

Jill P. Mesirov   Klaus Schulten   De Witt Sumners  
Editors

# Mathematical Approaches to Biomolecular Structure and Dynamics



Springer

# Mathematical Approaches To Biomolecular Structure And Dynamics

**Journal of Nonlinear Science**

## **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 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 Summer 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 Instrumentation and Resources and the Department of Energy DOE whose financial support made the summer program possible Aver 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 mechanisms 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, 1996-08-29

**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, 2002-05-02 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 proceedings of the two day tutorial which preceded the workshop Introduction to Epidemiology and Immunology appears as IMA Volume 125 Mathematical 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 BIOLOGY I would like to thank Carlos Castillo Chavez Director of the Mathematical and Theoretical Biology Institute and a member of the Departments 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 University 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 especially 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 Mathematics Howard University for serving as co editor of the proceedings I thank Simon A Levin Ecology and Evolutionary Biology Princeton University for providing an introduction *Mathematics of DNA Structure, Function and Interactions* Craig John Benham, Stephen Harvey, Wilma K. Olson, De Witt Sumners, David Swigon, 2009-07-30 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

**Mechanics: From Theory to Computation** Journal of Nonlinear Science, 2012-12-06 Starting in 1996 a sequence of articles appeared in the Journal of Nonlinear Science dedicated to the memory of one of its original editors Juan Carlos Simo Applied Mechanics Stanford University Sadly Juan Carlos passed away at an early age in 1994 We lost a brilliant colleague and a wonderful person These articles are collected in the present volume Many of them are updated and corrected

especially for this occasion These essays are in areas of scientific interest of Juan Carlos including mechanics particles rigid bodies fluids elasticity plasticity etc geometry applied dynamics and of course computation His interests were extremely broad he did not see boundaries between computation mathematics mechanics and dynamics and in that sense he ideally reflected the spirit of the journal and many of the most exciting areas of current scientific interest Juan Carlos was one of those select and gifted people who could cross interdisciplinary boundaries with extremely high quality and productive interactions of lasting value His contributions ranging from concrete engineering problems to fundamental mathematical theorems in geometric mechanics are remarkable In current conferences as well as in scientific books and articles and over a wide range of subjects one frequently hears how his ideas as well as specific results are often used and quoted this is one indication of just how profound and fundamental his work has impacted the community *Mechanics: From Theory to Computation* Juan Carlos Simo,2000 This collection of papers in honour of Juan Carlos Simo cover subjects including dynamical problems for geometrically exact theories of nonlinearly viscoelastic rods gravity waves on the surface of the sphere and problems and progress in microswimming *Smart Nanoconcretes and Cement-Based Materials* Mohd Shahir Liew,Phuong Nguyen-Tri,Tuan Anh Nguyen,Saeid Kakooei,2019-11-16 Smart Nanoconcretes and Cement Based Materials Properties Modelling and Applications explores the fundamental concepts and applications of smart nanoconcretes with self healing self cleaning photocatalytic antibacterial piezoelectrical heating and conducting properties and how they are used in modern high rise buildings hydraulic engineering highways tunnels and bridges This book is an important reference source for materials scientists and civil engineers who are looking to enhance the properties of smart nanomaterials to create stronger more durable concrete Explores the mechanisms through which active agents are released from nanocontainers inside concrete Shows how embedded smart nanosensors including carbon cement based smart sensors and micro nano strain sensors are used to increase concrete performance Discusses the major challenges of integrating smart nanomaterials into concrete composites

**Pacific Journal of Mathematics** ,2002-05 **A Mathematical Approach to Multilevel, Multiscale Health Interventions** Rodrick Wallace,Deborah Wallace,2013 This book based on published studies takes a unique perspective on the 30 year collapse of pharmaceutical industry productivity in the search for small molecule OC magic bulletOCO interventions The relentless escalation of inflation adjusted cost per approved medicine in the United States OCo from 200 million in 1950 to 1 2 billion in 2010 OCo has driven industry giants to at best slavish imitation in drug design and at worst abandonment of research and embracing of widespread fraud in consumer marketing The book adapts formalism across a number of disciplines to the strategy for design of multilevel interventions focusing first on molecular cellular and larger scale examples and then extending the argument to the simplifications provided by the dominant role of social and cultural structures and processes in individual and population patterns of health and illness In place of OC magic bulletsOCO we must now apply OC magic strategiesOCO that act across both the scale and level of organization This book

provides an introductory roadmap to the new tools that will be needed for the design of such strategies      **The Cumulative Book Index** ,1999      *Forthcoming Books* Rose Arny,1996-10      **Mathematical Approach To Multilevel, Multiscale Health Interventions, A: Pharmaceutical Industry Decline And Policy Response** Rodrick Wallace,Deborah

Wallace,2013-01-28 This book based on published studies takes a unique perspective on the 30 year collapse of pharmaceutical industry productivity in the search for small molecule magic bullet interventions The relentless escalation of inflation adjusted cost per approved medicine in the United States from 200 million in 1950 to 1 2 billion in 2010 has driven industry giants to at best slavish imitation in drug design and at worst abandonment of research and embracing of widespread fraud in consumer marketing The book adapts formalism across a number of disciplines to the strategy for design of mutilevel interventions focusing first on molecular cellular and larger scale examples and then extending the argument to the simplifications provided by the dominant role of social and cultural structures and processes in individual and population patterns of health and illness In place of magic bullets we must now apply magic strategies that act across both the scale and level of organization This book provides an introductory roadmap to the new tools that will be needed for the design of such strategies a      [SIAM Journal on Scientific Computing](#) ,2005      *Numerical Methods for Polymeric Systems* Stuart G.

Whittington,1998-08-13 This book contains contributions from a workshop on numerical methods for polymeric systems held at the IMA in May 1996 The workshop brought together chemists physicists mathematicians computer scientists and statisticians with a common interest in numerical methods This book is of interest to workers in polymer statistical at mechanics and also to a wider audience interested in numerical methods and their application in polymeric systems

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