

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	2.6.4	Liquid-Wall Interfaces	79
2.2.4	Binary Mixtures of Simple Fluids	45	2.6.5	Liquid-Solid Coexistence	81
2.3	Coulombic Systems	46	2.6.6	The Electrical Double Layer	81
2.3.1	Boundary Conditions	46	2.7	Conclusion	82
2.3.2	The One-Component Plasma (OCP)	47	References	83
2.3.3	Two-Dimensional Electron Layers	48			
2.3.4	Liquid Metals	49	3. Monte Carlo Studies of Critical and Multicritical Phenomena		
2.3.5	Primitive Model Electrolytes	50	By D.P. Landau (With 10 Figures)	93	
2.3.6	Simple Models of Polyelectrolytes	51	3.1 Two-Dimensional Lattice-Gas Ising Models	93	
2.3.7	Molten Salts and Superionic Conductors	51	3.1.1 Adsorbed Monolayers	93	
a)	KCl	52	3.1.2 Ising Model Critical and Multicritical Behavior	98	
b)	KCN	52	3.1.3 Models with Incommensurate Phases	100	
c)	Alkali Chlorides	52	3.2 Surfaces and Interfaces	101	
d)	Rb Halides	53	3.3 Three-Dimensional Binary-Alloy Ising Models	105	
e)	Cs Halides	53	3.4 Potts Models	109	
f)	Alkaline Earth Halides	53	3.5 Continuous Spin Models	111	
g)	Molten Salt Mixtures	53	3.6 Dynamic Critical Behavior	114	
h)	Superionic Conductors	53	3.7 Other Models	116	
2.4	Molecular Liquids	54	3.7.1 Miscellaneous Magnetic Models	116	
2.4.1	Hard Nonspherical Particles	55	3.7.2 Superconductors	117	
a)	Hard Spherocylinders	55	3.7.3 Interacting Electric Multipoles	118	
b)	Mixtures of Hard Spheres and Hard Spherocylinders	55	3.7.4 Liquid Crystals	119	
c)	Hard Diatomics	55	3.8 Conclusion and Outlook	120	
2.4.2	Two-Center Molecular Liquids	56	References	120
2.4.3	Simple Dipolar and Multipolar Liquids	56			
a)	Dipolar Hard-Sphere Systems	57	4. Few- and Many-Fermion Problems		
b)	Two- and Three-Dimensional Stockmayer Fluids	58	By K.E. Schmidt and M.H. Kalos (With 7 Figures)	125	
c)	Systems of Polarizable Particles	59	4.1 Review of the GFMC Method	126	
d)	Steric Effects in Polar Fluids	59	4.2 The Short Time Approximation	132	
2.4.4	Realistic Models of Molecular Liquids	59	4.3 The Fermion Problem and the Method of Transient Estimation	133	
2.4.5	Liquid Water	70	4.4 The Fixed Node Approximation	138	
2.5	Solutions	73	4.5 An Exact Solution for Few-Fermion Systems	139	
2.5.1	Dilute Aqueous Solutions of Nonelectrolytes	74	4.6 Speculations and Conclusions	141	
2.5.2	Solvation of Ions	76	References	142
2.5.3	Solvation of Large Dipoles	77			
2.5.4	Solvation of Biological Molecules	77	5. Simulations of Polymer Models. By A. Baumgärtner (With 21 Figures)	145	
2.6	Surfaces and Interfaces	77	5.1 Background	145	
2.6.1	Liquid-Vapor Interface of Simple Fluids	77	5.2 Variants of the Monte Carlo Sampling Techniques	148	
2.6.2	Liquid-Vapor Interface of Molecular Fluids	78	5.3 Equilibrium Configurations	151	
2.6.3	Density Profiles of the One-Component Plasma and Liquid Metals	79	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	8. Monte Carlo Studies of "Random" Systems	
5.3.4 Phase Transitions at High Concentrations	165	By K. Binder and D. Stauffer (With 5 Figures)	241
5.4 Polymer Dynamics	168	8.1 General Introduction	241
5.4.1 Brownian Dynamics of a Single Chain	168	8.2 Spin Glasses	244
5.4.2 Entanglement Effects	170	8.2.1 Short-Range Edwards-Anderson Ising Spin Glasses	244
5.5 Conclusions and Outlook	175	8.2.2 Short-Range Edwards-Anderson Heisenberg Spin Glasses	248
References	176	8.2.3 Site-Disorder Models	250
6. Simulation of Diffusion in Lattice Gases and Related Kinetic Phenomena		8.2.4 The Infinite-Range Model	252
By K.W. Kehr and K. Binder (With 26 Figures)	181	8.2.5 One-Dimensional Models	253
6.1 General Aspects of Monte Carlo Approaches to Dynamic Phenomena	181	8.3 Other Systems with Random Interactions	254
6.2 Diffusion in Lattice-Gas Systems in Equilibrium	183	8.4 Percolation Theory	255
6.2.1 Self-Diffusion in Noninteracting Two- and Three-Dimensional Lattice Gases	183	8.4.1 Cluster Numbers	255
6.2.2 Anomalous Diffusion in One-Dimensional Lattices	189	8.4.2 Computational Techniques	258
6.2.3 Tracer Particles with Different Jump Rates and the Percolation Conduction Problem	193	8.4.3 Cluster Structure	262
6.2.4 Self-Diffusion and Collective Diffusion in Interacting Lattice Gases, Including Systems with Order-Disorder Phase Transitions	198	8.4.4 Large-Cell Monte Carlo Renormalization	264
6.3 Diffusion and Domain Growth in Systems far from Equilibrium	209	8.4.5 Other Aspects	267
6.3.1 Nucleation, Spinodal Decomposition, and Lifshitz-Slyozov Growth	210	8.5 Conclusion	269
6.3.2 Late-Stage Scaling Behavior	213	References	270
6.3.3 Diffusion of Domain Walls and Ordering Kinetics	214	Note Added in Proof	275
6.3.4 Kinetics of Aggregation, Gelation and Related Phenomena	216	9. Monte Carlo Calculations in Lattice Gauge Theories	
6.4 Conclusion	217	By C. Rebbi (With 4 Figures)	277
References	218	9.1 Lattice Gauge Theories: Fundamental Notions	277
7. Roughening and Melting in Two Dimensions		9.2 General Monte Carlo Results for Lattice Gauge Systems	284
By Y. Saito and H. Müller-Krumbhaar (With 11 Figures)	223	9.3 Monte Carlo Determination of Physical Observables	288
7.1 Introductory Remarks	223	References	296
7.2 Roughening Transition	225	10. Recent Developments	
7.2.1 Solid-on-Solid (SOS) Model	225	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
7.2.2 Dual Coulomb Gas (CG) Model	227	10.1 Introduction and Some Specialized Topics	299
7.2.3 Step Free Energy and Crystal Morphology	231	10.1.1 Size Effects and Self-Averaging	299
7.3 Melting Transition	231	10.1.2 Slowing Down at Phase Transitions: Can we get Around it?	301
7.3.1 Theoretical Predictions	231	10.1.3 Pushing MC Calculations to their Limits: Superfast MC Programs on "Supercomputers"; Special Purpose Computers for MC Methods	303
7.3.2 Computer Experiments on Atomistic Systems	233	10.2 Simulation of Classical Fluids	304
7.3.3 Dislocation Vector System	235	10.3 Critical and Multicritical Phenomena	306
References	237	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