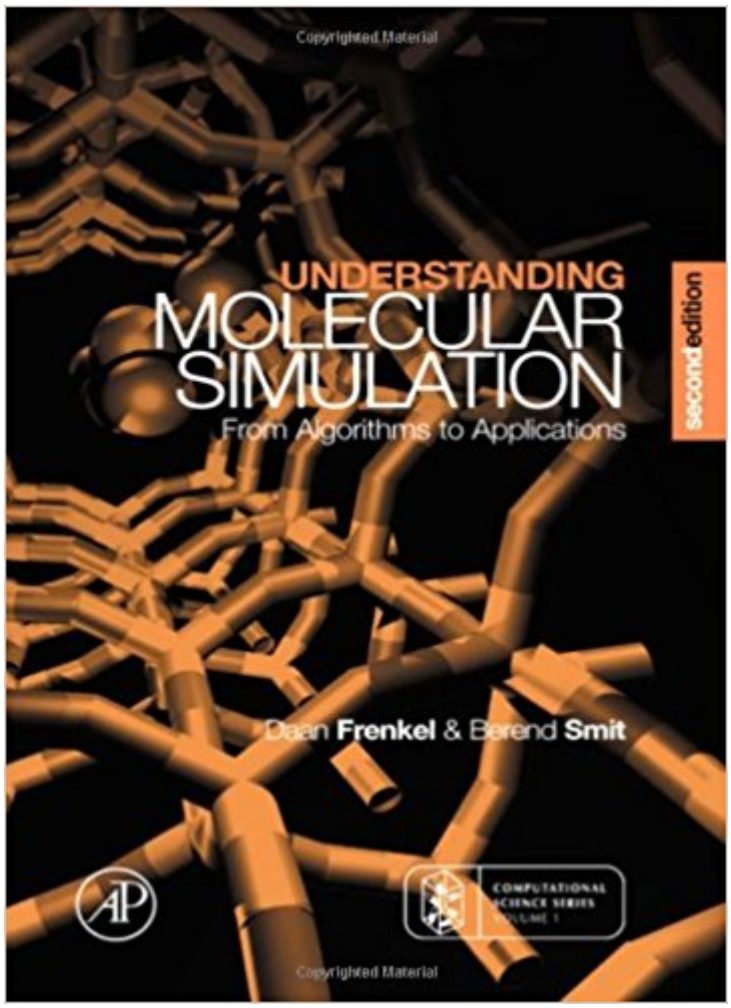
Understanding Molecular Simulation, Second Edition: From Algorithms To Applications (Computational Science Series, Vol 1)



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:Ã Â Transition path sampling and diffusive barrier crossing to simulaterare eventsÃ Â Dissipative particle dynamic as a course-grained simulation techniqueÃ Â Novel schemes to compute the long-ranged forcesÃ Â Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulationsÃ Â Multiple-time step algorithms as an alternative for constraintsÃ Â Defects in solidsÃ Â The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex moleculesÃ Â Parallel tempering for glassy HamiltoniansExamples 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

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Customer Reviews

"Ã¢â ¬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 continously 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.

Its an excellent book for those who are just beginners in MC & MD simulations. everything is very clearly explained with lot of examples and some related unsolved problems. the text explores this topic indetails with advanced chapters in later sections. Good for anybody int hsi 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.

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