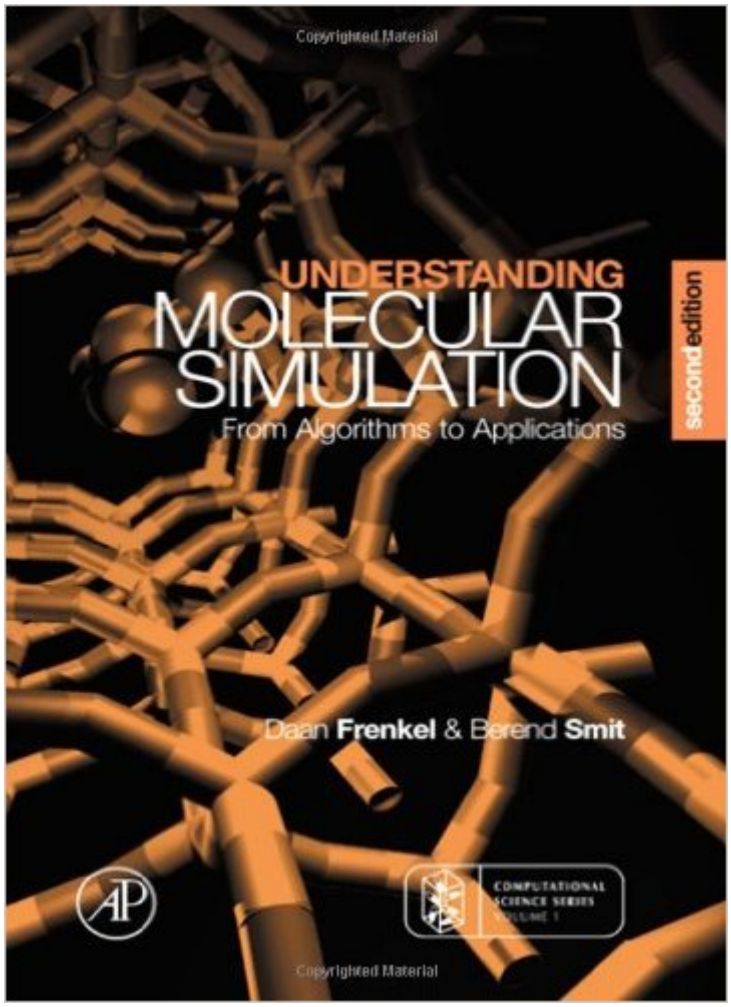
Understanding Molecular Simulation, Second Edition: From Algorithms To Applications (Computational Science)



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 simulaterare eventsÂ Dissipative particle dynamic as a course-grained simulation techniqueÂ Novel schemes to compute the long-ranged forcesÂ Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulationsÂ Multiple-time step algorithms as an alternative for constraintsÂ Defects in solidsÂ The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex moleculesÂ 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

The title of the book is overly ambitious and falls short on its promises. The book is a good introduction to Molecular Mechanics (MM), Molecular Dynamics (MD) and Monte Carlo (MC) methods, with detailed descriptions of the methods used and FORTRAN (pseudo)code, covering from the basics to some middle-level and some advanced algorithms.But it does NOT cover all the fields of Molecular Modelling, just the three mentioned (MM, MD and MC), there's no coverage of quantum mechanics methods, nor QSAR or other technologies. And, while it described the algorithms, I can't think of it going all the way through up to building applications. For this, Rapaport's makes a better job, and for a general intro to Molecular Modelling, Grant & Richards' Computational Chemistry is more comprehensive (albeit at a more superficial level). Nor does it provide much detail on the methods used in modelling biological macromolecules, an increasing application field for the methods discussed in the book.All in all, this book fails to satisfy its cover title, it won't introduce to the whole field (just the areas of MM, MD and MC) nor does it go up to application level. But it IS a REAL GOOD introduction to the subjects covered and their basic algorithms,with sample code, detailed descriptions and plenty of references to specialized articles, texts and resources.

This book covers many interesting topics in molecular simulation, both Monte Carlo and M.D. It focuses on understanding the main ideas rather than giving long codes. It's a good place to start, but it also covers some ideas not found in many other books. When I try to extend my molecular dynamics program I always check what Frenkel and Smit have to say about it.

This book is how I bootstrapped my way into being a molecular simulationist. Anyone who can program in some language can get started writing simple routines for the basic MD and MC simulations.I do Monte Carlo simulations at Princeton, and found this book to be the most helpful available for getting my research started. It is my most common reference, and is used extensively in writing background information for various research documents.However, after you have written your first few codes, you will pass the level of this book and need to move on. I use it less now than I did my first year.Every student in my group (Panagiotopoulos) has this book I think. And like me, they started with it, but moved on.

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).

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.

This book is an excellent introduction to the field of molecular dynamics simulation. It is easy to follow for a scientist entering the field and at the same time contains overview of most critical topics in MD simulation. The book's major goal is to describe how to simulate liquids, however it also mentions briefly the methods for gas and liquid simulations. List of references for further readings is very useful and complete.

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

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