Computational Methods for Macromolecules: Challenges and Applications

Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, October 12-14, 2000

Tamar Schlick and **Hin H. Gan,** both, New York University, New York (Eds.)

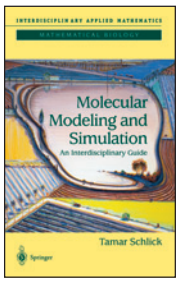
This special volume collects invited articles by participants of the Third International Workshop on Methods for Macromolecular Modeling , Courant Institute of Mathematical Sciences, Oct. 12-14, 2000. Leading developers of methods for biomolecular simulations review advances in Monte Carlo and molecular 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.

2002/513 PP./SOFTCOVER/$89.95
ISBN: 3-540-43756-8
LECTURE NOTES IN COMPUTATIONAL SCIENCE AND ENGINEERING, VOL. 24

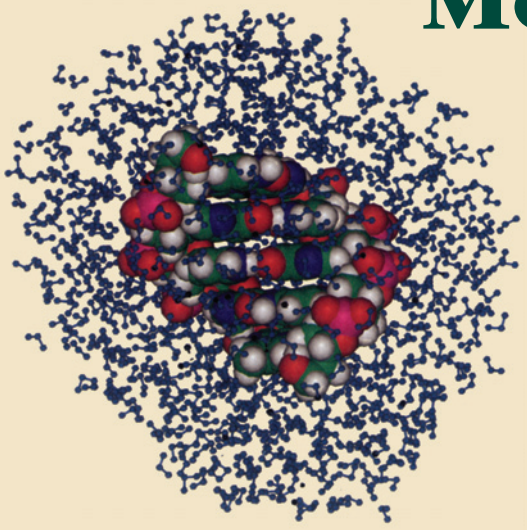
Springer

Springer

Springer-Verlag New York, Inc.
175 Fifth Avenue
New York, NY 10010



Molecular Modeling and Simulation

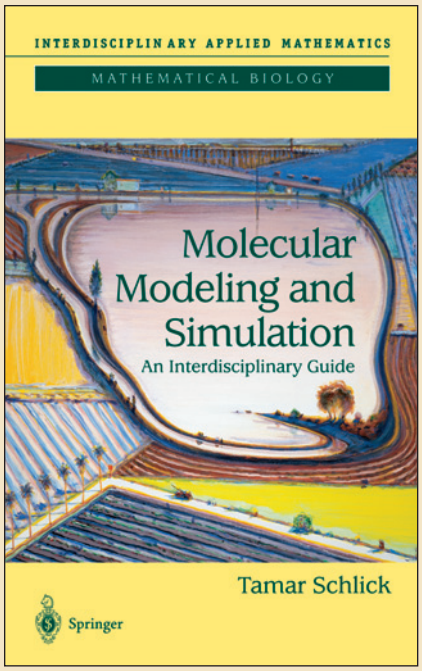


"The interdisciplinary structural biology community has waited long for a book of this kind which provides an excellent introduction to molecular modeling."

–HAROLD A. SCHERAGA, Todd Professor of Chemistry Emeritus, Cornell University

Springer

www.springer-ny.com



Molecular Modeling and Simulation

An Interdisciplinary Guide

Tamar Schlick, New York University, New York, NY

"A uniquely valuable introduction to the modeling of biomolecular structure and dynamics. A rigorous and up-to-date treatment of the foundations, enlivened by engaging anecdotes and historical notes."

–J. Andrew McCammon, Howard Hughes Medical Institute, University of California at San Diego

"I am often asked by physicists, mathematicians and engineers to recommend a book that would be useful to get them started in computational molecular biology. I am also often approached by my colleagues in computational biology to recommend a solid textbook for a graduate course in the area. Tamar Schlick has written the book that I will be recommending to both groups. Tamar has done an amazing job in writing a book that is both suitably accessible for beginners, and suitably rigorous for experts."

–J.J. Collins, Co-Director, Professor of Biomedical Engineering, Boston University

This book evolved from an interdisciplinary graduate course entitled Molecular Modeling developed at New York University. Its primary goal is to stimulate excitement for molecular modeling research while introducing readers to the wide range of biomolecular problems being solved by computational techniques and to those computational tools. The book is intended for beginning graduate students in medical schools and scientific fields such as biology, chemistry, physics, mathematics, and computer science. Other scientists who wish to enter, or become familiar, with the field of biomolecular modeling and simulation may also benefit from the broad coverage of problems and approaches.

The book surveys three broad areas: biomolecular structure and modeling: current problems and state of computations; molecular mechanics: force field origin, composition, and evaluation techniques; and simulation methods: geometry optimization, Monte Carlo, and molecular dynamics approaches. Appendices featuring homework assignments, reading lists, and other information useful for teaching molecular modeling complement the material in the main text. Extensive use of world wide web resources is encouraged, and additional course and text information may be found on a supplementary website.

Contents: Biomolecular Structure and Modeling: Historical Perspective • Biomolecular Structure and Modeling: Problem and Application Perspective • Protein Structure Introduction • Protein Structure Hierarchy • Nucleic Acids Structure Minitutorial • Topics in Nucleic Acids Structure • Theoretical and Computational Approaches to Biomolecular Structure • Force Fields • Nonbonded Computations • Multivariate Minimization in Computational Chemistry • Monte Carlo Techniques • Molecular Dynamics: Basics • Molecular Dynamics: Further Topics • Similarity and Diversity in Chemical Design • Epilogue • Appendices • Index

2002/620 PP., 160 ILLUS./HARDCOVER/ISBN 0-387-95404-X
LIST PRICE: $79.95
INTERDISCIPLINARY APPLIED MATHEMATICS, VOL. 21

INSTRUCTORS

Molecular Modeling and Simulation is an appropriate text for a variety of courses in molecular modeling, computational biology, bioinformatics, and molecular dynamics. It is available for examination under the 60-day approval policy, which enables instructors to peruse it at no charge (except return postage, if applicable) for 60 days.
To request: **Web:** www.springer-ny.com/textbooks
E-mail: textbook@springer-ny.com • **Fax:** 201-348-4505

ORDER FORM

ISBN	Qty.	Author	Title	Price
0-387-95404-X	____	Schlick	*Molecular Modeling and Simulation*	**$79.95**
3-540-43756-8	____	Schlick	*Computational Methods for Macromolecules*	**$89.95**

Subtotal . . $_____
Sales Tax . . $_____
Shipping . . $_____
TOTAL . . . $_____

CA, IL, MA, MO, NJ, NY, PA, TX, VA, and VT residents, please add sales tax. Canadian residents, please add 7% GST. Please add $5.00 for shipping one book and $1.00 for each additional book.

METHOD OF PAYMENT

❍ Check enclosed *(made payable to Springer-Verlag New York, Inc.)*
Charge my: ❍ Am Ex ❍ MasterCard ❍ Visa ❍ Discover

Card #:_____ Exp.Date:_____

Signature:_____ Date:_____

Name:_____

Group/Inst.:_____

Address:_____

City/State/Zip:_____

EASY WAYS TO ORDER:

Web www.springer-ny.com • **Call** Toll-Free 1-800-SPRINGER • **E-Mail** orders@springer-ny.com • **Mail** this flyer to Springer-Verlag New York, Inc., Order Dept. B5395, PO Box 2485, Secaucus, NJ 07096-2485 • **Visit** your local scientific bookstore • *Your 30-day return privilege is always guaranteed.* • **Outside the Americas:** Springer Customer Service, Haberstrasse 7, 69126, Heidelberg, Germany, Telephone: +49-6221-345-217/218, Fax: +49-6221-345-229, e-mail: orders@springer.de

6/03 Printed in USA Promotion #B5395