4. Some Important Recent Developments of the Monte Carlo Methodology

4.1 Introduction

Roughly at the time (1987) when the manuscript for the first three chapters of the present book was completed, several breakthroughs occurred. They had a profound influence on the scope of Monte Carlo simulations in statistical physics, particularly for the study of phase transitions in lattice models.

The first of these remarkable developments is the invention of the "cluster algorithms" [4.1-54] that reduce (or eliminate completely) the problem of "critical slowing down" (divergence of relaxation times near the critical point, see e.g. (2.3.26, 27) [2.59]) from which the single spin-flip algorithms suffer, since the increase of relaxation time means a dramatic increase of statistical errors; see, e.g., (2.3.28). The original version [4.1], proposed for the Ising model, is based on the mapping [4.55] between Potts models [2.106] and percolation [2.60], but meanwhile extensions exist to a wide variety of models, including also isotropic magnets [4.7, 9] and various quantum spin systems [4.54]. In this chapter, only the original version (for Ising and Potts problems) will be considered, however. Here we briefly outline the main physical idea: critical slowing down in the kinetic single-spin-flip Ising model [2.12] can be attributed to the fact that the long-range critical spin correlations correspond to the occurrence of large clusters of correlated spins. It takes a very long time until such a cluster disintegrates and finally disappears by many subsequent single spin flips. However, if the basic move is not a single spin flip but the overturning of a whole cluster, the cluster pattern changes rapidly and one thus can move much faster through phase space, even close to the critical point. Of course, the "art" is to construct the clusters that are considered for flipping such that at the same time one has a high acceptance rate for such a move, even if the cluster is very large, and that one destroys physical correlations by the successive action of the algorithm. There is no general recipe for how one can construct such an algorithm for a particular model – in some cases, where critical slowing down is very dramatic, like in spin glasses [2.41], intensive searches for efficient cluster algorithms have been made but have so far failed.

Another line of research, based on the idea that Monte Carlo updates should reduce the problem of critical slowing down if they operate on all length scales simultaneously, not only on the length scale of the lattice spa-
cing as the single spin-flip-type algorithms do, is known as “multigrid Monte Carlo”[4.56–61]. However, often the asymptotic behavior does not change qualitatively: i.e., the dynamic exponent $z$ in the relation between relaxation time $\tau$ and linear dimension $L$, $\tau \propto L^z$ (2.3.27), remains the same as in the single spin-flip-type algorithm. But the constant of proportionality in this relation may get markedly smaller (a decrease by a factor of 10 was often reported [4.60]). Nevertheless, we shall not deal with this approach here further, noting that it also lacks another advantage that the “cluster algorithms” have, namely that the latter yield in a very natural way “improved estimators” for various quantities: expressing quantities like susceptibilities [4.7, 96], pair correlation functions [4.7, 25], fourth-order cumulants [4.62], etc. in terms of “clusters” rather than using the original formulation in terms of spins, one exploits the fact that there are no correlations between different clusters, and hence the statistical noise is reduced.

The second important development that we shall discuss is the reanimation [4.63] of the old idea [4.64, 65] of “reweighting”: from a simulation at a single state point (characterized in an Ising model by choice of temperature $T$ and magnetic field $H$) one does not gain information on properties precisely at that point only, but also in the neighboring region. Extensions and variations of this concept are indeed very promising and powerful [4.46, 66–69]. The simplest approach, the “single histogram method” [4.63], starts from the observation that the distribution of the energy $P(E,T)$ at temperature $T$ can be obtained from the distribution $P(E,T_o)$ at a neighboring temperature $T_o$ by

$$P(E,T) = P(E,T_o) \exp[-(1/T - 1/T_o)E/k_B]/\sum_E P(E,T_o) \times \exp[-(1/T - 1/T_o)E/k_B].$$

(4.1.1)

Of course, in this simple form the method is useful only either for rather small systems [where $P(E,T_o)$ is sufficiently broad since the width of the distribution scales with $L^{-d/2}$, assuming a $d$-dimensional cubic box of linear dimension $L$ as the simulation volume] or at a critical point, as first recognized by Ferrenberg and Swendsen [4.63]: due to the critical fluctuations, the distribution is broadened over a width of order $L^{-1/\nu}$, where $\nu$ is the critical exponent of the correlation length. Since in a finite-size scaling analysis, see (2.3.20, 21), the region of interest is of the order of $|1 - T/T_c| \propto L^{-1/\nu}$, the region of interest in finite-size scaling is of the same order as the region in temperature accessible for reweighting. Of course, there still is a problem in the wings of the distribution, where due to reweighting statistical errors may get greatly magnified, but this problem is eased by the combined use of several histograms at suitably chosen neighboring temperatures (or other control parameters), the so-called “multiple histogram extrapolation” [4.46, 66, 70].

Particularly interesting are also reweighting schemes built into the simulation procedure: again this is an old idea under the name of “umbrella