

Contents

1. Introductory Examples	1
1.1 Percolation	1
1.2 A One-Particle Problem	4
Problems	6
2. Computer-Simulation Methods	8
Problems	12
3. Deterministic Methods	13
3.1 Molecular Dynamics	13
Integration Schemes	17
Calculating Thermodynamic Quantities	22
Organization of a Simulation	26
3.1.1 Microcanonical Ensemble Molecular Dynamics	27
3.1.2 Canonical Ensemble Molecular Dynamics	35
3.1.3 Isothermal-Isobaric Ensemble Molecular Dynamics	42
Problems	48
4. Stochastic Methods	51
4.1 Preliminaries	51
4.2 Brownian Dynamics	55
4.3 Monte-Carlo Method	61
4.3.1 Microcanonical Ensemble Monte-Carlo Method	73
4.3.2 Canonical Ensemble Monte-Carlo Method	78
4.3.3 Isothermal-Isobaric Ensemble Monte-Carlo Method	94
4.3.4 Grand Ensemble Monte-Carlo Method	96
Problems	100
Appendix	104
A1. Random Number Generators	104
A2. Program Listings	113
References	137
Subject Index	143