The Kavli Institute for Theoretical Physics University of California, Santa Barbara Knotted Fields Appreciation of the Classical Approach to Knots From 1833 to 1990

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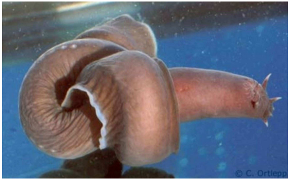
Outline

An appreciation of the classical approach to knotting in the mathematical and natural sciences with an eye on a few historical events.

- Origins of knotting, linking and, entanglement
- Mathematical knotting and linking: Gauss, Kelvin, Alexander
- The Jones era: Jones, HOMFLY, BLMH, Kauffman
- Applications in the natural sciences
- Discussion

In Nature

- Living organizimes employ knotting and entanglement to accomplish important tasks.
- The hagfish uses a knotted configuration to gain leverage in order to feed or as a defensive strategy.
- Vines use linking and entanglement to stabilize their positions during growth
- The presence of knotting, linking, and other forms of entanglement can be observed widely in nature.



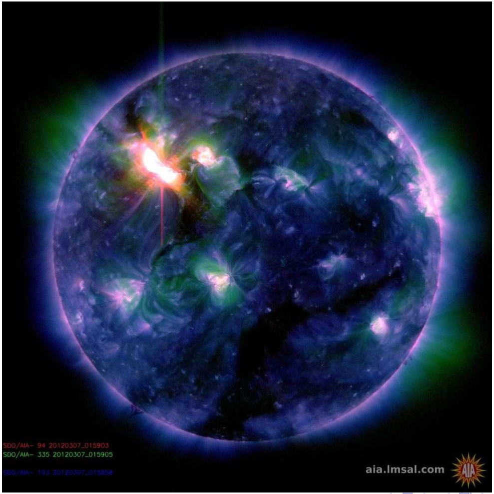
Human uses

- Knots can be found in the reminants of Finnish fish nets made of nettle fibers 10,000 years ago. The photo shows rock weights and bark floats.
- While some origins are utilitarian others, such as this Celtic knot, are decorative or have a religious interpertation.

Origins of knotting

An the earliest manifestations

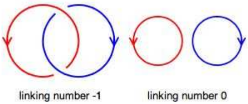
Entanglement of solar flares on March 6, 2012 (NASA/SDO/AIA)



Gauss Linking Number

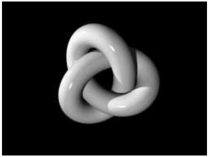
In 1833 Johann Carl Friedrich Gauss developed an integral formula that defined the linking number between two oriented simple closed curves in space, thereby initiating the mathematical study of knots and links.

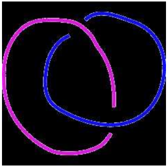
$$\text{linking number} = \frac{1}{4\pi}\oint_{\gamma_1}\oint_{\gamma_2}\frac{\mathbf{r}_1-\mathbf{r}_2}{|\mathbf{r}_1-\mathbf{r}_2|^3}\cdot(d\mathbf{r}_1\times d\mathbf{r}_2).$$



Vortex knots leads to knot identification and enumeration problems

Lord Kelvin (Sir William Thomson) and Peter Guthrie Tait were inspired by the work of Helmholtz and Maxwell to propose vortex tubes forming different knots and links as models for atomic structure. Building on the work of Gauss and his student, Listing, the classification of knots was undertaken. The unknotted ring was to represent oxygen while the simplest knot, the trefoil, was carbon and the Hopf link was to be sodium.
The absence of "ether" ended this vision.

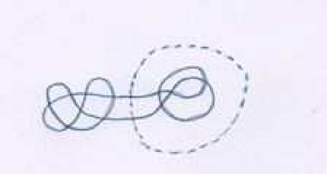


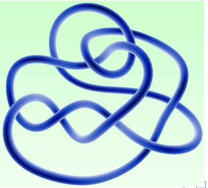


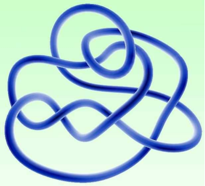
Nevertheless, the mathematical study of knotting and linking continued with its on life.

Enumeration

- Equality means we can move one configuration to the other in space
- Composition (connection sum) defines a monoid with the unknot as identity but without inverses.
- Enumeration focuses on irreducible, or prime, knots.
- P.G. Tait, in the late 1800's, began the systematic classification of prime knots with effort continuing to this day.

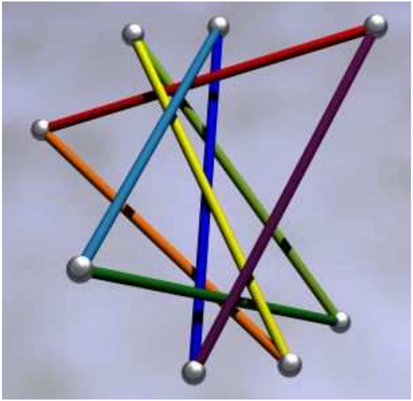






Polygonal Knots

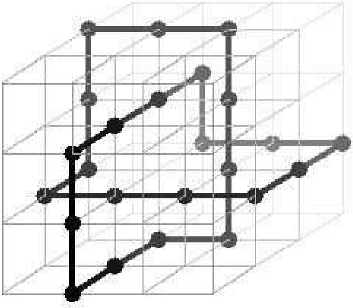
- Defined by an ordered sequence of n vertices in 3-space
- Connected cyclically by straight line segments called edges
- Two edges meet, if at all, at their common vertices



Mathematical Knotting and Linking

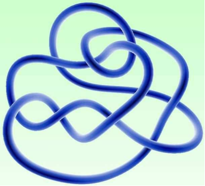
Lattice Knots

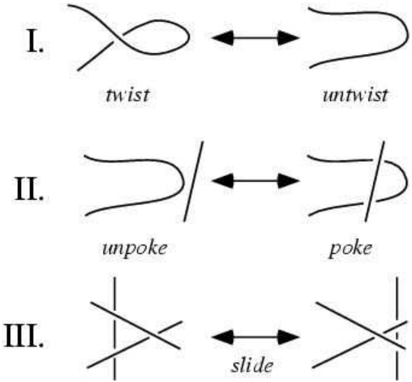
- Defined by an ordered sequence of *n* adjacent non-repeating vertices in simple cubic lattice
- Require the first vertex be adjacent to the last vertex
- Connect vertices cyclically by their adjoining edges



Knot and Link Presentations

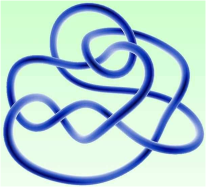
- Choose a projection of the knot or link orthogonally to a plane in 3-space
- which is generic:
  - For smooth knots: the projection does not annihilate any tangent vectors, at double points the images of the tangent vectors are distinct, and there are no triple points
  - For polygonal knots, vertices project 1-1, no edge interior image intersects a vertex, edge images intersect only in the interiors at discrete points, and there are no triple points





Theorem (Reidemeister 1926)

Two knots or links are ambient isotopic if and only there is a finite sequence of elementary Reidemeister moves, shown above, taking a presentation of the first to a presentation of the second.



But it's not so easy as one might hope

Indeed, determining whether an presentation represents the unknot is, in a very formal sense, a very hard problem!

Census organized by "complexity"

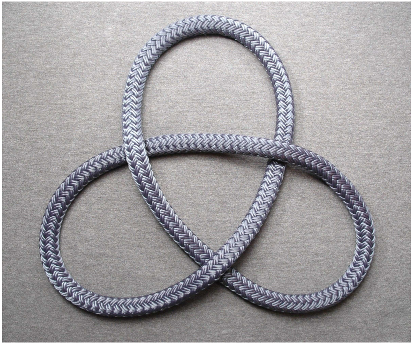
- The crossing number of a knot, *Cr(K)* is the fewest number of crossings appearing in a presentation of the knot

The "Unknot" or Trivial Knot

- Standard representative is a round circle
- Crossing number is 0. The unknot is designated by 0_1 denoting the first knot in the tabulation having 0 crossing

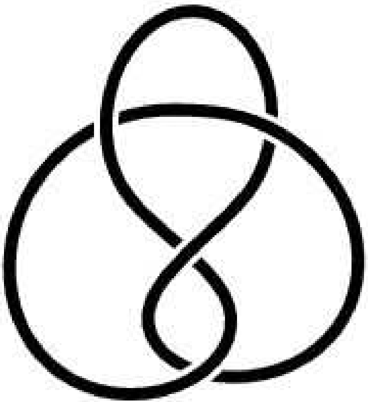
Three crossings

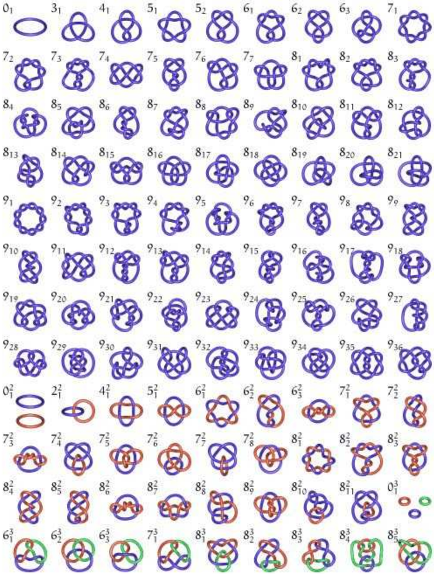
- The trefoil knot, 3_1



Four crossings

- The figure eight (or Listing's) knot, 4_1




0_1 3_1 4_1 5_1 5_2 6_1 6_2 6_3 7_1
7_2 7_3 7_4 7_5 7_6 7_7 8_1 8_2 8_3
8_4 8_5 8_6 8_7 8_8 8_9 8_{10} 8_{11} 8_{12}
8_{13} 8_{14} 8_{15} 8_{16} 8_{17} 8_{18} 8_{19} 8_{20} 8_{21}
9_1 9_2 9_3 9_4 9_5 9_6 9_7 9_8 9_9
9_{10} 9_{11} 9_{12} 9_{13} 9_{14} 9_{15} 9_{16} 9_{17} 9_{18}
9_{19} 9_{20} 9_{21} 9_{22} 9_{23} 9_{24} 9_{25} 9_{26} 9_{27}
9_{28} 9_{29} 9_{30} 9_{31} 9_{32} 9_{33} 9_{34} 9_{35} 9_{36}
0^2_1 2^2_1 4^2_1 5^2_1 6^2_1 6^2_2 6^2_3 7^2_1 7^2_2
7^2_3 7^2_4 7^2_5 7^2_6 7^2_7 7^2_8 8^2_1 8^2_2 8^2_3
8^2_4 8^2_5 8^2_6 8^2_7 8^2_8 8^2_9 8^2_{10} 8^2_{11} 0^3_1
6^3_1 6^3_2 6^3_3 7^3_1 8^3_1 8^3_2 8^3_3 8^3_4 8^3_5

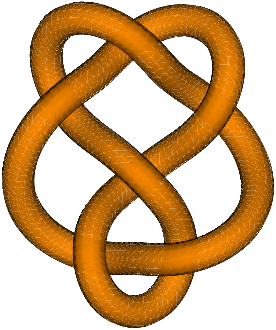
Alternating and Non-alternating Knots

- A knot or link is alternating if it has a presentation in which one alternates between crossing under and over when traversing the knot.
- Otherwise, a knot or link is non-alternating
- The "first" non-alternating prime knots are 8_{19}, 8_{20}, 8_{21}.
- Alternating knots are the most accessible to study but become proportionally rarer with increasing crossing number.

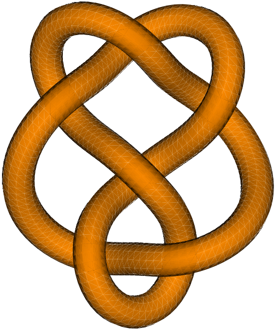
- (Minimal) Crossing number, $Cr(K)$, is the smallest number of crossings that must be occur in a presentation of the knot.

Crossings	Alternating Prime Knots	Non-Alternating Prime Knots
0	1	0
1	0	0
2	0	0
3	1	0
4	1	0
5	2	0
6	3	0
7	7	0
8	18	3
9	41	8
10	123	42
11	367	185
12	1288	888
13	4878	5110
14	19536	27436
15	85263	168030
16	379799	1008906
17	1769979	???
18	8400285	???
19	40619385	???
20	199631939	???
21	990623857	???
22	4976016485	???

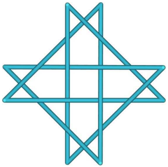
- Gordian or Unknotting number, $Un(K)$, is the smallest number of crossings that can be changed to get a presentation of the unknot, over all presentations of the knot.



- The Bridge number of a knot, $Br(K)$, is the smallest number of maxima (or minima) over all orthogonal projections to a line in 3-space over all presentations of the knot.
- Note, if there is a projection with a single maximum, the knot is trivial.
- Many of the simplest knots are two bridge knots. What is the first one that is not? How does one know?



- The Edge number of a knot, $Ed(K)$, is the smallest number of edges (or vertices) necessary to create a polygonal presentation of a knot.
- The Equilateral Edge number of a knot, $EEd(K)$, is the smallest number of edges (or vertices) necessary to create an equilateral polygonal presentation of a knot.
- The Lattice Edge number of a knot, $LEd(K)$, is the smallest number of edges (or vertices) necessary to have an simple cubic lattice presentation of a knot.



Mathematical Knotting and Linking: Linking Number of an Oriented Link

Figure: $+1$ **crossing**

Figure: -1 **crossing**

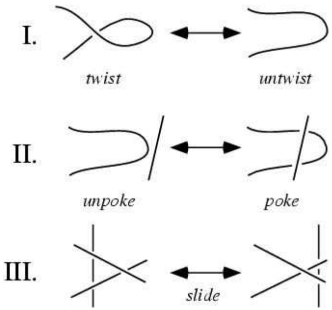
Definition

- A knot or link is oriented if a direction is assigned to each component.
- In an oriented link, the linking number, $Lk(L_1, L_2)$, between two components, L_1 and L_2 is defined to be half the sum of $\pm 1's$ associated to the crossings between the two components.

The linking number of an oriented link is a topological invariant

Must check invariance under Reidemeister Moves

- Type I
- Type II
- Type III



- The writhe of a knot or link presentation, $Wr(L)$, is defined to be the sum of the $\pm 1's$ in the diagram.
- The writhe of a minimal crossing diagram of a prime non-alternating knot is **NOT** an invariant, e.g. 10_{161} and 10_{162}, the Perko Pair, in old knot tables (pre 1974).
- But, if the knot is alternating, it is invariant.

Alexander/Conway Polynomial 1923/1969

Given an oriented link, **L**, there is a unique element, $\nabla(\mathbf{L})$ of $\mathbf{Z}[t, t^{-1}]$ such that

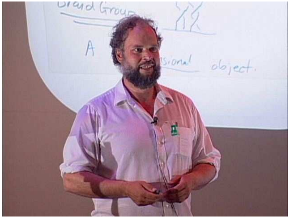
$$\nabla(\text{Unknot}) = 1$$

and, if $\mathbf{L}_-$, $\mathbf{L}_0$, $\mathbf{L}_+$ are link presentations that are identical outside the relation region where they are precisely as shown above, then

$$\nabla(\mathbf{L}_+) - \nabla(\mathbf{L}_-) - t\,\nabla(\mathbf{L}_0) = 0.$$

- The classical Alexander Polynomial is related to the Alexander-Conway polynomial by $\Delta\,(\mathbf{L})(t^2) = \nabla(\mathbf{L})(t - t^{-1})$

The Era of Jones



V. F. R. Jones Polynomial 1984

Given an oriented link, **L**, there is a unique element, $V(\mathbf{L})$ of $\mathbf{Z}[\mathrm{t}, t^{-1}]$ such that

$$V(\text{Unknot}) = 1$$

and, if $\mathbf{L}_-$, $\mathbf{L_0}$, $\mathbf{L}_+$ are link presentations that are identical outside the relation region where they are precisely as shown above, then

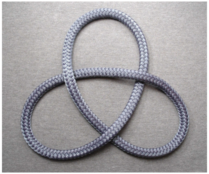
$$t^{-1}\ V(\mathbf{L}_+) \text{ - t } V(\mathbf{L}_-) + (t^{-\frac{1}{2}} - t^{\frac{1}{2}})V(\mathbf{L_0}) = 0.$$

Compare the calculations for the trefoil knot

- $\Delta\ (\mathbf{3_1})(t) = t^{-1} - 1 + t$
- $V(\mathbf{3_1})(\mathrm{t}) = t + t^3 - t^4$

What happens under mirror reflection?

- $\Delta\ (\overline{\mathbf{3_1}})(t) = t^{-1} - 1 + t$
- $V(\overline{\mathbf{3_1}})(\mathrm{t}) = -t^{-4} + t^{-3} + t^{-1}$



The Era of Jones: Alexander-Conway and Jones imply......

Berkeley, Summer 1985, Vaughan Jones with James **H**oste, Adrian **O**ceanu, Kenneth **M**illett, Peter **F**reyd, W. B. Raymond **L**ickorish, and David **Y**etter (HOMFLY) absent Przytycki and Traczyk

The Era of Jones: HOMFLY-PT Polynomial 1984

The HOMFLY Polynomial

Given an oriented link, **L**, there is a unique element, $P(\mathbf{L})$ of $\mathbf{Z}[\mathrm{l}, l^{-1}, \mathrm{m}, m^{-1}]$ such that

$$P(\text{Unknot}) = 1$$

and, if $\mathbf{L}_-$, $\mathbf{L_0}$, $\mathbf{L}_+$ are link presentations that are identical outside the relation region where they are precisely as shown above , then

$$l\ P(\mathbf{L}_+) + l^{-1}\ P(\mathbf{L}_-) + \mathrm{m}\ P(\mathbf{L_0}) = 0.$$

- $P(\mathbf{3_1})(l, m) = -2l^2 - l^4 + l^2 m^2$

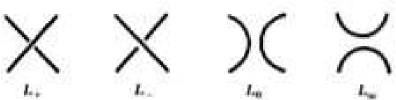
What happens under mirror reflection?

- $P(\overline{\mathbf{3_1}})(l, m) = -2l^{-2} - l^{-4} + l^{-2} m^2$

HOMFLY is an extension of both Conway-Alexander and Jones

- HOMFLY distinguishes knots that neither Conway-Alexander nor Jones can distinguish, e.g. 11_{388} and $\overline{11_{388}}$.
- HOMFLY is unable to distinguish "mutants" as well as other small families
- Beware, there is no agreement on the choice of variables and normalization.

The Jones Era: BLMH Polynomial Winter 1985



Brandt-Lickorish-Millett-Ho Polynomial

Given a link, **L**, there is a unique element, $Q(\mathbf{L})$ of $\mathbf{Z}[\mathrm{x}, x^{-1}]$ such that

$$Q(\mathrm{Unknot}) = 1$$

and, if $\mathbf{L}_+$, $\mathbf{L}_-$, $\mathbf{L_0}$, $\mathbf{L}_\infty$ are link presentations that are identical outside the relation region where they are precisely as shown above, then

$$Q(\mathbf{L}_+) + Q(\mathbf{L}_-) = \mathrm{x}\,(Q(\mathbf{L_0}) + Q(\mathbf{L}_\infty)).$$

For any presentation of an unoriented link, **L**, first define a Laurent polynomial, $\Lambda(L)$, in two variables, a and x, by
(i)

$$\Lambda(\text{Circle}) = 1;$$

(ii) If $\mathbf{L}_-$ contains a negative type I Reidemeister move and **L** denotes the result of its untwisting, then

$$\Lambda(\mathbf{L}_-) = a^{-1}\Lambda(\mathbf{L});$$

(iii) If $\mathbf{L}_+$ contains a positive type I Reidemeister move and **L** denotes the result of its untwisting, then

$$\Lambda(\mathbf{L}_+) = a\Lambda(\mathbf{L});$$

(iv)

$$\Lambda(\mathbf{L}_+) + \Lambda(\mathbf{L}_-) = x\left(\Lambda(\mathbf{L_0}) + \Lambda(\mathbf{L}_\infty)\right).$$

The Jones Era: Kauffman Polynomial

For any oriented link, **L**, the Laurent polynomial defined by

$$F(\mathbf{L}) = a^{-Wr(\mathbf{L})}\Lambda(\mathbf{L})$$

is an invariant of **L** in 3-space.

- $F(\mathbf{3_1})(a,z) = -2a^2 - a^4 + (a^3 + a^5)x + (a^2 + a^4)x^2$

What happens under mirror reflection?

- $F(\overline{\mathbf{3_1}})(a,z) = F(\mathbf{3_1})(a^{-1},z)$

Begin with an unoriented link diagram, **L**, for which we define a Laurent polynomial, $\langle \mathbf{L} \rangle$, in one variable, A, using the following rules:

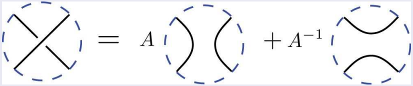
(i) if **O** denotes a planar circle,

$$\langle \mathbf{O} \rangle = 1;$$

(ii) the distant union of **L** and **O**, gives

$$\langle \mathbf{L} \sqcup \mathbf{O} \rangle = -(A^{-2} + A^{2})\langle \mathbf{L} \rangle;$$

(iii)

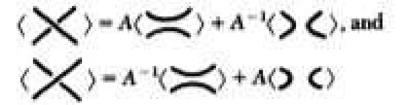


The Jones Era: Kauffman's Jones Polynomial

One defines a new polynomial: $X(\mathbf{L})$

$$X(\mathbf{L}) = (-A)^{-3Wr(\mathbf{L})}\langle \mathbf{L} \rangle$$

Taking the difference between the equations,

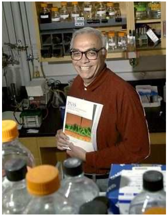


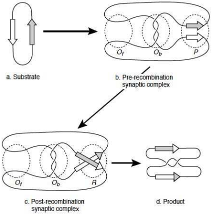
we get

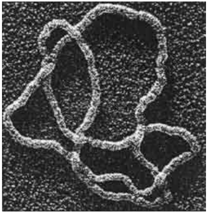
Accounting for the changes in the writhe and the normalization and letting $A = t^{\frac{-1}{4}}$, one has the Jones recursion equation.

Molecular Biology

Championed by Nick Cozzarelli, **Knot Theory** has been and is still being used to study the mechanism of enzymes that act upon DNA by changing their spatial structure thereby removing or creating knots.



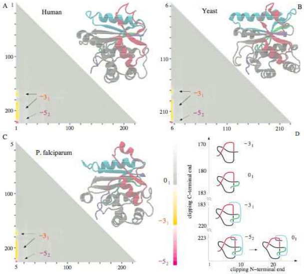




Nick Cozzarelli (Fall 1984)

Molecular Biology

Knot Theory is also being used to study the structure of proteins in order to give insight into the relationship between structure and function. But, its a somewhat different kind of "knot theory" that is exploited.



Sulkowska, Rawdon, Millett, Stasiak, Onuchic

Conservation of complex knotting and slip knotting patterns in proteins, PNAS June 2012

Knotting of open chains

Although for many objectives it is sufficient to consider only the knotting of closed curves, the knotting of open curves has important applications in the study of physicial and biological macromolecules, in the large, and for the study of knot localization in both open and closed curves.

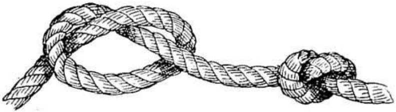


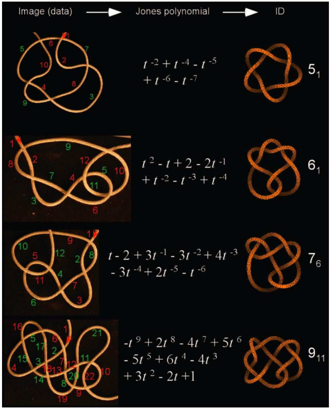
FIG. 7 FIG. 8

FIGS. 7 and 8.—Overhand knots.

Applications to the Natural Sciences

Raymer Smith Experiment

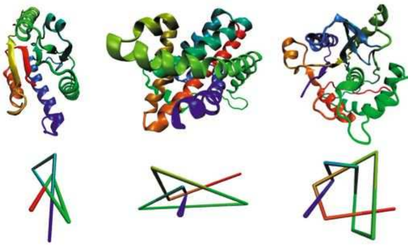
For example, in the 2007 Raymer-Smith study of the incidence of knotting by tumbling open strands of varying lengths and flexibility, a critical challenge was the notion of knotting in open strands.



Applications to the Natural Sciences

The "reasonable person" criterion

Mansfield (1994) "Nevertheless, to paraphrase Associate Justice Potter Stewart of the U.S. Supreme Court, we may not be able to define a knot in an open path, but we know one when we see one.....Since protein contours are not closed paths, it is only in the subjective sense of a 'reasonable-person' test that we can address the existence of knots in proteins."

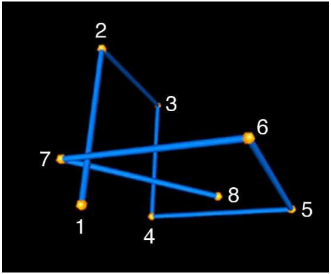


- PDB codes: 1*ns*5 1*yve* 1*xd*3

Applications to the Natural Sciences

Simplification of structure algorithms

In the study of polymers, the **primitive path analysis** has been employed since the 1970's (Edwards and others?)
Taylor's 2000 protein application kept the ends of the chain fixed and modified the interior conformation by means of permitted "triangle moves," a la Reidemeister (1926).

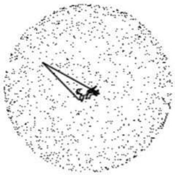


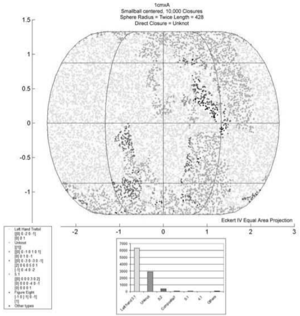
Millett-Dobay-Stasiak (Macromolecules 2005) example, above, shows how the result depends upon choices.

MDS propose another strategy to locate the knot.

MDS identification of knotting in open chains

MDS uses the statistics of the closure to the sphere at "infinity" to define the knot types defined for all except a set of measure 0 points on $\mathbf{S}^2$.

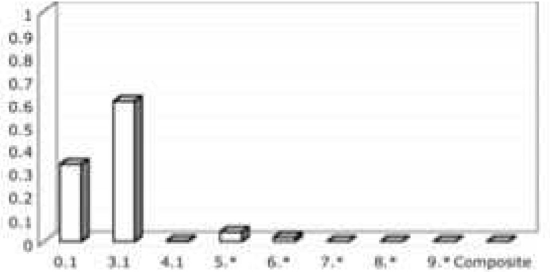




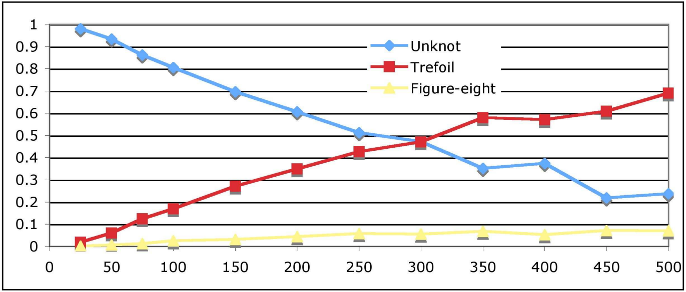
Millett-Dobay-Stasiak 2005 & Millett-Sheldon 2005

Estimation of knotting in open chains

This leads to the knotting spectrum of a configuration.

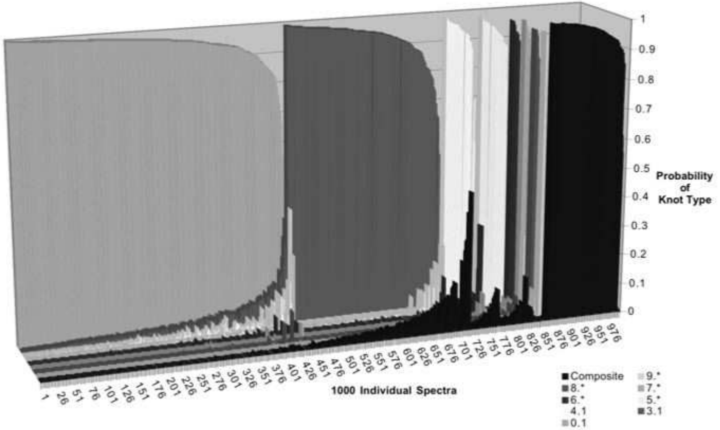


Estimation of knots and unknots in random walks



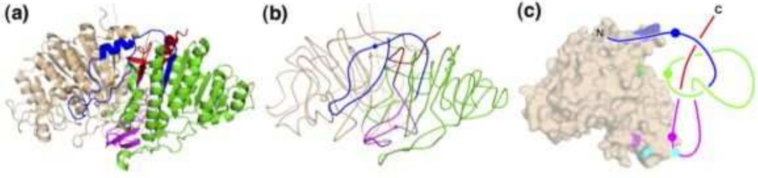
Random walks

What does this strategy tell us about knotting in 500 step random walks?



Slipknots: a protein example

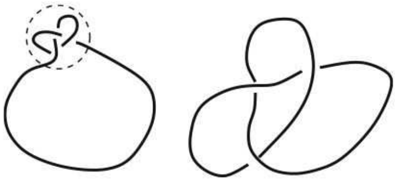
A slipknot is a knotted portion of a chain, an ephmeral knot, that is contained within an unknotted chain, the slipknot. Here is an example of a slipknot in alkaline phosphatase discovered by Todd Yeates (King et. al. J Mol Bio 2007).



Localization of knots in open and closed chains

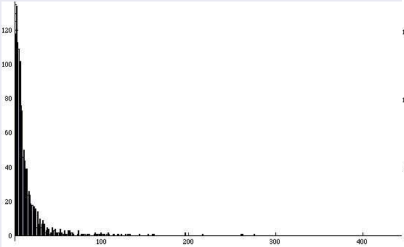
We can identify the locus of knots, ephemeral knots, and slipknots in an open or closed chains by testing segments of various lengths and starting points. This can illuminate questions concerning their size and location, for example:

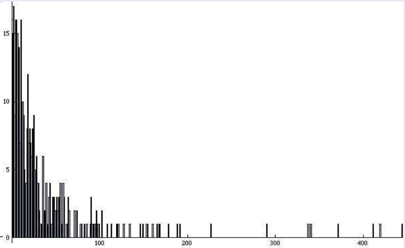
- The distribution of knot lengths in polygonal knots establishes the scale of knotting: *strongly local* knotting (of bounded length), *weakly local* knotting (sub-linear growth in length), and *global* knotting (growing asymptotically in proportion to the length).



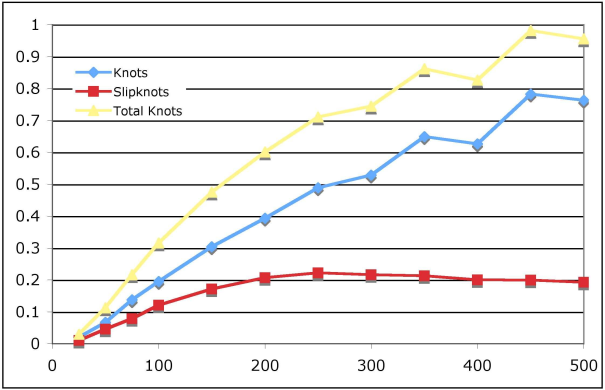
Estimation of knotting

The length distributions of knots and ephemeral knots in 500 step random walks

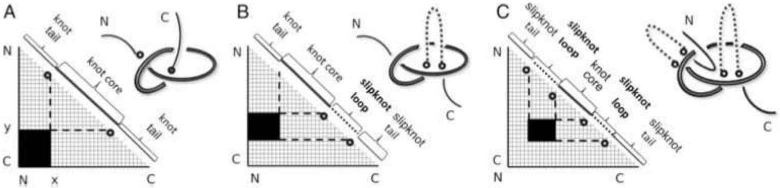




- How important is the presence of knots and slipknots to the overall structure of a random walk or random polygon?



Fingerprints of knots and slipknots in proteins



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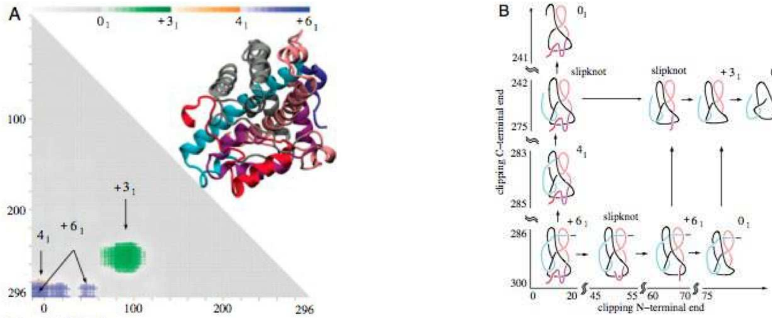
DehI protein forms a Stevedore's knot, 6_1, (Bolinger et al 2010) as well as slipknotted 3_1, 4_1 and 6_1



$74,223$ **structures analyzed,** 398 **knotted,** 222 **slipknotted**

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Applications to the Natural Sciences

Complex knotting fingerprints and their conservation

Table 1. Complex knotting patterns in proteins and their conservation

Motif	Family	Protein/PDB	Source
K $6_1,6_1,4_1,3_1$	α-haloacid dehalogenase	DehI/3bjx	*Arthrobacter sideroc aspulatus*
K $5_2,3_1,3_1$	ubiquitin C-terminal hydrolase	UCHL1/3irt UCHL3/1xd3 UCHL3/2wdt [n] UCHL5/3a7s* [n] Yuh1/1cmx*	Human Human *P. falciparum* Human Yeast
S $3_1,4_1,3_1$	SNF	LeuT(Aa)/2a65	*Aquifex aeolicus*
S $3_1,4_1,3_1$	NCS1	Mhp1/2jlo [n]	*M. liquefaciens*
S $3_1,4_1,3_1$	AA-permease	ApcT/3gia [n] AdiC/3l1l* [n] AdiC/3ncy [n]	*Methanocaldococcus* *E. coli* *Salmonella*
S $3_1,4_1,3_1$	SSF	vSGLT/3dh4 [n]	*Vibrio parahaemolyticus*
S $3_1,4_1,3_1$	BCCT	BetP/2wit* [n] PmCaiT/2wsw [n] EcCaiT/2wsx [n]	*Brevibacterium* *Proteus* *E. coli*
K $4_1,3_1$	KARI	KARI/1yve KARI/1yrl KARI/3fr8 [n]	Spinach *E. coli* Rice
K $4_1,4_1$	PHY	bphP/3c2w cph1/2vea	*Pseudomonas* *Synechocystis*
K $4_1,4_1$	PHY	bphP/1ztu bhyB2/2ool	*Deinococcus* *R. palustris*
S $3_1,3_1,3_1,3_1$	Cloacin	ColE7/2axc* [n] protein B/1rh1* [n]	*E. coli* *E. coli*
S $3_1,3_1,3_1,3_1$	S-pyocin	ColE3/1jch [n]	*E. coli*

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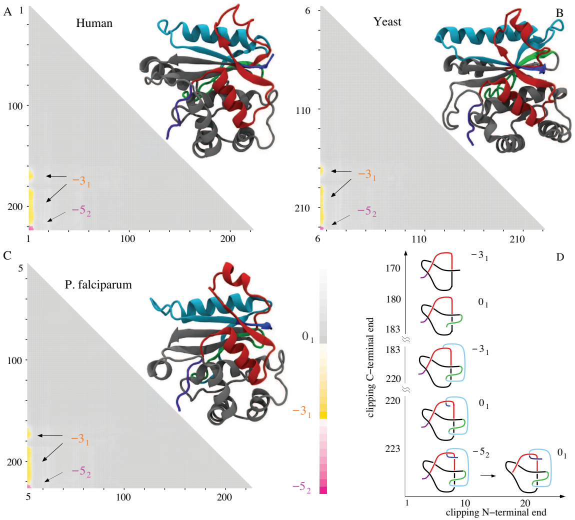
Applications to the Natural Sciences



Evolutionarily distant organisms: yeast, human, and plasmodium proteins: only 30% sequence identity

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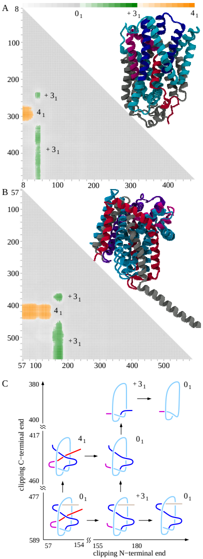
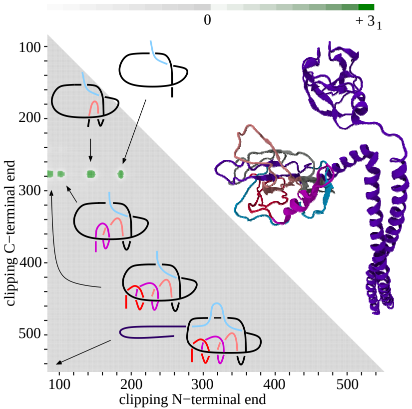


LeuT(Aa) and BetP proteins conserve structure despite large sequence divergence



Colcin E3 structure, motif $(S3_1 3_1 3_1 3_1)$ reveals structural complexity upon polypeptide chain clipping

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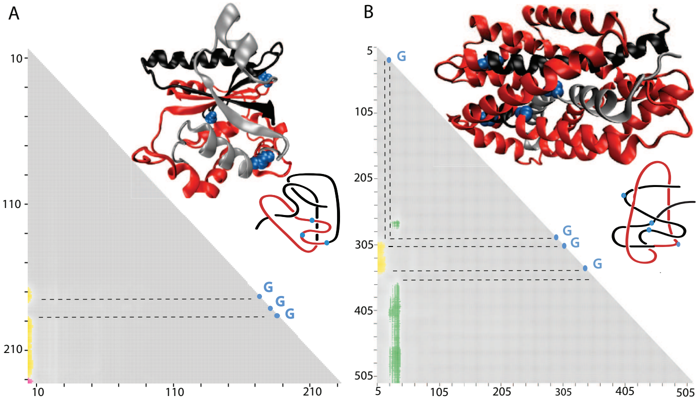

Yuh1 and LeuT illustrate observed strong conservation of glycines at knotting passage locations

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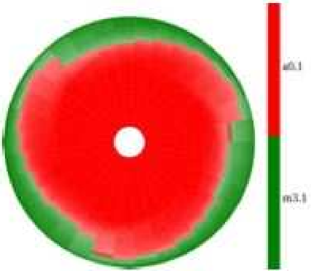
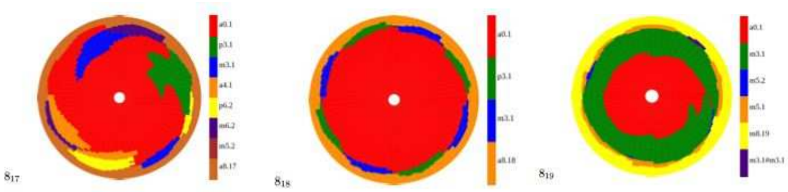
Localization structure of knots in ideal knots



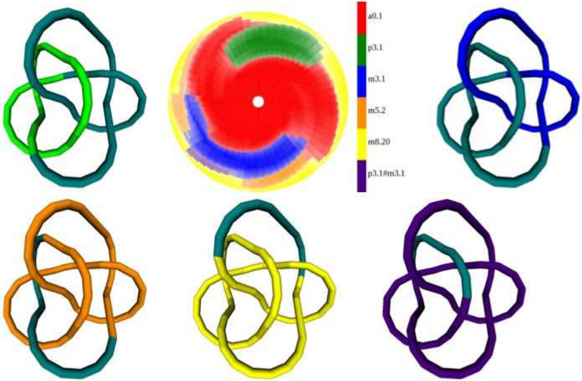
Structure of an ideal trefoil

Joint work with Heinrich, Hyde, Rawdon, and Stasiak



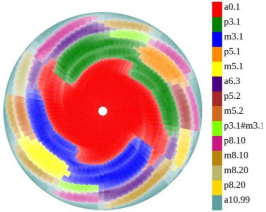
Structure of an ideal 8_{17}, 8_{18}, and 8_{19}

Joint work with Heinrich, Hyde, Rawdon, and Stasiak



Structure of an ideal 8_{20}

Joint work with Heinrich, Hyde, Rawdon, and Stasiak



Structure of an ideal 10_{99}

Joint work with Heinrich, Hyde, Rawdon, and Stasiak

Thank you for your attention

Happy Knotting in Santa Barbara