

Contents

Preface	x ⁱ
1 Introduction	
1.1 What is a Monte Carlo simulation?	2
1.2 What problems can we solve with it?	3
1.3 What difficulties will we encounter?	3
1.3.1 Limited computer time and memory	3
1.3.2 Statistical and other errors	3
1.4 What strategy should we follow in approaching a problem?	4
1.5 How do simulations relate to theory and experiment?	4
2 Some necessary background	7
2.1 Thermodynamics and statistical mechanics: a quick reminder	7
2.1.1 Basic notions	7
2.1.2 Phase transitions	13
2.1.3 Ergodicity and broken symmetry	24
2.1.4 Fluctuations and the Ginzburg criterion	25
2.1.5 A standard exercise: the ferromagnetic Ising model	25
2.2 Probability theory	27
2.2.1 Basic notions	27
2.2.2 Special probability distributions and the central limit theorem	29
2.2.3 Statistical errors	30
2.2.4 Markov chains and master equations	31
2.2.5 The ‘art’ of random number generation	32
2.3 Non-equilibrium and dynamics: some introductory comments	39
2.3.1 Physical applications of master equations	39
2.3.2 Conservation laws and their consequences	40
2.3.3 Critical slowing down at phase transitions	43
2.3.4 Transport coefficients	45
2.3.5 Concluding comments	45
References	46
3 Simple sampling Monte Carlo methods	48
3.1 Introduction	48
3.2 Comparisons of methods for numerical integration of given functions	48

3.2.1 Simple methods	48
3.2.2 Intelligent methods	50
3.3 Boundary value problems	51
3.4 Simulation of radioactive decay	53
3.5 Simulation of transport properties	54
3.5.1 Neutron transport	54
3.5.2 Fluid flow	55
3.6 The percolation problem	56
3.6.1 Site percolation	56
3.6.2 Cluster counting: the Hoshen-Kopelman algorithm	59
3.6.3 Other percolation models	60
3.7 Finding the groundstate of a Hamiltonian	60
3.8 Generation of ‘random’ walks	61
3.8.1 Introduction	61
3.8.2 Random walks	62
3.8.3 Self-avoiding walks	63
3.8.4 Growing walks and other models	65
3.9 Final remarks	66
References	66
4 Importance sampling Monte Carlo methods	68
4.1 Introduction	68
4.2 The simplest case: single spin-flip sampling for the simple Ising model	69
4.2.1 Algorithm	70
4.2.2 Boundary conditions	74
4.2.3 Finite size effects	77
4.2.4 Finite sampling time effects	90
4.2.5 Critical relaxation	98
4.3 Other discrete variable models	105
4.3.1 Ising models with competing interactions	105
4.3.2 q-state Potts models	109
4.3.3 Baxter and Baxter-Wu models	110
4.3.4 Clock models	112
4.3.5 Ising spin glass models	112
4.3.6 Complex fluid models	113
4.4 Spin-exchange sampling	114
4.4.1 Constant magnetization simulations	114
4.4.2 Phase separation	115
4.4.3 Diffusion	117
4.4.4 Hydrodynamic slowing down	119
4.5 Microcanonical methods	119
4.5.1 Demon algorithm	119
4.5.2 Dynamic ensemble	120
4.5.3 Q2R	120
4.6 General remarks, choice of ensemble	121

4.7 Statics and dynamics of polymer models on lattices	121
4.7.1 Background	121
4.7.2 Fixed length bond methods	122
4.7.3 Bond fluctuation method	123
4.7.4 Polymers in solutions of variable quality: Q-point, collapse transition, unmixing	124
4.7.5 Equilibrium polymers: a case study	127
4.8 Some advice	130
References	130
5 More on importance sampling Monte Carlo methods for lattice systems	133
5.1 Cluster flipping methods	133
5.1.1 Fortuin-Kasteleyn theorem	133
5.1.2 Swendsen-Wang method	134
5.1.3 Wolff method	137
5.1.4 ‘Improved estimators’	138
5.2 Specialized computational techniques	139
5.2.1 Expanded ensemble methods	139
5.2.2 Multispin coding	139
5.2.3 N-fold way and extensions	140
5.2.4 Hybrid algorithms	142
5.2.5 Multigrid algorithms	142
5.2.6 Monte Carlo on vector computers	143
5.2.7 Monte Carlo on parallel computers	143
5.3 Classical spin models	144
5.3.1 Introduction	144
5.3.2 Simple spin-flip method	144
5.3.3 Heatbath method	146
5.3.4 Low temperature techniques	147
5.3.5 Over-relaxation methods	147
5.3.6 Wolff embedding trick and cluster flipping	148
5.3.7 Hybrid methods	149
5.3.8 Monte Carlo dynamics vs. equation of motion dynamics	150
5.3.9 Topological excitations and solitons	150
5.4 Systems with quenched randomness	154
5.4.1 General comments: averaging in random systems	154
5.4.2 Random fields and random bonds	157
5.4.3 Spin glasses and optimization by simulated annealing	158
5.5 Models with mixed degrees of freedom: Si/Ge alloys, a case study	163
5.6 Sampling the free energy and entropy	164
5.6.1 Thermodynamic integration	164
5.6.2 Groundstate free energy determination	166
5.6.3 Estimation of intensive variables: the chemical potential	166
5.6.4 Lee-Kosterlitz method	167

5.6.5 Free energy from finite size dependence at T_c	167
5.7 Miscellaneous topics	168
5.7.1 Inhomogeneous systems: surfaces, interfaces, etc.	168
5.7.2 Other Monte Carlo schemes	173
5.7.3 Finite size effects: a review and summary	174
5.7.4 More about error estimation	175
5.7.5 Random number generators revisited	176
5.8 Summary and perspective	178
References	179
6 Off-lattice models	182
6.1 Fluids	182
6.1.1 <i>NVT</i> ensemble and the virial theorem	182
6.1.2 <i>NpT</i> ensemble	185
6.1.3 Grand canonical ensemble	189
6.1.4 Subsystems: a case study	192
6.1.5 Gibbs ensemble	197
6.1.6 Widom particle insertion method and variants	200
6.2 ‘Short range’ interactions	202
6.2.1 Cutoffs	202
6.2.2 Verlet tables and cell structure	202
6.2.3 Minimum image convention	202
6.2.4 Mixed degrees of freedom reconsidered	203
6.3 Treatment of long range forces	203
6.3.1 Reaction field method	203
6.3.2 Ewald method	204
6.3.3 Fast multipole method	204
6.4 Adsorbed monolayers	205
6.4.1 Smooth substrates	205
6.4.2 Periodic substrate potentials	206
6.5 Complex fluids	207
6.6 Polymers: an introduction	210
6.6.1 Length scales and models	210
6.6.2 Asymmetric polymer mixtures: a case study	216
6.6.3 Applications: dynamics of polymer melts; thin adsorbed polymeric films	219
6.7 Configurational bias and ‘smart Monte Carlo’	224
References	227
7 Reweighting methods	230
7.1 Background	230
7.1.1 Distribution functions	230
7.1.2 Umbrella sampling	230
7.2 Single histogram method: the <i>Ising</i> model as a case study	233
7.3 Multi-histogram method	240
7.4 Broad histogram method	240
7.5 Multicanonical sampling	241

7.5.1 The multicanonical approach and its relationship to canonical sampling	241
7.5.2 Near first order transitions	243
7.5.3 Groundstates in complicated energy landscapes	244
7.5.4 Interface free energy estimation	245
7.6 A case study: the Casimir effect in critical systems	246
References	248
8 Quantum Monte Carlo methods	250
8.1 Introduction	250
8.2 Feynman path integral formulation	252
8.2.1 Off-lattice problems: low-temperature properties of crystals	252
8.2.2 Bose statistics and superfluidity	258
8.2.3 Path integral formulation for rotational degrees of freedom	259
8.3 Lattice problems	261
8.3.1 The Ising model in a transverse field	261
8.3.2 Anisotropic Heisenberg chain	263
8.3.3 Fermions on a lattice	266
8.3.4 An intermezzo: the minus sign problem	269
8.3.5 Spinless fermions revisited	271
8.3.6 Cluster methods for quantum lattice models	274
8.3.7 Decoupled cell method	275
8.3.8 Handscomb's method	276
8.3.9 Fermion determinants	277
8.4 Monte Carlo methods for the study of groundstate properties	278
8.4.1 Variational Monte Carlo (VMC)	279
8.4.2 Green's function Monte Carlo methods (GFMC)	280
8.5 Concluding remarks	283
References	283
9 Monte Carlo renormalization group methods	286
9.1 Introduction to renormalization group theory	286
9.2 Real space renormalization group	290
9.3 Monte Carlo renormalization group	291
9.3.1 Large cell renormalization	291
9.3.2 Ma's method: finding critical exponents and the fixed point Hamiltonian	293
9.3.3 Swendsen's method	294
9.3.4 Location of phase boundaries	296
9.3.5 Dynamic problems: matching time-dependent correlation functions	297
References	298
10 Non-equilibrium and irreversible processes	299
10.1 Introduction and perspective	299
10.2 Driven diffusive systems (driven lattice gases)	299
10.3 Crystal growth	301

10.4 Domain growth	304
10.5 Polymer growth	306
10.5.1 Linear polymers	306
10.5.2 Gelation	306
10.6 Growth of structures and patterns	308
10.6.1 Eden model of cluster growth	308
10.6.2 Diffusion limited aggregation	308
10.6.3 Cluster-cluster aggregation	311
10.6.4 Cellular automata	311
10.7 Models for film growth	312
10.7.1 Background	312
10.7.2 Ballistic deposition	313
10.7.3 Sedimentation	314
10.7.4 Kinetic Monte Carlo and MBE growth	315
10.8 Outlook: variations on a theme	317
References	318
11 Lattice gauge models: a brief introduction	320
11.1 Introduction: gauge invariance and lattice gauge theory	320
11.2 Some technical matters	322
11.3 Results for $Z(N)$ lattice gauge models	322
11.4 Compact U(1) gauge theory	323
11.5 SU(2) lattice gauge theory	324
11.6 Introduction: quantum chromodynamics (QCD) and phase transitions of nuclear matter	325
11.7 The deconfinement transition of QCD	327
References	330
12 A brief review of other methods of computer simulation	332
12.1 Introduction	332
12.2 Molecular dynamics	332
12.2.1 Integration methods (microcanonical ensemble)	332
12.2.2 Other ensembles (constant temperature, constant pressure, etc.)	336
12.2.3 Non-equilibrium molecular dynamics	339
12.2.4 Hybrid methods (MD + MC)	339
12.2.5 <i>Ab initio</i> molecular dynamics	339
12.3 Quasi-classical spin dynamics	340
12.4 Langevin equations and variations (cell dynamics)	343
12.5 Lattice gas cellular automata	344
References	345
13 Outlook	346
Appendix: listing of programs mentioned in the text	348
Index	379