Preface

The primary motivation for new developments in Monte Carlo methods is the fact that they are widely used for those problems for which deterministic algorithms hopelessly break down. An important reason for this is that Monte Carlo methods do not require additional regularity of the problem's initial data. The main problem with the deterministic algorithms is that they normally need some additional approximation procedure, requiring additional regularity. Monte Carlo algorithms do not need such procedures. Nevertheless, if one can exploit the existing smoothness of the input data then normally Monte Carlo methods have a better convergence rate than the deterministic methods. At the same time, dealing with Monte Carlo algorithms one has to accept the fact that the result of the computation can be close to the true value only with a certain probability. Such a setting may not be acceptable if one needs a guaranteed accuracy or strictly reliable results. But in most cases it is reasonable to accept an error estimate with a probability smaller than 1. In fact, we shall see that this is a price paid by Monte Carlo methods to increase their convergence rate. The better convergence rate for Monte Carlo algorithms is reached with a given probability, so the advantage of Monte Carlo algorithms is a matter of definition of the probability error.

The second important motivation is that Monte Carlo is efficient in dealing with large and very large computational problems: multidimensional integration, very large linear algebra problems, integro-differential equations of high dimensions, boundary-value problems for differential equations in domains with complicated boundaries, simulation of turbulent flows, studying of chaotic structures, etc.. At the same time it is important to study applicability and acceleration analysis of Monte Carlo algorithms both theoretically and experimentally. Obviously the performance analysis of algorithms for people dealing with large-scale problems is a very important issue.

The third motivation for new developments of Monte Carlo methods is that they are very efficient when parallel processors or parallel computers are available. The reason for this is because Monte Carlo algorithms are inherently parallel and have minimum dependency. In addition, they are also naturally vectorizable when powerful vector processors are used. At the same time, the problem of parallelization of the Monte Carlo algorithms is not a trivial task because different kinds of parallelization can be used. To find the most efficient parallelization in order to obtain high speed-up of the algorithm is an extremely important practical problem in scientific computing. Another very important issue is the *scalability* of the algorithms. Scalability is a desirable property of algorithms that indicates their ability to handle growing amounts of computational work on systems with increasing number of processing nodes. With the latest developments of distributed and Grid computing during last ten years there is a serious motivation to prepare scalable large-scale Monte Carlo computational models as Grid applications.

One of most surprising findings is the absence of a systematic guide to Monte Carlo methods for applied scientists. This book differs from other existing Monte Carlo books by focusing on performance analysis of the algorithms and demonstrating some existing large scale applications in semiconductor device modeling. The reader will find description of some basic Monte Carlo algorithms as well as numerical results of implementations. Nevertheless, I found it important to give some known fundamental facts about Monte Carlo methods to help readers who want to know a little bit more about the theory. I also decided to include some exercises specially created for students participating in the course of *"Stochastic Methods and Algorithms for Computational Science"* at the University of Reading, UK. My experience working with students studying stochastic methods shows that the exercises chosen help in understanding the nature of Monte Carlo methods.

This book is primary addressed to applied scientists and students from Computer Science, Physics, Biology and Environmental Sciences dealing with Monte Carlo methods.

I. Dimov