Knots, random walks and biomolecules
Les Diablerets 2003
Abstracts

July 13, 2003

Eric Rawdon

Title: Polygonal Ropelength

Abstract:
The thickness” of a smooth knot is the ratio of the maximum radius of a non self- intersecting tube centered on the knot to its length; the ropelength energy is the reciprocal of the thickness, that is the length of unit-radius rope” needed to make the knot. When smooth ropelength was first defined, there was a desire to see ropelength minimizing conformations for different knot types. The speaker was one of the researchers who defined a polygonal version of ropelength with the goal of using computer simulations to approximate the smooth minima, the so-called ideal knots”. Subsequently, researchers have observed that minimum ropelength conformations predict behavior of knots tied with physical materials. In this talk, we review our current knowledge of polygon ropelength. In particular, we discuss approximation, a generalization of polygonal ropelength to model inflexible materials, shapes of ropelength minima, relationships with the Moebius energy, progress on simulating a gradient (i.e. a rigorous tightening algorithm), and future applications.

John Sullivan

Title: The Tight Clasp

Abstract:
We describe critical points (presumably the minimizers) for a (two-parameter) family of ropelength minimization problems, minimizing the length of two simply clasped ropes subject to a thickness constraint. The resulting configurations are piecewise analytic, but with as many as 11 pieces on each component.

Oguz Durumeric

Title: "Every ideal knot in R^3 must have a tight crossing"

Abstract:

The thickness, i(C) of a knot or link C is defined to be the radius of the largest tube one can put around the curve without any self intersections (= "normal injectivity radius of C" = "Global Radius of curvature by Gonzales and Maddocks in R^{3}"). For $C^{(1,1)}$ curves C, i(C) = min DCSD(C)/2, 1/(sup k(C)), where k(C) is the local curvature defined almost everywhere, and double critical self distance, DCSD(C) is the minimum of the distances between all double critical pairs (i.e. the segment between them is perpendicular to C at both end points) along the curve C. This is obtained by Litherland-Simon- Durumeric-Rawdon (for smooth case) and Cantarella-Kusner-Sullivan ($C^{(1,1)}$ case) in R^3. This result was later generalized to $C^{(1,1)}$ submanifolds of Riemannian manifolds by the author. The knots and links in ideal shapes are the minima of ropelength = length/thickness within a fixed knot class. Our intuition, as well as computer models tell us that an ideal knot thickened to the radius i(C) should look like a tightly wrapped ball of yarn/string with many "tight crossings" by which we mean i(C) = (1/2)DCSC(C). However, an analytical proof of this requires showing that focal points cannot occur earlier, which is not obvious intuitively. The Tight Clasp model by Sullivan indicates that (1/2)DCSC(C) = 1/(sup k(C)) = i(C) for certain type crossings. Theorem: i(C) = (1/2)DCSC(C), for every relative minimum C of ropelength in R^3. Hence, (1/2)DCSC(C)¡= 1/(sup k(C)) for relatively extremal knots and links. In the general case, with the possible exceptions of $C^{(1,1)}$ curves of constant curvature, the same result holds in R^n for all dimensions.

Heiko von der Mosel

Title: Necessary conditions for ideal knots

Abstract:

We present a characterization of ideal knots, i.e., of closed knotted curves of prescribed thickness with minimal length, where we use the notion of global curvature for the definition of thickness. We show with varational methods that for an ideal knot g, the normal vector g"(s) at a curve point g(s) is given by the integral over all vectors g(t)-g(s) against a Radon measure, where —g(t)-g(s)—/2 realizes the given thickness. As geometric consequences we obtain in particular, that points without contact lie on straight segments of g, and for points g(s) with exactly one contact point g(t) we have that g”(s) points exactly into the direction of g(t)-g(s). Moreover, isolated contact points lie on straight segments of g, and curved arcs of g consist of contact points only, all realizing the prescribed thickness with constant (maximal) global curvature.

Yuanan Diao

Title: The spectrum of the minimum ropelengths of nontrivial knots

Abstract:

For any given knot K, a thick realization K_0 of a knot type $\mathcal{K}$ is a knot of unit thickness which is of the knot type $\mathcal{K}$. The ropelength of $\mathcal{K}$ is defined as the arc length of the shortest thick realization of $\mathcal{K}$. A recent result shows that there exists a constant $b > 0$ such that for any knot type $\mathcal{K}$, its ropelength $L(\mathcal{K})$ is bounded above by $b \cdot (Cr(\mathcal{K}))^{3/2}$, where $Cr(\mathcal{K})$ is the crossing number of $\mathcal{K}$. It is also known that there exists a family of infinitely many knot types $\{\mathcal{K}_n\}$ such that $n = Cr(\mathcal{K}_n) \to \infty$ as $n \to \infty$ and $L(\mathcal{K}_n) = O(n)$. In this paper, we show that for each p with $3/4 \leq p \leq 1$, there exists a family of infinitely many knot types $\{\mathcal{K}_n\}$ with the property that $Cr(\mathcal{K}_n) \to \infty$ (as $n \to \infty$) such that $a_0 \cdot (Cr(\mathcal{K}_n))^p \leq L(\mathcal{K}_n) \leq b_0 \cdot (Cr(\mathcal{K}_n))^p$, where a_0 and b_0 are some positive constants. In other word, any power between 3/4 and 1 is realizable by some knot family.

Jason Cantarella

Title: The gradient flow for ropelength in theory and computation.

Abstract:

How do knots tighten in nature? The ”balance criterion” for ropelength-critical knots gives us a precise and attractive geometric picture for tight

configurations of knots: a knot is ropelength critical if the elastic force exerted by the tightening knot is balanced by a system of self-contact forces on the knot.

In this talk, we discuss extensions of this result to the case where the knot has not yet become fully tight. The same formalism provides a natural picture for the motion of the knot as it tightens; we'll discuss theory and numerical simulation of this flow. This work is joint with Fu, Kusner, Sullivan, and Wrinkle (balance criterion) and Rawdon and Piatek (numerical simulation of gradient flow).

Jana Smutny

Title: Computation of ideal shapes with Biarcs

Abstract:
We outline a discretization of a space curve with biarcs, i.e. a curve assembled from certain arcs of circles, and describe convergence results. The evaluation of the thickness of a biarc curve up to a prescribed error can be achieved via a bisection algorithm, an error estimate, and the necessary condition for points along the curve that are doubly critical for distance. Finally we describe output of a simulated annealing code (developed with B. Laurie and J. Maddocks) that implements these ideas to compute ideal shapes of knots. We will show graphs of various quantities such as radius of curvature, global radius of curvature, torsion angles for the computed ideal trefoil knot.

Eugene L. Starostin

Title: A constructive approach to modelling the ideal shapes of some linked structures

Abstract:
A variational approach is proposed to constructing tight shapes of linked perfect ropes each component of which is prescribed to have a planar centreline. Two particular examples are considered and explicit solutions are

presented. A concept of tight periodic structures is introduced and discussed. Both the method and the examples are hoped to provide an insight into the general properties of the ideal links and knots.

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Title: KNOTTING OF DNA REPLICATION INTERMEDIATES IN VIVO

Abstract:

As soon as DNA topoisomerases were discovered in the mid 60s, it was realized DNA knotting could occur in living cells. But experimental evidence for knotted molecules in vivo is still scarce. Most of what we currently know about DNA knotting comes from in vitro assays. In the course of studies dealing with the replication of bacterial plasmids containing two unidirectional ColE1 origins placed in opposite orientations, we found that initiation took place at only one of the two potential origins per replication round. The replication fork initiated at the active origin stalled as soon as it reached the other origin. Analyses of replication intermediates (RIs) of these plasmids by two-dimensional (2D) agarose gel electrophoresis after linearization with a restriction enzyme that cut the plasmid only once and outside the putative replication bubble, revealed a "beads-on-a-string" signal, which electron microscopy showed were due to knotted bubbles. Further studies indicated that during DNA replication the probability of knotting behind the fork is inversely proportional to precatenane density. As RIs progressively relax as the replication fork advances, the number and complexity of knotted bubbles increases. It is well known that the electrophoretic mobility of knots is a function of the number of nodes. We confirmed this observation for the first dimension of our 2D gels, which occurred at low voltage in 0.3 to 0.5second dimension, which took place at high voltage in 0.8 to 1.5electrophoretic behaviour of knotted bubbles varied depending on their molecular mass. For small molecules it was still a function of the number of nodes. But for large molecules, the mobility of knotted bubbles could even diminish as the number of nodes increased.–

Giovanni Dietler

Title: Numerical simulation of gel electrophoresis of DNA knots

Abstract:

Gel electrophoresis experiments of DNA knots of equal string length allow to separate the knots by their type. We present a numerical simulation of the experiments using knotted and charged polymer drifting in an electric field. The gel is simulated by obstacles made with rods arranged in a square lattice. Using a simple Monte Carlo algorithm, the dependence of the electrophoretic mobility as a function of the knot type and as a function of the intensity of the electric field can be studied. The results are in agreement with the experiments. Namely, at low electric field the most complex knots travel faster in the gel, while at high electric field the behavior is reversed, with the simpler knots traveling faster than the complex knots. We conclude that the topology of the DNA is playing a major role in the transport properties of DNA.

Oscar Gonzalez

Title: Sedimentation dynamics of rigid, knotted filaments

Abstract:

Recent experiments have shown that there is an approximate linear relationship between the gel migration speeds of different DNA knots and the average crossing number of their ideal geometrical forms. Here we consider the sedimentation dynamics of rigid knots in a Stokes fluid and show that an approximate linear relation between migration speed and crossing number also holds for different knots in their ideal forms. These results suggest that a population of rigid, knotted filaments might be separated by sedimentation in much the same way that DNA knots are separated by electrophoresis

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Alexander Grosberg

Title: Knots and Scaling: recent and not-so-recent results

Abstract:
How do knot constraints affect properties of polymers? How do polymer physics experience illuminates the problems of knots theory? A review of these and related questions will be presented.

Corinne Cerf (joint work with Andrzej Stasiak)

Title: Linear relations between writhe and minimal crossing number in Conway families of ideal knots and links

Abstract:
Whereas there is no general relation between the writhe of a knot in its ideal configuration (Wrideal) and the minimal crossing number of this knot (n), linear relations between Wrideal and n have been observed in some families of knots [1]. We were able to predict Wrideal of any rational knot or link using invariants of alternating knots and links, giving rise to a value called PWr [2]. We define here Conway families of knots and links such that for every such family, PWr presents a linear behavior versus n. The slope of the lines and the shift between any two lines with the same slope can be computed using parameters of the considered Conway families [3,4]. [1] V. Katritch et al., Nature 384 (1996) 142. [2] C. Cerf & A. Stasiak, Proc. Natl. Acad. Sci. USA 97 (2000) 3795. [3] C. Cerf & A. Stasiak, to appear in the Proceedings of the Workshop on Applications of Topology to Biology, Max Planck Institute, Dresden, July 1-5, 2002. [4] C. Cerf & A. Stasiak, New Journal of Physics, submitted.

Tetsuo Deguchi

Title: Topological expansion of random links.

Abstract:
In statistical mechanics, entropic effects can be explained in terms of some

effective potentials or forces. If the number of possible configurations of a system are reduced due to some constraint, then its effect can be expressed as an effective entropic force on the system.

In fact, we can show that self-avoiding polygons (SAPs) with a fixed knot, which we call random knots, are larger in size than those of no topological constraint, when the number of polygonal nodes is large enough. The effective swelling is derived from topological entropic repulsion among the segments of random knots. In this talk, we discuss the entropic force arising from topological constraints of random links.

We introduce an approximate analytic formula describing the entropic force between two random knots as a function of their distance. Through numerical simulations we show that the average sizes of random links are enhanced due to their topological constraints.

Akos Dobay

Title: The Average Crossing Number of Equilateral Random Polygons.

Abstract:

We show that the mean of the average crossing numbers (ACN) of all equilateral random walks of length n is of the form $\frac{3}{16} \cdot n \cdot \ln n + O(n)$. Similar result holds for equilateral random polygons. These results are confirmed by our numerical studies. Random knots of increasing length n show, in addition, that when analysed configurations are divided into individual knot types then $\langle \mathrm{ACN}(\mathcal{K}) \rangle$ of each analysed knot type can be described by a function $\langle \mathrm{ACN}(\mathcal{K}) \rangle = a \cdot (n - n_0) \cdot \ln(n - n_0) + b \cdot (n - n_0) + c$ where a, b and c are constants typical for different knots and where n_0 is the minimal number of segments required to form a given knot type. $\langle \mathrm{ACN}(\mathcal{K}) \rangle$ profiles of individual knot types diverge from each other with more complex knots showing higher $\langle \mathrm{ACN}(\mathcal{K}) \rangle$ than less complex knots. $\langle \mathrm{ACN}(\mathcal{K}) \rangle$ profiles of individual knot types intersect however with the $\langle \mathrm{ACN}(\mathcal{K}) \rangle$ profile of all closed walks. These points of intersections define the equilibrium length of a respective knot types, i.e., the chain length at which a statistical ensemble of configurations of a given knot type upon cutting, equilibration and reclosure does not show a tendency to increase or decrease its $\langle \mathrm{ACN}(\mathcal{K}) \rangle$. The concept of equilibrium length seems to be universal and applies also to other characteristics of random knots that continuously change with the chain size such as the mean radius of gyration $\langle \mathrm{R_g} \rangle$.

Kenneth C. Millett
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Title: Local Scaling Transitions near Equilateral Knots

Abstract:

Preliminary results of a study of the local structure of knot space near equilateral knots will be presented and contrasted with data reflecting the global structure of knot space. These data give insight into the transitions arising with increasing edge numbers, scaling phenomena, as well as the effect of small pertrubations that do not necessarily perserve the knot type.

Stephen C. Harvey

Title: Knots in RNA and DNA Viruses: When Are They Useful, and When Do They Need to Be Avoided?

Abstract:

Viral genomes must be packaged without knotting or tangling. RNA viruses have to avoid knotted genomes because there are no cellular RNA topoisomerases that could unknot them. DNA viruses have to avoid knotted genomes because of the way they inject DNA into the host cell upon infection. But knots are not always undesirable. In vitro assays on tailless mutants of DNA bacteriophage reveal a distribution of DNA knots that provide clues to the nature of the packaged DNA structure. And there is a remarkable case of protein knotting in bacteriophage HK97 that serves to strengthen and stabilize the structure of the viral capsid. This talk will describe these phenomena and present our efforts at developing three-dimensional models for the structure of viral RNA and DNA genomes.

Cristian Micheletti

Title: Thermodynamics of DNA packaging inside a viral capsid: the role of DNA intrinsic thickness

Abstract:

We discuss some aspects of theequilibrium thermodynamics of a thick polymer confined in a spherical region of space. This is used to gain insight into the DNA packaging process. The experimental reference system for the present study is the recent characterization of the loading process of the genome inside the $\phi 29$ bacteriophage capsid. Our emphasis is on the modelling of double-stranded DNA as a flexible thick polymer (tube) instead of a beads-and-springs chain. By using finite-size scaling to extrapolate our results to genome lengths appropriate for $\phi 29$, we find that the thickness-induced force may account for up to half the one measured experimentally at high packing densities. An analogous agreement is found for the total work that has to be spent in the packaging process. Remarkably, such agreement can be obtained in the absence of any tunable parameters and is a mere consequence of the DNA thickness. Furthermore, we provide a quantitative estimate of how the persistence length of a polymer depends on its thickness. The expression accounts for the significant difference in the persistence lengths of single- and double-stranded DNA (again with the sole input of their respective sections and natural nucleotide/base-pair spacing).

Gustavo A. Arteca
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Title: Polymer shape dynamics during folding-unfolding transitions.

Abstract:

We discuss the interplay between molecular size and chain entanglements (measured in terms of the statistics of bond-bond projected crossings) during polymer configurational transitions. Particular attention is given to descriptors of mean size for "inner" and "outer" regions of a polymer chain, and entanglement descriptors relative to chains in folded native conformations. Two cases are considered: (a) folding-unfolding transitions in anhydrous proteins and protein ions, and (b) stretching transitions in grafted polymers with transient loop entanglements. In all cases, we monitor the evolution over time in conformer populations within the parameter space for large-scale molecular shape features. What emerges is an insight into mechanisms underlying these transitions, as well as their dependence on relevant control variables (e.g., temperature and ion charge). Also interestingly, the method provides an estimate on the nonrandom nature of the unfolded (or denatured) state of realistic polymers.

Francesco Valle

Title: Atomic Force Microscopy of complex DNA knots

Abstract:

We have imaged complex DNA knots deposited onto a surface by atomic force microscopy. The deposition technique used allows a fast trapping of the molecules on the surface. By this technique the DNA conformation on the surface reflects its three dimensional bulk one. Some preliminary results will be shown, with particular attention to the conformation of knotted circular closed DNA and to the confinement of the crossings to a relatively small portion of the chain.

Xiaoyan Robert Bao

Title: Behaviour of complex knots in single DNA molecules

Abstract:

Knots appear naturally in long polymers. In molecular biology topological constraints arise during DNA replication; knots also occur in some proteins. Knotting can profoundly impact the dynamics of systems in which they appear, and the magnitudes of these effects depend strongly on the complexity of the knot. Using optical tweezers, we have tied knots of known complexity into single DNA molecules and discovered that, in contrast to rigid polymers, knots in long DNA molecules are mobile and undergo thermal diffusion. We show that this behaviour is consistent with "self-reptation" of the knot along a polymer, that it depends on the complexity of knot that was tied, and that this dependence can be explained by a simple hydrodynamical model.

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Title: Topisomerase-inspired approach explains why distinct types of random knots with similar complexity form with different probability.

Abstract:

Probability of random knots formation was investigated in numerous studies [1-4]. It was observed that in general more complex knots form with a lower probability than less complex knots. However, some knots do not follow this rule of thumb and for example 51torus and 52twist knots that have the same minimal number of crossings and thus have a similar complexity in fact form with an almost two-fold difference in their probability [2,3,5]. An approach based on predicting the entropy of different knots did not explain the probability difference between 51 and 52 knots [5]. We investigate here how different knot types react to internal random strand passages (topoisomerase-like reaction) and what is the probability that such a strand passage leads to a maintenance of original knot type or to creation of another type of knot. We observed for example that upon a random passage 51 and 52 knots maintain their respective original knot type with practically the same probability. This observation strongly suggests that entropy of 51 and 52 knots are practically equal. Why then 52 knots are observed almost twice more frequent than 51 knots among random knots of the same chain length? We propose that the reason for the disparity in their relative probability of formation lies in the fact that 52 knots can be directly generated by one strand passage from unknotted circle while this is not possible for 51 knot. Therefore 52 knots have two pathways that lead to their formation from simpler knots: one direct from unknotted circle and an indirect one through trefoils. 51 knots however can be only formed by the indirect way through trefoils. Thus the probability to form a random knot of a given type is not only related to the available conformational space of a given knot type but also to the number of ways this space can be reached.

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[4] J. Arsuaga, M. Vazquez, S. Trigueros, D. W. Sumners and J. Roca, Proc. Nat. Acad. Sci. , 99, 5373-5377, 2002.
[5] A. Y. Grosberg, Ideal Knots, World Scientific, Singapore, 129-141, 1998.

John H. Maddocks

Title: Real knots

Abstract:

I will discuss work with J.B. Keller (Ropes in Equilibrium, SIAM J. Applied Math **47** 1987) which describes the mechanics of how a completely flexible (but possibly resistant to twist) rope interacts with surfaces and other segments of rope, both in the presence and absence of friction. Remarks will then be made on how this old work relates to the more recent computations of ideal shapes.
