Mathematical Approaches To Polymer Sequence Analysis And Related Problems

This book covers the most recent advances in the deformation and fracture behaviour of polymer material. It provides deeper insight into related morphology–property correlations of thermoplastics, elastomers and polymer resins. Each chapter of this book gives a comprehensive review of state-of-the-art methods of materials testing and diagnostics, tailored for plastic pipes, films and adhesive systems as well as elastomeric components and others. The investigation of deformation and fracture behaviour using the experimental methods of fracture mechanics has been the subject of intense research during the last decade. In a systematic manner, modern aspects of fracture mechanics in the industrial application of polymers for bridging basic research and industrial development are illustrated by multifarious examples of innovative materials usage. This book will be of value to scientists, engineers and in polymer materials science.

The idea of this book grew out of a symposium that was held at Stony Brook in September 2012 in celebration of David S.Warren's fundamental contributions to Computer Science and the area of Logic Programming in particular. Logic Programming (LP) is at the nexus of Knowledge Representation, Artificial Intelligence, Mathematical Logic, Databases, and Programming Languages. It is fascinating and intellectually stimulating due to the fundamental interplay among theory, systems, and applications brought about by logic. Logic programs are more declarative in the sense that they strive to be logical specifications of "what" to do rather

than "how" to do it, and thus they are high-level and easier to understand and maintain. Yet, without being given an actual algorithm, LP systems implement the logical specifications automatically. Several books cover the basics of LP but focus mostly on the Prolog language with its incomplete control strategy and non-logical features. At the same time, there is generally a lack of accessible yet comprehensive collections of articles covering the key aspects in declarative LP. These aspects include, among others, well-founded vs. stable model semantics for negation, constraints, object-oriented LP, updates, probabilistic LP, and evaluation methods, including top-down vs. bottom-up, and tabling. For systems, the situation is even less satisfactory, lacking accessible literature that can help train the new crop of developers, practitioners, and researchers. There are a few guides onWarren's Abstract Machine (WAM), which underlies most implementations of Prolog, but very little exists on what is needed for constructing a state-of-the-art declarative LP inference engine. Contrast this with the literature on, say, Compilers, where one can first study a book on the general principles and algorithms and then dive in the particulars of a specific compiler. Such resources greatly facilitate the ability to start making meaningful contributions quickly. There is also a dearth of articles about systems that support truly declarative languages, especially those that tie into first-order logic, mathematical programming, and constraint solving. LP helps solve challenging problems in a wide range of application areas, but in-depth analysis of their connection with LP language abstractions and LP implementation methods is lacking. Also, rare are surveys of challenging application areas of LP, such as Bioinformatics, Natural Language Processing, Verification, and Planning. The goal of this book is to help fill in the previously mentioned void in the LP literature. It offers a number of overviews on key aspects

of LP that are suitable for researchers and practitioners as well as graduate students. The following chapters in theory, systems, and applications of LP are included.

This book explores quantitative aspects of protein biophysics and attempts to delineate certain rules of molecular behavior that make atomic scale objects behave in a digital way. This book will help readers to understand how certain biological systems involving proteins function as digital information systems despite the fact that underlying processes are analog in nature. The in-depth explanation of proteins from a quantitative point of view and the variety of level of exercises (including physical experiments) at the end of each chapter will appeal to graduate and senior undergraduate students in mathematics, computer science, mechanical engineering, and physics, wanting to learn about the biophysics of proteins. L. Ridgway Scott has been Professor of Computer Science and of Mathematics at the University of Chicago since 1998, and the Louis Block Professor since 2001. He obtained a B.S. degree (Magna Cum Laude) from Tulane University in 1969 and a PhD degree in Mathematics from the Massachusetts Institute of Technology in 1973. Professor Scott has published over 130 papers and three books, extending over biophysics, parallel computing and fundamental computing aspects of structural mechanics, fluid dynamics, nuclear engineering, and computational chemistry. Ariel Fernández (born Ariel Fernández Stigliano) is an Argentinian-American physical chemist and mathematician. He obtained his Ph. D. degree in Chemical Physics from Yale University and held the Karl F. Hasselmann Endowed Chair Professorship in Bioengineering at Rice University. He is currently involved in research and entrepreneurial activities at various consultancy firms. Ariel Fernández authored three books on translational medicine and biophysics, and published 360 papers in professional journals. He holds two patents in the field of

biotechnology.

Polymer chains that interact with themselves and/or with their environment are fascinating objects, displaying a range of interesting physical and chemical phenomena. The focus in this monograph is on the mathematical description of some of these phenomena, with particular emphasis on phase transitions as a function of interaction parameters, associated critical behavior and space-time scaling. Topics include: self-repellent polymers, self-attracting polymers, polymers interacting with interfaces, charged polymers, copolymers near linear or random selective interfaces, polymers interacting with random substrate and directed polymers in random environment. Different techniques are exposed, including the method of local times, large deviations, the lace expansion, generating functions, the method of excursions, ergodic theory, partial annealing estimates, coarse-graining techniques and martingales. Thus, this monograph offers a mathematical panorama of polymer chains, which even today holds plenty of challenges.

Polymer Solutions: An Introduction to Physical Properties offers a fresh, inclusive approach to teaching the fundamentals of physical polymer science. Students, instructors, and professionals in polymer chemistry, analytical chemistry, organic chemistry, engineering, materials, and textiles will find Iwao Teraoka's text at once accessible and highly detailed in its treatment of the properties of polymers in the solution phase. Teraoka's purpose in writing Polymer Solutions is twofold: to familiarize the advanced undergraduate and beginning graduate student with basic concepts, theories, models, and experimental techniques for polymer solutions; and to provide a reference for researchers working in the area of polymer solutions as well as those in charge of chromatographic characterization of polymers. The author's incorporation of recent advances in the

instrumentation of size-exclusion chromatography, the method by which polymers are analyzed, renders the text particularly topical. Subjects discussed include: Real, ideal, Gaussian, semirigid, and branched polymer chains Polymer solutions and thermodynamics Static light scattering of a polymer solution Dynamic light scattering and diffusion of polymers Dynamics of dilute and semidilute polymer solutions Study questions at the end of each chapter not only provide students with the opportunity to test their understanding, but also introduce topics relevant to polymer solutions not included in the main text. With over 250 geometrical model diagrams, Polymer Solutions is a necessary reference for students and for scientists pursuing a broader understanding of polymers.

Biomarker discovery is an important area of biomedical research that may lead to significant breakthroughs in disease analysis and targeted therapy. Biomarkers are biological entities whose alterations are measurable and are characteristic of a particular biological condition. Discovering, managing, and interpreting knowledge of new biomarkers are challenging and attractive problems in the emerging field of biomedical informatics. This volume is a collection of state-of-the-art research into the application of data mining to the discovery and analysis of new biomarkers. Presenting new results, models and algorithms, the included contributions focus on biomarker data integration, information retrieval methods, and statistical machine learning techniques. This volume is intended for students, and researchers in bioinformatics, proteomics, and genomics, as well engineers and applied scientists interested in the interdisciplinary application of data mining techniques.

The ability of condensation polymers to undergo additional chemical reactions, so-called transreactions, is really fascinating. These processes lead to novel copolymers with

desired composition and sequential order, allow to enhance the compatibility and to minimize molecular weight fluctuations during polycondensation and processing and to provide for chemical healing of laminates of condensation polymers. An international team of highly reputated polymer chemists and physicists discusses here, first of all, various types of transreactions, but additional condensations are also detailed in many cases. - A comprehensive book of high interest to any polymer scientist in academia and industry! This series presents critical reviews of the present and future trends in polymer and biopolymer science including chemistry, physical chemistry, physics and materials science. It is addressed to all scientists at universities and in industry who wish to keep abreast of advances in the topics covered. Impact Factor Ranking: Always number one in Polymer Science. More information as well as the electronic version of the whole content available at: www.springerlink.com

Written by experts in both mathematics and biology, Algebraic and Discrete Mathematical Methods for Modern Biology offers a bridge between math and biology, providing a framework for simulating, analyzing, predicting, and modulating the behavior of complex biological systems. Each chapter begins with a question from modern biology, followed by the description of certain mathematical methods and theory appropriate in the search of answers. Every topic provides a fast-track pathway through the problem by presenting the biological foundation, covering the relevant mathematical theory, and highlighting connections between them. Many of the projects and exercises embedded in each chapter utilize specialized software, providing students with much-needed familiarity and experience with

computing applications, critical components of the "modern biology" skill set. This book is appropriate for mathematics courses such as finite mathematics, discrete structures, linear algebra, abstract/modern algebra, graph theory, probability, bioinformatics, statistics, biostatistics, and modeling, as well as for biology courses such as genetics, cell and molecular biology, biochemistry, ecology, and evolution. Examines significant questions in modern biology and their mathematical treatments Presents important mathematical concepts and tools in the context of essential biology Features material of interest to students in both mathematics and biology Presents chapters in modular format so coverage need not follow the Table of Contents Introduces projects appropriate for undergraduate research Utilizes freely accessible software for visualization, simulation, and analysis in modern biology Requires no calculus as a prerequisite Provides a complete Solutions Manual Features a companion website with supplementary resources
Drug discovery is an expensive, time-consuming process and the modern drug discovery community is constantly challenged not only with discovering novel bioactive agents to combat resistance from known diseases and fight against new ones, but to do so in a way that is economically effective. Advances in both experimental and theoretical/computational methods envisage that the greatest challenges in drug discovery can be most successfully addressed by using a multi-scale approach, drawing on the specialties of a whole host of different disciplines. Multi-Scale Approaches to Drug Discovery

furnishes chemists with the detail they need to identify drug leads with the highest potential before isolating and synthesizing them to produce effective drugs with greater swiftness than classical methods may allow. This significantly speeds up the search for more efficient therapeutic agents. After an introduction to multi-scale approaches outlining the need for and benefits of their use, the book goes on to explore a range of useful techniques and research areas, and their potential applications to this process. Profiling drug binding by thermodynamics, machine learning for predicting enzyme sub-classes, and multitasking models for computer-aided design and virtual compound screening are discussed, before the book goes on to review Alkaloid Menispermaceae leads, natural chemotherapeutic agents and methods for speeding up the design and virtual screening of therapeutic peptides. Flavonoids as multi-target compounds are then explored, before the book concludes with a review of Quasi-SMILES as a novel tool. Collecting together reviews and original research contributions written by leading experts in the field, Multi-Scale Approaches to Drug Discovery highlights cutting-edge approaches and practical examples of their implementation for those involved in the drug discovery process at many different levels. Using the combined knowledge of medicinal, computational, pharmaceutical and bio- chemists, it aims to support growth in the multi-scale approach to promote greater success in the development of new drugs. Offers practical guidance on ways to implement multiscale approaches for increased efficiency in drug discovery

Draws on the experience of a highly skilled team of authors under the editorial guidance of one of the field's leading experts Includes cutting-edge techniques at the forefront of medicinal chemistry and drug discovery optimization

Propelled by the success of the sequencing of the human and many related genomes, molecular and cellular biology has delivered significant scientific breakthroughs. Mathematics (broadly defined) continues to play a major role in this effort, helping to discover the secrets of life by working collaboratively with bench biologists, chemists and physicists. Because of its outstanding record of interdisciplinary research and training, the IMA was an ideal venue for the 2007-2008 IMA thematic year on Mathematics of Molecular and Cellular Biology. The kickoff event for this thematic year was a tutorial on Mathematics of Nucleic Acids, followed by the workshop Mathematics of Molecular and Cellular Biology, held September 15--21 at the IMA. This volume is dedicated to the memory of Nicholas R. Cozzarelli, a dynamic leader who fostered research and training at the interface between mathematics and molecular biology. It contains a personal remembrance of Nick Cozzarelli, plus 15 papers contributed by workshop speakers. The papers give an overview of state-of-the-art mathematical approaches to the understanding of DNA structure and function, and the interaction of DNA with proteins that mediate vital life processes.

The papers collected in this volume reproduce contributions by leading sch- arstoaninternationalschoola ndworkshopwhichwasorganizedandheldwith

thegoaloftakinga snapshotofadiscipline undertumultuous growth. Indeed, the area of protein folding, docking and alignment is developing in response to needs for a mix of heterogeneous expertise spanning biology, chemistry, mathematics, computer science, and statistics, among others. Some of the problems encountered in this area are not only important for the scienti?c challenges they pose, but also for the opportunities they disclose intermsofmedicalandindustrialexploitation. Atypicalexampleiso?eredby protein-drug interaction (docking), a problem posing daunting computational problems at the crossroads of geometry, physics and chemistry, and, at the same time, a problem with unimaginable implications for the pharmacopoeia of the future. The schoolfocused on problems posed by the study of the mechanisms - hind protein folding, and explored di?erent ways of attacking these problems under objective evaluations of the methods. Together with a relatively small core of consolidated knowledge and tools, important re?ections were brought to this e?ort by studies in a multitude of directions and approaches. It is obviously impossible to predict which, if any, among these techniques will prove completely successful, but it is precisely the implicit dialectic among them that best conveys the current ?avor of the ?eld. Such unique diversity and richness inspired the format of the meeting, and also explains the slight departure of the present volume from the typical format in this series: the exposition of the current sediment is complemented here by a selection of quali?ed specialized contributions.

This first comprehensive overview of reactive extrusion

technology for over a decade combines the views of contributors from both academia and industry who share their experiences and highlight possible applications and markets. They also provide updated information on the underlying chemical and physical concepts, summarizing recent developments in terms of the material and machinery used. As a result, readers will find here a compilation of potential applications for reactive extrusion to access new and cost-effective polymeric materials, while using existing compounding machines.
Graph Theory (as a recognized discipline) is a relative newcomer to Mathematics. The first formal paper is found in the work of Leonhard Euler in 1736. In recent years the subject has grown so rapidly that in today's literature, graph theory papers abound with new mathematical developments and significant applications. As with any academic field, it is good to step back occasionally and ask Where is all this activity taking us?, What are the outstanding fundamental problems?, What are the next important steps to take?. In short, Quo Vadis, Graph Theory?. The contributors to this volume have together provided a comprehensive reference source for future directions and open questions in the field.
Scientific theories that explain how physical systems behave are described by mathematical models which provide the basis for computer simulations of events that occur in the physical universe. These models, being only mathematical characterizations of actual phenomena, are obviously subject to error because of the inherent limitations of all mathematical abstractions. In this work,

new theory and methodologies are developed to quantify such modeling error in a special way that resolves a fundamental and standing issue: multiscale modeling, the development of models of events that transcend many spatial and temporal scales. Specifically, we devise the machinery for a posteriori estimates of relative modeling error between a model of fine scale and another of coarser scale, and we use this methodology as a general approach to multiscale problems. The target application is one of critical importance to nanomanufacturing: imprint lithography of semiconductor devices. The development of numerical methods for multiscale modeling has become one of the most important areas of computational science. Technological developments in the manufacturing of semiconductors hinge upon the ability to understand physical phenomena from the nanoscale to the microscale and beyond. Predictive simulation tools are critical to the advancement of nanomanufacturing semiconductor devices. In principle, they can displace expensive experiments and testing and optimize the design of the manufacturing process. The development of such tools rest on the edge of contemporary methods and high-performance computing capabilities and is a major open problem in computational science. In this dissertation, a molecular model is used to simulate the deformation of polymeric materials used in the fabrication of semiconductor devices. Algorithms are described which lead to a complex molecular model of polymer materials designed to produce an etch barrier, a critical component in imprint lithography approaches to semiconductor

manufacturing. Each application of this so-called polymerization process leads to one realization of a lattice-type model of the polymer, a molecular statics model of enormous size and complexity. This is referred to as the base model for analyzing the deformation of the etch barrier, a critical feature of the manufacturing process. To reduce the size and complexity of this model, a sequence of coarser surrogate models is generated. These surrogates are the multiscale models critical to the successful computer simulation of the entire manufacturing process. The surrogate involves a combination of particle models, the molecular model of the polymer, and a coarse-scale model of the polymer as a nonlinear hyperelastic material. Coefficients for the nonlinear elastic continuum model are determined using numerical experiments on representative volume elements of the polymer model. Furthermore, a simple model of initial strain is incorporated in the continuum equations to model the inherit shrinking of the A coupled particle and continuum model is constructed using a special algorithm designed to provide constraints on a region of overlap between the continuum and particle models. This coupled model is based on the so-called Arlequin method that was introduced in the context of coupling two continuum models with differing levels of discretization. It is shown that the Arlequin problem for the particle-tocontinuum model is well posed in a one-dimensional setting involving linear harmonic springs coupled with a linearly elastic continuum. Several numerical examples are presented. Numerical experiments in three dimensions are also discussed in

which the polymer model is coupled to a nonlinear elastic continuum. Error estimates in local quantities of interest are constructed in order to estimate the modeling error due to the approximation of the particle model by the coupled multiscale surrogate model. The estimates of the error are computed by solving an auxiliary adjoint, or dual, problem that incorporates as data the quantity of interest or its derivatives. The solution of the adjoint problem indicates how the error in the approximation of the polymer model inferences the error in the quantity of interest. The error in the quantity of interest represents the relative error between the value of the quantity evaluated for the base model, a quantity typically unavailable or intractable, and the value of the quantity of interest provided by the multiscale surrogate model. To estimate the error in the quantity of interest, a theorem is employed that establishes that the error coincides with the value of the residual functional acting on the adjoint solution plus a higher-order remainder. For each surrogate in a sequence of surrogates generated, the residual functional acting on various approximations of the adjoint is computed. These error estimates are used to construct an adaptive algorithm whereby the model is adapted by supplying additional fine-scale data in certain subdomains in order to reduce the error in the quantity of interest. The adaptation algorithm involves partitioning the domain and selecting which subdomains are to use the particle model, the continuum model, and where the two overlap. When the algorithm identifies that a region contributes a relatively large amount to the error in the quantity of interest, it is scheduled for refinement

by switching the model for that region to the particle model. Numerical experiments on several configurations representative of nano-features in semiconductor device fabrication demonstrate the effectiveness of the error estimate in controlling the modeling error as well as the ability of the adaptive algorithm to reduce the error in the quantity of interest. There are two major conclusions of this study: 1. an effective and well posed multiscale model that couples particle and continuum models can be constructed as a surrogate to molecular statics models of polymer networks and 2. an error estimate of the modeling error for such systems can be estimated with sufficient accuracy to provide the basis for very effective multiscale modeling procedures. The methodology developed in this study provides a general approach to multiscale modeling. The computational procedures, computer codes, and results could provide a powerful tool in understanding, designing, and optimizing an important class of semiconductormanufacturing processes. The study in this dissertation involves all three components of the CAM graduate program requirements: Area A, Applicable Mathematics; Area B, Numerical Analysis and Scientific Computation; and Area C, Mathematical Modeling and Applications. The multiscale modeling approach developed here is based on the construction of continuum surrogates and coupling them to molecular statics models of polymer as well as a posteriori estimates of error and their adaptive control. A detailed mathematical analysis is provided for the Arlequin method in the context of coupling particle and continuum models for a class of one-dimensional

model problems. Algorithms are described and implemented that solve the adaptive, nonlinear problem proposed in the multiscale surrogate problem. Large scale, parallel computations for the base model are also shown. Finally, detailed studies of models relevant to applications to semiconductor manufacturing are presented.

Polymer and cell dynamics play an important role in processes like tumor growth, metastasis, embryogenesis, immune reactions and regeneration. Based on an international workshop on numerical simulations of polymer and cell dynamics in Bad Honnef (Germany) in 2000, this volume provides an overview of the relevant mathematical and numerical methods, their applications and limits. Polymer and Cell Dynamics will be of interest to scientists and advanced undergraduates.

An edited volume describing the latest developments in approaching the problem of polymer sequence analysis, with special emphasis on the most relevant biopolymers (peptides and DNA) but not limited to them. The chapters will include peptide sequence analysis, DNA sequence analysis, analysis of biopolymers and nonpolymers, sequence alignment problems, and more.

Natural and synthetic water soluble polymers are used in a wide range of familiar industrial and consumer products, including coatings and inks, papers, adhesives, cosmetics and personal care products. They perform a variety of functions without which these products would be significantly more expensive, less effective or both. Written for research, development and formulation chemists, technologists and engineers at graduate level and beyond in the fine and

specialty chemicals, polymers, food and pharmaceutical industries, the Handbook of Industrial Water Soluble Polymers deals specifically with the functional properties of both natural and synthetic water soluble polymers. By taking a function based approach, rather than a “polymer specific” approach the book illustrates how polymer structure leads to effect, and shows how different polymer types can be employed to achieve appropriate product properties. Polymers are used in everything from nylon stockings to commercial aircraft to artificial heart valves, and they have a key role in addressing international competitiveness and other national issues. Polymer Science and Engineering explores the universe of polymers, describing their properties and wide-ranging potential, and presents the state of the science, with a hard look at downward trends in research support. Leading experts offer findings, recommendations, and research directions. Lively vignettes provide snapshots of polymers in everyday applications. The volume includes an overview of the use of polymers in such fields as medicine and biotechnology, information and communication, housing and construction, energy and transportation, national defense, and environmental protection. The committee looks at the various classes of polymers--plastics, fibers, composites, and other materials, as well as polymers used as membranes and coatings--and how their composition and specific methods of processing result in unparalleled usefulness. The reader can also learn the science behind the technology, including efforts to model polymer synthesis after nature's methods, and breakthroughs in characterizing polymer properties needed for twenty-first-century applications. This informative volume will be important to chemists, engineers, materials scientists, researchers, industrialists, and policymakers interested in the role of polymers, as well as to science and engineering educators and students.

This book describes fruitful past collaborations between the mathematical and materials sciences and indicates future challenges. It seeks both to encourage mathematical sciences research that will complement vital research in materials science and to raise awareness of the value of quantitative methods. The volume encourages both communities to increase cross-disciplinary collaborations, emphasizing that each has much to gain from such an increase, and it presents recommendations for facilitating such work. This book is written for both mathematical and materials science researchers interested in advancing research at this interface; for federal and state agency representatives interested in encouraging such collaborations; and for anyone wanting information on how such cross-disciplinary, collaborative efforts can be accomplished successfully.

This book is a collection of representative and novel works done in Data Mining, Knowledge Discovery, Clustering and Classification that were originally presented in French at the EGC'2012 Conference held in Bordeaux, France, on January 2012. This conference was the 12th edition of this event, which takes place each year and which is now successful and well-known in the French-speaking community. This community was structured in 2003 by the foundation of the French-speaking EGC society (EGC in French stands for ``Extraction et Gestion des Connaissances'' and means ``Knowledge Discovery and Management'', or KDM). This book is intended to be read by all researchers interested in these fields, including PhD or MSc students, and researchers from public or private laboratories. It concerns both theoretical and practical aspects of KDM. The book is structured in two parts called ``Knowledge Discovery and Data Mining'' and ``Classification and Feature Extraction or Selection''. The first part (6 chapters) deals with data clustering and data mining.

The three remaining chapters of the second part are related to classification and feature extraction or feature selection. This volume presents a collection of courses introducing the reader to the recent progress with attention being paid to laying solid grounds and developing various basic tools. An introductory chapter on lattice spin models is useful as a background for other lectures of the collection. The topics include new results on phase transitions for gradient lattice models (with introduction to the techniques of the reflection positivity), stochastic geometry reformulation of classical and quantum Ising models, the localization/delocalization transition for directed polymers. A general rigorous framework for theory of metastability is presented and particular applications in the context of Glauber and Kawasaki dynamics of lattice models are discussed. A pedagogical account of several recently discussed topics in nonequilibrium statistical mechanics with an emphasis on general principles is followed by a discussion of kinetically constrained spin models that are reflecting important peculiar features of glassy dynamics.

This book primarily focuses on rigorous mathematical formulation and treatment of static problems arising in continuum mechanics of solids at large or small strains, as well as their various evolutionary variants, including thermodynamics. As such, the theory of boundary- or initial-boundary-value problems for linear or quasilinear elliptic, parabolic or hyperbolic partial differential equations is the main underlying mathematical tool, along with the calculus of variations. Modern concepts of these disciplines as weak solutions, polyconvexity, quasiconvexity, nonsimple materials, materials with various rheologies or with internal variables are exploited. This book is accompanied by exercises with solutions, and appendices briefly presenting the basic mathematical concepts and results needed. It serves as an

advanced resource and introductory scientific monograph for undergraduate or PhD students in programs such as mathematical modeling, applied mathematics, computational continuum physics and engineering, as well as for professionals working in these fields.

Physical Chemistry: An Advanced Treatise, Volume XIB: Mathematical Methods focuses on mathematical techniques that consist of concepts relating to differentiation and integration. This book discusses the methods in lattice statistics, Pfaffian solution of the planar Ising problem, and probability theory and stochastic processes. The random variables and probability distributions, non-equilibrium problems, Brownian motion, and scattering theory are also elaborated. This text likewise covers the elastic scattering from atoms, solution of integral and differential equations, concepts in graph theory, and theory of operator equations. This volume provides graduate and physical chemistry students a basic understanding of mathematical techniques important in chemistry.

This IMA Volume in Mathematics and its Applications MATHEMATICAL APPROACHES TO BIOMOLECULAR STRUCTURE AND DYNAMICS is one of the two volumes based on the proceedings of the 1994 IMA Sum mer Program on "Molecular Biology" and comprises Weeks 3 and 4 of the four-week program. Weeks 1 and 2 appeared as Volume 81: Genetic Mapping and DNA Sequencing. We thank Jill P. Mesirov, Klaus Schulten, and De Witt Sumners for organizing Weeks 3 and 4 of the workshop and for editing the proceedings. We also take this opportunity to thank the National Institutes of Health (NIH) (National Center for Human Genome Research), the National Science Foundation (NSF)

(Biological Instrumen tation and Resources), and the Department of Energy (DOE), whose fi nancial support made the summer program possible. A vner Friedman Robert Gulliver v PREFACE The revolutionary progress in molecular biology within the last 30 years opens the way to full understanding of the molecular structures and mech anisms of living organisms. Interdisciplinary research in mathematics and molecular biology is driven by ever growing experimental, theoretical and computational power. The mathematical sciences accompany and support much of the progress achieved by experiment and computation as well as provide insight into geometric and topological properties of biomolecular structure and processes. This volume consists of a representative sample of the papers presented during the last two weeks of the month-long Institute for Mathematics and Its Applications Summer 1994 Program in Molecular Biology.

Propositional logic has been recognized throughout the centuries as one of the cornerstones of reasoning in philosophy and mathematics. Over time, its formalization into Boolean algebra was accompanied by the recognition that a wide range of combinatorial problems can be expressed as propositional satisfiability (SAT) problems. Because of this dual role, SAT developed into a mature, multi-faceted scientific discipline, and from the earliest days of computing a search was underway to discover how to solve SAT problems in an automated fashion. This book, the Handbook of Satisfiability, is the second, updated and revised edition of the book first published in 2009 under the same name. The handbook

aims to capture the full breadth and depth of SAT and to bring together significant progress and advances in automated solving. Topics covered span practical and theoretical research on SAT and its applications and include search algorithms, heuristics, analysis of algorithms, hard instances, randomized formulae, problem encodings, industrial applications, solvers, simplifiers, tools, case studies and empirical results. SAT is interpreted in a broad sense, so as well as propositional satisfiability, there are chapters covering the domain of quantified Boolean formulae (QBF), constraints programming techniques (CSP) for word-level problems and their propositional encoding, and satisfiability modulo theories (SMT). An extensive bibliography completes each chapter. This second edition of the handbook will be of interest to researchers, graduate students, final-year undergraduates, and practitioners using or contributing to SAT, and will provide both an inspiration and a rich resource for their work. Edmund Clarke, 2007 ACM Turing Award Recipient: "SAT solving is a key technology for 21st century computer science." Donald Knuth, 1974 ACM Turing Award Recipient: "SAT is evidently a killer app, because it is key to the solution of so many other problems." Stephen Cook, 1982 ACM Turing Award Recipient: "The SAT problem is at the core of arguably the most fundamental question in computer science: What makes a problem hard?"

Presents basic principles and experimental techniques for the analysis of the chemical microstructure of homo- and copolymer chains. Provides mathematical methods

for calculating microstructure based on chemical models of the polymerization process. The basis of chemical and physical methods (i. e., vibrational and NMR) are presented with special emphasis on their role in determining repeating units and sequencing units in polymer chains. A detailed analysis of the copolymerization processes is presented and the microstructure of a copolymer is used for the determination of the copolymerization mechanism.

This IMA Volume in Mathematics and its Applications TOPOLOGY AND GEOMETRY IN POLYMER SCIENCE is based on the proceedings of a very successful one-week workshop with the same title. This workshop was an integral part of the 1995-1996 IMA program on "Mathematical Methods in Materials Science." We would like to thank Stuart G. Whittington, De Witt Sumners, and Timothy Lodge for their excellent work as organizers of the meeting and for editing the proceedings. We also take this opportunity to thank the National Science Foun dation (NSF), the Army Research Office (ARO) and the Office of Naval Research (ONR), whose financial support made the workshop possible. A vner Friedman Robert Gulliver v PREFACE This book is the product of a workshop on Topology and Geometry of Polymers, held at the IMA in June 1996. The workshop brought together topologists, combinatorialists, theoretical physicists and polymer scientists, who share an interest in characterizing and predicting the microscopic en tanglement properties of polymers, and their effect on macroscopic physical properties.

Approximately half of the world production of the

petrochemical industry (more than 100 million tonnes) is in the form of polymers, yet it would probably surprise most people to learn how much their lifestyle depends on polymers ranging, as they do, from detergents, kitchenware and electrical appliances to furnishings and a myriad other domestic goods. Still less are they likely to be aware of the extensive part they play in engineering applications for mechanical machine components and advanced high performance aircraft. This versatility derives from the fact that polymeric materials are made up of a range of molecules of varying length, whose properties are related to molecular structure and the proportions of the chains in the mixture. For example, polypropylene is a commodity polymer which is produced in hun dreds of different grades to meet specific market requirements. This depends on the catalyst as well as the operating conditions and reactor design. A major area for growth is in substituting polymers for conventional materials such as ceramics and metals. Not only can they match these materials in terms of mechanical strength and robustness but they have very good resistance to chemical attack. Polyamides, for example, are widely used for car bumpers and new polymers are being developed for engine manifolds and covers. In 1993 there is, typically, 100 kg of various polymers used in cars and this is continually increasing, giving a net weight reduction and hence better fuel economy.

1 V.O. Aseyev, H. Tenhu, F. Winnik: Temperature Dependence of the Colloidal Stability of Neutral Amphiphilic Polymers in Water.- 2 V.I. Lozinsky:

Approaches to Chemical Synthesis of Protein-Like Copolymers.- 3 S.I. Kuchanov, A.R. Khokhlov: Role of Physical Factors in the Processes of Obtaining of Copolymers.- 4 A.Y. Grosberg, A.R. Khokhlov: "After-Action" of the Ideas of O.M. Lifshitz in Polymer and Biopolymer Physics.-

This book describes the theories, applications, and challenges for different oral controlled release formulations. This book differs from most in its focus on oral controlled release formulation design and process development. It also covers the related areas like preformulation, biopharmaceutics, in vitro-in vivo correlations (IVIVC), quality by design (QbD), and regulatory issues.

A new edition explaining the underlying science and applications of liquid crystalline polymers.

Offers new strategies to optimize polymer reactions With contributions from leading macromolecular scientists and engineers, this book provides a practical guide to polymerization monitoring. It enables laboratory researchers to optimize polymer reactions by providing them with a better understanding of the underlying reaction kinetics and mechanisms. Moreover, it opens the door to improved industrial-scale reactions, including enhanced product quality and reduced harmful emissions. Monitoring Polymerization Reactions begins with a review of the basic elements of polymer reactions and their kinetics, including an overview of stimuli-responsive polymers. Next, it explains why certain polymer and reaction characteristics need to be monitored. The book then explores a variety of practical

topics, including: Principles and applications of important polymer characterization tools, such as light scattering, gel permeation chromatography, calorimetry, rheology, and spectroscopy Automatic continuous online monitoring of polymerization (ACOMP) reactions, a flexible platform that enables characterization tools to be employed simultaneously during reactions in order to obtain a complete record of multiple reaction features Modeling of polymerization reactions and numerical approaches Applications that optimize the manufacture of industrially important polymers Throughout the book, the authors provide step-by-step strategies for implementation. In addition, ample use of case studies helps readers understand the benefits of various monitoring strategies and approaches, enabling them to choose the best one to match their needs. As new stimuli-responsive and "intelligent" polymers continue to be developed, the ability to monitor reactions will become increasingly important. With this book as their guide, polymer scientists and engineers can take full advantage of the latest monitoring strategies to optimize reactions in both the lab and the manufacturing plant.

Polymer Sequence Determination: Carbon-13 NMR Method covers the principles, practice, and application of 13C NMR to polymer structure determination. This book is divided into six chapters that highlight spectral interpretations, applications, and experimental considerations. Chapter 1 examines the polymer structure, with special emphasis on those structural features delineated by 13C NMR, along with the assignment techniques used during 13C NMR

interpretations of polymer spectra. Chapters 2 and 3 present the methods for measuring sequence distributions and number-average sequence lengths for configurational sequences in vinyl homopolymers and for the comonomer distribution in copolymers and terpolymers. Chapter 4 discusses the statistical approaches to polymer characterization, while Chapter 5 contains practical experimental considerations when designing an NMR experiment to obtain quantitative structural information. Chapter 6 reviews 13C NMR studies for various vinyl homopolymers and copolymers. This book will be of great value to polymer scientists, NMR spectroscopists, and researchers.

This revised and updated Second Edition of the best-selling reference/text is essential reading for students and scientists who seek a thorough and practical introduction to the field of polymer spectroscopy. Eleven chapters cover the fundamental aspects and experimental applications of the primary spectroscopic methods. The advantages and disadvantages of the various techniques for particular polymer systems are also discussed. The goal of the author is not to make the reader an expert in the field, but rather to provide enough information about the different spectroscopic methods that the reader can determine how the available techniques can be used to solve a particular polymer problem. This Second Edition contains new and updated information on techniques in IR and NMR, as well as an all-new chapter on Mass Spectrometry.

Imposingly thick text derived from a one-semester course intended to acquaint advanced undergraduate

(and beginning graduate) students with the concepts and methods of linear mathematics. Though physics is referred to in the title, the book is in almost every organizational and notational respect

This book offers a comprehensive range of mathematical approaches to the solution of problems in modern organic, physical, and macromolecular chemistry. A variety of mathematical methods, including graph theory, topology, qualitative theory of ordinary and partial differential equations, probability theory and random processes, and computer simulations, is presented using straightforward chemical examples. Each chapter contains a thorough review of the subject, with a balanced progression from the elementary to more advanced topics. For the novice reader, basic concepts and terms are introduced, general problems are formulated, and solutions are discussed using the results of numerous studies in the literature. For the experienced researcher, the contributors present the results of their original research as well as those from other recent works.

This IMA Volume in Mathematics and its Applications Applications of Combinatorics and Graph Theory to the Biological and Social Sciences is based on the proceedings of a workshop which was an integral part of the 1987-88 IMA program on APPLIED COMBINATORICS. We are grateful to the Scientific Committee: Victor Klee (Chairman), Daniel Kleitman, Dijen Ray-Chaudhuri and Dennis Stanton for planning and implementing an exciting and stimulating year long program. We especially thank the Workshop Organizers,

Joel Cohen and Fred Roberts, for organizing a workshop which brought together many of the major figures in a variety of research fields connected with the application of combinatorial ideas to the social and biological sciences. A vner Friedman Willard Miller
APPLICATIONS OF COMBINATORICS AND GRAPH THEORY TO THE BIOLOGICAL AND SOCIAL SCIENCES: SEVEN FUNDAMENTAL IDEAS FRED S. RoBERTS* Abstract. To set the stage for the other papers in this volume, seven fundamental concepts which arise in the applications of combinatorics and graph theory in the biological and social sciences are described. These ideas are: RNA chains as "words" in a 4 letter alphabet; interval graphs; competition graphs or niche overlap graphs; qualitative stability; balanced signed graphs; social welfare functions; and semiorders. For each idea, some basic results are presented, some recent results are given, and some open problems are mentioned.

Advances in computer science and technology and in biology over the last several years have opened up the possibility for computing to help answer fundamental questions in biology and for biology to help with new approaches to computing. Making the most of the research opportunities at the interface of computing and biology requires the active participation of people from both fields. While past attempts have been made in this direction, circumstances today appear to be much more favorable for progress. To help take advantage of these opportunities, this study was requested of the NRC by the National Science Foundation, the Department of

Defense, the National Institutes of Health, and the Department of Energy. The report provides the basis for establishing cross-disciplinary collaboration between biology and computing including an analysis of potential impediments and strategies for overcoming them. The report also presents a wealth of examples that should encourage students in the biological sciences to look for ways to enable them to be more effective users of computing in their studies.