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Jill P. Mesirov Klaus Schulten De Witt Sumners
Editors

Mathematical Approaches to Biomolecular Structure and Dynamics

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Carlos Castillo-Chavez,Sally Blower,Pauline van den Driessche,Denise Kirschner,Abdul-Aziz Yakubu

Mathematical Approaches To Biomolecular Structure And Dynamics:

Mathematical Approaches to Biomolecular Structure and Dynamics Jill P Mesirov,Klaus Schulten,De Witt Sumners,1996-08-29 **Mathematical Approaches to Biomolecular Structure and Dynamics** Jill P. Mesirov,Klaus Schulten,De Witt Sumners,1996-08-29 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 **Mathematical Approaches to Biomolecular Structure and Dynamics** Jill P. Mesirov,Klaus Schulten,De Witt Sumners,2012-12-06 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

Mathematical Approaches to Molecular Structural Biology Subrata Pal,2022-11-19 Mathematical Approaches to Molecular Structural Biology offers a comprehensive overview of the mathematical foundations behind the study of biomolecular structure Initial chapters provide an introduction to the mathematics associated with the study of molecular structure such as vector spaces and matrices linear systems matrix decomposition vector calculus probability and statistics The book then moves on to more advanced areas of molecular structural biology based on the mathematical concepts discussed in earlier chapters Here key methods such as X ray crystallography and cryo electron microscopy are explored in addition to biomolecular structure dynamics within the context of mathematics and physics This book equips readers with an understanding of the fundamental principles behind structural biology providing researchers with a strong groundwork for further investigation in both this and related fields Includes a detailed introduction to key mathematical principles and their application to molecular structural biology Explores the mathematical underpinnings behind advanced techniques such as X ray crystallography and Cryo electron microscopy Features step by step protocols that illustrate mathematical and statistical principles for studying molecular structure and dynamics Provides a basis for further investigation into the field of computational molecular biology Includes figures and graphs throughout to visually demonstrate the concepts discussed

Mathematical Approaches for Emerging and Reemerging Infectious Diseases: Models, Methods, and Theory Carlos Castillo-Chavez,Sally Blower,Pauline van den Driessche,Denise Kirschner,Abdul-Aziz Yakubu,2012-12-06 This IMA Volume in Mathematics and its Applications MATHEMATICAL APPROACHES FOR EMERGING AND REEMERGING INFECTIOUS DISEASES MODELS AND THEORY METHODS is based on the proceedings of a successful one week workshop The pro ceedings of the two day tutorial which preceded the workshop Introduction to Epidemiology and Immunology appears as IMA Volume 125 Math ematical Approaches for Emerging and Reemerging Infectious Diseases An Introduction The tutorial and the workshop are integral parts of the September 1998 to June 1999 IMA program on MATHEMATICS IN BI OLOGY I would like to thank Carlos Castillo Chavez Director of the Math ematical and Theoretical Biology Institute and a member of the Depart ments of Biometrics Statistics and Theoretical and Applied Mechanics Cornell University Sally M Blower Biomathematics UCLA School of Medicine Pauline van den Driessche Mathematics and Statistics Uni versity of Victoria and Denise Kirschner Microbiology and Immunology University of Michigan Medical School for their superb roles as organizers of the meetings and editors of the proceedings Carlos Castillo Chavez es pecially made a major contribution by spearheading the editing process I am also grateful to Kenneth L Cooke Mathematics Pomona College for being one of the workshop organizers and to Abdul Aziz Yakubu Mathe matics Howard University for serving as co editor of the proceedings I thank Simon A Levin Ecology and Evolutionary Biology Princeton Uni versity for providing an introduction

Mathematical Approaches for Emerging and Reemerging Infectious Diseases: An Introduction Carlos

Castillo-Chavez,2002-05-02 This book grew out of the discussions and presentations that began during the Workshop on Emerging and Reemerging Diseases May 17 21 1999 sponsored by the Institute for Mathematics and its Application IMA at the University of Minnesota with the support of NIH and NSF The workshop started with a two day tutorial session directed at ecologists epidemiologists immunologists mathematicians and scientists interested in the study of disease dynamics The core of this first volume Volume 125 covers tutorial and research contributions on the use of dynamical systems deterministic discrete delay PDEs and ODEs models and stochastic models in disease dynamics The volume includes the study of cancer HIV pertussis and tuberculosis Beginning graduate students in applied mathematics scientists in the natural social or health sciences or mathematicians who want to enter the fields of mathematical and theoretical epidemiology will find this book useful **Mathematical Modelling of Biosystems** Rubem P. Mondaini,Panos M. Pardalos,2008-02-23 This volume is an interdisciplinary book which introduces in a very readable way state of the art research in the fundamental topics of mathematical modelling of Biosystems In short the book offers an overview of mathematical and computational modelling of biosystems including biological phenomena in general There is also a special introduction to Protein Physics which aims to explain the all or none first order phase transitions from native to denatured states Multiparticle Quantum Scattering with Applications to Nuclear, Atomic and Molecular Physics Donald G. Truhlar,Barry Simon,2012-12-06 This IMA Volume in Mathematics and its Applications MULTIPARTICLE QUANTUM SCATTERING WITH APPLICATIONS TO NUCLEAR ATOMIC AND MOLECULAR PHYSICS is based on the proceedings of a workshop with the same title which was an integral part of the 1994 1995 IMA program on Waves and Scattering We would like to thank Donald G Truhlar and Barry Simon for their ex cellent work as organizers of this meeting and as editors of the proceedings We also take this opportunity to thank the National Science Foundation 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 The workshop on Multiparticle Quantum Scattering with Applications to Nuclear Atomic and Molecular Physics was held June 12 16 1995 at the Institute for Mathematics and Its Applications in the University of Min nesota Twin Cities campus as part of the 1994 95 Program on Waves and Scattering There were about seventy participants including the plenary lecturers whose contributions are included in this volume The workshop was preceded by a two day tutorial featuring lectures by Donald J Kouri and Gian Michele Graf and we are pleased that both Professors Graf and Kouri were able to write up their tutorials as opening chapters of this volume **Molecular Modeling and Simulation** Tamar Schlick,2013-04-18 Science is a way of looking reverencing And the purpose of all science like living which amounts to the same thing is not the ac cumulation of gnostic power the fixing of formulas for the name of God the stockpiling of brutal efficiency accomplishing the sadistic myth of progress The purpose of science is to revive and cultivate a perpetual state of wonder For nothing deserves wonder so much as our capacity to experience it Roald Hoffman and Shira Leibowitz Schmidt in Old Wine New Flasks Re flections on Science

and Jewish Tradition W H Freeman 1997 Challenges in Teaching Molecular Modeling This textbook evolved from a graduate course termed Molecular Modeling intro duced in the fall of 1996 at New York University The primary goal of the course is to stimulate excitement for molecular modeling research much in the spirit of Hoffman and Leibowitz Schmidt above while providing grounding in the discipline Such knowledge is valuable for research dealing with many practical problems in both the acadernic and industrial sectors from developing treatments for AIDS via inhibitors to the protease enzyme of the human imrnunodeficiency virus HIV 1 to designing potatoes that yie1d spot free potato chips via trans genic potatoes with altered carbohydrate metabolism In the course of writing xii Preface this text the notes have expanded to function also as an introduction to the field for scientists in other disciplines by providing a global perspective into problems and approaches rather than a comprehensive survey **High Performance Computing in Science and Engineering '20** Wolfgang E. Nagel,Dietmar H. Kröner,Michael M. Resch,2022-01-01 This book presents the state of the art in supercomputer simulation It includes the latest findings from leading researchers using systems from the High Performance Computing Center Stuttgart HLRS in 2020 The reports cover all fields of computational science and engineering ranging from CFD to computational physics and from chemistry to computer science with a special emphasis on industrially relevant applications Presenting findings of one of Europe s leading systems this volume covers a wide variety of applications that deliver a high level of sustained performance The book covers the main methods in high performance computing Its outstanding results in achieving the best performance for production codes are of particular interest for both scientists and engineers The book comes with a wealth of color illustrations and tables of results Computational Methods for Macromolecules: Challenges and Applications Tamar Schlick,Hin H. Gan,2012-12-06 This special volume collects invited articles by participants of the Third International Workshop on Methods for Macromolecular Modeling Courant Institute of Mathematical Sciences Oct 12 14 2000 Leading developers of methods for biomolecular simulations review advances in Monte Carlo and molecular dynamics methods free energy computational methods fast electrostatics particle mesh Ewald and fast multipole methods mathematics and molecular neurobiology nucleic acid simulations enzyme reactions and other essential applications in biomolecular simulations A Perspectives article by the editors assesses the directions and impact of macromolecular modeling research including genomics and proteomics These reviews and original papers by applied mathematicians theoretical chemists biomedical researchers and physicists are of interest to interdisciplinary research students developers and users of biomolecular methods in academia and industry Large-Scale Optimization with Applications Lorenz T. Biegler,1997-07-31 With contributions by specialists in optimization and practitioners in the fields of aerospace engineering chemical engineering and fluid and solid mechanics the major themes include an assessment of the state of the art in optimization algorithms as well as challenging applications in design and control in the areas of process engineering and systems with partial differential equation models *Evolutionary Algorithms* Lawrence D. Davis,Kenneth De Jong,Michael D.

Vose,L.Darrell Whitley,2012-12-06 This IMA Volume in Mathematics and its Applications EVOLUTIONARY ALGORITHMS is based on the proceedings of a workshop that was an integral part of the 1996 97 IMA program on MATHEMATICS IN HIGH PERFORMANCE COMPUTING I thank Lawrence David Davis Tica Associates Kenneth De Jong Computer Science George Mason University Michael D Vose Computer Science The University of Tennessee and L Darrell Whitley Computer Science Colorado State University for their excellent work in organizing the workshop and for editing the proceedings Further appreciation is ex tended to Donald G Truhlar Chemistry and Supercomputing Institute University of Minnesota who was also one of the workshop organizers In addition I also take this opportunity to thank the National Science Foundation NSF Minnesota Supercomputing Institute MSI and the Army Research Office ARO whose financial support made the workshop possible Willard Miller Jr Professor and Director v PREFACE The IMA Workshop on Evolutionary Algorithms brought together many of the top researchers working in the area of Evolutionary Com putation for a week of intensive interaction The field of Evolutionary Computation has developed significantly over the past 30 years and today consists a variety of subfields such as genetic algorithms evolution strate gies evolutionary programming and genetic programming each with their own algorithmic perspectives and goals Nonlinear Optical Materials Jerome V. Moloney,2012-12-06 Mathematical methods play a significant role in the rapidly growing field of nonlinear optical materials This volume discusses a number of successful or promising contributions The overall theme of this volume is twofold 1 the challenges faced in computing and optimizing nonlinear optical material properties and 2 the exploitation of these properties in important areas of application These include the design of optical amplifiers and lasers as well as novel optical switches Research topics in this volume include how to exploit the magnetooptic effect how to work with the nonlinear optical response of materials how to predict laser induced breakdown in efficient optical devices and how to handle electron cloud distortion in femtosecond processes

Pattern Formation in Continuous and Coupled Systems Martin Golubitsky,Dan Luss,Steven H. Strogatz,2012-12-06 This IMA Volume in Mathematics and its Applications PATTERN FORMATION IN CONTINUOUS AND COUPLED SYSTEMS is based on the proceedings of a workshop with the same title but goes be yond the proceedings by presenting a series of mini review articles that sur vey and provide an introduction to interesting problems in the field The workshop was an integral part of the 1997 98 IMA program on EMERG ING APPLICATIONS OF DYNAMICAL SYSTEMS I would like to thank Martin Golubitsky University of Houston Math ematics Dan Luss University of Houston Chemical Engineering and Steven H Strogatz Cornell University Theoretical and Applied Mechan ics for their excellent work as organizers of the meeting and for editing the proceedings I also take this opportunity to thank the National Science Foundation NSF and the Army Research Office ARO whose financial support made the workshop possible Willard Miller Jr Professor and Director v PREFACE Pattern formation has been studied intensively for most of this cen tury by both experimentalists and theoreticians and there have been many workshops and conferences devoted to the subject In the IMA workshop on Pattern Formation in Continuous and

Coupled Systems held May 11 15 1998 we attempted to focus on new directions in the patterns literature **Singularities and Oscillations** Jeffrey Rauch,Michael Taylor,2012-12-06 This IMA Volume in Mathematics and its Applications SINGULARITIES AND OSCILLATIONS is based on the proceedings of a very successful one week workshop with the same title which was an integral part of the 1994 1995 IMA program on Waves and Scattering We would like to thank Joseph Keller Jeffrey Rauch and Michael Taylor for their excellent work as organizers of the meeting We would like to express our further gratitude to Rauch and Taylor who served as editors of 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 Avner Friedman Robert Gulliver v PREFACE Thestudyofsingularitiesand oscillationsofwaves has progressed along several fronts A key common feature is the presence of a small scale in the solutions Recent emphasis has been on nonlinear waves Nonlinear problems are generally less amenable than linear problems to broad unified approaches As a result there is a justifiable tendency to concentrate on problems of particular geometric or physical interest This volume con tains a multiplicity of approaches brought to bear on problems varying from the formation ofcaustics and the propagation ofwaves at a boundary to the examination ofviscous boundary layers There is an examination of the foundations of the theory of high frequency electromagnetic waves in a dielectric or semiconducting medium Unifying themes are not entirely absent from nonlinear analysis **Parallel Solution of Partial Differential Equations** Petter Bjorstad,Mitchell Luskin,2012-12-06 This IMA Volume in Mathematics and its Applications PARALLEL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS is based on the proceedings of a workshop with the same title The work shop was an integral part of the 1996 97IMA program on MATHEMAT ICS IN HIGH PERFORMANCE COMPUTING I would like to thank Petter Bj0rstad of the Institutt for Informatikk University of Bergen and Mitchell Luskin of the School of Mathematics University of Minnesota for their excellent work as organizers of the meeting and for editing the proceedings I also take this opportunity to thank the National Science Founda tion NSF Department of Energy DOE and the Army Research Office ARO whose financial support made the workshop possible Willard Miller Jr Professor and Director v PREFACE The numerical solution of partial differential equations has been of major importance to the development of many technologies and has been the target of much of the development of parallel computer hardware and software Parallel computers offer the promise of greatly increased perfor mance and the routine calculation of previously intractable problems The papers in this volume were presented at the IMA workshop on the Paral lel Solution of PDE held during June 9 13 1997 The workshop brought together leading numerical analysts computer scientists and engineers to assess the state of the art and to consider future directions *Grid Generation and Adaptive Algorithms* Marshall W. Bern,Joseph E. Flaherty,Mitchell Luskin,2012-12-06 This IMA Volume in Mathematics and its Applications GRID GENERATION AND ADAPTIVE ALGORITHMS is based on the proceedings of a workshop with the same title The work shop was an integral part of the 1996 97 IMA

program on MATHEMAT ICS IN HIGH PERFORMANCE COMPUTING I would like to thank Marshall Bern Xerox Palo Alto Research Cen ter Joseph E Flaherty Department of Computer Science Rensselaer Polytechnic Institute and Mitchell Luskin School of Mathematics Uni versity of Minnesota for their excellent work as organizers of the meeting and for editing the proceedings I also take this opportunity to thank the National Science Founda tion NSF Department of Energy DOE and the Army Research Office ARO whose financial support made the workshop possible Willard Miller Jr Professor and Director v PREFACE Scientific and engineering computation has become so complex that traditional numerical computation on uniform meshes is generally not pos sible or too expensive Mesh generation must reflect both the domain geometry and the expected solution characteristics Meshes should fur thermore be related to the solution through computable estimates of dis cretization errors This suggests an automatic and adaptive process where an initial mesh is enriched with the goal of computing a solution with prescribed accuracy specifications in an optimal manner While automatic mesh generation procedures and adaptive strategies are becoming available major computational challenges remain Three dimensional mesh genera tion is still far from automatic Statistics in Genetics M.Elizabeth Halloran,Seymour Geisser,1999-06-04 Though the Genome Project will eventually result in the sequencing of the human genome as well as the genomes of several other organisms there will still be a need for good statistics for family studies of complex diseases The papers in this volume are contributions by some of the leading researchers in the field to the current topics in statistical genetics One section deals with DNA sequence matching and issues related to forensics while another deals with statistical problems of modeling phylogenies and inferential difficulties related to the complex tree structures produced as well as the method of coalescence

Parallel Processing of Discrete Problems Panos M. Pardalos,2012-12-06 In the past two decades breakthroughs in computer technology have made a tremendous impact on optimization In particular availability of parallel computers has created substantial interest in exploring the use of parallel processing for solving discrete and global optimization problems The chapters in this volume cover a broad spectrum of recent research in parallel processing of discrete and related problems The topics discussed include distributed branch and bound algorithms parallel genetic algorithms for large scale discrete problems simulated annealing parallel branch and bound search under limited memory constraints parallelization of greedy randomized adaptive search procedures parallel optical models of computing randomized parallel algorithms general techniques for the design of parallel discrete algorithms parallel algorithms for the solution of quadratic assignment and satisfiability problems The book will be a valuable source of information to faculty students and researchers in combinatorial optimization and related areas

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Mathematical Approaches To Biomolecular Structure And Dynamics Introduction

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