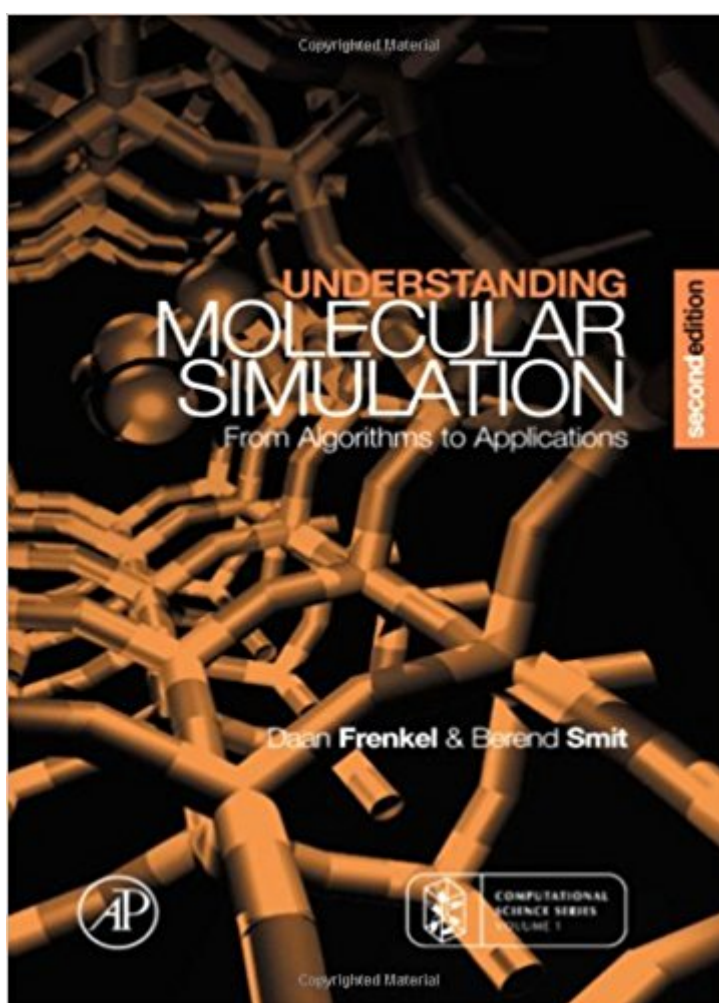


The book was found

Understanding Molecular Simulation, Second Edition: From Algorithms To Applications (Computational Science Series, Vol 1)



Synopsis

Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Since the first edition only five years ago, the simulation world has changed significantly -- current techniques have matured and new ones have appeared. This new edition deals with these new developments; in particular, there are sections on:Â

- Transition path sampling and diffusive barrier crossing to simulate rare events
- Dissipative particle dynamic as a coarse-grained simulation technique
- Novel schemes to compute the long-ranged forces
- Hamiltonian and non-Hamiltonian dynamics in the context of constant-temperature and constant-pressure molecular dynamics simulations
- Multiple-time step algorithms as an alternative for constraints
- Defects in solids
- The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex molecules
- Parallel tempering for glassy Hamiltonians

Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web. Several new examples have been added since the first edition to illustrate recent applications. Questions are included in this new edition. No prior knowledge of computer simulation is assumed.

Book Information

Series: Computational Science Series, Vol 1

Hardcover: 664 pages

Publisher: Academic Press; 2 edition (November 7, 2001)

Language: English

ISBN-10: 0122673514

ISBN-13: 978-0122673511

Product Dimensions: 1.5 x 6 x 9 inches

Shipping Weight: 2.2 pounds (View shipping rates and policies)

Average Customer Review: 4.1 out of 5 stars 18 customer reviews

Best Sellers Rank: #178,227 in Books (See Top 100 in Books) #30 in Books > Science & Math > Chemistry > Molecular Chemistry #50 in Books > Engineering & Transportation > Engineering >

Customer Reviews

"â brilliantly maintains a balance between explaining the physical phenomena and performing computations. Its marvelous writing style invites scientists and students to deepen their knowledge of MD simulations."--ComputingReviews.com, January 11, 2013 "... this book brilliantly lays down the scientific foundations of the simulational approach ..."--Prof. Kurt Binder in Physics World, 1997 "... a treasure. The book is a marvellous mix of just enough formalism with an informal and readable style, sufficient detail to understand methodological advances, appropriate mathematics ..."--Prof. Mark A. Ratner in Physics Today, 1997

This book explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. Since a wide variety of computational tools exists, the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Examples are included that highlight current applications, and the codes of the case studies are available on the World Wide Web. No prior knowledge of computer simulation is assumed.

The book is a very good reference, but the digital quality is very bad. Letters are missing from words, and it features nonsensical overtype and missing symbols from formulae. It is the lowest quality e-book I've seen; all of the equations that aren't overtyped or missing variables look like they were copied and pasted images (there is blur/cutoff evidence).

The textbook is great starting point to understand the classical molecular simulation. However, it lacks the understanding of quantum molecular dynamics. Otherwise, it is a solid textbook to use

My holy book:)

Nice book, and the delivery was fast. It actually looked better than I expected.

It's an excellent book for those who are just beginners in MC & MD simulations. Everything is very clearly explained with a lot of examples and some related unsolved problems. The text explores this topic in detail with advanced chapters in later sections. Good for anybody in this field be it in materials science, physics or related fields.

When I have any question about simulations, this book is my first choice and it usually doesn't disappoint me. Best part of this book is crystal theory and algorithm. I know how to run a simulation, how to choose a parameter WITH CONFIDENCE after reading it. However, codes in it are not always helpful, I usually need to implement in my own way. In brief, this book is very good on basic principle and algorithm of molecular simulations, but not how to write a piece of code.

Exactly as described; quick delivery!

First it looks good, and then apparently it's new and in good quality with every page. I will read it and use it carefully, cos I want keep for very long time.

[Download to continue reading...](#)

Understanding Molecular Simulation, Second Edition: From Algorithms to Applications
(Computational Science Series, Vol 1) Biological Modeling and Simulation: A Survey of Practical Models, Algorithms, and Numerical Methods (Computational Molecular Biology) Molecular Simulation Studies on Thermophysical Properties: With Application to Working Fluids (Molecular Modeling and Simulation) Current Topics in Computational Molecular Biology (Computational Molecular Biology) Introduction to Computational Science: Modeling and Simulation for the Sciences, Second Edition An Introduction to Bioinformatics Algorithms (Computational Molecular Biology) Molecular Gas Dynamics: Theory, Techniques, and Applications (Modeling and Simulation in Science, Engineering and Technology) Computational Geometry: Algorithms and Applications Atmospheric and Space Flight Dynamics: Modeling and Simulation with MATLAB® and Simulink® (Modeling and Simulation in Science, Engineering and Technology) Computational Fluid Dynamics Simulation of Spray Dryers: An Engineer's Guide (Advances in Drying Science and Technology) Computational Ergodic Theory (Algorithms and Computation in Mathematics, Vol. 13) Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Molecular Gas Dynamics and the Direct Simulation of Gas Flows (Oxford Engineering Science Series) Theoretical Neuroscience:

Computational and Mathematical Modeling of Neural Systems (Computational Neuroscience Series)
Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis (Theoretical and
Computational Chemistry Series) Computational Approaches to Protein Dynamics: From Quantum
to Coarse-Grained Methods (Series in Computational Biophysics) Practical Algorithms in Pediatric
Nephrology: (Practical Algorithms in Pediatrics. Series Editor: Z. Hochberg) Practical Algorithms in
Pediatric Gastroenterology: (Practical Algorithms in Pediatrics. Series Editor: Z. Hochberg) Practical
Algorithms in Pediatric Endocrinology: (Practical Algorithms in Pediatrics. Series Editor: Z.
Hochberg)

[Contact Us](#)

[DMCA](#)

[Privacy](#)

[FAQ & Help](#)