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LECTURE NOTES PREPARED FOR THE
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APPLICATIONS OF KNOT THEORY
HELD IN SAN DIEGO, CALIFORNIA
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10 9 8 7 6 5 4 3 2 1 14 13 12 11 10 09

# Contents

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# Preface

The original motivation for understanding and classifying knots was due to Lord Kelvin who theorized in the 1880s that atoms were knotted or linked vortex rings in the "ether", and that different elements were determined by the knot or link type of the vortex ring. By the early 1900s, Kelvin's theory had been proven wrong. However topologists continued to study the knot theory as an area of pure mathematics. Over the past 20-30 years, knot theory has rekindled its historic ties with biology, chemistry, and physics as a means of creating more sophisticated descriptions of the entanglements and properties of natural phenomena—from strings to organic compounds to DNA.

For example, DNA knots and links have been implicated in a number of cellular processes since their discovery in the late 1960s. In particular, they have been found during replication and recombination, and as the products of protein actions, notably with topoisomerases, recombinases, and transposases. The variety of DNA knots and links observed makes biologically separating and distinguishing these molecules a critical issue. While DNA knots and links can be visualized via electron microscopy, this process can be both difficult and time-consuming. So topological methods of characterizing and predicting their behavior can be helpful.

Chemists have been interested in molecular chirality since Pasteur first described it in 1848. For example, since the two mirror forms of the same molecule can interact with a host's metabolism very differently, predicting whether or not a molecule will be chiral is important to pharmaceutical companies as they develop new medications. While the geometry of a rigid molecule determines whether or not it is chiral, for flexible or even partially flexible molecules, knot theory can play a role in determining chirality.

In addition to the examples described above, there are many other deep interactions between knot theory and various areas of scientific investigation. The 2008 AMS Short Course *Applications of Knot Theory*, on which this volume is based, was intended to introduce the area of applied knot theory to a broad mathematical audience. The aim of the Short Course and this volume, while not covering all aspects of applied knot theory, is to provide the reader with a mathematical appetizer, in order to stimulate the mathematical appetite for further study of this exciting field.

No prior knowledge of topology, biology, chemistry, or physics is assumed. In particular, the first three chapters of this volume introduce the reader to knot theory (by Colin Adams), topological chirality and molecular symmetry (by Erica Flapan), and DNA topology (by Dorothy Buck). The second half of this volume is focused on three particular applications of knot theory. Lou Kauffman presents a chapter on applications of knot theory to physics, Ned Seeman presents a chapter on how topology is used in DNA nanotechnology, and Jon Simon presents a chapter on the statistical and energetic properties of knots and their relation to molecular biology. The articles and their authors are described in more detail below.

### Description of articles and their authors

**Chapter 1: A Brief Introduction to Knot Theory from the Physical Point of View by Colin Adams**

This article introduces the mathematical theory of knots, including Reidemeister moves, surfaces, types of knots, and various invariants associated to knots, including the new superinvariants. It also touches on the stick number for knots and its implications for chemistry.

Colin Adams is the Thomas T. Read Professor of Mathematics at Williams College. He authored the now-standard undergraduate knot theory text, "The Knot Book", and is renowned for his witty and deceptively sophisticated introductory geometry and topology talks. His own research focuses on hyperbolic knots and 3-manifolds. He has involved numerous undergraduates in annual summer research projects at Williams. He is a recipient of the Deborah and Franklin Tepper Haimo Distinguished Teaching Award from the MAA, and has been selected as a Polya Lecturer for the MAA as well as a Sigma Xi Distinguished Lecturer.

**Chapter 2: Topological Chirality and Symmetries of Non-rigid Molecules by Erica Flapan**

This article explains the concept of chirality and why it is important, and discusses the differences between chemical, geometric, topological, and intrinsic chirality. It then introduces four different techniques to show that a molecule is topologically chiral. The article concludes by presenting different approaches to classifying molecular symmetries. In particular, it compares the point group to the topological symmetry group, and explains how the topological symmetry group can be used to analyze the symmetries of non-rigid molecules.

Erica Flapan is the Lingurn H. Burkhead Professor of Mathematics at Pomona College. Her research is in knot theory, 3-dimensional topology, and applications of topology to chemistry and biology. Her book "When Topology Meets Chemistry", is jointly published by the Mathematical Association of America and Cambridge University Press. From 2000 to 2004, she was the principal investigator on an NSF-CCLI grant entitled "Enhancing the mathematical understanding of students in chemistry". As part of this grant, she developed a course entitled "Problem Solving in the Sciences", to help students with weak math skills succeed in general chemistry, and together with Daniel O'Leary (an organic chemist), she developed an interdisciplinary upper division course entitled "Symmetry and Chirality".

**Chapter 3: DNA Topology by Dorothy Buck**

This article introduces DNA, and explains the contributions of knot theory to its study. In particular, it explores the topological techniques used to understand both DNA itself, and how it interacts with proteins in the cell. As an extended example, it gives an overview of the tangle model and its variations to understand the molecular process of site-specific recombination. It also discusses various mathematical contributions to several open questions involving DNA, including how a protein can effectively unknot DNA.

Dorothy Buck is a Mathematical Biologist at Imperial College, London in the Department of Mathematics and Centre for Bioinformatics. She specializes in 3-manifold topology and its applications to mathematical biology. Her training is in both mathematics and microbiology. She spent six years working in molecular biology labs at the University of Texas at Austin and Johns Hopkins Medical School. Before joining the faculty at Imperial, she was an NSF Postdoctoral Fellow with Craig Benham at the Genome Center at the University of California at Davis, and an Assistant Professor in the Applied Mathematics Department at Brown University.

**Chapter 4: Knots and Physics by Louis H. Kauffman**

Knots are mathematical abstractions of the topological properties of rope in physical space. As such, there are immediate relationships of knots with the physics of ropes, weaves, long-chain molecules and other knotting phenomena in nature. There are also beautiful and surprising relationships of knot theory with the structures and methods of statistical mechanics and quantum theory. This article surveys some of the author's favorite interactions between knots and physics.

Louis Kauffman is Professor of Mathematics at University of Illinois-Chicago. He authored the interdisciplinary text "Knots and Physics". He discovered the bracket polynomial state model for the Jones polynomial, and the first direct relationship between statistical mechanics models and knot invariants. As a topologist, he is omnivorous, working in knot theory and its relationships with statistical mechanics, quantum theory, algebra, combinatorics, and more recently, biology. He is the Editor of the Journal of Knot Theory and its Ramifications.

**Chapter 5: Synthetic Single-Stranded DNA Topology by Nadrian C. Seeman**

The double helical nature of the DNA molecule has a wide variety of topological implications. Most biologists are familiar with the notion that circular DNA molecules are catenanes/links, so that the strands are linked about once every 10 nucleotides. Consequently, biological systems contain topoisomerases which change the linking topology of the molecule, thereby solving a variety of problems in the metabolism of the genetic material. Today, the realm of DNA extends beyond its biological role as a molecule with an unbranched helix axis. Branched DNA molecules exist as intermediates in genetic recombination, but for 25 years synthetic branched DNA molecules have been built for a variety of purposes that are important for nanotechnology and for molecular computation. The ability to assemble branched DNA backbones has enabled the deliberate construction of single-stranded knots, polyhedral catenanes and Borromean rings. New branched DNA motifs have been derived by using techniques from knot theory. Branched DNA molecules have enabled the deliberate construction of periodic and aperiodic DNA crystals. The applications of these systems include analysis of biological systems, nanoelectronics and nanorobotics.

This article presents the features of synthetic DNA topology, from the design of branched, knotted and linked motifs, to the construction of objects, arrays and devices.

Ned Seeman is the Margaret and Herman Sokol Professor of Chemistry at New York University. He founded the field of structural DNA nanotechnology. His lab has characterized the interactions of synthetic DNA knots with topoisomerases, developed a general algorithm for the construction of any DNA knot, synthesized a DNA molecule that can be built to yield four different topological species, and discovered an RNA topoisomerase. For his innovation, he was awarded the Feynman Prize in Nanotechnology, the Emerging Technology Award from Discover Magazine and elected Fellow of the Royal Society of Chemistry. He is the Founding President of the International Society for Nanoscale Science, Computation and Engineering. Most impressively, in 2008 he was awarded the Nichols Medal from the American Chemical Society.

**Chapter 6: Long Tangled Filaments by Jonathan Simon**

This article considers filaments, from rope and string and hair to DNA and proteins, anything that might be understood as one-dimensional strands wiggling and tangling in three-dimensional space.

If the filaments are short, we can try to describe their exact geometric shape and understand how their shape relates to physical behavior. If the filaments are somewhat long and flexible, then topological knot type can be very useful, as evidenced by the success of topological methods for studying the actions of DNA enzymes. But if the filaments are very long (think of a complicated 3-dimensional scribble) or somehow random (think of a lot of complicated 3-dimensional scribbles) then it may be impractical to try to describe the exact shapes or even knot types. We need to develop a vocabulary of ideas and models that describe physically important geometric/topological properties of long tangled things.

This article presents ideas, experiments, and theorems dealing with packing, curvature, tangling, and knotting of individual complicated filaments as well as statistical ensembles. It explores some of the work that has been done, some open research problems, and some topics that seem well-suited for undergraduate research activities.

Jon Simon is Professor of Mathematics at the University of Iowa. He pioneered the rigorous applications of knot theory to chemistry, in particular by proving the topological chirality of molecular Möbius ladders. He co-developed the idea of Möbius energy of thick knots. His current research also includes particular knotting and tangling of filaments; "energy" of knots; and applications to molecular biology, in particular, knotted DNA loops.

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Dorothy Buck, Erica Flapan

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# Index

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