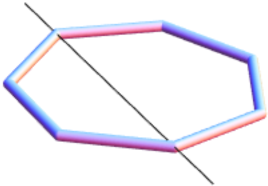
Definition

Given an (abstract) triangulation of the n-gon, the folds on any two chords commute. A *dihedral angle* move rotates around all of these chords by independently selected angles.



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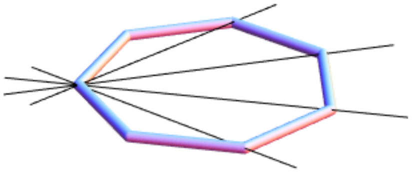
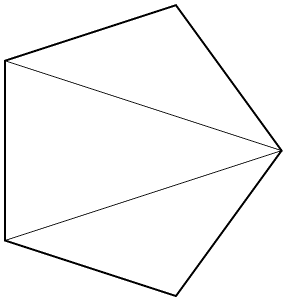
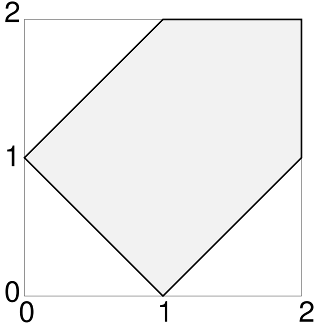


Definition

A abstract triangulation T of the n-gon picks out $n-3$ nonintersecting chords. The lengths of these chords obey triangle inequalities, so they lie in a convex polytope in $\mathbb{R}^{n-3}$ called the *triangulation polytope* $\mathcal{P}$.





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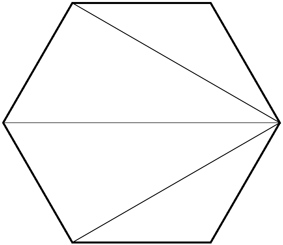
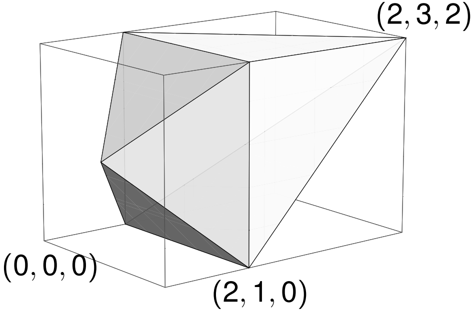
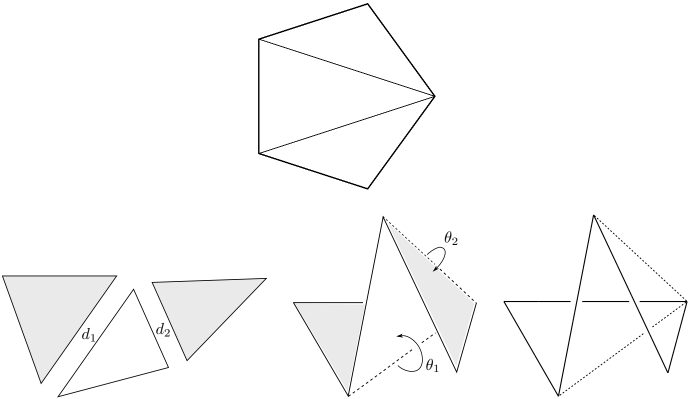




Definition

If $\mathcal{P}$ is the triangulation polytope and T^{n-3} is the torus of $n-3$ dihedral angles, then there are *action-angle coordinates*:

$$\alpha\colon\ \mathcal{P} \times T^{n-3} \to \mathrm{Pol}(n)/\,\mathrm{SO}(3)$$



Theorem (with Cantarella)

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Corollary

Any sampling algorithm for convex polytopes is a sampling algorithm for closed equilateral polygons.

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The joint pdf of the $n - 3$ chord lengths in an abstract triangulation of the n-gon in a closed random equilateral polygon is Lesbesgue measure on the triangulation polytope.

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Corollary (with Cantarella)

The expectation of any function of a collection of non-intersecting chordlengths can be computed by integrating over the triangulation polytope.

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	$\frac{461}{385}$	$\frac{506}{385}$	$\frac{506}{385}$	$\frac{461}{385}$			
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A Bound on Knot Probability

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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.

Using a result of Calvo, in either this triangulation or the 2–4–6 triangulation, 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

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

$\square$

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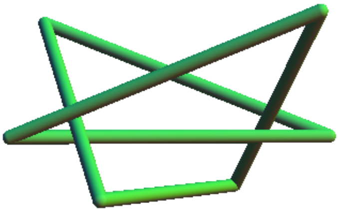

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Action-angle coordinates reduce sampling equilateral polygon space to the (solved) problem of sampling a convex polytope.

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A Markov Chain for Convex Polytopes

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Theorem (Smith, 1984)

The m-step transition probability of hit-and-run starting at any point $\vec{p}$ in the interior of $\mathcal{P}$ converges geometrically to Lesbegue measure on $\mathcal{P}$ as $m \to \infty$.

A (new) Markov Chain for Polygon Spaces

Definition (TSMCMC(β))

Given a triangulation T of the n-gon and associated polytope $\mathcal{P}$. If $x_k = (\vec{p}_k, \vec{\theta}_k) \in \mathcal{P} \times T^{n-3}$, define x_{k+1} by

- Update $\vec{p}_k$ by a hit-and-run step on $\mathcal{P}$ with probability β.
- Replace $\vec{\theta}_k$ with a new uniformly sampled point in T^{n-3} with probability $1 - \beta$.

At each step, construct the corresponding polygon $\alpha(x_k)$ using action-angle coordinates.

Definition (TSMCMC(β))

Given a triangulation T of the n-gon and associated polytope $\mathcal{P}$. If $x_k = (\vec{p}_k, \vec{\theta}_k) \in \mathcal{P} \times T^{n-3}$, define x_{k+1} by

- Update $\vec{p}_k$ by a hit-and-run step on $\mathcal{P}$ with probability β.
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At each step, construct the corresponding polygon $\alpha(x_k)$ using action-angle coordinates.

Proposition (with Cantarella)

Starting at any polygon, the m-step transition probability of TSMCMC(β) converges geometrically to the standard probability measure on $\mathrm{Pol}(n)/SO(3)$.

Error Analysis for Integration with TSMCMC(β)

Suppose f is a function on polygons. If a run R of TSMCMC(β) produces $x_1, \ldots, x_m$, let

$$\mathrm{SampleMean}(f; R, m) := \frac{1}{m} \sum_{k=1}^{m} f(\alpha(x_k))$$

be the sample average of the values of f over the run.

Because TSMCMC(β) converges geometrically, we have

[1] w denotes weak convergence, $E(f)$ is the expectation of f

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Theorem (Markov Chain Central Limit Theorem)

If f is square-integrable, there exists a real number $\sigma(f)$ so that[1]

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

the Gaussian with mean 0 and standard deviation $\sigma(f)^2$.

[1] w denotes weak convergence, $E(f)$ is the expectation of f

Given a length-m run R of TSMCMC and a square integrable function f, we can compute SampleMean$(f; R, m)$. There is a statistically consistent estimator called the **Geyer IPS Estimator** $\bar{\sigma}_m(f)$ for $\sigma(f)$.

According to the estimator, a 95% confidence interval for the expectation of f is given by

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

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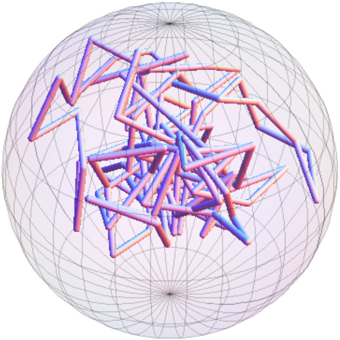
Experimental Observation

With 95% confidence, we can say that the fraction of knotted equilateral hexagons is between 1.1 and 1.5 in 10,000.

Definition

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



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*

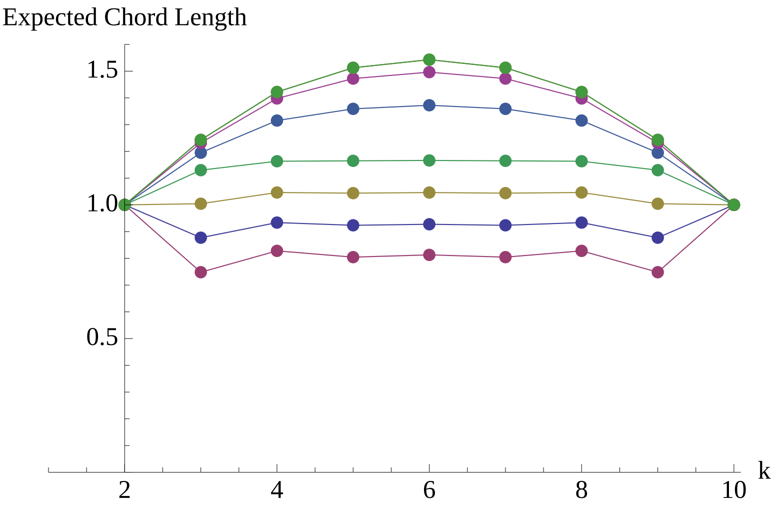
$$0 \leq d_1 \leq 2 \qquad \begin{array}{c} 1 \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq 1 \end{array} \qquad 0 \leq d_{n-3} \leq 2$$

together with the additional linear inequalities

$$d_i \leq R.$$

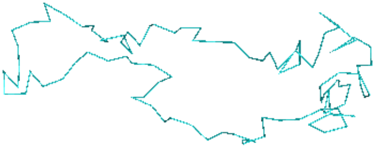
These polytopes are simply subpolytopes of the fan triangulation polytopes. Many other confinement models are possible!

Expected Chordlengths for Confined 10-gons



Confinement radii are 1.25, 1.5, 1.75, 2, 2.5, 3, 4, and 5.

Unconfined 100-gons



Unconfined 100-gons

Unconfined 100-gons

20-confined 100-gons

20-confined 100-gons

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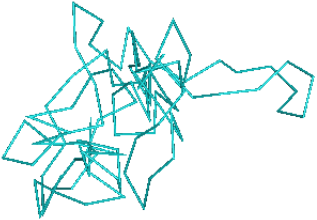
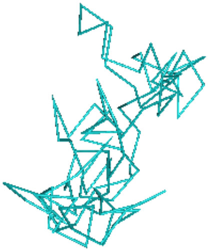
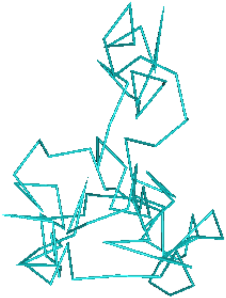


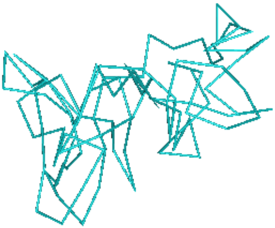
10-confined 100-gons





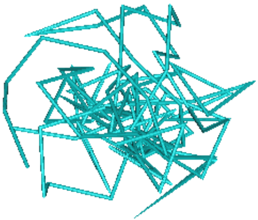
5-confined 100-gons

5-confined 100-gons

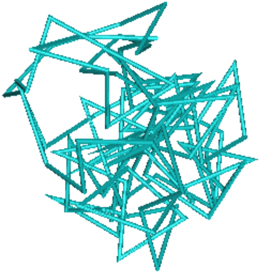


5-confined 100-gons

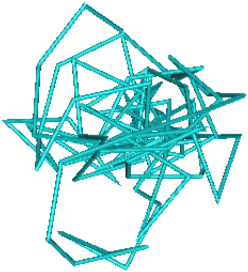
2-confined 100-gons



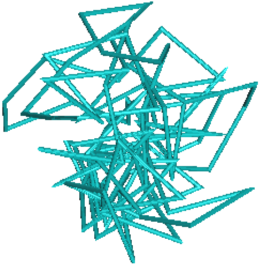
2-confined 100-gons

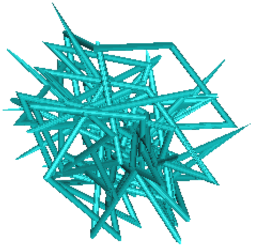


2-confined 100-gons

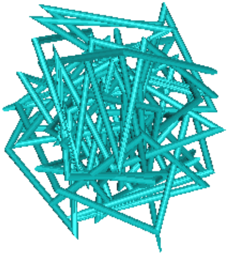


2-confined 100-gons





1.1-confined 100-gons



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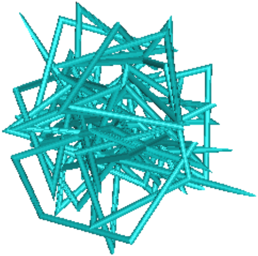

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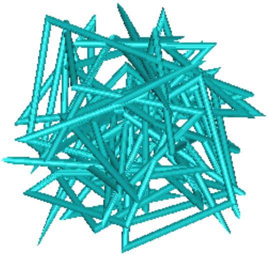

Thank you!

Thank you for listening!

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