13 Monte Carlo simulations at the periphery of physics and beyond

13.1 COMMENTARY

In the preceding chapters we described the application of Monte Carlo methods in numerous areas that can be clearly identified as belonging to physics. Although the exposition was far from complete, it should have sufficed to give the reader an appreciation of the broad impact that Monte Carlo studies has already had in statistical physics. A more recent occurrence is the application of these methods in non-traditional areas of physics related research. More explicitly, we mean subject areas that are not normally considered to be physics at all but which make use of physics principles at their core. In some cases physicists have entered these arenas by introducing quite simplified models that represent a 'physicist's view' of a particular problem. Often such descriptions are oversimplified, but the hope is that some essential insight can be gained as is the case in many traditional physics studies. (A provocative perspective of the role of statistical physics outside physics has been presented by Stauffer (2004).) In other cases, however, Monte Carlo methods are being applied by non-physicists (or 'recent physicists') to problems that, at best, have a tenuous relationship to physics. This chapter is to serve as a brief glimpse of applications of Monte Carlo methods 'outside' physics. The number of such studies will surely grow rapidly; and even now, we wish to emphasize that we will make no attempt to be complete in our treatment.

In recent years the simulation of relatively realistic models of proteins has become a 'self-sufficient' enterprise. For this reason, such studies will be found in a separate, new chapter (Chapter 14), and in this chapter we will only consider models that are primarily of interest to statistical physicists.

13.2 ASTROPHYSICS

Because of the complexity of astrophysical processes, the utility of analytic calculations is quite limited. Given the power of modern computational resources, however, computer simulations offer the hope of being able to make quantitative comparisons between calculated spectra and observational results. One simple example is the use of a Monte Carlo simulation routine to study a high mass X-ray binary system (Watanabe *et al.*, 2004; Nagase and Watanabe, 2006).

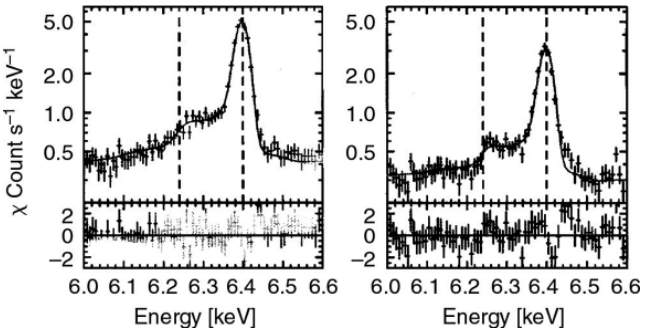

Fig. 13.1 Two spectra (left and right) of the iron Kα region. Superimposed on the data are lines showing 'best fits' to the Monte Carlo data. From Watanabe *et al.* (2004).

This approach bears some resemblance to the use of simple sampling Monte Carlo to study reactor design mentioned in Chapter 3. Here, individual, incident photons (instead of neutrons) are followed as they move through a fully three-dimensional geometry, as are other photons that are produced by the physical interactions that are included, until they escape from the simulation volume or are destroyed by some physical process. The simulator includes photoionization, photoexcitation, and Compton scattering as the physical processes that may occur. X-ray spectra are then computed and compared with observational spectra for the iron Kα region obtained from the Chandra High Energy Transmission Grating Spectrometer. As shown in Fig. 13.1, the agreement is impressive.

Other simulation packages exist; for example, SOPHIA (Mücke *et al.*, 2000), which calculates photohadronic interactions of relativistic nucleons with an ambient photon radiation field, can also be used for radiation and background studies at high energy colliders.

A distinct application of Monte Carlo simulations is typified by the development of a framework for the scientific analysis of spatially and spectroscopically complex celestial sources using the X-Ray Telescope (XRT) and X-ray Imaging Spectrometer (XIS) on board *Suzaku* (Ishisaki *et al.*, 2007). A photon-by-photon instrumental simulator was built using a ray-tracing library, while the XIS simulation utilized a spectral 'Redistribution Matrix' File (RMF), generated separately by other tools. Instrumental characteristics and calibration were incorporated to make the simulations as realistic as possible.

There are numerous other applications of simulations in this field, and these examples are only intended to provide a taste of how Monte Carlo methods are used in modern astrophysics.

13.3 MATERIALS SCIENCE

Monte Carlo simulations are now finding increased utility in a broad range of studies that are more applied than those typically referred to under the rubric of 'condensed matter physics'. Broadly termed 'materials science', these activities actually run the gamut from rather basic research to topics that

are often termed 'engineering'. Early Monte Carlo studies often focused on phase separation in materials. An example was the simulation of thin film codeposition (Adams *et al*., 1993) in which resultant microstructures for a simple lattice model were compared with those from experimental studies of Al–Ge alloys. Monte Carlo studies have also explored more theoretical aspects of phase separation (see, e.g., Section 10.4), and recent Monte Carlo studies have probed new horizons. Certainly one important goal of materials science is the study of novel materials, and one such example is the Monte Carlo simulation of graphene using a sophisticated, many-body potential for carbon (Fasolino *et al*., 2007). (The electron transport properties of graphene give it great potential technological value and understanding its properties would be of value.) These simulations found ripples that result from thermal fluctuations with a size distribution that is peaked at about 80 A, in good agreement with experiment. This behavior appears to result from the special ability of carbon to form different types of bonds; hence, graphene is different from a generic two-dimensional crystal.

Whereas materials science has traditionally been associated with materials with potential engineering application, interest has been growing in the study of soft materials with potential applications as pharmaceutical materials. There are a host of unresolved issues in this field, including manufacture and control of drug/dosage form plus improving drug delivery through improved understanding of structure and properties of micro/nanoparticles, bulk powders, and their assemblies. For a recent overview, see the *MRS Bulletin* edited by Elliot and Hancock (2006).

Monte Carlo simulation can also be a valuable tool for the study of imperfections in materials, including both chemical impurities and structural defects, including undesirable microstructure, creep failure, etc. Typically, quite standard Monte Carlo methods (described in earlier chapters) are used, but the models examined reflect the materials of interest far more closely than do simple systems, such as the Ising model, that are usually considered in statistical physics.

In this interdisciplinary area between physics and engineering, one is often interested in modeling properties and phenomena occurring over vastly different scales of space and time. Monte Carlo methods have found their place as one of the different items in the 'toolbox' of computational materials science (Yip, 2005).

13.4 CHEMISTRY

A fundamental area of chemistry where Monte Carlo simulations play a key role is the field of heterogeneously catalyzed chemical reactions. In this context, one experimentally observes a wealth of complex phenomena: pattern formation and self-organization, regular and irregular kinetic oscillations of these patterns (see, e.g., Ertl (1990) and Imbiehl (1993)), propagation and interference of chemical waves and spatio-temporal structures, chaotic temporal behavior,

and irreversible phase transitions in chemical reaction systems (Marro and Dickman, 1999; Loscar and Albano, 2003).

It turns out that Monte Carlo studies of such irreversible phase transitions have much in common with Monte Carlo studies of phase transitions which occur in thermal equilibrium systems, e.g. concepts such as finite size scaling analyses can be carried over to such problems; moreover, the models formulated for these chemical reaction systems are often motivated by models in physics (Loscar and Albano, 2003).

To mention a specific system as an example, we consider the catalytic oxidation of carbon monoxide, $2CO + O_2 \rightarrow 2CO_2$. This reaction proceeds according to the well known Langmuir–Hinshelwood mechanism, i.e. both reactants are adsorbed on the surface of a catalyst (e.g. noble metals such as Pt):

$$\begin{aligned} &CO\,(g) + S \rightarrow CO\,(a)\,, \\ &O_2\,(g) + 2S \rightarrow 2O\,(a)\,, \\ &CO\,(a) + O\,(a) \rightarrow CO_2\,(g)\,. \end{aligned}$$

Here S stands for an empty adsorption site on the surface, while (a) and (g) refer to the adsorbed and gas phases of the respective molecules. This reaction takes place when the catalyst is held in contact with a reservoir of both gases CO and O_2 at partial pressures p_{CO} and p_{O_2}, respectively.

Apart from the reaction steps of the above reaction equations, the simulation then takes into account surface diffusion (i.e. random hops of an adatom to empty neighboring adsorption sites), desorption, etc. A simple model for such a system that was much studied by Monte Carlo methods is the Ziff–Gulari–Barshad (ZGB) model. (See Ziff *et al.* (1986), which showed that a transition to an inactive state of the surface can occur ('poisoning' the surface), where the reaction has stopped. Since this early work, much research on this model and related models has been carried out; see Marro and Dickmann (1999) and Loscar and Albano (2003) for reviews.)

Another area of very active research is the kinetics of irreversible polymerization where one wishes to understand the distribution of molecular weight of linear and branched macromolecules. Early applications of Monte Carlo simulations of polymerization kinetics can be found in Johnson and O'Driscoll (1984) and Chaumont *et al.* (1985), for example. Sometimes chemical reactions and physical processes need to be simulated together (e.g. phase separation process of a polymer blend can be 'arrested' by suitable chemical reactions, and thus the reactive formation of co-continuous nanostructures can be studied (John and Sommer, 2008)). A related subject at the borderline of chemistry and physics of polymers is the formation of 'living polymers', which is discussed elsewhere in this book. Also, for small molecules the interplay between chemical reactions and their equation of state is a subject of Monte Carlo study (Johnson, 1999). Lastly, we mention that concepts such as percolation and fractals, etc., which we have already discussed in Chapter 3 of this book, also play a role within the context of chemistry (Kopelman, 1989).

A much cited paper in the literature (Northrup and McCammon, 1980) reported that Monte Carlo sampling yielded 10 times less atomic diffusion than molecular dynamics for the same amount of CPU time in simulations of bovine pancreatic trypsin inhibitor (BPTI). This result was then sometimes used to justify the use of molecular dynamics instead of Monte Carlo. However, Jorgensen and Tirado-Rives (1996) later challenged this result by directly comparing Metropolis sampling with leap-frog molecular dynamics simulations for 267 hexane molecules in the NPT ensemble. They used a united atom model, keeping C=C bonds fixed in the Monte Carlo sampling and using SHAKE in the molecular dynamics simulation. The generation of new trial configurations did not simply attempt to move a single atom, as did Northrup and McCammon (1980), but rather involved translation of the entire molecule and changes in the internal degrees of freedom. The conclusion was that, with this move set, molecular dynamics requires 1.6–3.8 times *more* CPU time than does Monte Carlo. We have pointed out earlier that inventive algorithms can make Monte Carlo simulations exceedingly effective, and Jorgensen and Tirado-Rives (1996) provided an excellent example of the need for such approaches when they estimated that molecular dynamics would require 300 000 years to simulate liquid hexane for 1s on a fast workstation of the day. While this estimate would be substantially reduced on today's computers, the CPU time required would still render such a study untenable.

13.5 'BIOLOGICALLY INSPIRED' PHYSICS

13.5.1 Commentary and perspective

A number of interesting problems that have been examined by Monte Carlo simulation can be loosely viewed as part of biology, but since the formulation is closer to that of statistical physics instead of 'real' biology we will term them as 'biologically inspired' physics. Intriguing examples of such work include the study of genealogical trees for simple neutral models of a closed population with sexual reproduction and clearly separated generations (Derrida *et al.*, 2000) and investigations of inherently non-equilibrium models for self-propelled particles in biological systems (such as schools of fish) as described by Czirók and Vicsek (2000). These latter systems have been studied using finite difference equations with stochastic noise, as described in the previous chapter, but provide a glimpse of another kind of 'biologically inspired' system. Yet another example is provided by the simple bit string models for reproduction that have also been examined via simulation (de Oliveira *et al.*, 2003). These investigations yield fascinating results, although, as indicated earlier, the connection to real biology is somewhat tenuous.

13.5.2 Lattice proteins

The entire problem of finding native states and folding pathways for protein has become an industry unto itself, with contributions coming from physics,

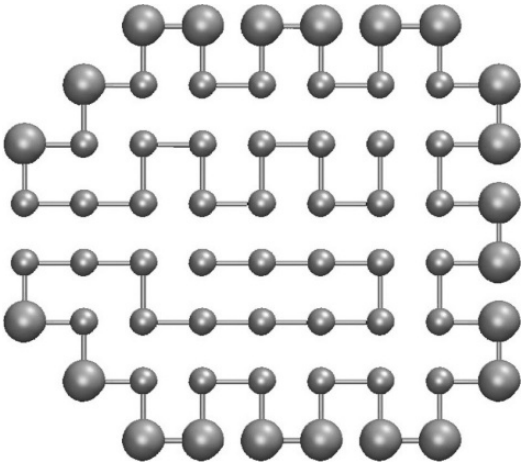

Fig. 13.2 Ground-state configuration for a 64mer HP model on a square lattice determined from Wang–Landau sampling. Large spheres are polar (P) monomers and small spheres are hydrophobic (H) monomers. After Wüst and Landau (unpublished data).

mathematics, and statistics in addition to biology. It has, in part, become a 'yardstick' against which the performance of various methods is measured with respect to their ability to find the low-lying groundstate that corresponds to the folded conformation of the protein model. Because of the growth in sophistication of simulations of such systems, Chapter 14 will be devoted to Monte Carlo simulations of protein folding using 'realistic' models. Nonetheless, much can be learned from over-simplified models that are at the intersection between statistical physics and biochemistry. The simplistic HP model (Dill, 1985; Lau and Dill, 1989) on the simple cubic lattice is already adequate to serve as a 'testing ground'. In this model, the protein is described as a heteropolymer composed of two kinds of monomers (hydrophobic, H, and polar, P) that form a self-avoiding walk on the lattice, with an attractive interaction between hydrophobic segments that we take to be unity. The groundstate, which is often degenerate, typically has a hydrophobic core and a hydrophilic (polar) outer surface. An example is the 64mer HP model on a square lattice, whose groundstate is shown in Fig. 13.2.

A famous HP model example is the 103mer (Lattmann *et al.*, 1994), whose groundstate energy was initially believed to be $E_{\min} = -49$ (Toma and Toma, 1996), until recent refinements of the PERM algorithm, see Chapters 4 and 6) due to Hsu *et al.* (2003a, 2003b) found distinctly lower energies, namely $E_{\min} = -54$ and $E_{\min} = -55$, respectively. Then, a combination of these refined PERM methods with multicanonical sampling (see Chapter 7) due to Bachmann and Janke (2004) achieved a still lower value, namely $E_{\min} = -56$, for this particular sequence of the 103mer HP model. More recently, Wüst and Landau (2008) used Wang–Landau sampling (Chapter 7) with 'pull-moves' (Lesh *et al.*, 2003) and found a yet lower groundstate, $E_{\min} = -58$. They also determined the thermodynamic properties. This is another indication of how the use of improved trial moves can be more effective than the use of raw computer power. In the Second Edition of this book we ended the brief discussion of the HP model with the following sentence: *Therefore, it is likely*

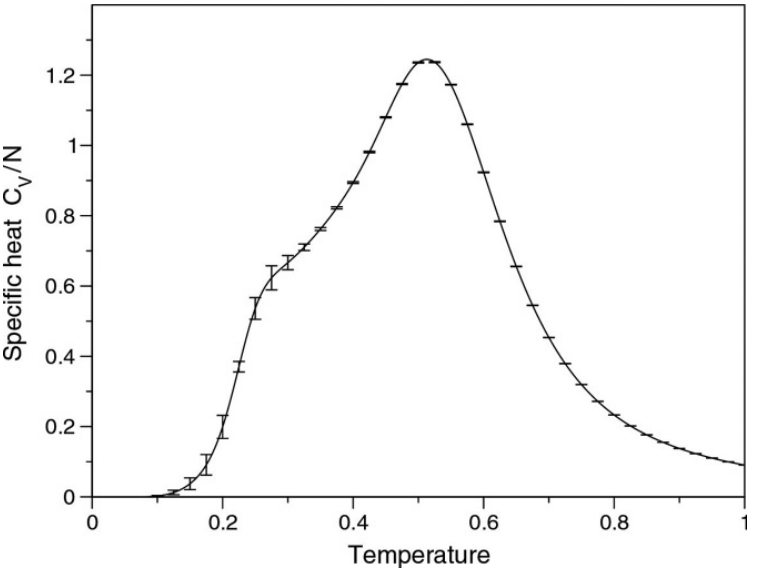

Fig. 13.3 Specific heat of the 103mer HP model determined by Wang–Landau sampling. After Wüst and Landau (unpublished data).

that lower-lying states exist and remain to be discovered. This prediction was quickly shown to be true.

From the density of states it was possible to calculate the temperature dependence of the specific heat of the 103mer, and this is shown in Fig. 13.3. The specific heat shows a peak at higher temperatures caused by the collapse of the protein, and at lower temperature there is a shoulder that appears as the collapsed globule rearranges itself into the native state. This behavior is characteristic of what is seen in much more realistic protein models in the continuum.

13.5.3 Cell sorting

The sorting of a mixture of two types of biological cells has been studied using a modified version of the large state Potts model (Graner and Glazier, 1992). The model describes a collection of N cells by defining N degenerate spins $\sigma(i, j) = 1, 2, N$, where i, j identifies a lattice site. A cell σ consists of all sites in the lattice with spin a. A second variable is introduced, the cell 'type' τ, which may have different values, and there may be many cells of each type. A trial move then consists of attempting to change the spin value at a given site to that of one of its nearest neighbors. This modified Potts model Hamiltonian includes surface energies between neighboring cell types and an area constraint (since cells cannot disappear). The characteristic cell sorting behavior can be seen in Fig. 13.4. They found that long-distance cell movement led to sorting with a logarithmic increase in the length scale of homogeneous clusters with time. A recent parallel version of this algorithm permits large-scale simulations of cell morphogenesis with 10^7 or more cells (Chen *et al.*, 2007).

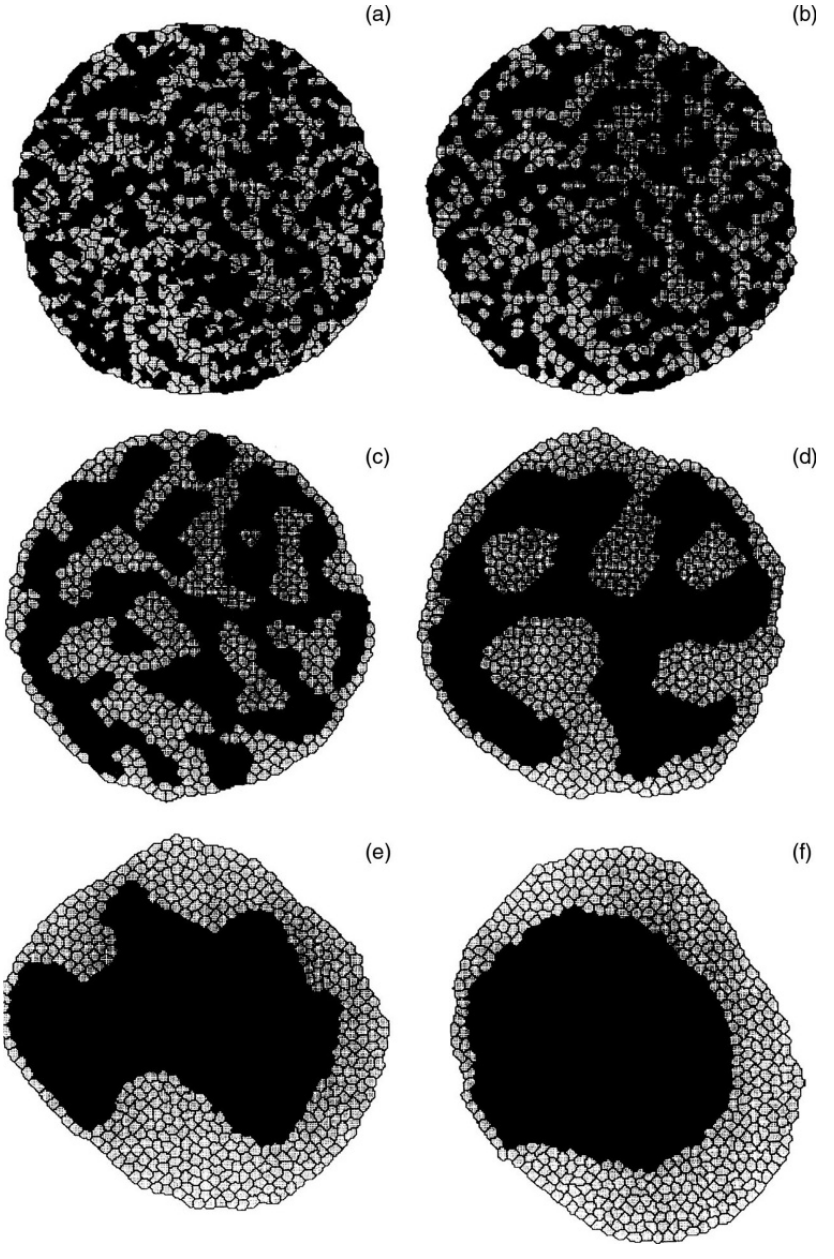

Fig. 13.4 Time dependence of cell sorting for two different cell types: (a) initial, randomly assigned cell type; (b) 1 MCS; (c) 100 MCS; (d) 1000 MCS; (e) 4000 MCS; (f) 10 000 MCS. From Graner and Glazier (1992).

13.6 BIOLOGY

Monte Carlo methods have found their way into use in a variety of ways in modern biology in addition to the protein folding problem. To whet the reader's appetite, we will describe just a few examples of the application to 'real' biological problems.

A relatively early example was the use of simulated annealing (Chapter 5) to order clones in a library with respect to their order along a chromosome

(Cuticchia *et al.*, 1992). Some initial order is chosen and the total distance between clones is calculated. Clones are then randomly interchanged so as to minimize the difference with respect to the true linking distance. The Metropolis algorithm is used with the difference in energy in a model in statistical physics translating to the difference in the total linking distance. Temperature is introduced as a fictitious variable, and is increased and then decreased in the same manner as for spin glasses. Both a simulated chromosome as well as one real genome could be easily reconstructed using a VAX 2000 (a computer which is quite slow by today's standards).

Within the context of functional genomics, the determination of the topology and kinetics of a living cell's full biochemical and gene regulatory circuitry is a major challenge. Monte Carlo methods have now been devised to walk through the parameter space of possible chemical reaction networks to identify an ensemble of deterministic kinetics models with rate constants that are consistent with RNA and protein profiling data (Battogtokh *et al.*, 2002; Yu *et al.*, 2007). The initial rate constants are chosen randomly and a Metropolis method is then used to adjust them so as to improve a figure of merit that describes the consistency with the data. A large number of different sets of choices, i.e. an ensemble, fulfill the desired conditions. The method was successfully applied to *Neurospora crassa* and used to identify an ensemble of oscillating network models that were quantitatively consistent with RNA and protein profiling data on the biological clock of the system.

A quite different kind of application of Monte Carlo methods lies at the intersection between biology, medicine, and nuclear engineering. Monte Carlo transport codes, e.g. the MCNP4B transport code that was developed for reactor design (see Section 3.5), can be used to evaluate neutron doses in radiotherapy treatments. Richardson and Dubeau (2003) used this approach to study the age-dependent steady-state dose from beta decay of ^{14}C to marrow and bone. The simulation assumes that the ^{14}C beta particles originate from uniformly distributed point sources in the fat cells in marrow and models the bone cavities as spherical cavities with 10 μm thick walls. Different parameters were used to model the bone volume and fat fraction, and they concluded that the increase in the fat fraction of the marrow with age rather than the bone morphology was the dominant factor governing the ^{14}C dose to marrow and bone surface. While the details are certainly dependent upon explicit choices that are made for, e.g., fat cell distribution, bone geometry, thickness, etc., it is clear that Monte Carlo simulations can provide a view that is impossible to obtain by analytic means in such complex, biological environments.

13.7 MATHEMATICS/STATISTICS

There has been interest in the mathematics community about various forms of Monte Carlo algorithms with the early work by Hastings (1970) on Markov Chain Monte Carlo. Of course, the nomenclature is somewhat different in mathematics, but many of the same questions remain to be answered. (For

example, the classic approach is referred to as the 'Metropolis–Hastings' algorithm, and the non-linear relaxation time is termed the 'burn in' time.) In a recent article, Hitchcock (2003) described the history of the 'infiltration' of Monte Carlo simulations into the statistics community. (The article also referred to the first serious Monte Carlo 'experiment' of which we are aware: in 1777, Georges Louis Comte de Buffon attempted to estimate the value of π by repeatedly throwing a needle onto a grid of parallel lines and measuring how often the needle landed on a line.) For a nice overview of Monte Carlo methods with a distinctly statistics flavor (Gibbs sampler, Bayesian inference, parametric statistical modeling, etc.), see Liu (2001). Recently, Mustonen and Rajesh (2003) have used Wang–Landau sampling (see Section 7.8) to solve a problem in combinatorial number theory. Simulations allowed the treatment of integers that were 40 times larger than those amenable to study by exact enumeration. A more general description of the use of Monte Carlo simulations in statistics can be found in the book by Gilks *et al.* (1996).

The HP model (see Section 13.5) has also become a topic of substantial interest in the statistics community, and there are now high quality results that have been obtained using a variety of innovative Monte Carlo techniques (Kou *et al.*, 2006; Zhang *et al.*, 2007). This is another example of how Monte Carlo is aiding cross-fertilization between disciplines.

13.8 SOCIOPHYSICS

It has become somewhat fashionable to use Monte Carlo simulations to attempt to predict, or at least understand, sociological phenomena. As a simple example, Stauffer (2002) has described the use of the Sznajd model (Sznajd-Weron and Sznajd, 2000) as a simple approach to studying how opinions are changed by contact between different individuals. Each site of a lattice carries an Ising spin, i.e. can be up or down, and two parallel neighbors 'convince' their neighbors to have the same direction. One can begin with different distributions (possibly random) of up and down spins and, of course, there may be modification of the rules used to determine how neighbors are 'convinced', including spins that cannot be convinced at all. Whether or not this model, or similar variants, can truly add to our understanding of social behavior, including voter opinions, is arguably uncertain. A summary of recent simulations in sociophysics, along with some specific examples that have an emphasis on hierarchical and consensus models, has been provided by Stauffer (2003) and Stauffer *et al.* (2006).

13.9 ECONOPHYSICS

Over the past 25 years numerous physicists have entered the world of finance in substantial number, but much of the work that is done in that area seems to have little relationship to physics. Here we adopt the term 'econophysics' to have the broad meaning that Stanley *et al.* (1999) gave to the phrase:

'Econophysics describes work being done by physicists in which financial and economic systems are treated as complex systems.' Indeed, power laws and universal behavior, two of the hallmarks of statistical physics, can be identified in analyses of existing financial data. For a general overview of the nature of the state of 'econophysics' we direct the interested reader to the proceedings of the 2002 International Econophysics Conference (Stanley *et al.*, 2003).

A number of research studies have attempted to directly apply some of the lessons learned in the earlier part of this textbook to problems of economics. For example, a modification of the Cont–Bouchaud model (Cont and Bouchard, 2000; Stauffer, 2001) identified clusters of parallel spins in an Ising square lattice as groups of traders acting together within the context of a particular stock market model. They produced their data by performing standard Metropolis simulations but emphasized finite size effects by fixing spins at the upper and lower system boundaries. Early simulations treated this as a percolation model (see Chapter 3); consequently there were no correlations between traders. By averaging over results for all temperatures they were able to get return distributions that were in reasonable agreement with reality.

Hammel and Paul (2002) performed simple sampling Monte Carlo simulations of a trader-based model for stock market dynamics and found a 'stationary state' of the model. The model used differs quite substantially from the Ising model and attempts to represent, at least in some simple way, the 'dynamics' expected on the trading floor. (Attempts to describe the behavior by a simple reaction-diffusion equation produced results that were incompatible with market phenomenology.) The model used by Hammel and Paul (2002) includes equal populations of buyers and sellers which perform random walks on discrete prices that they bid and ask. The price idea of a trader changes with a given probability that is one of the input parameters. The size of the change in price idea depends upon recent history, and whenever a trade occurs the buyer and seller exchange identities. They found a log-normal distribution of bid and asked prices relative to the current market price and determined that time dependence (in Monte Carlo time) for the parameters that characterized the distribution.

While intriguing in many ways, the simulations that have been performed using models of statistical physics may prove to be little more than academic exercises. They could nonetheless eventually lead to a better understanding of the complex issues involved in real world economics and finance. Of course, simulations of more sophisticated models are already finding direct application in real investment situations. As a tangible example we cite the case of a major investment bank that advertised guidance under the general rubric of 'Monte Carlo for the Masses' and offered a yearly subscription to a modeling program.

13.10 'TRAFFIC' SIMULATIONS

The use of computers to study automobile traffic is far from new, but the influence of Monte Carlo simulations in areas emanating from a more liberal

interpretation of the word 'traffic' are becoming plentiful. Of course, simulations of automobile traffic flow are probably best known in the statistical physics community within the context of the Nagel–Schreckenberg model (Nagel and Schreckenberg, 1992). The model introduces a number of vehicles, N_{veh}, moving in the same directions with different, discrete values of the speed. At each time step the arrangement of the vehicles is updated, in parallel, including acceleration, deceleration (due to other vehicles), randomization of speed, and a stepwise forward motion of the vehicles. Depending on the values of the parameters used, free-flowing traffic, traffic jams, or the coexistence of the two may be found. (For a more complete treatment of this subject, see Chowdury *et al*. (2000) and references therein.) Direct simulation Monte Carlo simulations have also been used to study vehicular traffic flow (Waldeer, 2003). Flow is modeled by a Boltzmann-like master equation and different possible interaction profiles and algorithms are evaluated. In several cases comparison could be made with analytic theory, with good agreement resulting; and, using a two velocity dependent distance threshold, comparison could be made with measured data. Agreement is qualitative at medium and high densities, but at low densities non-interacting driver behavior is not taken into account with sufficient detail.

An intriguing simulational study of a traffic related problem was made by Tang and Ong (1988) who examined the damping of road noise by foliage lining the streets of Singapore. A simple model was constructed that included both the reflection of noise between the buildings on opposite sides of the road and noise attenuation by the leaf canopy lining the road. Sound waves are regarded as a shower of particles and both reflection and absorption might occur in the canopy. Both test and measured noise spectra could be used and different approximations were used for leaf vibrational resonance modes. (The characteristics of the leaf canopy were chosen to closely mimic that of the giant angsana trees normally found lining the roads in Singapore.) They followed up to 10^6 randomly directed sound waves in determining overall reflection and attenuation of noise. The conclusion that they reached was that the trees do not substantially affect traffic noise at ground level because the reflection dominates, but at higher building stories the leaf canopy does reduce traffic noise, particularly at the high end of the spectrum.

Monte Carlo simulations have also been applied to the examination of different kinds of airport traffic. The simulation of airplane takeoffs and (randomized) landings for a mixture of different kinds of aircraft was used to help optimize the scheduling patterns (Pitfield and Jerrard, 1999). This approach was applied to Rome Fiumicino International Airport, and by segregating the landings by aircraft type, capacity could be increased to the point that airport expansion could be shelved. Pitfield *et al*. (1998) also applied Monte Carlo simulation to look for potentially conflicting ground movements at a new (Seoul) airport. Their goal was to use random events, drawn from a 'realistic' cumulative distribution, to simulate the movement of aircraft on the ground, both for takeoffs and landings. The goal was to determine the amount of conflict between towed aircraft and departing and arriving flights. The results showed

that neither the number of conflicts nor the holding time was very high for the planned pattern and that more costly alternatives were unnecessary.

A somewhat related but quite different 'traffic' problem relates to flow of electricity through a telephone company electronic switching system whose components were subject to failure. Monte Carlo simulations were already playing a role in this area several decades ago. For example, Malec (1971) performed simulations of a simple 'Tri-switch' (redundant) model to assess the likelihood of a system failure assuming a given distribution of random failure of individual components and availability of only a single repairman. Multiple kinds of random number distributions were chosen for comparison including uniform, exponential, normal, and log-normal (see Section 2.2.5 for a description of how to generate different types of random number distributions). He was able to estimate the mean time to system outage as a function of the mean time to repair of the individual components. Although a large number of trials was not made, the data were already adequate to show that simulations were useful as predictive tools and for testing proposed design changes.

13.11 MEDICINE

Understanding gene expression data from newly developed gene chips, with the subsequent potential benefits to medical technology, is a daunting task. To overcome the inherent complexity of the data analysis 'superparamagnetic clustering techniques' that exploit the properties of phase transitions in disordered Potts ferromagnets have been developed. A quantitative measure of topological inhomogeneity, Λ, was developed by Agrawal (2002) and was used to determine the interaction neighborhood from colon cancer data (Agrawal and Domany, 2003). This information was used to construct a $q = 20$ Potts model that was then studied using Monte Carlo simulations. They found that the width of the superparamagnetic domain coincides with the minimum in Λ. The clustering solutions obtained by superparamagnetic clustering are robust against noise inherent in the data.

Another area in medicine in which Monte Carlo simulations are playing a significant role is in the development of physics research tools for medical use. One such example is in the design of medical imaging devices for emission tomography. Assié *et al.* (2004) provide an overview of the validation of Monte Carlo generated data against real data obtained from PET (positron emission tomography) and SPECT (single photon emission computerized tomography) cameras. Clearly, in this area Monte Carlo is useful only if it can produce quantitatively reliable data under quite realistic circumstances. Monte Carlo simulations have also been developed for the assessment of radiotherapy distribution (Leal *et al.*, 2004). Complete with its own graphical user interface, the program runs on a Beowulf cluster using PVM for parallelization.

A more recently developed Maplet (programmed with Maple 10) running on a PC can now be used to simulate the transport of radiation in biological tissues (Yip and Carvalho, 2007).

The cell sorting approach described in Section 13.5.3 has been adapted to form a simple model of choroidal neovascularization in the eye which is then studied with Monte Carlo simulations (Shirinifard *et al.*, 2012). This process leads to macular degeneration which causes blindness, a medical condition that is obviously of significance but which cannot yet be studied in full atomistic detail. But the combination of coarse grained model building and Monte Carlo simulation is beginning to shed light on the processes involved.

13.12 NETWORKS: WHAT CONNECTIONS REALLY MATTER?

Many collections of objects, either man-made or naturally occurring, are connected together in what sometimes appears to be a rather chaotic manner. Over the past several decades many studies have originated in different disciplines, but they can now be grouped together under the general rubric of 'networks'. There appears to be a certain commonality whether the 'object' of the study is social interaction or data transfer between nodes in a massively parallel computer, so we have chosen to group all such efforts together in a single sub-section.

Broadly speaking, we can place Monte Carlo studies involving networks into two different classes. One set of studies encompasses 'traditional' simulations of magnetic systems, e.g. the Ising model, on a complex interaction topology, e.g. small world networks (Watts and Strogatz, 1998). A second sub-area is the study of network topologies and their characterization in their own right.

The thermodynamic behavior of a number of different magnetic models has been studied on small world networks. In these models, bonds on a regular lattice are rewired on a regular lattice with a probability p, and p can be varied to look for changes in characteristic behavior. Simple examples include Ising and XY-models. Guclu *et al.* (2006) even drew a comparison with the synchronization problem in distributed computing and found KPZ-like kinetic roughening of the synchronization landscape.

Because of advances in technology, vast amounts of data have now become available for study, e.g. mobile phone records, and the connectivity between individual nodes allows the researcher to construct a network. (Such data are kept anonymous to preserve personal privacy.) The important question that then arises is 'what really matters' in the structure of the network? Thus, most early work focused on the study of existing data; more recently, a number of models have been proposed that can then be simulated using Monte Carlo methods. Monte Carlo construction of networks based upon existing cell phone data (Kumpula *et al.*, 2007; Onnela *et al.*, 2007) or upon 'known' community structure (Newman and Girvan, 2004) have allowed the first simulational analysis of social networks. Since real networks often depend upon many uncontrollable features, it is likely that Monte Carlo simulations of well defined models will play an increasingly valuable role in the future.

13.13 FINANCE

Monte Carlo methods have also found their way into practical application in finance. Here we are no longer talking about 'universal laws' but rather about the very practical question of 'how do we make a profit'? In many cases this means optimizing options pricing, in particular derivatives pricing, but in a finite amount of time so that the result can actually be used in the marketplace. For a general overview, see Jäckel (2002) or McLeish (2005).

A glance at any newspaper, where a time series of the financial value of some investment on the stock market is depicted, reveals that such investment values undergo large and seemingly random stochastic fluctuations. Clearly, Monte Carlo methods can be used to simulate large classes of stochastic processes, described by some underlying master equations; it is, hence, plausible that Monte Carlo simulations of fluctuations in the prices of financial instruments that are traded should be useful to quantify market rules. Risk factors that need to be taken into account include foreign currency exchange rates, interest rates, and prices of commodities and stocks. The basic assumption in the mathematical modeling of the time evolution of a 'risk factor' $S(t)$ is written qualitatively as (Deutsch, 2002)

$$dS(t) = a(S, t)dt + b\,(S, t)\,X\sqrt{dt}, \tag{13.1}$$

where dt is a time increment, $a(S, t)$ is the drift rate, X is a normally distributed random variable, and the scale for the fluctuations is set by the so-called 'volatility' of the process $b(S, t)$. Of course, in reality, the time evolution of many coupled risk factors must be considered. Therefore, the practical usefulness of analytical approximations based on Eqn. (13.1) describing the time evolution of the value of financial investments, such as the famous Black–Scholes differential equation, are somewhat limited, and it is useful to complement them by extensive simulations of models that describe how the risk factors are interrelated. Although there is still need for much research (note that there is evidence that large fluctuations in the stock market do not follow a normal distribution, unlike the above assumption, etc.), Monte Carlo methods are now accepted and widely used as a tool in the management of financial risks of various investments.

Monte Carlo simulations in finance differ from Monte Carlo simulations in physics in two important aspects: (i) while in physics, the error bars of a result can be made smaller and smaller by suitably increasing the statistical effort, this often is not possible in actual applications to the evaluation of risks of financial investments, where, e.g., an answer needs to be given to a client after a short time; (ii) while most models simulated in physics use, in some way or another, well established laws of nature (such as conservation laws, exact relations of statistical thermodynamics, etc.), in economics, or finance, much less is known about basic underlying 'laws', and hence the models that can be studied are highly phenomenological.

On a more mundane level, Monte Carlo simulations have already been incorporated into various commercial packages that are designed for investment risk assessment and to be used by individuals with modest investment portfolios. These programs, or applets, are intended for use on PCs and, in some cases, to work with standard PC software such as Excel.

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