

Contents

1. A Simple Introduction to Monte Carlo Simulation and Some Specialized Topics.	
By K. Binder and D. Stauffer (With 6 Figures)	1
1.1 A First Guide to Monte Carlo Sampling	2
1.1.1 Random Numbers	2
1.1.2 An Example of "Simple Sampling": The Percolation Problem	4
1.1.3 An Example of "Importance Sampling": The Ising Model	5
1.1.4 An Example of Continuous Degrees of Freedom: The Heisenberg Model	9
1.1.5 A First Warning: Finite-Size Effects, Metastability, Slowing Down	13
1.2 Special Topics	17
1.2.1 What can be Learned from Distribution Functions; Finite-Size Scaling	17
1.2.2 Estimation of Free Energy and Entropy	23
1.2.3 Estimation of Intensive Thermodynamic Quantities	26
1.2.4 Interface Free Energy	27
1.2.5 Methods of Locating First-Order Phase Changes	28
1.2.6 Linear Response, Susceptibilities and Transport Coefficients	30
1.3 Conclusion	31
Appendix. 1.A. Multispin Coding	32
References	33
Notes Added in Proof	36
 2. Recent Developments in the Simulation of Classical Fluids	
By D. Levesque, J.J. Weis, and J.P. Hansen	37
2.1 Some Recent Methodological Developments	37
2.1.1 Modified Metropolis Algorithms	38
2.1.2 Sampling in the Grand-Canonical Ensemble	39
2.1.3 Evaluation of the Chemical Potential	40
2.1.4 Variations on a Theme	42
2.2 Simple Monatomic Fluids	43
2.2.1 Hard-Core Systems in Two and Three Dimensions	43
2.2.2 Soft-Core and Lennard-Jones Systems in Two Dimensions	43

2.2.3	Rare-Gas Fluids in Three Dimensions	44
2.2.4	Binary Mixtures of Simple Fluids	45
2.3	Coulombic Systems	46
2.3.1	Boundary Conditions	46
2.3.2	The One-Component Plasma (OCP)	47
2.3.3	Two-Dimensional Electron Layers	48
2.3.4	Liquid Metals	49
2.3.5	Primitive Model Electrolytes	50
2.3.6	Simple Models of Polyelectrolytes	51
2.3.7	Molten Salts and Superionic Conductors	51
	a) KCl	52
	b) KCN	52
	c) Alkali Chlorides	52
	d) Rb Halides	53
	e) Cs Halides	53
	f) Alkaline Earth Halides	53
	g) Molten Salt Mixtures	53
	h) Superionic Conductors	53
2.4	Molecular Liquids	54
2.4.1	Hard Nonspherical Particles	55
	a) Hard Spherocylinders	55
	b) Mixtures of Hard Spheres and Hard Spherocylinders	55
	c) Hard Diatomics	55
2.4.2	Two-Center Molecular Liquids	56
2.4.3	Simple Dipolar and Multipolar Liquids	56
	a) Dipolar Hard-Sphere Systems	57
	b) Two- and Three-Dimensional Stockmayer Fluids	58
	c) Systems of Polarizable Particles	59
	d) Steric Effects in Polar Fluids	59
2.4.4	Realistic Models of Molecular Liquids	59
2.4.5	Liquid Water	70
2.5	Solutions	73
2.5.1	Dilute Aqueous Solutions of Nonelectrolytes	74
2.5.2	Solvation of Ions	76
2.5.3	Solvation of Large Dipoles	77
2.5.4	Solvation of Biological Molecules	77
2.6	Surfaces and Interfaces	77
2.6.1	Liquid-Vapor Interface of Simple Fluids	77
2.6.2	Liquid-Vapor Interface of Molecular Fluids	78
2.6.3	Density Profiles of the One-Component Plasma and Liquid Metals	79

2.6.4	Liquid-Wall Interfaces	79
2.6.5	Liquid-Solid Coexistence	81
2.6.6	The Electrical Double Layer	81
2.7	Conclusion	82
	References	83
3.	Monte Carlo Studies of Critical and Multicritical Phenomena	
	By D.P. Landau (With 10 Figures)	93
3.1	Two-Dimensional Lattice-Gas Ising Models	93
3.1.1	Adsorbed Monolayers	93
3.1.2	Ising Model Critical and Multicritical Behavior	98
3.1.3	Models with Incommensurate Phases	100
3.2	Surfaces and Interfaces	101
3.3	Three-Dimensional Binary-Alloy Ising Models	105
3.4	Potts Models	109
3.5	Continuous Spin Models	111
3.6	Dynamic Critical Behavior	114
3.7	Other Models	116
3.7.1	Miscellaneous Magnetic Models	116
3.7.2	Superconductors	117
3.7.3	Interacting Electric Multipoles	118
3.7.4	Liquid Crystals	119
3.8	Conclusion and Outlook	120
	References	120
4.	Few- and Many-Fermion Problems	
	By K.E. Schmidt and M.H. Kalos (With 7 Figures)	125
4.1	Review of the GFMC Method	126
4.2	The Short Time Approximation	132
4.3	The Fermion Problem and the Method of Transient Estimation	133
4.4	The Fixed Node Approximation	138
4.5	An Exact Solution for Few-Fermion Systems	139
4.6	Speculations and Conclusions	141
	References	142
5.	Simulations of Polymer Models. By A. Baumgärtner (With 21 Figures)	145
5.1	Background	145
5.2	Variants of the Monte Carlo Sampling Techniques	148
5.3	Equilibrium Configurations	151
5.3.1	Asymptotic Properties of Single Chains in Good Solvents ...	151
5.3.2	Phase Transitions of Single Chains	156

5.3.3	Chain Morphology in Concentrated Solutions and in the Bulk	163
5.3.4	Phase Transitions at High Concentrations	165
5.4	Polymer Dynamics	168
5.4.1	Brownian Dynamics of a Single Chain	168
5.4.2	Entanglement Effects	170
5.5	Conclusions and Outlook	175
	References	176
6.	Simulation of Diffusion in Lattice Gases and Related Kinetic Phenomena	
	By K.W. Kehr and K. Binder (With 26 Figures)	181
6.1	General Aspects of Monte Carlo Approaches to Dynamic Phenomena	181
6.2	Diffusion in Lattice-Gas Systems in Equilibrium	183
6.2.1	Self-Diffusion in Noninteracting Two- and Three-Dimensional Lattice Gases	183
6.2.2	Anomalous Diffusion in One-Dimensional Lattices	189
6.2.3	Tracer Particles with Different Jump Rates and the Percolation Conduction Problem	193
6.2.4	Self-Diffusion and Collective Diffusion in Interacting Lattice Gases, Including Systems with Order-Disorder Phase Transitions	198
6.3	Diffusion and Domain Growth in Systems far from Equilibrium	209
6.3.1	Nucleation, Spinodal Decomposition, and Lifshitz-Slyozov Growth	210
6.3.2	Late-Stage Scaling Behavior	213
6.3.3	Diffusion of Domain Walls and Ordering Kinetics	214
6.3.4	Kinetics of Aggregation, Gelation and Related Phenomena	216
6.4	Conclusion	217
	References	218
7.	Roughening and Melting in Two Dimensions	
	By Y. Saito and H. Müller-Krumbhaar (With 11 Figures)	223
7.1	Introductory Remarks	223
7.2	Roughening Transition	225
7.2.1	Solid-on-Solid (SOS) Model	225
7.2.2	Dual Coulomb Gas (CG) Model	227
7.2.3	Step Free Energy and Crystal Morphology	231
7.3	Melting Transition	231
7.3.1	Theoretical Predictions	231
7.3.2	Computer Experiments on Atomistic Systems	233
7.3.3	Dislocation Vector System	235
	References	237

8. Monte Carlo Studies of "Random" Systems	
By K. Binder and D. Stauffer (With 5 Figures)	241
8.1 General Introduction	241
8.2 Spin Glasses	244
8.2.1 Short-Range Edwards-Anderson Ising Spin Glasses	244
8.2.2 Short-Range Edwards-Anderson Heisenberg Spin Glasses	248
8.2.3 Site-Disorder Models	250
8.2.4 The Infinite-Range Model	252
8.2.5 One-Dimensional Models	253
8.3 Other Systems with Random Interactions	254
8.4 Percolation Theory	255
8.4.1 Cluster Numbers	255
8.4.2 Computational Techniques	258
8.4.3 Cluster Structure	262
8.4.4 Large-Cell Monte Carlo Renormalization	264
8.4.5 Other Aspects	267
8.5 Conclusion	269
References	270
Note Added in Proof	275
 9. Monte Carlo Calculations in Lattice Gauge Theories	
By C. Rebbi (With 4 Figures)	277
9.1 Lattice Gauge Theories: Fundamental Notions	277
9.2 General Monte Carlo Results for Lattice Gauge Systems	284
9.3 Monte Carlo Determination of Physical Observables	288
References	296
 10. Recent Developments	
By K. Binder, A. Baumgärtner, J.-P. Hansen, M.H. Kalos, K.W. Kehr, D.P. Landau, D. Levesque, H. Müller-Krumbhaar, C. Rebbi, Y. Saito, K.E. Schmidt, D. Stauffer, J.-J. Weis	299
10.1 Introduction and Some Specialized Topics	299
10.1.1 Size Effects and Self-Averaging	299
10.1.2 Slowing Down at Phase Transitions: Can we get Around it?	301
10.1.3 Pushing MC Calculations to their Limits: Superfast MC Programs on "Supercomputers"; Special Purpose Computers for MC Methods	303
10.2 Simulation of Classical Fluids	304
10.3 Critical and Multicritical Phenomena	306
10.4 Few- and Many-Fermion Problems	307
10.5 Simulation of Polymer Models	309
10.5.1 Monte-Carlo Techniques	309

10.5.2	Polymer Networks	309
10.5.3	Polymer Blends	310
10.5.4	Polymer Melting	310
10.5.5	Dynamics of Polymers	310
10.6	Diffusion in Lattice Gases and Related Kinetic Phenomena	310
10.7	Roughening and Melting in Two Dimensions	313
10.7.1	Two-Dimensional Melting	313
10.7.2	Roughening Transition	314
10.8	"Random" Systems: Spin Glasses, Percolation, etc.	314
10.8.1	Spin Glasses	314
10.8.2	Random Fields, Random Impurities, etc.	315
10.8.3	Percolation	315
10.9	Lattice Gauge Theories	315
10.10	Concluding Remarks	317
	References	318
Additional References with Titles		325
Subject Index		333