A Guide to
Monte Carlo Simulations in
Statistical Physics
Fourth Edition

David P. Landau
Center for Simulational Physics, University of Georgia, USA

Kurt Binder
Institut für Physik, Johannes-Gutenberg-Universität, Germany

CAMBRIDGE UNIVERSITY PRESS
Contents

Preface xv

1 Introduction 1
1.1 What is a Monte Carlo simulation? 1
1.2 What problems can we solve with it? 2
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
1.6 Perspective 5
References 6

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 15
2.1.3 Ergodicity and broken symmetry 27
2.1.4 Fluctuations and the Ginzburg criterion 27
2.1.5 A standard exercise: the ferromagnetic Ising model 28
2.2 Probability theory 30
2.2.1 Basic notions 30
2.2.2 Special probability distributions and the central limit theorem 31
2.2.3 Statistical errors 33
2.2.4 Markov chains and master equations 33
2.2.5 The 'art' of random number generation 35
2.3 Non-equilibrium and dynamics: some introductory comments 41
2.3.1 Physical applications of master equations 41
2.3.2 Conservation laws and their consequences 43
2.3.3 Critical slowing down at phase transitions 46
2.3.4 Transport coefficients 48
2.3.5 Conclusion: comments: why bother about dynamics when doing Monte Carlo for statics? 48

References 48

3 Simple sampling Monte Carlo methods 51
3.1 Introduction 51
3.2 Comparisons of methods for numerical integration of given functions 51
3.2.1 Simple methods 51
3.2.2 Intelligent methods 53
3.3 Boundary value problems 54
3.4 Simulation of radioactive decay 56
3.5 Simulation of transport properties 57
3.5.1 Neutron transport 57
3.5.2 Fluid flow 58
3.6 The percolation problem 58
3.6.1 Site percolation 59
3.6.2 Cluster counting: the Hoshen–Kopelman algorithm 62
3.6.3 Other percolation models 63
3.7 Finding the ground state of a Hamiltonian 63
3.8 Generation of ‘random’ walks 64
3.8.1 Introduction 64
3.8.2 Random walks 65
3.8.3 Self-avoiding walks 66
3.8.4 Growing walks and other models 68
3.9 Final remarks 69

References 69

4 Importance sampling Monte Carlo methods 71
4.1 Introduction 71
4.2 The simplest case: single spin-flip sampling for the simple Ising model 72
4.2.1 Algorithm 73
4.2.2 Boundary conditions 76
4.2.3 Finite size effects 79
4.2.4 Finite sampling time effects 93
4.2.5 Critical relaxation 100
4.3 Other discrete variable models 108
4.3.1 Ising models with competing interactions 108
4.3.2 q-state Potts models 112
4.3.3 Baxter and Baxter–Wu models 113
4.3.4 Clock models 114
4.3.5 Ising spin glass models 115
4.3.6 Complex fluid models 116
4.4 Spin-exchange sampling 117
4.4.1 Constant magnetization simulations 117
4.4.2 Phase separation 118
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3.6</td>
<td>Wolff embedding trick and cluster flipping</td>
<td>162</td>
</tr>
<tr>
<td>5.3.7</td>
<td>Hybrid methods</td>
<td>163</td>
</tr>
<tr>
<td>5.3.8</td>
<td>Monte Carlo dynamics vs. equation of motion dynamics</td>
<td>163</td>
</tr>
<tr>
<td>5.3.9</td>
<td>Topological excitations and solitons</td>
<td>164</td>
</tr>
<tr>
<td>5.4</td>
<td>Systems with quenched randomness</td>
<td>166</td>
</tr>
<tr>
<td>5.4.1</td>
<td>General comments: averaging in random systems</td>
<td>166</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Parallel tempering: a general method to better equilibrate systems with complex energy landscapes</td>
<td>171</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Random fields and random bonds</td>
<td>172</td>
</tr>
<tr>
<td>5.4.4</td>
<td>Spin glasses and optimization by simulated annealing</td>
<td>173</td>
</tr>
<tr>
<td>5.4.5</td>
<td>Ageing in spin glasses and related systems</td>
<td>178</td>
</tr>
<tr>
<td>5.4.6</td>
<td>Vector spin glasses: developments and surprises</td>
<td>178</td>
</tr>
<tr>
<td>5.5</td>
<td>Models with mixed degrees of freedom: Si/Ge alloys, a case study</td>
<td>179</td>
</tr>
<tr>
<td>5.6</td>
<td>Methods for systems with long range interactions</td>
<td>181</td>
</tr>
<tr>
<td>5.7</td>
<td>Parallel tempering, simulated tempering, and related methods: accuracy considerations</td>
<td>183</td>
</tr>
<tr>
<td>5.8</td>
<td>Sampling the free energy and entropy</td>
<td>186</td>
</tr>
<tr>
<td>5.8.1</td>
<td>Thermodynamic integration</td>
<td>186</td>
</tr>
<tr>
<td>5.8.2</td>
<td>Groundstate free energy determination</td>
<td>187</td>
</tr>
<tr>
<td>5.8.3</td>
<td>Estimation of intensive variables: the chemical potential</td>
<td>188</td>
</tr>
<tr>
<td>5.8.4</td>
<td>Lee–Kosterlitz method</td>
<td>189</td>
</tr>
<tr>
<td>5.8.5</td>
<td>Free energy from finite size dependence at $T_c$</td>
<td>189</td>
</tr>
<tr>
<td>5.9</td>
<td>Miscellaneous topics</td>
<td>190</td>
</tr>
<tr>
<td>5.9.1</td>
<td>Inhomogeneous systems: surfaces, interfaces, etc.</td>
<td>190</td>
</tr>
<tr>
<td>5.9.2</td>
<td>Anisotropic critical phenomena: simulation boxes with arbitrary aspect ratio</td>
<td>196</td>
</tr>
<tr>
<td>5.9.3</td>
<td>Other Monte Carlo schemes</td>
<td>198</td>
</tr>
<tr>
<td>5.9.4</td>
<td>Inverse and reverse Monte Carlo methods</td>
<td>200</td>
</tr>
<tr>
<td>5.9.5</td>
<td>Finite size effects: review and summary</td>
<td>202</td>
</tr>
<tr>
<td>5.9.6</td>
<td>More about error estimation</td>
<td>202</td>
</tr>
<tr>
<td>5.9.7</td>
<td>Random number generators revisited</td>
<td>204</td>
</tr>
<tr>
<td>5.10</td>
<td>Summary and perspective</td>
<td>207</td>
</tr>
<tr>
<td>References</td>
<td></td>
<td>208</td>
</tr>
<tr>
<td>6</td>
<td>Off-lattice models</td>
<td>212</td>
</tr>
<tr>
<td>6.1</td>
<td>Fluids</td>
<td>212</td>
</tr>
<tr>
<td>6.1.1</td>
<td>$NVT$ ensemble and the virial theorem</td>
<td>212</td>
</tr>
<tr>
<td>6.1.2</td>
<td>$NpT$ ensemble</td>
<td>216</td>
</tr>
<tr>
<td>6.1.3</td>
<td>Grand canonical ensemble</td>
<td>220</td>
</tr>
<tr>
<td>6.1.4</td>
<td>Near critical coexistence: a case study</td>
<td>224</td>
</tr>
<tr>
<td>6.1.5</td>
<td>Subsystems: a case study</td>
<td>226</td>
</tr>
<tr>
<td>6.1.6</td>
<td>Gibbs ensemble</td>
<td>231</td>
</tr>
</tbody>
</table>
6.1.7 Widom particle insertion method and variants 234
6.1.8 Monte Carlo phase switch 236
6.1.9 Cluster algorithm for fluids 239
6.1.10 Event chain algorithms 241
6.2 'Short range' interactions 242
6.2.1 Cutoffs 242
6.2.2 Verlet tables and cell structure 242
6.2.3 Minimum image convention 243
6.2.4 Mixed degrees of freedom reconsidered 243
6.3 Treatment of long range forces 243
6.3.1 Reaction field method 243
6.3.2 Ewald method 244
6.3.3 Fast multipole method 245
6.4 Adsorbed monolayers 246
6.4.1 Smooth substrates 246
6.4.2 Periodic substrate potentials 246
6.5 Complex fluids 247
6.5.1 Application of the Liu–Luijten algorithm to a binary fluid mixture 250
6.6 Polymers: an introduction 251
6.6.1 Length scales and models 251
6.6.2 Asymmetric polymer mixtures: a case study 257
6.6.3 Applications: dynamics of polymer melts; thin adsorbed polymeric films 261
6.6.4 Polymer melts: speeding up bond fluctuation model simulations 265
6.7 Configurational bias and 'smart Monte Carlo' 267
6.8 Estimation of excess free energies due to walls for fluids and solids 270
6.9 A symmetric, Lennard–Jones mixture: a case study 272
6.10 Finite size effects on interfacial properties: a case study 275
6.11 Outlook 277
References 278

7 Reweighting methods 282
7.1 Background 282
7.1.1 Distribution functions 282
7.1.2 Umbrella sampling 282
7.2 Single histogram method 285
7.2.1 The Ising model as a case study 286
7.2.2 The surface–bulk multicritical point: another case study 292
7.3 Multihistogram method 295
7.4 Broad histogram method 296
7.5 Transition matrix Monte Carlo 296
7.6 Multicanonical sampling 297
7.6.1 The multicanonical approach and its relationship to canonical sampling 297
7.6.2 Near first order transitions 299
7.6.3 Groundstates in complicated energy landscapes 300
7.6.4 Interface free energy estimation 301
7.7 A case study: the Casimir effect in critical systems 302
7.8 Wang–Landau sampling 303
7.8.1 Basic algorithm 303
7.8.2 Applications to models with continuous variables 307
7.8.3 A simple example of two-dimensional Wang–Landau sampling 307
7.8.4 Microcanonical entropy inflection points 308
7.8.5 Back to numerical integration 309
7.8.6 Replica exchange Wang–Landau sampling 310
7.9 A case study: evaporation/condensation transition of droplets 314
References 316

8 Quantum Monte Carlo methods 319
8.1 Introduction 319
8.2 Feynman path integral formulation 320
8.2.1 Off-lattice problems: low temperature properties of crystals 320
8.2.2 Bose statistics and superfluidity 327
8.2.3 Path integral formulation for rotational degrees of freedom 328
8.3 Lattice problems 331
8.3.1 The Ising model in a transverse field 331
8.3.2 Anisotropic Heisenberg chain 332
8.3.3 Fermions on a lattice 336
8.3.4 An intermezzo: the minus sign problem 338
8.3.5 Spinless fermions revisited 340
8.3.6 Cluster methods for quantum lattice models 342
8.3.7 Continuous time simulations 344
8.3.8 Decoupled cell method 345
8.3.9 Handscomb’s method and the stochastic series expansion (SSE) approach 346
8.3.10 Wang–Landau sampling for quantum models 347
8.3.11 Fermion determinants 349
8.4 Monte Carlo methods for the study of groundstate properties 350
8.4.1 Variational Monte Carlo (VMC) 351
8.4.2 Green’s function Monte Carlo methods (GFMC) 353
8.5 Towards constructing the nodal surface of off-lattice, many-Fermion systems: the ‘survival of the fittest’ algorithm 355
8.6 Concluding remarks 359
References 360

9 Monte Carlo renormalization group methods 364
9.1 Introduction to renormalization group theory 364
9.2 Real space renormalization group 368
9.3 Monte Carlo renormalization group 369
  9.3.1 Large cell renormalization 369
  9.3.2 Ma's method: finding critical exponents and
       the fixed point Hamiltonian 371
  9.3.3 Swendsen's method 372
  9.3.4 Location of phase boundaries 374
  9.3.5 Dynamic problems: matching time-dependent
       correlation functions 375
  9.3.6 Inverse Monte Carlo renormalization group
       transformations 376
References 376

10 Non-equilibrium and irreversible processes 378
10.1 Introduction and perspective 378
10.2 Driven diffusive systems (driven lattice gases) 378
10.3 Crystal growth 381
10.4 Domain growth 384
10.5 Polymer growth 387
  10.5.1 Linear polymers 387
  10.5.2 Gelation 387
10.6 Growth of structures and patterns 389
  10.6.1 Eden model of cluster growth 389
  10.6.2 Diffusion limited aggregation 389
  10.6.3 Cluster–cluster aggregation 392
  10.6.4 Cellular automata 392
10.7 Models for film growth 393
  10.7.1 Background 393
  10.7.2 Ballistic deposition 394
  10.7.3 Sedimentation 395
  10.7.4 Kinetic Monte Carlo and MBE growth 396
10.8 Transition path sampling 398
10.9 Forced polymer pore translocation: a case study 399
10.10 The Jarzynski non-equilibrium work theorem and its
     application to obtain free energy differences from
     trajectories 402
10.11 Outlook: variations on a theme 404
References 404

11 Lattice gauge models: a brief introduction 408
11.1 Introduction: gauge invariance and lattice gauge theory 408
11.2 Some technical matters 410
# Contents

11.3 Results for $Z(N)$ lattice gauge models 410  
11.4 Compact U(1) gauge theory 411  
11.5 SU(2) lattice gauge theory 412  
11.6 Introduction: quantum chromodynamics (QCD) and phase transitions of nuclear matter 413  
11.7 The deconfinement transition of QCD 415  
11.8 Towards quantitative predictions 418  
11.9 Density of states in gauge theories 420  
11.10 Perspective 421  
References 421

12 A brief review of other methods of computer simulation 423  
12.1 Introduction 423  
12.2 Molecular dynamics 423  
12.2.1 Integration methods (microcanonical ensemble) 423  
12.2.2 Other ensembles (constant temperature, constant pressure, etc.) 427  
12.2.3 Non-equilibrium molecular dynamics 430  
12.2.4 Hybrid methods (MD + MC) 430  
12.2.5 *Ab initio* molecular dynamics 431  
12.2.6 Hyperdynamics and metadynamics 432  
12.3 Quasi-classical spin dynamics 432  
12.4 Langevin equations and variations (cell dynamics) 436  
12.5 Micromagnetics 437  
12.6 Dissipative particle dynamics (DPD) 438  
12.7 Lattice gas cellular automata 439  
12.8 Lattice Boltzmann equation 440  
12.9 Multiscale simulation 440  
12.10 Multiparticle collision dynamics 442  
References 444

13 Monte Carlo simulations at the periphery of physics and beyond 447  
13.1 Commentary 447  
13.2 Astrophysics 447  
13.3 Materials science 448  
13.4 Chemistry 449  
13.5 'Biologically inspired' physics 451  
13.5.1 Commentary and perspective 451  
13.5.2 Lattice proteins 451  
13.5.3 Cell sorting 453  
13.6 Biology 454  
13.7 Mathematics/statistics 455  
13.8 Sociophysics 456  
13.9 Econophysics 456  
13.10 'Traffic' simulations 457  
13.11 Medicine 459
<table>
<thead>
<tr>
<th>Contents</th>
<th>xiii</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.12 Networks: what connections really matter?</td>
<td>460</td>
</tr>
<tr>
<td>13.13 Finance</td>
<td>461</td>
</tr>
<tr>
<td>References</td>
<td>462</td>
</tr>
<tr>
<td>14 Monte Carlo studies of biological molecules</td>
<td>465</td>
</tr>
<tr>
<td>14.1 Introduction</td>
<td>465</td>
</tr>
<tr>
<td>14.2 Protein folding</td>
<td>466</td>
</tr>
<tr>
<td>14.2.1 Introduction</td>
<td>466</td>
</tr>
<tr>
<td>14.2.2 How to best simulate proteins: Monte Carlo or molecular dynamics?</td>
<td>467</td>
</tr>
<tr>
<td>14.2.3 Generalized ensemble methods</td>
<td>467</td>
</tr>
<tr>
<td>14.2.4 Globular proteins: a case study</td>
<td>469</td>
</tr>
<tr>
<td>14.2.5 Simulations of membrane proteins</td>
<td>470</td>
</tr>
<tr>
<td>14.3 Monte Carlo simulations of RNA structures</td>
<td>472</td>
</tr>
<tr>
<td>14.4 Monte Carlo simulations of carbohydrates</td>
<td>472</td>
</tr>
<tr>
<td>14.5 Determining macromolecular structures</td>
<td>474</td>
</tr>
<tr>
<td>14.6 Outlook</td>
<td>475</td>
</tr>
<tr>
<td>References</td>
<td>475</td>
</tr>
<tr>
<td>15 Outlook</td>
<td>477</td>
</tr>
<tr>
<td>Appendix: Listing of programs mentioned in the text</td>
<td>479</td>
</tr>
<tr>
<td>Index</td>
<td>511</td>
</tr>
</tbody>
</table>