

Contents

1. Introduction	1
2. Computer Simulation Methods	5
2.1 Essential Features of Simulation Methods	5
2.1.1 Ensemble Averages on a Computer	6
2.1.2 Simulation Algorithms	6
2.2 The Monte Carlo Algorithm	8
2.2.1 Simple Sampling	8
2.2.2 Importance Sampling	9
2.2.3 Interpretation of the Monte Carlo Process as a Dynamical Process	11
2.3 Molecular Dynamics	13
2.3.1 The Microcanonical Ensemble	14
2.3.2 Discretization and Systematic Effects	15
2.3.3 Molecular Dynamics Algorithms	17
2.4 Hybrid Molecular Dynamics	18
2.5 Accuracy Considerations and Finite-Size Problems	21
2.5.1 Choosing the Boundary Conditions	21
2.5.2 Effects of Finite Simulation Time	22
2.5.3 Statistical Errors and Self-Averaging	23
2.5.4 Finite-Size Scaling: Using Finite-Size Effects	24
2.6 Monte Carlo Algorithm for the Ising Model	25
2.6.1 The Ising Model	26
2.6.2 Implementing the Monte Carlo Algorithm for the Ising Model	27
2.6.3 The Swendsen-Wang Algorithm and the Equivalence Between the Ising Model and Percolation	28
2.6.4 Cluster Identification	32
2.6.5 Other Cluster Update Algorithms	33
3. Physics and Parallelism	37
4. Concepts of Parallelism	43
4.1 Some Basic Definitions	43
4.2 The Complexity of Computation	45

4.3	More on Models and Methods	46
4.4	Performance Measurements	49
5.	Parallel Machines and Languages	51
5.1	General Purpose Parallel Computers	51
5.1.1	Processor Concepts	51
5.1.2	Communication Networks	53
5.2	Parallel Machines for Special Physics Problems	58
5.2.1	Monte Carlo Machines	59
5.2.2	Molecular Dynamics Computers	63
5.3	Languages for Parallel Computers	64
5.4	The Matching Problem	66
6.	Replication Algorithms	71
7.	Geometrically Parallel Algorithms	75
7.1	Geometric Parallelization	76
7.2	Strips, Squares and Checker-Boards	79
7.2.1	Detailed Balance and the Checker-Board	79
7.2.2	Strips	80
7.2.3	Squares	82
7.2.4	Communication Procedures	83
7.2.5	Timing and Efficiency Considerations	84
7.2.6	Geometric Parallelism in Higher Dimensions	85
7.3	Non-local and Cluster Algorithms	87
7.3.1	Parallel Algorithms for Cluster Identification	87
7.3.2	The Public Stack Cluster Algorithm	88
7.3.3	The Binary Tree Cluster Algorithm	89
7.3.4	Performance Measurements	90
7.4	Parallel Molecular Dynamics Algorithms	91
7.4.1	Short-Range vs Long-Range Interactions	91
7.4.2	A Geometrically Parallelized Algorithm for Molecular Dynamics	93
7.5	Hybrid Molecular Dynamics	94
7.6	Polymers on the Lattice	95
7.6.1	Single Polymers	96
7.6.2	Dense Polymer Systems	97
7.7	Off-Lattice Polymers	100
7.8	Hybrid Molecular Dynamics for Polymers	101
7.9	Limits of Geometric Parallelization	101
8.	Data Parallel Algorithms	105
8.1	Data Parallel Algorithm for Long-Range Interactions	105
8.2	Polymers	106

9. Introduction to a Parallel Language	111
9.1 Transputer-Based Parallel Machines	111
9.2 Parallel Programming in Occam	113
9.2.1 The Process and the Channel Concepts	115
9.2.2 Two Elementary Processes	119
9.2.3 A Trivial Example	120
9.2.4 Repetition and the Conditional	121
9.2.5 An Occam Program for the Ising Model	127
9.2.6 More on Choices and Selection	133
9.2.7 Further Language Elements	136
9.2.8 Arithmetic	140
9.2.9 Placements	144
Appendices	149
A. A Parallel Ising Model Program	149
B. Random Number Generator	156
C. A Parallel Molecular Dynamics Program	159
References	171
Subject Index	179