PREFACE

The physical properties of knotted and linked configurations in space have long been of interest to mathematicians. More recently, these properties have become significant to biologists, physicists, and engineers among others. Their depth of importance and breadth of application are now widely appreciated, and valuable progress continues to be made each year. Nevertheless, many fundamental and basic questions in the general domain of modeling physical knotting remain completely unanswered or at least are not fully or satisfactorily answered.

This volume consists primarily of chapters by researchers who spoke at two conferences: a special session on "Numerical Methods, Calculations, and Simulations in Knot Theory and its Applications" held at the Western Sectional meeting of the AMS in San Francisco in May 2003, and a conference on "Knots, Random Walks and Biomolecules" sponsored by the Bernoulli Centre of the Swiss Federal Institute of Technology in Lausanne and held in Les Diablerets, Switzerland, in July 2003.

The special session produced several contributions from researchers who are using computers to study problems that would otherwise be intractable. While computations have long been used to analyze problems, formulate conjectures, and search for special structures in knot theory, increased computational power has made them a staple in many facets of the field. From properties of knot invariants, to knot tabulation, studies of hyperbolic structures, knot energies, and the exploration of spaces of knots, computers have opened the doors to problems that would have otherwise been too difficult to do by hand.

The conference in Switzerland produced chapters concentrating on the models that researchers use to understand knotting, linking, and entanglement in physical and biological systems. Topics range from knotted umbilical cords, to studies of DNA knots, knots in proteins, and the structure of tight knots.

Together, the chapters in this volume present a unique arrangement of treatises exploring, in broad terms, four major themes: physical knot theory, knot theory in the life sciences, computational knot theory, and geometric knot theory.

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Part 1. Physical Knot Theory

Physical knot theory encompasses the study of knotting in structures composed of "real" materials, as well as the mathematical modeling of such structures. Knot energy, ropelength, and thickness (all of which measure the compactness of an embedding), and in particular the configurations that optimize these quantities, play a central role in this area. Chapters in this section discuss the dynamics of knots slipping off the end of a metal chain, the energy spectrum of tightly-knotted Quantum Chromodynamic (QDC) flux tubes, and the search for ideal configurations of knots. We begin with an article which, despite being one of the first papers ever written on physical knots, remains essentially unknown.

1. **On the Theory of Solid Knots**
   by Otto Krötenheerdt and Sigrid Veit; translated by Ted Ashton.

   Originally published in 1974 in the *Wissenschaftliche Beiträge der Martin-Luther-Universität Halle-Wittenberg* and translated by Ted Ashton, this appears to be the earliest treatise on thick knots and knots formed from identical beads.

2. **A Tutorial on Knot Energies**
   by E. J. J. van Rensburg.

   This chapter looks at different properties of knot energies defined for lattice knots, polygonal knots, and smooth knots. Several energies are analyzed with respect to these properties.

3. **Universal Energy Spectrum of Tight Knots and Links in Physics**
   by R. Buniy and T. Kephart.

   A system of tightly knotted, linked, or braided flux tubes can be given a universal mass-energy spectrum as the lengths of the fixed radius tubes depend only on the topology of the configuration. This proposal is motivated by examples from plasma physics, but the principal focus is on the model of glueballs as knotted QCD flux tubes.

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4. **Knot Dynamics in a Driven Hanging Chain: Experimental Results**
   by A. Belmonte.

   The author investigates the formation and motion of knots in a linear hanging chain shaken vertically with varying amplitude and frequency. An interesting phase diagram is presented that defines the optimal ratios between the amplitude and frequency required to generate knots. In addition, the complicated dynamics of the unknotting of different knots are analyzed.

5. **Biarcs, Global Radius of Curvature, and the Computation of Ideal Knot Shapes**
   by M. Carlen, B. Laurie, J. Maddocks, and J. Smutny.

   The authors introduce and exploit a $C^{1,1}$ biarc discretization to compute approximations to the ideal shapes of the trefoil and figure-eight knots with a tight control of numerical error. Geometric and parametric contact and approximate contact sets of thickened configurations are rigorously defined and carefully analyzed on the two approximately ideal shapes that are computed.

Part 2. Knot Theory in the Life Sciences

The chapters in this section explore knotting, linking, and folding in a biological setting. The issues addressed by these chapters include the dynamics of DNA gel-electrophoresis, DNA elasticity and packing, statistical models for protein folding, and the entangling of umbilical cords in the womb.

6. **Knotted Umbilical Cords**
   by Alain Goriely.

   In about 1% of newborn babies, the umbilical cord is knotted. The author reviews the medical literature on knotted umbilical cords, starting with the 1609 work of Louise Bourgois, and then offers a detailed explanation of the conditions required for the formation of knots in umbilical cords.

7. **Modelling DNA as a Thick Polymer: Application to DNA Elasticity and Packaging Thermodynamics**
   by C. Micheletti and D. Marenduzzo.

   The authors consider a thick polymer model to provide a coarse-grained description for double-stranded DNA. They use the model to gain insight into how the intrinsic thickness of DNA affects the behavior of the biomolecule subject to compaction.

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8. **Monte Carlo Simulations of Gel-Electrophoresis of DNA Knots**
   by C. Weber, M. Fleurant, P. De Los Rios, and G. Dietler.

   Circular DNA molecules of the same size but forming different knot types can be separated by gel electrophoresis according to their knot type. The authors present a numerical simulation that mimics the physical behavior of knotted DNA molecules during the process of gel electrophoresis.

9. **Atomic Force Microscopy of Complex DNA Knots**
   by F. Valle, M. Favre, J. Roca, and G. Dietler.

   This chapter analyzes DNA knots formed by circularization within intact phage particles in order to answer the long-standing question of how DNA is packed in phage heads. The authors apply atomic force microscopy imaging to investigate such DNA knots.

10. **Protein Folds, Knots and Tangles**
    by W. Taylor.

    The author introduces some interesting topological concepts to describe the structure and topology of properly folded protein chains. Applying one of these concepts, it is possible to detect whether or not a linear protein chain is knotted.

11. **Tying Down Open Knots: A Statistical Method For Identifying Open Knots With Applications To Proteins**
    by K. C. Millett and B. M. Sheldon.

    A new strategy of describing the nature of knotting that occurs in open random walks or proteins of varying lengths is investigated. Random walk and protein data are presented in a novel manner that gives deeper spatial information about the associated knotting spectrum and suggest new directions of research.

12. **Scaling of the Average Crossing Number in Equilateral Random Walks, Knots and Proteins**
    by A. Dobay, J. Dubochet, A. Stasiak, and Y. Diao.

    The authors compare configurations of properly folded proteins with those of random walks. They observe that, with respect to scaling behavior, small proteins (up to 300 amino acids) resemble self-attracting random walks while large proteins behave like ideal random walks in which independent segments neither attract nor repel each other.

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13. **Folding Complexity in a Random-Walk Copolymer Model**
by G. Arteca.

Physical properties of polymers are frequently approximated using a rather simple model of equilateral chains. More complex models are needed to describe correctly the effect of varying segment lengths in natural polymers like polysaccharides and proteins. The author investigates, both analytically and numerically, the potential effects of varying the segment lengths on selected physical properties of modeled polymers.

Part 3. Computational Knot Theory

This section highlights computational aspects of knot theory. These chapters utilize statistical methods (such as Monte Carlo explorations) and deterministic algorithms to measure the probability of knotting, the average crossing number in different types of random polygons, the ropelength of a knot, and to analyze properties of polymers modeled as random walks.

14. **Universal Characteristics of Polygonal Knot Probabilities**
by K. Millett and E. Rawdon.

The authors explore several functions for fitting probability graphs of different knotting models with the hopes of finding a single function that works for both the unknot and non-trivial knots. Of particular interest is the finite-range of knotting in the models.

15. **The Average Crossing Number of Gaussian Random Walks and Polygons**
by Y. Diao and C. Ernst.

Prior results on the average crossing number of equilateral random walks and polygons are extended to Gaussian random walks and polygons. The mean average crossing number, ACN, for Gaussian random walks and polygons of length n is of the form $\frac{1}{2\pi} n \ln n + O(n)$.

16. **Ropelength of Tight Polygonal Knots**
by J. Baranska, P. Pieranski, and E. Rawdon.

The authors analyze polygonal knots provided by the SONO algorithm arriving at upper bounds for the minimum smooth ropelength of a few knots. The analysis suggests another formula allowing one to estimate the minimum ropelength of smooth knots from the data obtained for polygons with fewer edges.

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17. **A Fast Octree-Based Algorithm for Computing Ropelength**
by T. Ashton and J. Cantarella.

This chapter presents an algorithm using octrees for computing the polygonal ropelength in (expected) $O(n \log n)$ time. This improves on the standard algorithm, which runs in $O(n^2)$ time. Some performance results for the authors' implementation are included.

18. **Topological Entropic Force Between a Pair of Random Knots Forming a Fixed Link**
by T. Deguchi.

The author explores the probability that two unknotted components are linked as a function of the distance between their centers of mass. Physical arguments are presented to derive an analytic expression for the cases of the trivial and Hopf link.

19. **Under-Knotted and Over-Knotted Polymers: 1. Unrestricted Loops**
by N. Moore, R. Lua, and A. Grosberg.

The authors present computer simulations to examine the probability distributions of the gyration radius for zero-thickness random equilateral knots. Of particular interest is the dependence of the distributions on length and topology.

20. **Under-Knotted and Over-Knotted Polymers: 2. Compact Self-Avoiding Loops**
by R. Lua, N. Moore, and A. Grosberg.

The authors explore compact random knots, namely those forming Hamiltonian closed paths on the 3-dimensional cubic lattice. In particular, they analyze the effect of topology and the size of the knotted regions.

21. **On the Mean Gyration Radius and the Radial Distribution Function of Ring Polymers With Excluded Volume Under a Topological Constraint**
by M. Shimamura and T. Deguchi.

The competition between topological effects and those of excluded volume on the average size of ring polymers is studied in this chapter. In addition, radial distribution functions of segments of ring polymers with fixed knotting are discussed. Numerical results suggest that topological constraints on ring polymers lead to entropic repulsion among polymer segments.

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22. **Thermodynamics and Topology of Disordered Knots. Correlations in Trivial Lattice Knot Diagrams**
by S. Nechaev and O. Vasilyev.

In this investigation of the statistical properties of random lattice knots, the focus is on the "knottedness" of densely packed knots as measured by the Jones-Kauffman polynomial. The results of this study provide support for a conjecture that collapsed closed polymer chains form systems of densely packed mutually segregated folds.

23. **Generating Large Random Knot Projections**
by Y. Diao, C. Ernst, and Uta Ziegler.

This chapter addresses the difficult problem of randomly generating knot projections with a large number of crossings. Two approaches to generate diagrams of large knots are presented, and even though they both have the drawback of lack of control over the resulting probability distribution, they are of undeniable interest.

Part 4. Geometric Knot Theory

The central questions of the chapters in this final section address a variety of topics, all of which focus on the geometry of knotting and folding. These include knot enumeration, flat ribbons, quadrisecants, writhe of non-closed curves, ropelength-critical clasps, hyperbolic invariants, and thick surfaces.

24. **Minimal Flat Knotted Ribbons**
by L. Kauffman.

The author obtains upper bounds for the minimal length required to make a flat knotted ribbon by examining the configurations which naturally arise when a flat ribbon is tied as a trefoil or figure-eight knot and pulled tight. In the case of a trefoil, the conjectured optimal configuration takes on the shape of a regular pentagon; in the case of the figure-eight knot, it has a hexagonal shape.

25. **Quadrisecants of Knots with Small Crossing Number**
by G. T. Jin.

This chapter examines the set of quadrisecants for several embeddings of the knots with five crossings or fewer. It also conjectures that the "quadrisecant approximation" of a knot K – that is, the piecewise-linear knot whose vertices are the intersection points of K with each of its quadrisecants – has the same knot type as K.

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26. **On the Writhe of Non-Closed Curves**
by E. Starostin.

The author defines the writhe of an open space curve and explores its computation. The approach is based on closing the tangent indicatrix with a geodesic. A relationship connecting the writhe with the Gauss integral over the open curve is also studied.

27. **On a Mathematical Model for Thick Surfaces**
by P. Strzelecki and H. von del Mosel.

The authors of this paper extend the concept of thick knots to surfaces by using a quantity – known as the global radius of curvature $\Delta[X]$ – which is defined over a large class of non-smooth parametric surfaces. The main result is that a surface X is in fact a continuously differentiable manifold and can be "thickened" by a constant magnitude of θ whenever $\Delta[X] \geq \theta > 0$.

28. **Some Ropelength-Critical Clasps**
by J. Sullivan and N. Wrinkle.

The Gehring ropelength problem asks to minimize the length of a link whose components stay at a unit distance from each other; a balance criterion describes which configurations are critical. Several explicit configurations of clasped ropes which are balanced, and hence critical, are presented.

29. **Remarks on Some Hyperbolic Invariants of 2-Bridge Knots**
by J. Hoste and P. Shanahan.

The authors describe a recursive technique suitable for computing several hyperbolic invariants of a class of 2-bridge knots. These include the representation and character varieties, the trace and cusp fields, and the A-polynomial. Applications and generalizations of this computational technique are also discussed.

30. **Conjectures on the Enumeration of Alternating Links**
by P. Zinn-Justin.

This chapter parallels the enumeration of alternating links and tangles with statistical models on random lattices. The insight provided by this parallelism leads to conjectures on asymptotic counting as the number of crossings becomes large.

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We believe that this collection provides the reader with an excellent entry to the foundations of work in these areas and to the broad spectrum of new questions, techniques, and research progress. Without the extraordinary efforts of the large number of researchers whose work is presented in the collection, we would never have been able to bring the project to a timely conclusion. The editors thank all the authors and referees for their dedication to this project.

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