Preface

The dawn of the modern computer age brought about a revolution in our methods for addressing problems in physics and in the physical sciences in general. There are two aspects to this revolution.

The first is quantitative. Problems can be treated now using classical methods that would have been ineffective before. In cases where decades were spent on the development of approximation schemes to allow complex physics problems to be reduced to simplified (often oversimplified) models which could be envisioned and calculated, it is now possible to solve the complex problem directly. This does not mean that the analytic methods and approximations should be discarded. On the contrary, in many cases the numerical technique functions best if it is provided with a good starting "guess". A good approximate starting solution may be essential to timely completion of the algorithm. In this sense computer methods may often be regarded as a modern "perturbation theory".

The second facet of the revolution is qualitative. There are methods now being used for which the formulation itself did not predate the existence of rapid calculating devices. This remark applies to most of the field of Monte Carlo computation (although the subject of probability distributions, on which it is based, existed long before) but especially to the rapidly developing area of the Monte Carlo Green's Function method for treating several and many-body problems. This method is leading into new conceptual areas such as the representation of multi-dimensional functions by a collection of points. It would seem that Monte Carlo provides the only practical technique for the numerical treatment of such functions and the development of techniques for their manipulation and use provide an ongoing challenge. The fact that many of the Monte Carlo techniques are still under development should not prevent workers in all areas of the physical sciences from making use of these methods today.

While many of the algorithms used in this book date from the last century (or even well before) the majority have been developed within the last 50 years and many within the last two decades. It is easy to imagine that this explosion of intellectual activity in the solution of problems in science will be regarded by historians in the same light as other great breakthroughs in science.

The distribution of subjects is quite varied corresponding to the eclectic nature of computational physics. The first eight chapters treat techniques of value to many fields of science, while the final sections deal primarily with the solutions to problems in quantum mechanics taken from the recent literature.

Chapter 4 may seem disjunct to some but, in fact, is an essential part of the *present endeavor to present a fairly complete picture of computational science at the student level. In order to obtain the maximum result in any field it is necessary to adapt the methods used to the facilities available, and* vice versa. *The relationship between the solutions of problems in physics and computers is no exception to this rule. The present (very conscious) movement is to create systems where the programmer can run the code on any machine which supports the appropriate language. This aspect of portability is certainly to be desired. However, to write a program on a scalar machine and run it on a vector machine without realizing that some simple changes in the coding would lead to an order of magnitude increase in speed is failing to take advantage of the facility. This aspect goes much deeper, however, in that the techniques for the solution of scientific problems are varied, so that the machine architecture will (or at least should) influence the fundamental representation of our resolution of problems in physics, and indeed our approach to intellectual understanding itself.*

This book is intended for first-year graduate students (or seniors) as a preparation for research in the physical sciences (especially physics) with an orientation toward computational aspects. Indeed, there are few fields of science today which do not require a certain degree of expertise in the use of computers to solve the complex mathematical problems which arise.

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