

<<分子模拟入门>>

图书基本信息

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前言

Why did we write a second edition ?

A minor revision of the first edition would have been adequate to correct the (admittedly many) typographical mistakes. However, many of the nice comments that we received from students and colleagues alike, ended with a remark of the type: "unfortunately, you don't discuss topic x". And indeed, we feel that, after only five years, the simulation world has changed so much that the title of the book was no longer covered by the contents. The first edition was written in 1995 and since then several new techniques have appeared or matured. Most (but not all) of the major changes in the second edition deal with these new developments. In particular, we have included a section on.

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内容概要

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书籍目录

Preface to the Second Edition
Preface
List of Symbols
1 Introduction
Part 1 Basics
2 Statistical Mechanics
2.1 Entropy and Temperature
2.2 Classical Statistical Mechanics
2.2.1 Ergodicity
2.3 Questions and Exercises
3 Monte Carlo Simulations
3.1 The Monte Carlo Method
3.1.1 Importance Sampling
3.1.2 The Metropolis Method
3.2 A Basic Monte Carlo Algorithm
3.2.1 The Algorithm
3.2.2 Technical Details
3.2.3 Detailed Balance versus Balance
3.3 Trial Moves
3.3.1 Translational Moves
3.3.2 Orientational Moves
3.4 Applications
3.5 Questions and Exercises
4 Molecular Dynamics Simulations
4.1 Molecular Dynamics: The Idea
4.2 Molecular Dynamics: A Program
4.2.1 Initialization
4.2.2 The Force Calculation
4.2.3 Integrating the Equations of Motion
4.3 Equations of Motion
4.3.1 Other Algorithms
4.3.2 Higher-Order Schemes
4.3.3 Liouville Formulation of Time-Reversible Algorithms
4.3.4 Lyapunov Instability
4.3.5 One More Way to Look at the Verlet Algorithm
4.4 Computer Experiments
4.4.1 Diffusion
4.4.2 Order-Algorithm to Measure Correlations
4.5 Some Applications
4.6 Questions and Exercises
Part 2 Ensembles
5 Monte Carlo Simulations in Various Ensembles
5.1 General Approach
5.2 Canonical Ensemble
5.2.1 Monte Carlo Simulations
5.2.2 Justification of the Algorithm
5.3 Microcanonical Monte Carlo
5.4 Isobaric-Isothermal Ensemble
5.4.1 Statistical Mechanical Basis
5.4.2 Monte Carlo Simulations
5.4.3 Applications
5.5 Isotension-Isothermal Ensemble
5.6 Grand-Canonical Ensemble
5.6.1 Statistical Mechanical Basis
5.6.2 Monte Carlo Simulations
5.6.3 Justification of the Algorithm
5.6.4 Applications
5.7 Questions and Exercises
6 Molecular Dynamics in Various Ensembles
6.1 Molecular Dynamics at Constant Temperature
6.1.1 The Andersen Thermostat
6.1.2 Nos Hoover Thermostat.
Part 3 Free Energies and Phase Equilibria
Part 4 Advanced Techniques
Part 5 Appendices

章节摘录

插图：It is difficult to talk about Monte Carlo or Molecular Dynamics programs in abstract terms. The best way to explain how such programs work is to write them down. This will be done in the present section. Most Monte Carlo or Molecular Dynamics programs are only a few hundred to several thousand lines long. This is very short compared to, for instance, a typical quantum-chemistry code. For this reason, it is not uncommon that a simulator will write many different programs that are tailor-made for specific applications. The result is that there is no such thing as a standard Monte Carlo or Molecular Dynamics program. However, the cores of most MD/MC programs are, if not identical, at least very similar. Next, we shall construct such a core. It will be very rudimentary, and efficiency has been traded for clarity. But it should demonstrate how the Monte Carlo method works.

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