Average Geometric and Topological Properties of Open and Closed Equilateral Polygonal Chains

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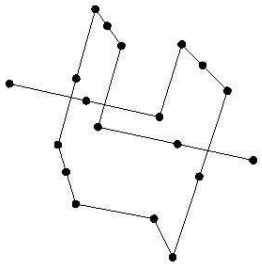
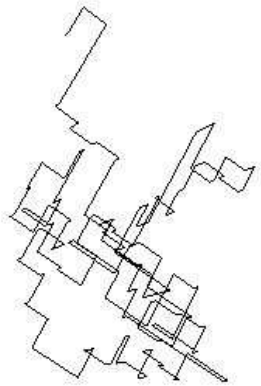


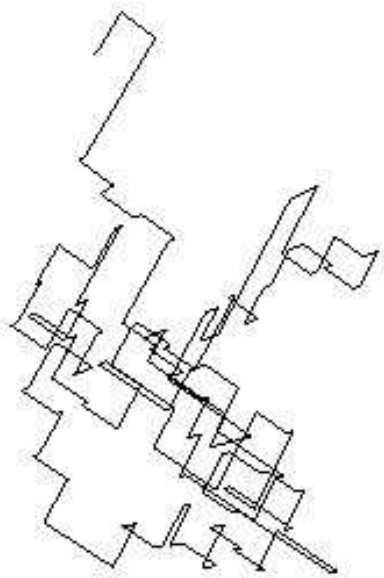


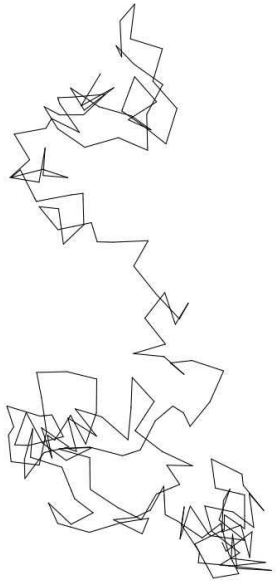
Topological Dynamics in the Physical and Biological Sciences Program

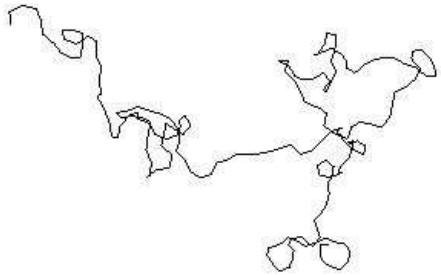
Plan

- Self-Avoiding Random Walks on the Cubic Lattice and in 3-space
- Geometric and Topological Properties: ETE, SRGN, Knots and Slipknots
- Frisch-Wasserman Delbruck Conjecture: Sumners-Whittington, Pippenger, Millett Theorems
- Monte Carlo Markov Chain Sampling
- Ergodicity: Kron, Lal, Madras-Sokal, Reiter
  - Naive, Reptation, Pivot, Local vrs Multilocal Methods, Inchworm (Reiter + M)
  - Thickness Preserving (Zirbel 2012)

Random walks on the cubic lattice and in 3-space







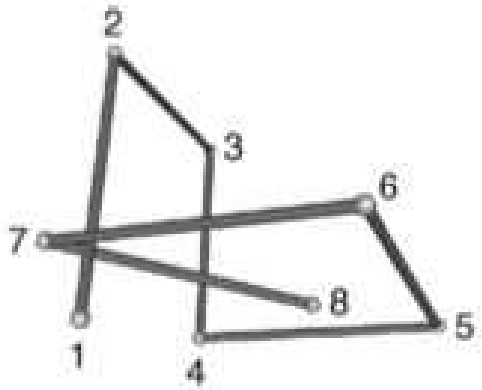
Quantities of Interest

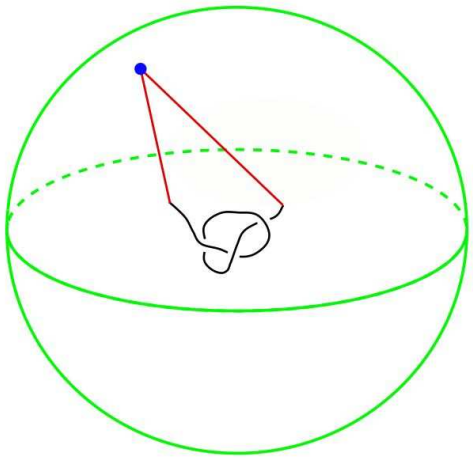
- End-To-End Distance
- Squared Radius of Gyration
- Size and Shape of Knot Locus

Knots in open curves

Reference: Millett, Dobay and Stasiak, "Linear Random Knots and Their Scaling Behavior". *Macromolecules*, **2005**, 38, 601–606.

- Center of mass of open curve at origin (vertices have unit mass)
- Close ends of open curve to random points on "sphere at infinity"

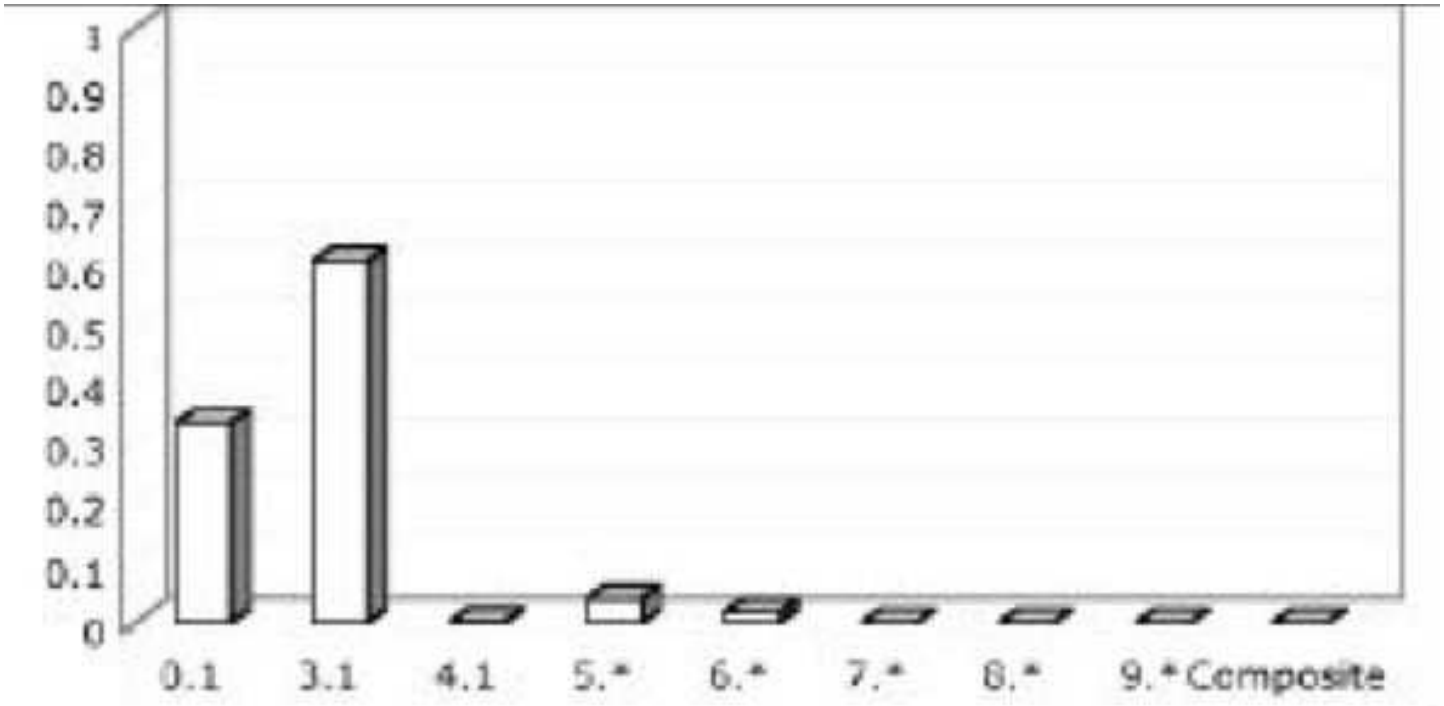




Knots in open curves

Definition

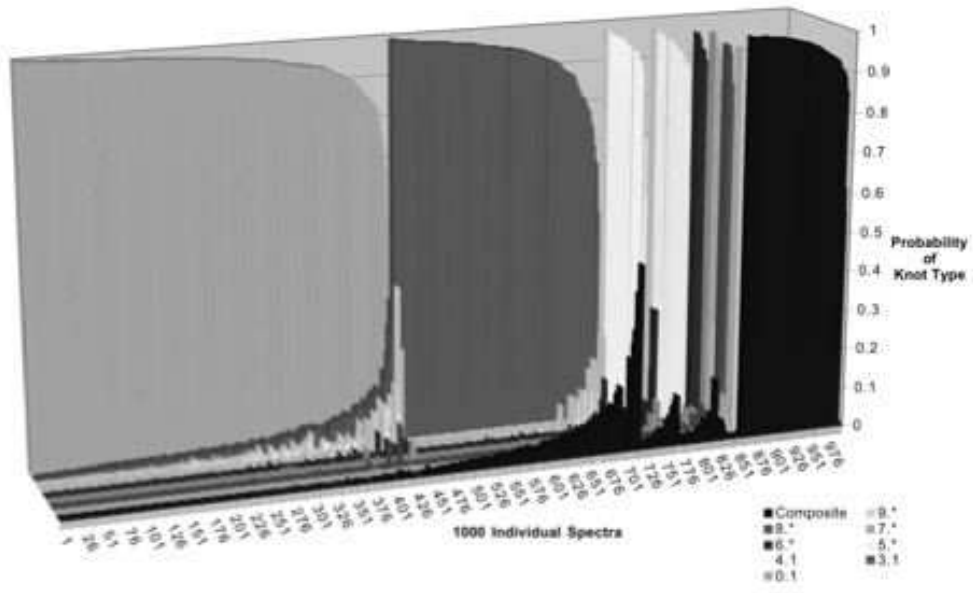
- Analyze statistics of resulting HOMFLY polynomials to determine the "spectrum"
- A knot type is determined by plurality, i.e. the "winner'" is the one with the most votes
  - Alternatively, one may require a majority selection, i.e. 50%



Knots in open curves

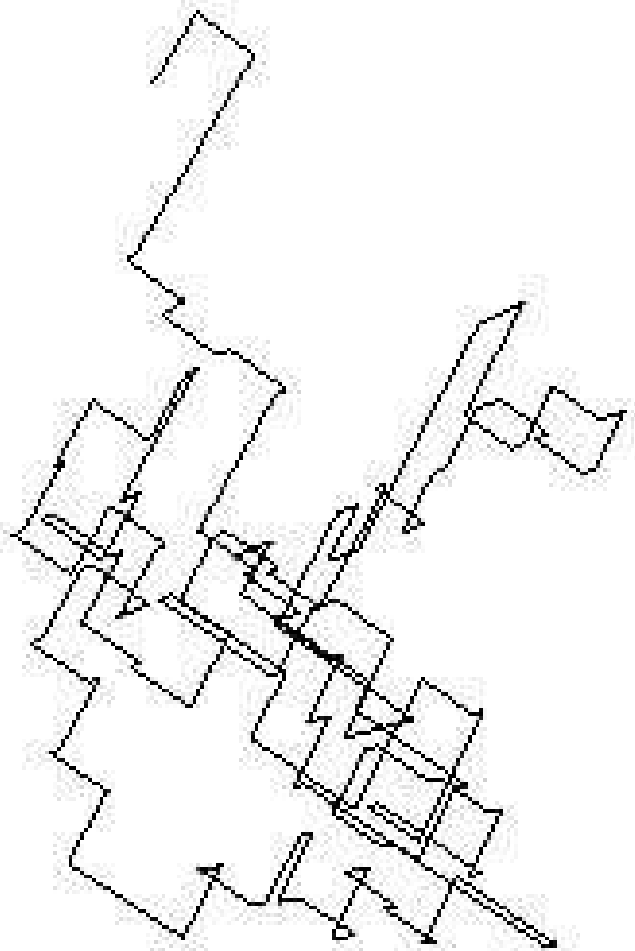
How well does this work in practice? Millett & Sheldon, Physical and numerical models in knot theory, Ser. Knots Everything, (36) 2005, World Scientific Pub, pp 203-217.

- Captures the principal knotting: only 4 cases of 1000 of length 50 failed to have a knot type appearing more than 50%
- 86.1% of the walks showed the same knot type for more than 90% of random closures



Frisch-Wasserman Delbruck Conjecture (1961-2)

With increasing length, the probability that a random walk or polygon contains a knot goes to one.



Sumners-Whittington, Knots in self-avoiding walks, J Phys A, 1998, 21(7), 1689-1694.
Pippenger, Knots in random walks, Discrete Appl Math, 1989, 25(3), 273-278.

Theorem

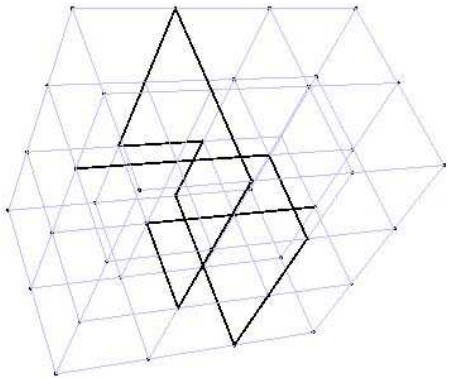
All except exponentially few sufficiently long self-avoiding polygons and random walks on the simple cubic lattice contain a knot of any given topological type.

Corollary

The probability that a random walk or polygon in the simple cubic lattice contains a knot goes to one as the number of edges goes to infinity.

Key idea of the proof

- There is a "tight trefoil" knot in the simple cubic lattice (31.4% 0_1 *and* 68.6% 3_1):



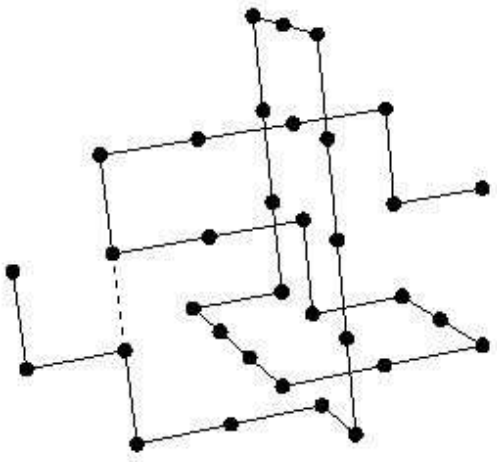
- Once a tight knot is tied in the simple cubic lattice it can't be untied.

"Open" Knots, Ephemeral Knots, and Slipknots

- A segment in a random walk or polygon whose knotting spectrum contains a knot type occurring a plurality of the time is said to have that *open knot type*.
- A segment in a random walk or polygon which is knotted and is contained in an unknotted segment is an *ephemeral knot*.
- An unknotted segment in a random walk or polygon containing an ephemeral knot is a *slipknot*.

A Tight Lattice Slipknot

- There is a "tight trefoil slipknot" in the simple cubic lattice
  slipknot : $86.7\%\ 0_1,\ 13.1\%\ 3_1$
  ephemeral knot : $6.3\%\ 0_1, 92.76\%\ 3_1, 0.44\%\ 4_1, 0.47\%\ 5_1$



Millett, Knots, slipknots, and ephemeral knots in random walks and equilateral polygons, JKTR, 2010, 19(5),6-1-615.

Theorem

All except exponentially few sufficiently long (self-avoiding) walks or polygons in the simple cubic lattice (or $\mathbf{R}^3$) contain an ephemeral knot and its associated slipknot, of any fixed topological type,.

Corollary

The probability that a (self-avoiding) random walk or polygon in the simple cubic lattice (or $\mathbf{R}^3$) contains an ephemeral knot and its associated slipknot, of any fixed topological type, goes to one as the length goes to infinity.

A Curious Consequence

Corollary

The probability that a knotted self-avoiding random walk or polygon in the simple cubic lattice (or 3-space) contains a slipknot goes to one as the length goes to infinity.

Theorem Opportunity

But we don't know how to prove the clearly true statement: "The probability that an unknotted self-avoiding random walk or polygon in the simple cubic lattice (or 3-space) contains a slipknot goes to one as the length goes to infinity."

Monte Carlo Markov Chain Sampling of Configuration Space

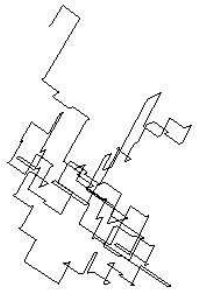
$(MC)^2$ Sampling

One seeks an algorithm, including a random walk, for sampling the configuration space by creating a Markov chain having the probability distribution as its equilibrium distribution. Among the key issues are the precise distribution on the configuration space and the knowing the algorithm gives a Markov chain, e.g. knowing that the samples do not depend upon the previous samples. In a random walk this translates into know the number of steps one must take in order to have independence.

Ergodicity

Superficially, one must know that every configuration is accessible and a bit more concerning the probabilities of steps, e.g. "detailed balance."

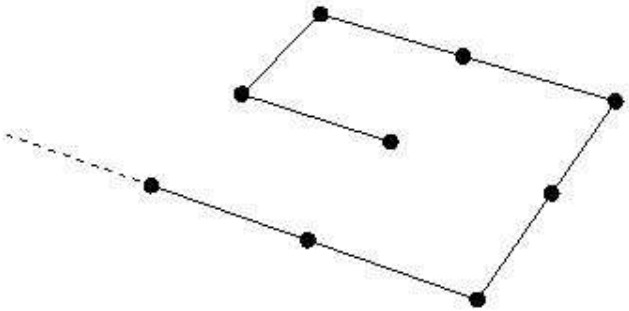
Self-avoiding Walks (SAWs) on the cubic lattice



Generation of SAWs

- Naive Growth Method (random growth of SAW til length n)
- Reptation: Kron et al (1965) (replace the initial step with an additional random step at terminus)
- Pivot: Lal (1969) (apply a lattice symmetry to random terminal segment), Madras-Sokal (1988)
- Local/non-local: Madras-Sokal (1987) (simultaneous moves in two or more subsegments)
- Bilocal: Reiter (1990) ("kink move" plus extension/truncation)

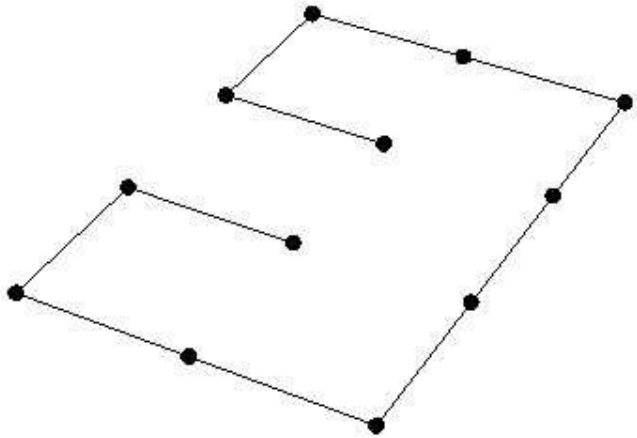
SAWs on the cubic lattice



Generation of SAWs: Naive Growth Method

- Random growth of SAW from origin until target length n
- While every SAW can be reached, the likelihood of barrier conformations increases and renders the Naive Growth Method worrisome.
- Estimations of the proportion of barrier conformations are known.

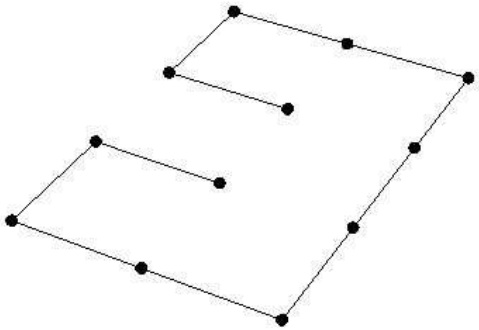
SAWs on the cubic lattice

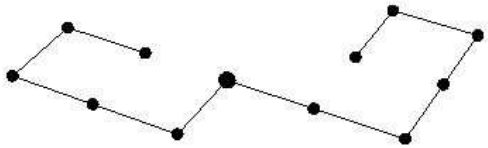


Generation of SAWs: Reptation Method (Kron 1965)

- Successive replacement of the initial step by an additional random step at the terminus.
- The Reptation Method begins with a configuration of the desired length but can encounter obstacles.
- There are SAWs which can not reached.

SAWs on the cubic lattice





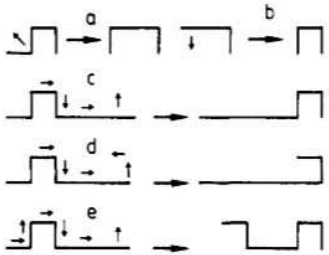
Generation of SAWs: Pivot Method (Lal 1969)

- Apply a lattice symmetry to random terminal segment if allowed.
- The Pivot Method begins with a configuration of the desired length and applies a sequence of pivots.
- Madras & Sokal (1988) prove that the Pivot Method is ergodic.

SAWs on the cubic lattice

Generation of SAWs: Local versus Non-local Moves

- Madras & Sokal (1987) prove that local modifications of a SAW can not be egrodic. The Pivot Method is not local.
- In order to overcome this problem, methods must include distal modifications. Key example is found in Reiter (1990).

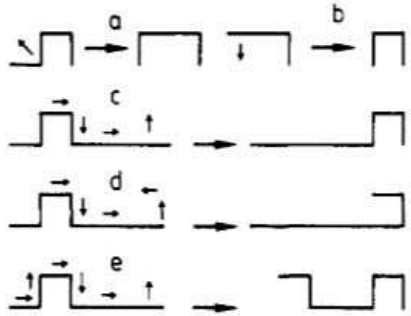


- These bilocal methods begin with a configuration of the desired length and apply a sequence of permitted moves.
- By extending the methods of Madras & Sokal (1988), Reiter proved that they are ergodic.
- In this algorithm, removals occur first leaving space for growth;-{

SAWs on the cubic lattice

Generation of SAWs (Millett 2011)

One must take care to insure that the moves correspond to "physical" movements of chains. Movement prior to the elimination of conformational barriers should not be allowed.

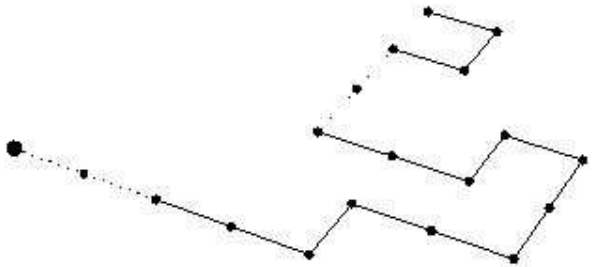


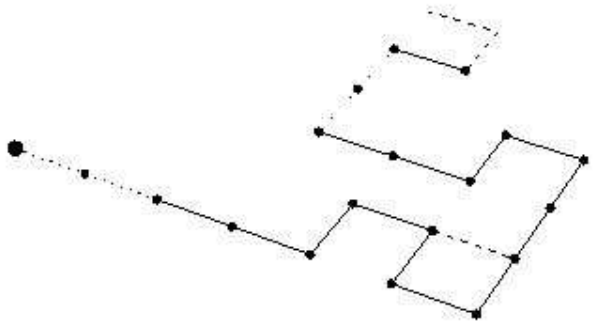
- A new algorithm avoiding these problems follows from a few observations;
  - reptation moves are not necessary and
  - requiring growth before or simultaneously with removal still provides an ergodic method so we are once again happy.;-}

SAWs on the cubic lattice

Generation of SAWs

Inchworm Method consist in the creation of a permitted "kink" with an associated two step shortening of the terminus of the walk or it's inverse, i.e. the elimination of a "kink" and the permitted random addition of two steps at the terminus of walk if the space is available in the initial configuration.

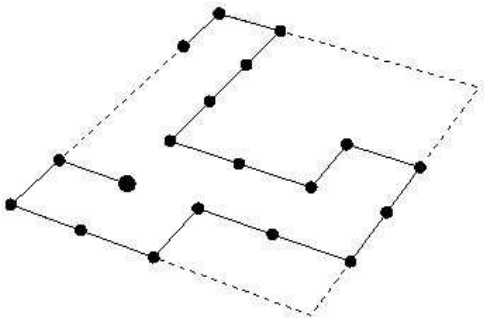


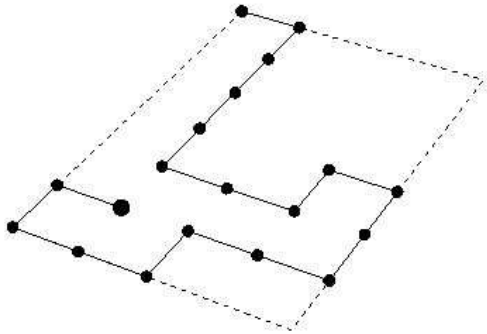


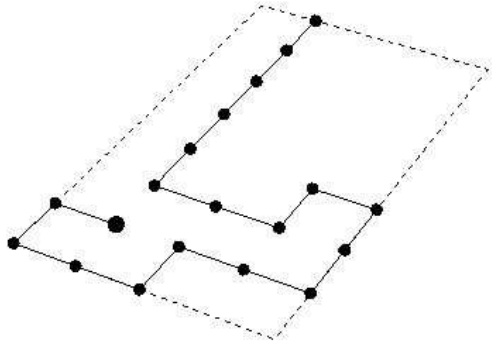
SAWs on the cubic lattice

Generation of SAWs: The Inchworm Observations (KCM 2011)

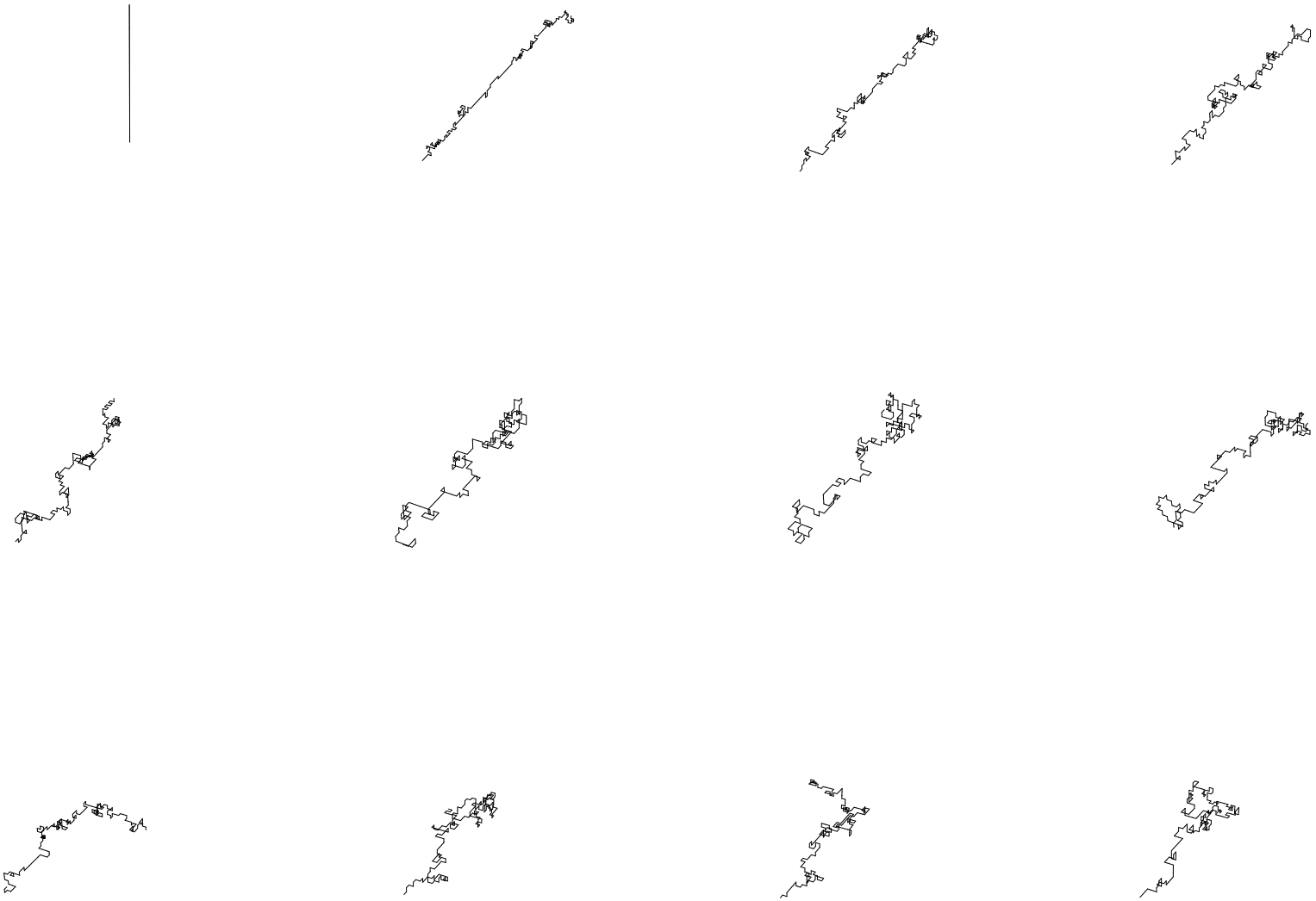
- Inchworms mimic physical movements.
- Inchworms are ergodic.
- Proof works in all dimensions.



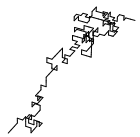


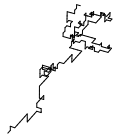


Watching the Inchworm in action I



Watching the Inchworm in action II





Ergodic inchworm on the cubic lattice

We are hoping to have a movie of an inchworm in action here

Eventually, inchworms tie themselves in knots. What kind of knots? They must also "unknot." How long do these take, on average?

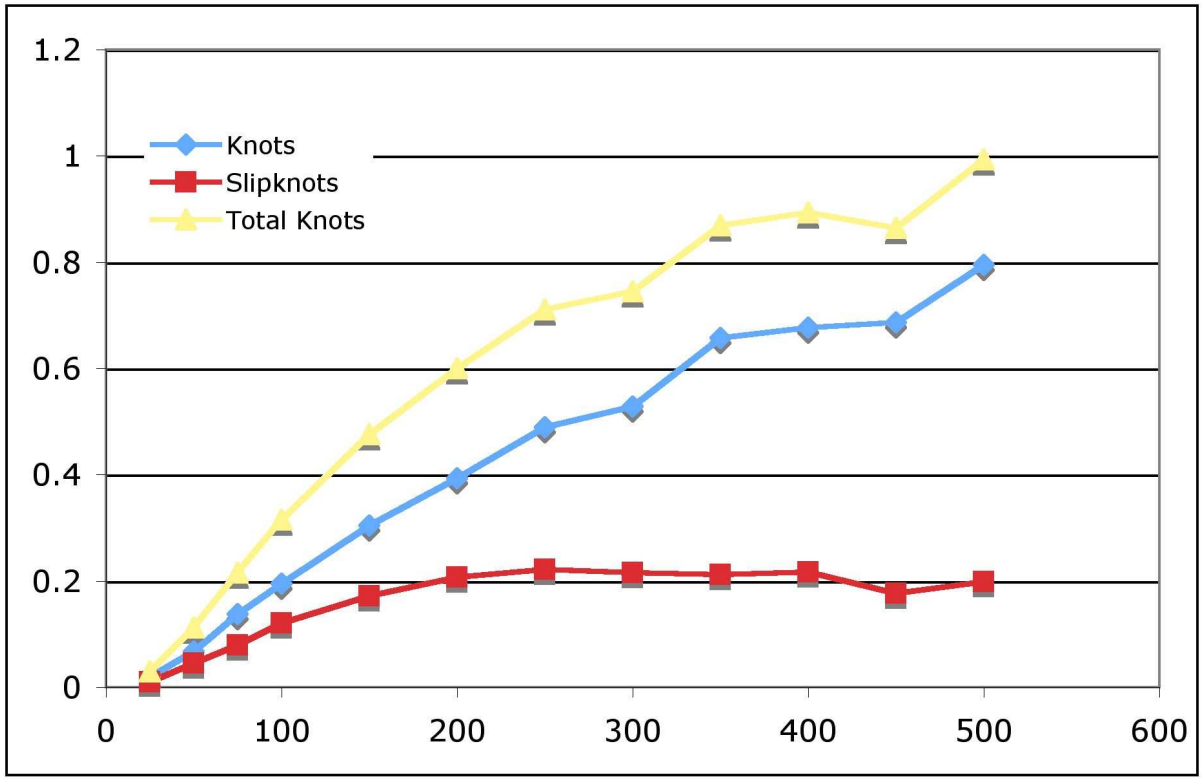
- Very roughly, there are 3328 distinct 22-step open lattice trefoils and there are $1.1x10^{15}$ 22-step SAW's.
- The autocorrelation time seems to be approximately $2.0x10^{6}$ for a 200-step SAW.
- Or 10^{4} if operations were restricted to the 22-step tail.

In mildly constrained 200 step SAW's we have observed knot persistences of, on average, 34.76 steps:

$$14, 1, 18, 4, 1, 16, 102, 1, 10, 11, 2, 60, 147, 9, 151, 9$$

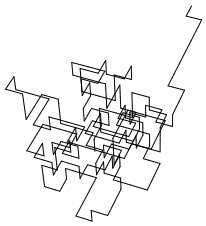
Knots and Slipknots in 3-Space Random Walks

The proportion of walks containing a knot or a slipknot as a function of the number of steps.



SAWs on the cubic lattice

Knotty 200-step mildly constrained Inchworms



3-space random walks

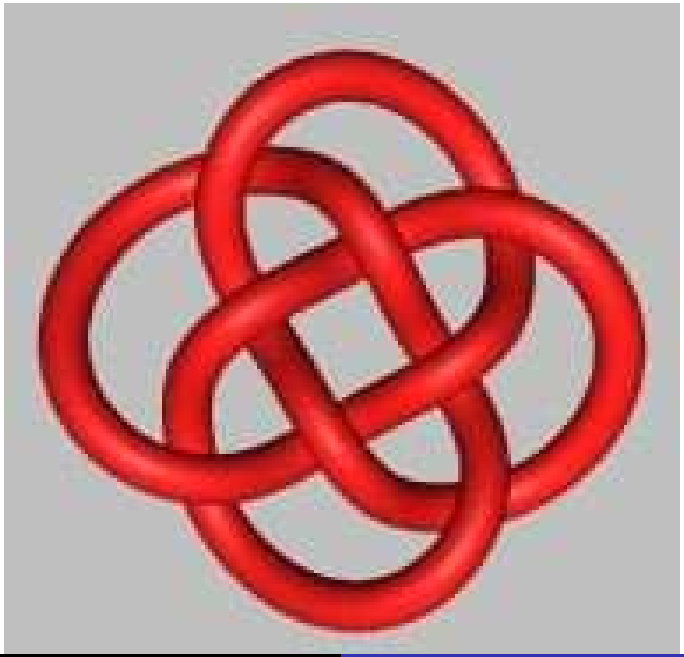
In order to reflect some of the structure explicit in lattice SAW's, we must impose an excluded volume constraint. This will be our next topic.

Excluded volume of a chain or polygon

Embedded Normal Tube

The key idea is that of an embedded solid tube centered on the conformation. Its maximum radius gives the (unnormalized) thickness of the chain or polygon. It depends upon, and is determined by,

- the minimal vertex curvature (to prevent local pinching)
- the distance between distant segments



The Space of Thick Random Walks and Polygons

Polygonal Knot Space, PKS, can be partitioned by "thickness"

- Thickness is continuous on PKS
- Define PKS_τ to be those conformations whose thickness is not smaller than τ.

Objective: Randomly Sample PKS_τ

- What is the average geometry of thick conformations?
- How does knotting and slip knotting depend upon τ?
  - Thick short conformations are never knotted.
- How does the "shape" of knots and slipknots depend upon τ?

Randomly Sample PKS_τ

For closed polygons

- this is a really hard problem.
- The "naive" method (using polygonal folds or crankshafts) works asymptotically but it can be and likely is a very very long wait for statistically significant results.
- Other "faster" approaches lack rigorous theoretical foundation.

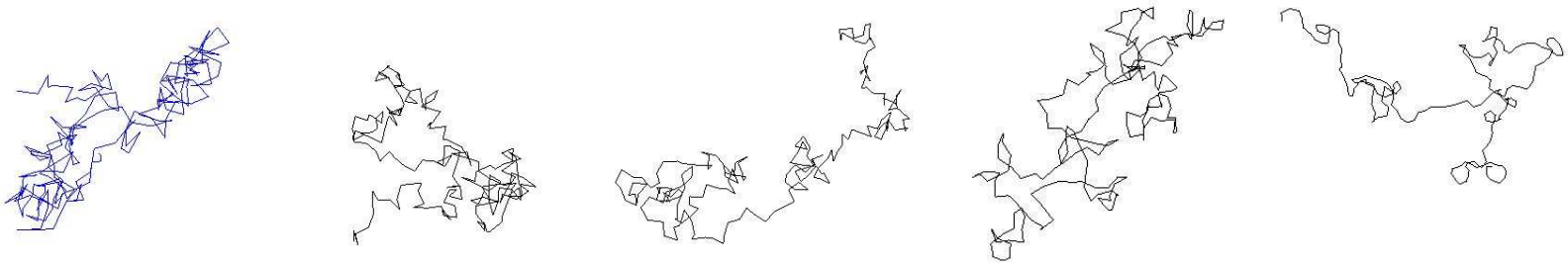
For random walks

- the "naive" method works asymptotically as above, but fortunately we have new strategy: Laura Zirbel's ergodic 3-space reflection method.

Thick Random Walks in 3-space

Some different types of random walks

Ideal random walks have no constraint other than being self-avoiding. As soon as a thickness constraint is imposed, one expects significantly different average structures as measured by the radius of gyration, end-to-end distance, and the presence and nature of knots. Here are examples of ideal walks and those with thickness at least $0.1, 0.2, 0.3, \textit{and}\ 0.4$, respectively



Laura Zirbel's 3-Space Walk Reflection Method

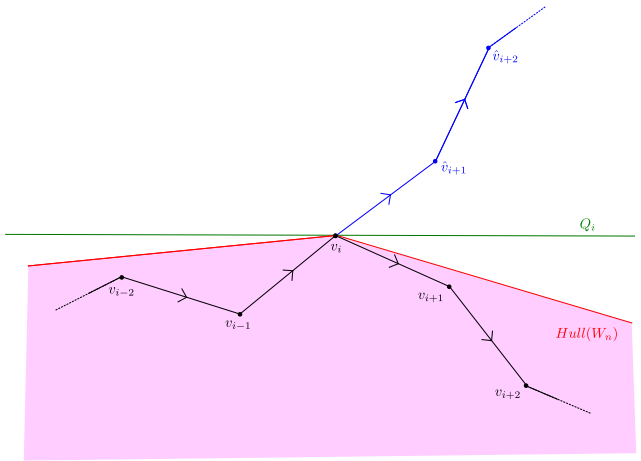
Outline

- Suppose one is given any walk, W, of n steps of thickness τ, i.e. a conformation in PKS_τ
- We describe a finite sequence of elementary operations on walks that never decrease τ and which we then prove ends at the straight rod conformation.
- We show that these operations give a Markov Chain Random Walk that never decreases thickness thereby defining a walk in PKS_τ.

Laura Zirbel's 3-Space Walk Reflection Method

Single Reflection Moves

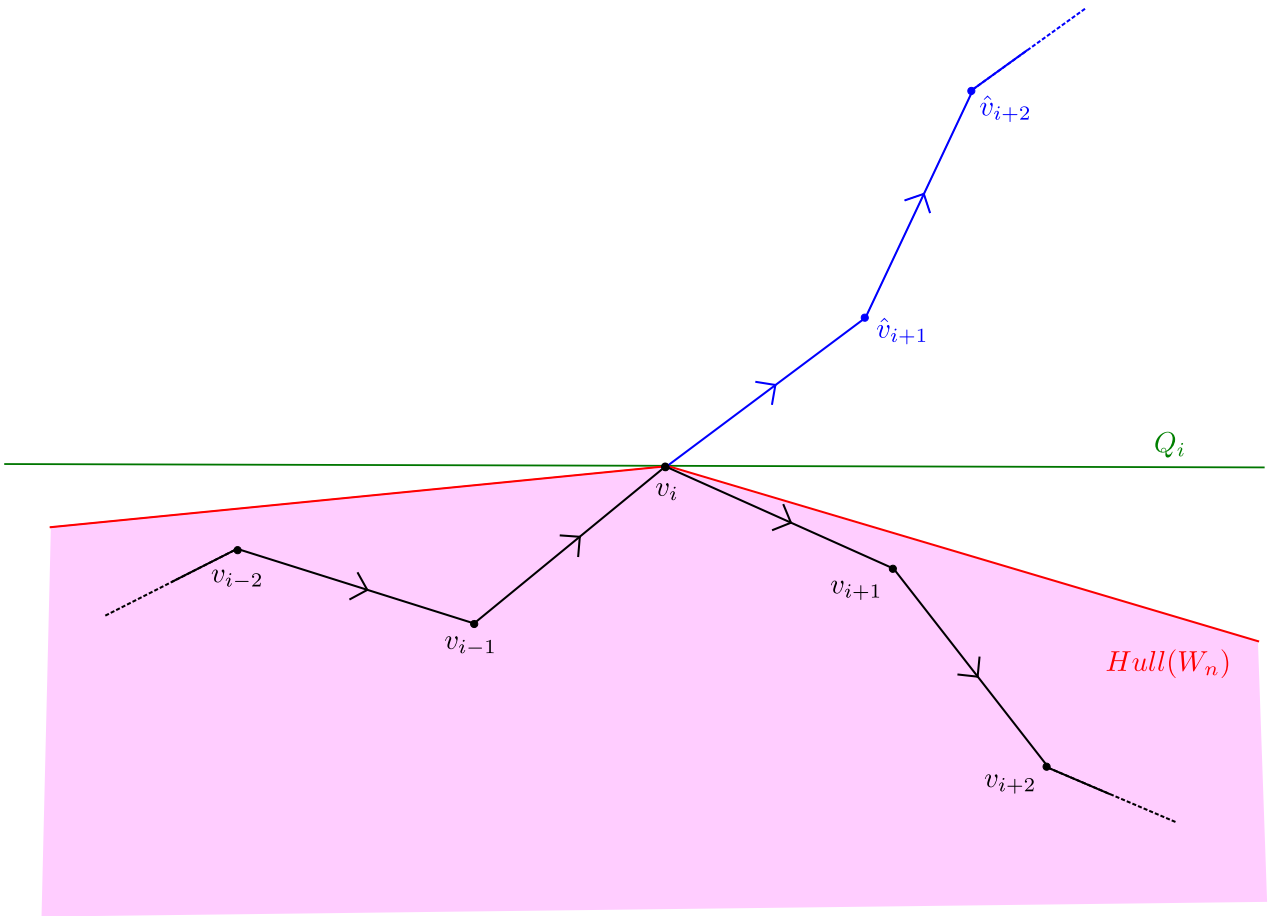
- On the surface of the *convex hull of W*, select a vertex v_i and consider the plane, P, determined by $v_{i-1}, v_i, and\ v_{i+1}$
- Select a plane, Q_i, containing v_i and having the convex hull on one side.
- Define the associated "single reflection move" by taking the vertices $v_{i+1}, v_{i+2}, \ldots$ to their mirror images through the plane Q_i thereby defining a new configuration W'



Laura Zirbel's 3-Space Walk Reflection Method

Single Reflection Moves

The thickness of W' is not smaller than that of W



Laura Zirbel's 3-Space Walk Reflection Method

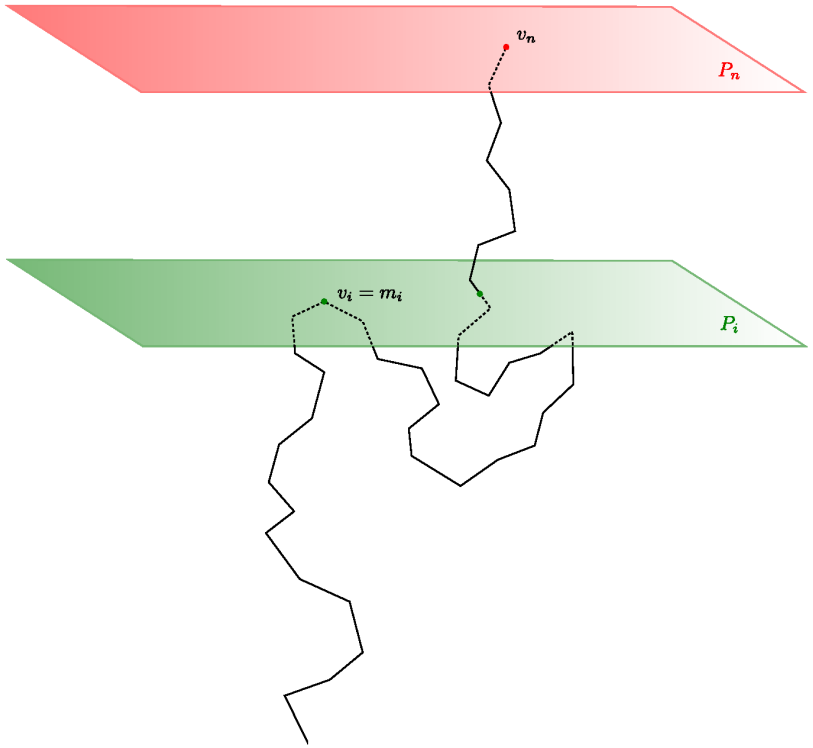
Double Reflection Moves

As in sports, mastery of a single move is not sufficient. One must master the double move as well. Using a series of "single reflection moves" we the two termini on the surface of the convex hull determining its diameter. The diameter is, of course, bounded by the number of steps....we wish to increase the diameter until there are no longer any local maxima or minima with respect to the axis determined by the termini. Such conformations, though not yet linear, are can be made so by careful adjustments to the turning angles that do not decrease thickness.

Laura Zirbel's 3-Space Walk Reflection Method

Double Reflection Moves

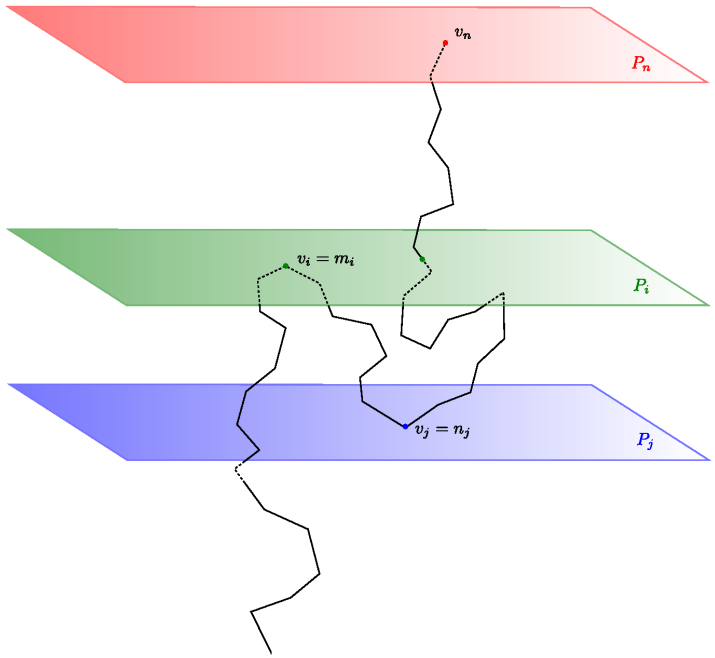
Let P_n be the separating plane containing the terminal vertex v_n and P_i be the parallel plane containing the local maximum vertex such the distance between the planes is the smallest.



Laura Zirbel's 3-Space Walk Reflection Method

Double Reflection Moves

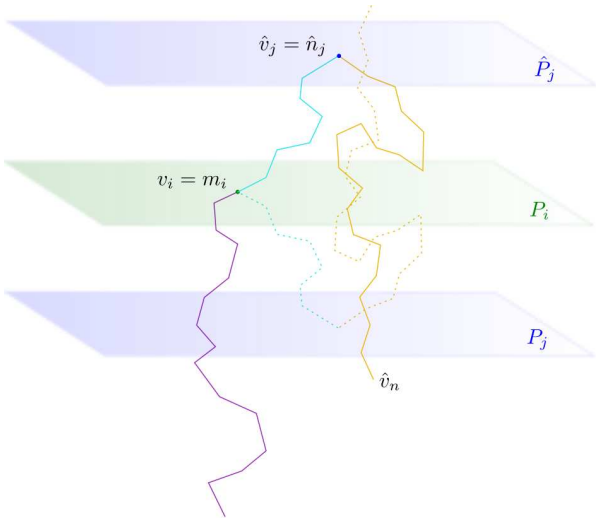
Between v_n and v_i there must be a local minimum vertex v_j whose parallel plane P_j is furthest from P_n among such. The first step in defining the double reflection is to reflect the terminal segment through P_i.



Laura Zirbel's 3-Space Walk Reflection Method

Double Reflection Moves

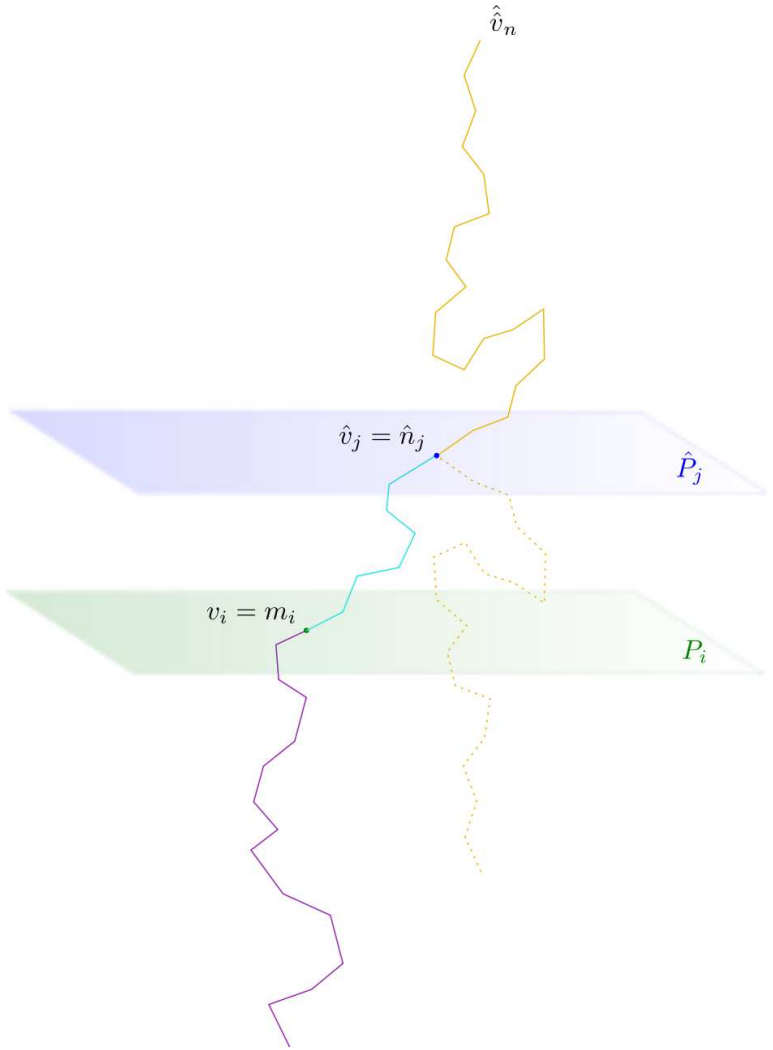
The second step in defining the double reflection is to reflect the terminal segment of the result of the first reflection through the plane defined by the reflected image of P_j from the first step. The result is the "double reflection" of our initial configuration.



Laura Zirbel's 3-Space Walk Reflection Method

Double Reflection Moves

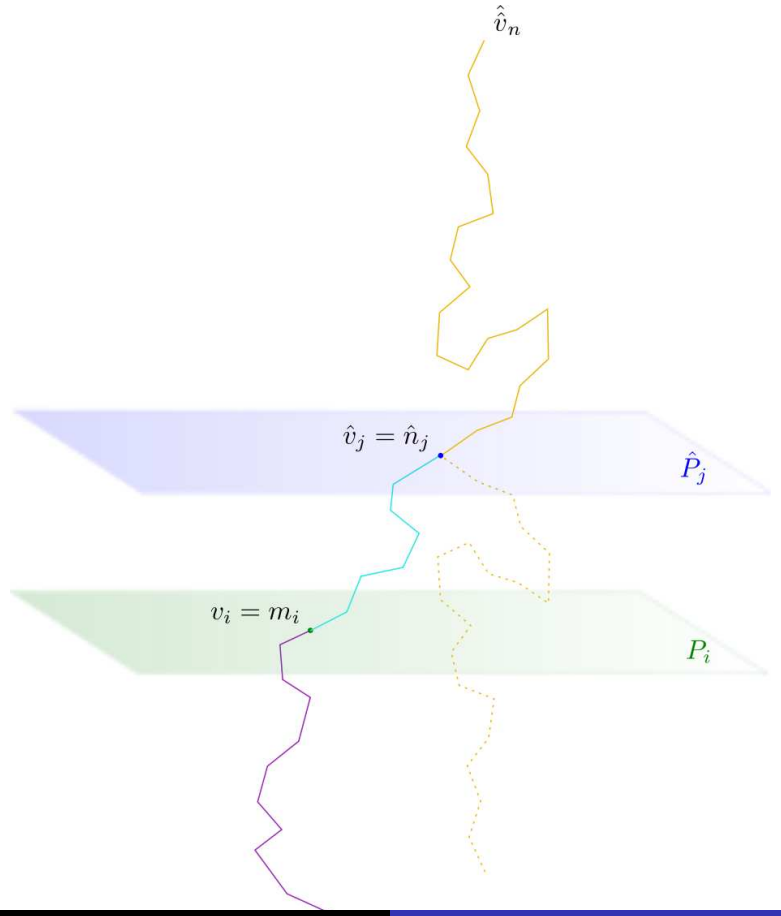
The thickness of the result is no smaller than that of the start.



Laura Zirbel's 3-Space Walk Reflection Method

Single and Double Reflection Moves

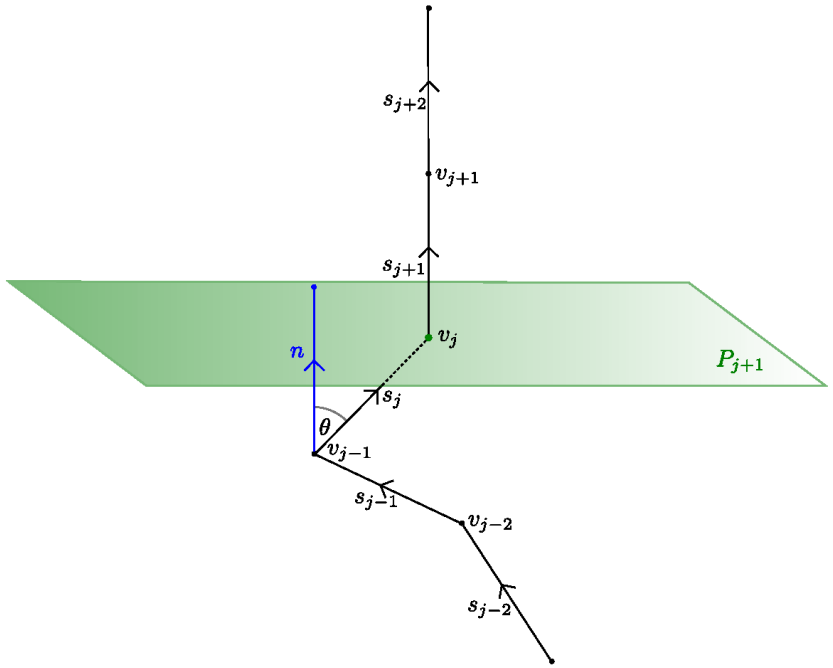
By employing these, one arrives at conformations with termini on the surface of the convex hull and without critical points with respect to the diameter connecting the termini.



Laura Zirbel's 3-Space Walk Reflection Method

Single and Double Reflection Moves

By employing these, one now straightens the walk to a rod.



Laura Zirbel's 3-Space Walk Reflection Method

Single and Double Reflection Moves

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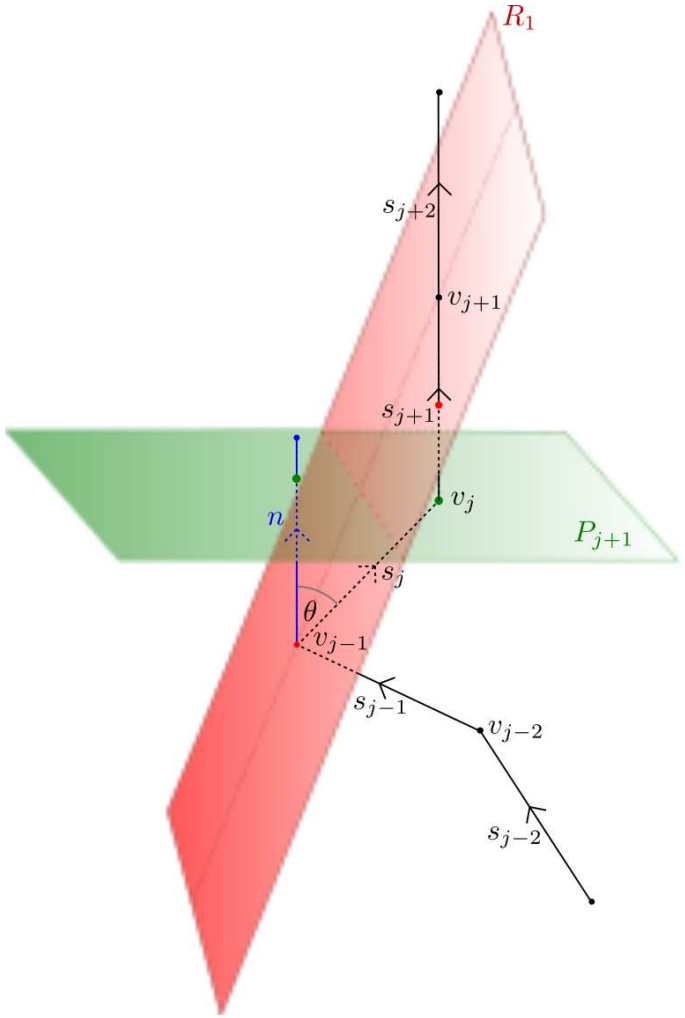

Laura Zirbel's 3-Space Walk Reflection Method

Single and Double Reflection Moves

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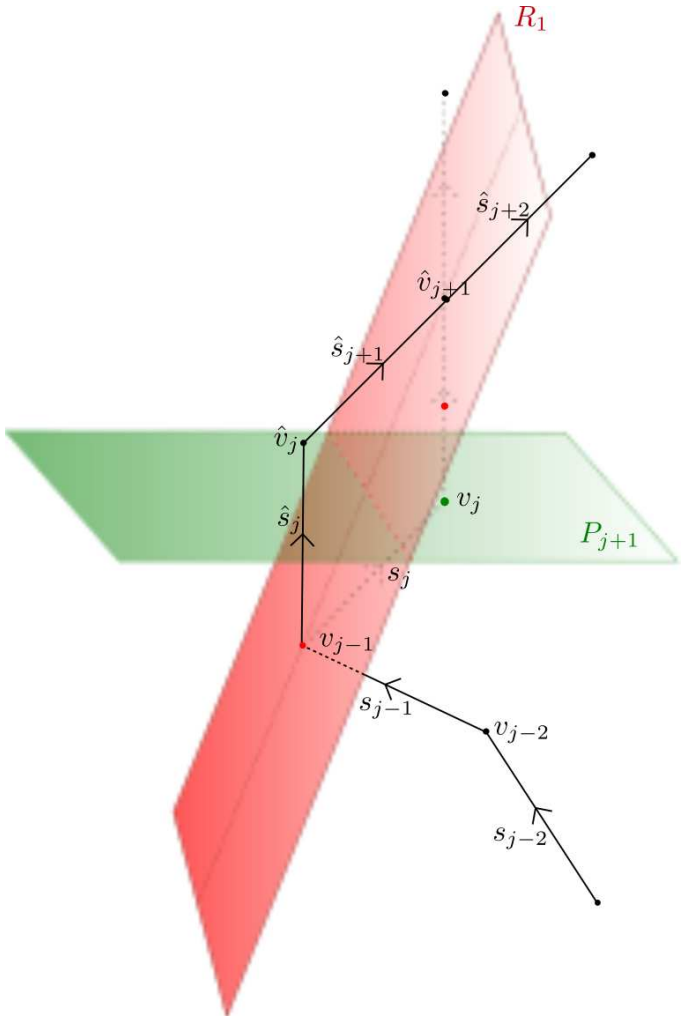

Laura Zirbel's 3-Space Walk Reflection Method

Single and Double Reflection Moves

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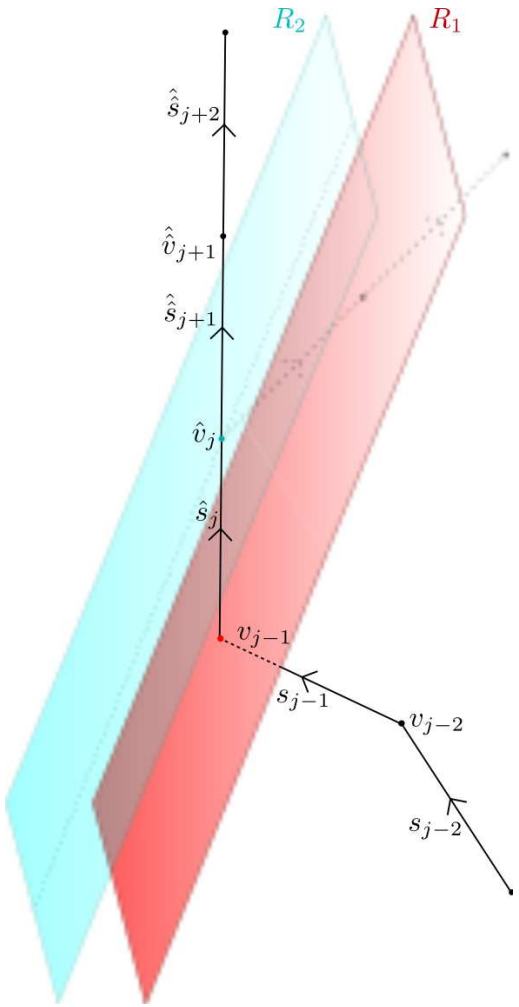


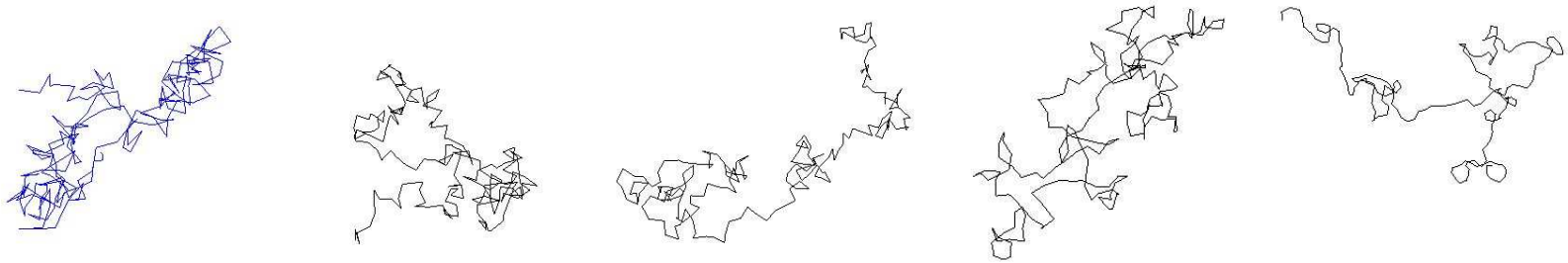
Laura Zirbel's 3-Space Walk Reflection Method

Theorem: L Zirbel 2012

The reflection method is ergodic.

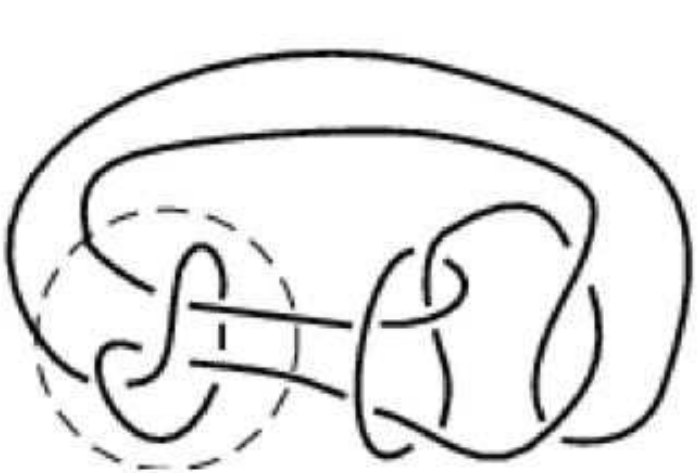
Thick Walk Generation Algorithm

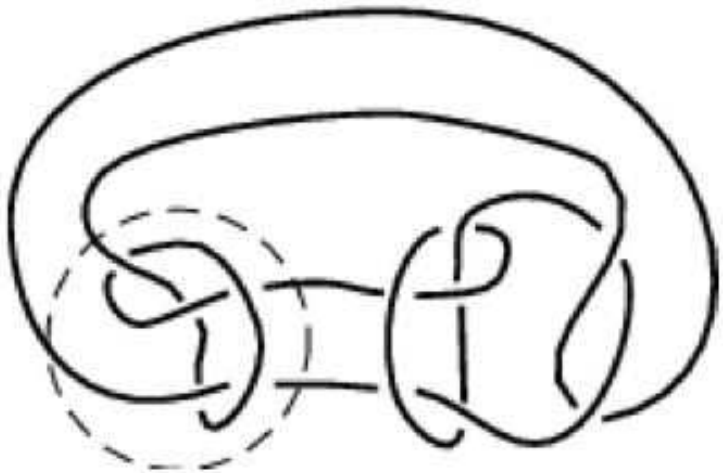
The basic step consists of randomly selecting one or two vertices of a conformation, determining the locally allowable reflection plane (in order to not violate the target thickness constraint), and checking that the resulting conformations do not violate the distal thickness constraints.



Trefoil Slipknots: Two trefoil slipknots in 12 crossing presentations of the Conway and Kinoshita-Terasaka knots

The Kinoshita-Tereasaka and Conway Knots





are constructed from two trefoil slipknots

Thanks to my collaborators on this research

- Laura Zirbel
- Alex Lin
- Eric Rawdon
- Akos Dobay
- Andrzej Stasiak

Thank you

- to the Isaac Newton Institute for Mathematics Sciences
- to the Topological Dynamics in the Physical and Biological Sciences Program for making my splendid visit possible
- and to you, for your attention.