

15 Outlook

Within this book we have attempted to elucidate the essential features of Monte Carlo simulations and their application to problems in statistical physics. We have attempted to give the reader practical advice as well as to present theoretically based background for the methodology of the simulations as well as the tools of analysis. New Monte Carlo methods will be devised and will be used with more powerful computers, but we believe that the advice given to the reader in Section 4.8 will remain valid.

In general terms we can expect that progress in Monte Carlo studies in the future will take place along two different routes. First, there will be a continued advancement towards ultra high resolution studies of relatively simple models in which critical temperatures and exponents, phase boundaries, etc., will be examined with increasing precision and accuracy. As a consequence, high numerical resolution as well as the physical interpretation of simulational results may well provide hints to the theorist who is interested in analytic investigation. On the other hand, we expect that there will be a tendency to increase the examination of much more complicated models which provide a better approximation to physical materials. As the general area of materials science blossoms, we anticipate that Monte Carlo methods will be used to probe the often complex behavior of real materials. This is a challenge indeed, since there are usually phenomena which are occurring at different length and time scales. As a result, it will not be surprising if multiscale methods are developed and Monte Carlo methods will be used within multiple regions of length and time scales. We encourage the reader to think of new problems which are amenable to Monte Carlo simulation but which have not yet been approached with this method.

Lastly, it is likely that an enhanced understanding of the significance of numerical results can be obtained using techniques of scientific visualization. The general trend in Monte Carlo simulations is to ever larger systems studied for longer and longer times. The mere interpretation of the data is becoming a problem of increasing magnitude, and visual techniques for probing the system (again over different scales of time and length) must be developed. Coarse-graining techniques can be used to clarify features of the results which are not immediately obvious from inspection of columns of numbers. ‘Windows’ of various size can be used to scan the system looking for patterns which develop

in both space and time; and the development of such methods may well profit from interaction with computer science.

Clearly improved computer performance is moving swiftly in the direction of parallel computing. Because of the inherent complexity of message passing, it is likely that we shall see the development of hybrid computers in which large arrays of symmetric (shared memory) multiprocessors appear. (Until much higher speeds are achieved on the Internet, it is unlikely that non-local assemblies of machines will prove useful for the majority of Monte Carlo simulations.) We must continue to examine the algorithms and codes which are used for Monte Carlo simulations to insure that they remain well suited to the available computational resources.

We strongly believe that the utility of Monte Carlo simulations will continue to grow quite rapidly, but the directions may not always be predictable. We hope that the material in this book will prove useful to the reader who wanders into unfamiliar scientific territory and must be able to create new tools instead of merely copying those that can be found in many places in the literature. If so, our efforts in developing this textbook will have been worthwhile.