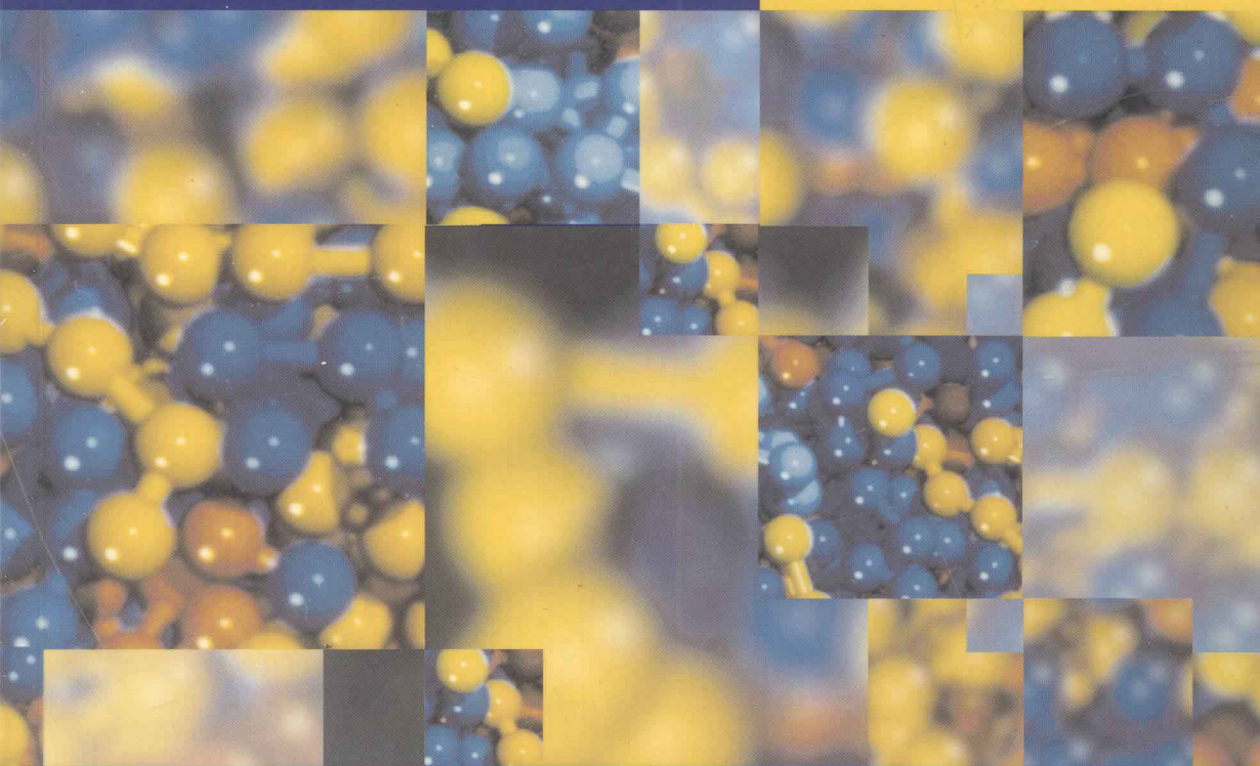


A Guide to
**Monte Carlo Simulations in
Statistical Physics**

**David P. Landau &
Kurt Binder**



A Guide to Monte Carlo Simulations in Statistical Physics

David P. Landau

Center for Simulation Physics, The University of Georgia

Kurt Binder

Institut für Physik, Johannes-Gutenberg-Universität Mainz



CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS

The Edinburgh Building, Cambridge CB2 2RU, UK <http://www.cup.cam.ac.uk>
40 West 20th Street, New York, NY 10011-4211, USA <http://www.cup.org>
10 Stamford Road, Oakleigh, Melbourne 3166, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain

© David P. Landau and Kurt Binder 2000

This book is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without
the written permission of Cambridge University Press.

First published 2000

Printed in the United Kingdom at the University Press, Cambridge

Typeface Ehrhardt 10.25/12.5pt *System* Advent 3B2 [KT]

A catalogue record for this book is available from the British Library

Library of Congress Cataloging in Publication data

Landau, David P.

A guide to Monte Carlo simulations in statistical physics / David P. Landau, Kurt Binder.
p. cm.

Includes index.

ISBN 0 521 65314 2 (hardbound)

1. Monte Carlo method. 2. Statistical physics. I. Binder, K. (Kurt), 1944– . II. Title.

QC174.85.M64L36 2000

530.13–dc21 99-38308CIP

ISBN 0 521 65314 2 hardback

ISBN 0 521 65366 5 paperback

A Guide to Monte Carlo Simulations in Statistical Physics

This book deals with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics as well as in related fields, for example polymer science and lattice gauge theory.

After briefly recalling essential background in statistical mechanics and probability theory, the authors give a succinct overview of simple sampling methods. The next several chapters develop the importance sampling method, both for lattice models and for systems in continuum space. The concepts behind the various simulation algorithms are explained in a comprehensive fashion, as are the techniques for efficient evaluation of system configurations generated by simulation (histogram extrapolation, multicanonical sampling, thermodynamic integration and so forth). The fact that simulations deal with small systems is emphasized, and the text incorporates various finite size scaling concepts to show how a careful analysis of finite size effects can be a useful tool for the analysis of simulation results. Other chapters also provide introductions to quantum Monte Carlo methods, aspects of simulations of growth phenomena and other systems far from equilibrium, and the Monte Carlo renormalization group approach to critical phenomena. Throughout the book there are many applications, examples, and exercises to help the reader in a thorough study of this book; furthermore, many up-to-date references to more specialized literature are also provided.

This book will be bought by graduate students who have to deal with computer simulations in their research, as well as by postdoctoral researchers, in both physics and physical chemistry. It can be used as a textbook for graduate courses on computer simulations in physics and related disciplines.

DAVID P. LANDAU was born on June 22, 1941 in St. Louis, MO, USA. He received a B.A. in Physics from Princeton University in 1963 and a Ph.D. in Physics from Yale University in 1967. His Ph.D. research involved experimental studies of magnetic phase transitions as did his postdoctoral research at the CNRS in Grenoble, France. After teaching at Yale for a year he moved to the University of Georgia and initiated a research program of Monte Carlo studies in statistical physics. He is currently the Research Professor of Physics and founding Director of the Center for Simulation Physics at the University of Georgia. He has been teaching graduate courses in computer simulations since 1982. David Landau has authored/co-authored almost 300 research publications and is editor/co-editor of more than a dozen books. The University of Georgia awarded him a Creative Research Medal in 1981 and named him a Senior Teaching Fellow in 1993. In 1998 he also became an Adjunct Professor at the Helsinki University of Technology. He is a Fellow of the American Physical Society and a past Chair of the Division of Computational Physics of the APS. He received the Jesse W. Beams award from SESAPS in 1987, and a Humboldt Fellowship and Humboldt Senior U.S. Scientist award in 1975 and 1988 respectively. In 1999 he was named a Fellow of the Japan Society for the Promotion of Science. He is currently a Principal Editor for the journal *Computer Physics Communications*.

KURT BINDER was born on February 10, 1944 in Korneuburg, Austria and then lived in Vienna, where he received his Ph.D. in 1969 at the Technical University of Vienna. Even then his thesis dealt with Monte Carlo simulations of Ising and Heisenberg magnets, and since then he has pioneered the development of Monte Carlo simulation methods in statistical physics. From 1969 until 1974 Kurt Binder worked at the Technical University in Munich, where he defended his Habilitation thesis in 1973 after a stay as IBM postdoctoral fellow in Zurich in 1972/73. Further key times in his career were spent at Bell Laboratories, Murray Hill, NJ (1974) and a first appointment as Professor of Theoretical Physics at the University of Saarbrücken back in Germany (1974–1977), followed by a joint appointment as full professor at the University of Cologne and the position as one of the directors of the Institute of Solid State Research at Jülich (1977–1983). He has held his present position as Professor of Theoretical Physics at the University of Mainz, Germany since 1983, and since 1989 he has also been an external member of the Max-Planck-Institut for Polymer Research at Mainz. Kurt Binder has written more than 600 research publications and edited five books dealing with computer simulation. His book (with Dieter W. Hermann) *Monte Carlo Simulation in Statistical Physics: An Introduction*, first published in 1988, is in its 3rd edition. Kurt Binder has been a corresponding member of the Austrian Academy of Sciences in Vienna since 1992 and received the Max Planck Medal of the German Physical Society in 1993. He also acts as Editorial Board member of several journals and presently serves as chairman of the IUPAP Commission on Statistical Physics.

Preface

Historically physics was first known as ‘natural philosophy’ and research was carried out by purely theoretical (or philosophical) investigation. True progress was obviously limited by the lack of real knowledge of whether or not a given theory really applied to nature. Eventually experimental investigation became an accepted form of research although it was always limited by the physicist’s ability to prepare a sample for study or to devise techniques to probe for the desired properties. With the advent of computers it became possible to carry out simulations of models which were intractable using ‘classical’ theoretical techniques. In many cases computers have, for the first time in history, enabled physicists not only to invent new models for various aspects of nature but also to solve those same models without substantial simplification. In recent years computer power has increased quite dramatically, with access to computers becoming both easier and more common (e.g. with personal computers and workstations), and computer simulation methods have also been steadily refined. As a result computer simulations have become another way of doing physics research. They provide another perspective; in some cases simulations provide a theoretical basis for understanding experimental results, and in other instances simulations provide ‘experimental’ data with which theory may be compared. There are numerous situations in which direct comparison between analytical theory and experiment is inconclusive. For example, the theory of phase transitions in condensed matter must begin with the choice of a Hamiltonian, and it is seldom clear to what extent a particular model actually represents a real material on which experiments are done. Since analytical treatments also usually require mathematical approximations whose accuracy is difficult to assess or control, one does not know whether discrepancies between theory and experiment should be attributed to shortcomings of the model, the approximations, or both. The goal of this text is to provide a basic understanding of the methods and philosophy of computer simulations research with an emphasis on problems in statistical thermodynamics as applied to condensed matter physics or materials science. There exist many other simulation problems in physics (e.g. simulating the spectral intensity reaching a detector in a scattering experiment) which are more straightforward and which will only occasionally be mentioned. We shall use many specific examples and, in some cases, give explicit computer programs, but we wish to

emphasize that these methods are applicable to a wide variety of systems including those which are not treated here at all. As computer architecture changes the methods presented here will in some cases require relatively minor reprogramming and in other instances will require new algorithm development in order to be truly efficient. We hope that this material will prepare the reader for studying new and different problems using both existing as well as new computers.

At this juncture we wish to emphasize that it is important that the simulation algorithm and conditions be chosen with the physics problem at hand in mind. The *interpretation* of the resultant output is critical to the success of any simulational project, and we thus include substantial information about various aspects of thermodynamics and statistical physics to help strengthen this connection. We also wish to draw the reader's attention to the rapid development of scientific visualization and the important role that it can play in producing *understanding* of the results of some simulations.

This book is intended to serve as an introduction to Monte Carlo methods for graduate students, and advanced undergraduates, as well as more senior researchers who are not yet experienced in computer simulations. The book is divided up in such a way that it will be useful for courses which only wish to deal with a restricted number of topics. Some of the later chapters may simply be skipped without affecting the understanding of the chapters which follow. Because of the immensity of the subject, as well as the existence of a number of very good monographs and articles on advanced topics which have become quite technical, we will limit our discussion in certain areas, e.g. polymers, to an introductory level. The examples which are given are in FORTRAN, not because it is necessarily the best scientific computer language, but because it is certainly the most widespread. Many existing Monte Carlo programs and related subprograms are in FORTRAN and will be available to the student from libraries, journals, etc. A number of sample problems are suggested in the various chapters; these may be assigned by course instructors or worked out by students on their own. Our experience in assigning problems to students taking a graduate course in simulations at the University of Georgia over a 15 year period suggests that for maximum pedagogical benefit, students should be required to prepare cogent reports after completing each assigned simulational problem. Students were required to complete seven 'projects' in the course of the quarter for which they needed to write and debug programs, take and analyze data, and prepare a report. Each report should briefly describe the algorithm used, provide sample data and data analysis, draw conclusions and add comments. (A sample program/output should be included.) In this way, the students obtain practice in the summary and presentation of simulational results, a skill which will prove to be valuable later in their careers. For convenience, the case studies that are described have been simply taken from the research of the authors of this book – the reader should be aware that this is by no means meant as a negative statement on the quality of the research of numerous other groups in the field. Similarly, selected references are given to aid the reader in finding

more detailed information, but because of length restrictions it is simply not possible to provide a complete list of relevant literature. Many coworkers have been involved in the work which is mentioned here, and it is a pleasure to thank them for their fruitful collaboration. We have also benefited from the stimulating comments of many of our colleagues and we wish to express our thanks to them as well.

Contents

Preface	xi
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
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: θ -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 NVT ensemble and the virial theorem	182
6.1.2 NpT 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 Ising 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

1 Introduction

1.1 WHAT IS A MONTE CARLO SIMULATION?

In a Monte Carlo simulation we attempt to follow the ‘time dependence’ of a model for which change, or growth, does not proceed in some rigorously predefined fashion (e.g. according to Newton’s equations of motion) but rather in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation. With a second, different sequence of random numbers the simulation will not give identical results but will yield values which agree with those obtained from the first sequence to within some ‘statistical error’. A very large number of different problems fall into this category: in percolation an empty lattice is gradually filled with particles by placing a particle on the lattice randomly with each ‘tick of the clock’. Lots of questions may then be asked about the resulting ‘clusters’ which are formed of neighboring occupied sites. Particular attention has been paid to the determination of the ‘percolation threshold’, i.e. the critical concentration of occupied sites for which an ‘infinite percolating cluster’ first appears. A percolating cluster is one which reaches from one boundary of a (macroscopic) system to the opposite one. The properties of such objects are of interest in the context of diverse physical problems such as conductivity of random mixtures, flow through porous rocks, behavior of dilute magnets, etc. Another example is diffusion limited aggregation (DLA) where a particle executes a random walk in space, taking one step at each time interval, until it encounters a ‘seed’ mass and sticks to it. The growth of this mass may then be studied as many random walkers are turned loose. The ‘fractal’ properties of the resulting object are of real interest, and while there is no accepted analytical theory of DLA to date, computer simulation is the method of choice. In fact, the phenomenon of DLA was first discovered by Monte Carlo simulation!

Considering problems of statistical mechanics, we may be attempting to sample a region of phase space in order to estimate certain properties of the model, although we may not be moving in phase space along the same path which an exact solution to the time dependence of the model would yield. Remember that the task of equilibrium statistical mechanics is to calculate thermal averages of (interacting) many-particle systems: Monte Carlo simulations can do that, taking proper account of statistical fluctuations and their

effects in such systems. Many of these models will be discussed in more detail in later chapters so we shall not provide further details here. Since the accuracy of a Monte Carlo estimate depends upon the thoroughness with which phase space is probed, improvement may be obtained by simply running the calculation a little longer to increase the number of samples. Unlike in the application of many analytic techniques (e.g. perturbation theory for which the extension to higher order may be prohibitively difficult), the improvement of the accuracy of Monte Carlo results is possible not just in principle but also in practice!

1.2. WHAT PROBLEMS CAN WE SOLVE WITH IT?

The range of different physical phenomena which can be explored using Monte Carlo methods is exceedingly broad. Models which either naturally or through approximation can be discretized can be considered. The motion of individual atoms may be examined directly; e.g. in a binary (AB) metallic alloy where one is interested in interdiffusion or unmixing kinetics (if the alloy was prepared in a thermodynamically unstable state) the random hopping of atoms to neighboring sites can be modeled directly. This problem is complicated because the jump rates of the different atoms depend on the locally differing environment. Of course, in this description the quantum mechanics of atoms with potential barriers in the eV range is not explicitly considered, and the sole effect of phonons (lattice vibrations) is to provide a ‘heat bath’ which provides the excitation energy for the jump events. Because of a separation of time scales (the characteristic times between jumps are orders of magnitude larger than atomic vibration periods) this approach provides very good approximation. The same kind of arguments hold true for growth phenomena involving macroscopic objects, such as DLA growth of colloidal particles; since their masses are orders of magnitude larger than atomic masses, the motion of colloidal particles in fluids is well described by classical, random Brownian motion. These systems are hence well suited to study by Monte Carlo simulations which use random numbers to realize random walks. The motion of a fluid may be studied by considering ‘blocks’ of fluid as individual particles, but these blocks will be far larger than individual molecules. As an example, we consider ‘micelle formation’ in lattice models of microemulsions (water–oil–surfactant fluid mixtures) in which each surfactant molecule may be modeled by two ‘dimers’ on the lattice (two occupied nearest neighbor sites on the lattice). Different effective interactions allow one dimer to mimic the hydrophilic group and the other dimer the hydrophobic group of the surfactant molecule. This model then allows the study of the size and shape of the aggregates of surfactant molecules (the micelles) as well as the kinetic aspects of their formation. In reality, this process is quite slow so that a deterministic molecular dynamics simulation (i.e. numerical integration of Newton’s second law) is not feasible. This example shows that part of the ‘art’ of simulation is the appropriate choice

(or invention!) of a suitable (coarse-grained) model. Large collections of interacting classical particles are directly amenable to Monte Carlo simulation, and the behavior of interacting quantized particles is being studied either by transforming the system into a pseudo-classical model or by considering permutation properties directly. These considerations will be discussed in more detail in later chapters. Equilibrium properties of systems of interacting atoms have been extensively studied as have a wide range of models for simple and complex fluids, magnetic materials, metallic alloys, adsorbed surface layers, etc. More recently polymer models have been studied with increasing frequency; note that the simplest model of a flexible polymer is a random walk, an object which is well suited for Monte Carlo simulation. Furthermore, some of the most significant advances in understanding the theory of elementary particles have been made using Monte Carlo simulations of lattice gauge models.

1.3 WHAT DIFFICULTIES WILL WE ENCOUNTER?

1.3.1 Limited computer time and memory

Because of limits on computer speed there are some problems which are inherently not suited to computer simulation, at this time. A simulation which requires years of cpu time on whatever machine is available is simply impractical. Similarly a calculation which requires memory which far exceeds that which is available can be carried out only by using very sophisticated programming techniques which slow down running speeds and greatly increase the probability of errors. It is therefore important that the user first consider the requirements of both memory and cpu time *before* embarking on a project to ascertain whether or not there is a realistic possibility of obtaining the resources to simulate a problem properly. Of course, with the rapid advances being made by the computer industry, it may be necessary to wait only a few years for computer facilities to catch up to your needs. Sometimes the tractability of a problem may require the invention of a new, more efficient simulation algorithm. Of course, developing new strategies to overcome such difficulties constitutes an exciting field of research by itself.

1.3.2 Statistical and other errors

Assuming that the project can be done, there are still potential sources of error which must be considered. These difficulties will arise in many different situations with different algorithms so we wish to mention them briefly at this time without reference to any specific simulation approach. All computers operate with limited word length and hence limited precision for numerical values of any variable. Truncation and round-off errors may in some cases lead to serious problems. In addition there are statistical errors which arise as