Malvin H. Kalos, Paula A. Whitlock

Monte Carlo Methods

Second Revised and Enlarged Edition

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Monte Carlo Methods

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Library of Congress Card No.: applied for

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

Bibliographic information published by the Deutsche Nationalbibliothek
Die Deutsche Nationalbibliothek lists this publication in the Deutsche National-bibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de

Typesetting Laserwords Private Ltd, Chennai, India
Printing betz-druck GmbH, Darmstadt
Bookbinding Litges & Dopf GmbH, Heppenheim

Printed in the Federal Republic of Germany
Printed on acid-free paper

ISBN: 978-3-527-40760-6

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Preface to the Second Edition

We began our preface to the first edition with the sentence, ''This book has had a long gestation period.'' The gestation of our second edition has been equally long.

In a sense, more has changed in the last twenty-two years in the theory and practice of Monte Carlo methods than in the twenty-two years before that. Tremendous strides have been made in the development of new techniques and applications. This is of course primarily a testament to the power of the methods and the breadth of their applicability, but it is also a testament to the breathtaking evolution of computing power which has made possible much wider and deeper experimentation and studies. More computing power enables more challenging applications, which exposes the need for more effective methods. In particular, the appearance of massively parallel computers – with as many as 200 000 processors – and for which many Monte Carlo calculations are well suited, has accelerated the evolution.

We have also seen new fields – such as financial computing – for which Monte Carlo methods are an essential tool.

As with almost all intellectual efforts, the synergy between widespread applicability and widespread interest has produced an exponential growth in new ideas.

It seemed to us that the aims of our previous edition – to give a short but unified approach to the field, limiting ourselves to applications in the physical sciences – is needed now as much, or perhaps more than before. We have corrected, revised, and extended the material in the first edition, and we have added new material on various quantum MC techniques, on Brownian motion, Poisson processes, simulated annealing, adaptive MC, and on quasi-MC.

As always, we have benefited from the collaboration and advice of many people. Our decades of friendship and research with Geoffrey Chester were essential and inspirational. We have continued to learn much from David Ceperley and Kevin Schmidt. In more recent times, MHK has had the privilege of working with Vasily Bulatov, Jaime Marian and Enrique Martinez,

Monte Carlo Methods. Second Edition. M.H. Kalos and P.A. Whitlock

ISBN: 978-3-527-40760-6

and long term interactions with Francesco Pederiva and Randolph Hood. PAW has enjoyed working with Marvin Bishop, Silvio Vitiello and Todor Gurov.

New York, July 2008

Malvin H. Kalos
Paula A. Whitlock

Preface to the First Edition

This book has had a long gestation period. While it simmered on the back burner, we pursued research in various aspects of Monte Carlo methods and their application to the simulation of physical systems. Out of this diversity we believe we see a basic way of looking at the field. It is unfortunate that some observers and even some specialists of Monte Carlo methods seem to regard Monte Carlo as a bag of miscellaneous devices. Often it comes across that way when applied. It is true that like many other technical endeavors, especially those with as intensely practical an outlook as Monte Carlo methods, a body of ingenious tricks has arisen, awaiting invocation as needed. But we believe – and hope that our book is successful in conveying both in a general and a practical sense – that there are a number of unifying ideas that underlie the study and use of good Monte Carlo methods.

The first is the importance of random walks – on the one hand as they occur in natural stochastic systems, and on the other, in their relation to integral and differential equations.

The other basic theme is that of variance reduction and, above all, of importance sampling as a technical means of achieving variance reduction. Importance sampling is the transformation of a basically straight-forward random sampling method by changing variables or, what amounts to the same thing, by changing the underlying probability distribution while leaving a required mean unchanged. It is by no means the only method, nor in particular cases the best method, for variance reduction. But it offers a coherent point of view about variance reduction. In important cases it offers the theoretical possibility of zero variance. The use of approximations to variance minimizing transformations is a powerful technique for the introduction of a priori knowledge based on experience or approximate solution of the problem at hand into a still exact numerical treatment based on Monte Carlo methods.

We believe that these ideas have stood us well in our research in radiation transport, in statistical physics, and in quantum mechanics and have served to unify them intellectually. We offer them to our readers in the hope that our point of view will make the theory and practice of Monte Carlo more interesting and more effective.

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This book is a distillation of some years of practice and thought about Monte Carlo methods. As such it has benefited from the ideas and suggestions of many friends and colleagues, too numerous to list in full. It would be remiss not to mention some of them, however, starting with Gerald Goertzel, who first introduced one of us (MHK) to the mixed joys of Monte Carlo on primitive computers, and to many of the basic ideas expressed in our book. Others from whom we have learned include particularly Harry Soodak, Eugene Troubetzkoy, Herbert Steinberg, Loup Verlet, Robert Coveyou, Phillip Mittleman, Herbert Goldstein, David Ceperley, Kevin Schmidt, and Geoffrey Chester. Notes of early lectures taken by Jacob Celnik were very helpful.

We gratefully acknowledge the help and encouragement of our many colleagues and students during the time this book was being written. We especially thank David Ceperley for giving the original lecture on which Chapter 5 was based. Youqin Zhong and John Halton gave numerous suggestions for improving earlier versions of the manuscript. We thank them for their efforts and hope the final book lives up to their expectations.

New York, August 1986

Malvin H. Kalos
Paula A. Whitlock

1
What is Monte Carlo?

1.1
Introduction

The name *Monte Carlo* was applied to a class of mathematical methods first used by scientists working on the development of nuclear weapons in Los Alamos in the 1940s. The essence of the method is the invention of games of chance whose behavior and outcome can be used to study some interesting phenomena. While there is no essential link to computers, the effectiveness of numerical or simulated gambling as a serious scientific pursuit is enormously enhanced by the availability of modern digital computers.

It is interesting, and may strike some as remarkable, that carrying out games of chance or random sampling will produce anything worthwhile. Indeed, some authors have claimed that Monte Carlo will never be a method of choice for other than rough estimates of numerical quantities.

Before asserting the contrary, we shall give a few examples of what we mean and do not mean by Monte Carlo calculations. Consider a circle and its circumscribed square. The ratio of the area of the circle to the area of the square is $\pi/4$. It is plausible that if points were placed at random in the square, the fraction $\pi/4$ would also lie inside the circle. If that is true (and we shall prove later that in a certain sense it is), then one could measure $\pi l4$ by putting a round cake pan with diameter L inside a square cake pan with side L and collecting rain in both. It is also possible to program a computer to generate random pairs of Cartesian coordinates to represent random points in the square and count the fraction that lies in the circle. This fraction as determined from many experiments should be close to $\pi/4$, and the fraction would be called an *estimate for* $\pi/4$. In 1 000 000 experiments, it is very likely (95% chance) that the number of points inside the circle would range between 784 600 and 786 200, yielding estimates of $\pi/4$ that are between 0.7846 and 0.7862, compared with the true value of 0.785398.

The example illustrates that random sampling may be used to solve a mathematical problem, in this case, evaluation of a definite integral,

$$I = \int_0^1 \int_0^{\sqrt{1-x^2}} \mathrm{d}x\, \mathrm{d}y. \tag{1.1}$$

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The answers obtained by the above procedure are statistical in nature and subject to the laws of chance. This aspect of Monte Carlo is a drawback, but not a fatal one, since one can determine how accurate the answer is, and obtain a more accurate answer, if needed, by conducting more experiments. Sometimes, in spite of the random character of the answer, it is the most accurate answer that can be obtained for a given investment of computer time. The determination of the value of π can of course be done faster and more accurately by non–Monte Carlo methods. In many dimensions, however, Monte Carlo methods are often the only effective means of evaluating integrals.

A second and complementary example of a Monte Carlo calculation is one that Ulam [1] cited in his autobiography. Suppose one wished to estimate the chances of winning at solitaire, assuming the deck is perfectly shuffled before laying out the cards. Once we have chosen a particular strategy for placing one pile of cards on another, the problem is a straightforward one in elementary probability theory, but is also a very tedious one. It would not be difficult to program a computer to randomize lists representing the 52 cards of a deck, prepare lists representing the different piles, and then simulate the playing of the game to completion. Observation over many repetitions would lead to a Monte Carlo estimate of the chance of success. This method would in fact be the easiest way of making any such estimate. We can regard the computer gambling as a faithful simulation of the real random process, namely, the card shuffling.

Nowadays, random numbers are used in many ways associated with computers. These include, for example, computer games and generation of synthetic data for testing. These are of course interesting, but not what we consider Monte Carlos, since they do not produce numerical results. A definition of a Monte Carlo method would be one that involves deliberate use of random numbers in a calculation that has the structure of a stochastic process. By *stochastic process*, we mean a sequence of states whose evolution is determined by random events. In a computer, these are generated by a deterministic algorithm that generates a sequence of pseudorandom numbers, which mimics the properties of truly random numbers.

A distinction is sometimes made between simulation and Monte Carlo. In this view, simulation is a rather direct transcription into computing terms of a natural stochastic process (as in the example of solitaire). Monte Carlo, by contrast, is the solution by probabilistic methods of nonprobabilistic problems (as in the example of π). The distinction is somewhat useful, but often impossible to maintain. The emission of radiation from atoms and its interaction with matter is an example of a natural stochastic process, since each event is to some degree unpredictable (Chapter 6). It lends itself very well to a rather straightforward stochastic simulation, but the average behavior of such radiations can also be described by mathematical equations whose numerical solution can be obtained using Monte Carlo methods. Indeed, the same computer code can be viewed simultaneously as a ''natural simulation'' or as a solution of the equations by random sampling. As we shall also see, the latter point of view

is essential in formulating efficient schemes. The main point we wish to stress here is that the same techniques directly yield both powerful and expressive simulation and powerful and efficient numerical methods for a wide class of problems.

We would like to return to the issue of whether Monte Carlo calculations are in fact worth carrying out. This can be answered in a very pragmatic way: many people use them and they have become an accepted part of scientific practice in many fields. The reasons do not always depend on pure computational economy. As in our solitaire example, convenience, ease, directness, and expressiveness of the method are important assets–increasingly so as pure computational power becomes cheaper. In addition, as asserted in discussing π, Monte Carlo methods are in fact computationally effective, compared with deterministic methods when treating many-dimensional problems. That is why partly their use is so widespread in operations research, in radiation transport (where problems up to seven dimensions must be dealt with), and especially in statistical physics and chemistry (where systems of thousands of particles can now be treated quite routinely). An exciting development in the past few years is the use of Monte Carlo methods to evaluate path integrals associated with field theories as in quantum chromodynamics.

1.2 Topics to be Covered

This book focuses on several major areas. The first topic addressed is a review of some simple probability ideas with emphasis on concepts central to Monte Carlo theory. For more rigorous information on probability theory, references to standard texts are given. Further chapters deal with the crucial question of how random events (or reasonable facsimiles) are programmed on a computer. Techniques for sampling complicated distributions are necessary for applications and, equally important, serve as a basis for illustrating the concepts of probability theory that are used throughout.

Then we consider quadratures in finite-dimensional spaces. Attention is paid to the important and interesting case of singular integrands, especially those for which the variance of a straightforward estimate does not exist so that the usual central limit theorems do not apply. These are cases for which variance reduction methods have an immediate and direct payoff. Also explored are quasi-Monte Carlo methods, which use low-discrepancy sequences that uniformly fill the multidimensional space.

Finally, applications of Monte Carlo methods are discussed. An introduction to current uses in statistical physics is given. The simulation of a simple example of radiation transport is developed, and this naturally leads to the solution of integral equations by Monte Carlo. The ideas are then used as a framework upon which a relationship between random walks and integral equations could be constructed and also to introduce the fundamentals of variance reduction for the simulation of random walks.

1.3 A Short History of Monte Carlo

Perhaps the earliest documented use of random sampling to find the solution to an integral is that of Comte de Buffon [2]. In 1777, he described the following experiment. A needle of length L is thrown at random onto a horizontal plane ruled with straight lines a distance $d(d > L)$ apart. What is the probability, P, that the needle will intersect one of these lines? Comte de Buffon performed the experiment of throwing the needle many times to determine P. He also carried out the mathematical analysis of the problem and showed that

$$P = \frac{2L}{\pi d}. \tag{1.2}$$

Some years later, Laplace [3] suggested that this idea could be used to evaluate π from throws of the needle. This is indeed a Monte Carlo determination of π; however, as in the first example of this chapter, the rate of convergence is slow. It is very much in the spirit of inverting a probabilistic result to get a stochastic computation. We would call it an *analog* computation nowadays [4].

Lord Kelvin [5] appears to have used random sampling to aid in evaluating some time integrals of the kinetic energy that appear in the kinetic theory of gases. His random sampling consisted of drawing numbered pieces of paper from a bowl. He worried about the bias introduced by insufficient mixing of the papers and by static electricity. Gossett (as ''Student'' [6]) used similar random sampling to assist in his discovery of the distribution of the correlation coefficient.

Many advances were being made in probability theory and the theory of random walks that would be used in the foundations of Monte Carlo theory. For example, Courant *et al.* [7] showed the equivalence of the behavior of certain random walks to solutions of certain partial differential equations. In the 1930s, Enrico Fermi made some numerical experiments that would now be called *Monte Carlo calculations*.[1)] In studying the behavior of the newly discovered neutron, he carried out sampling experiments about how a neutral particle might be expected to interact with condensed matter. These led to substantial physical insight and to the analytical theory of neutron diffusion and transport.

During the Second World War, the bringing together of such people as von Neumann, Fermi, Ulam, and Metropolis and the beginnings of modern digital computers gave a strong impetus to the advancement of Monte Carlo. In the late 1940s and early 1950s, there was a surge of interest. Papers appeared that described the new method and how it could be used to solve problems in statistical mechanics, radiation transport, economic modeling, and other fields [8–10]. Unfortunately, the computers of that time were not really adequate to carry out more than pilot studies in many areas. The later growth of computer power made

1) This information was communicated privately to MHK by Segre and Anderson.

it possible to carry through more and more ambitious calculations and to learn from failures.

At the same time, theoretical advances and putting into practice powerful error-reduction methods meant that applications advanced far faster than implied by sheer computing speed and memory size. The two most influential developments of that kind were the improvements in methods for the transport equation, especially reliable methods of "importance sampling" [11] and the invention of the algorithm of Metropolis *et al*. [12]. The resulting successes have borne out the optimistic expectations of the pioneers of the 1940s.

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2
A Bit of Probability

2.1
Random Events

As explained in Chapter 1, a Monte Carlo calculation is a numerical stochastic process, that is, a sequence of random events. While we shall not discuss the philosophical question of what random events are [1, 2], we shall assume that they do exist and that it is possible and useful to develop a computer program to produce effective equivalents of natural random events.

We must distinguish between elementary and composite events. Elementary events are those that we cannot (or do not choose to) analyze into still simpler events. Normally the result (head or tail) of flipping a coin or the result (1–6) of rolling a die are thought of as elementary events. In the case of a die, however, we might interest ourselves only in whether the number was even or odd, in which case there are two outcomes. Composite events are those defined from a number of elementary events. Examples include flipping a coin twice (with four outcomes, head–head, head–tail, tail–head, tail–tail). It is sometimes useful to talk of this pair as a single ''event''.

As far as one knows, random events occur in nature [3]; for example, the physical outcome of the scattering of an electron by an atom cannot be predicted with certainty. It is difficult to be sure which natural random events are ''elementary,'' although we will simplify models of physical processes by treating some events as elementary, and on that basis build up composite events. The distinction between an elementary random event and others depends on one's state of knowledge and the depth of the analysis given to the problem. Thus, one important kind of event, ''compound elastic scattering'' of neutrons by nuclei, is usefully analyzed for theoretical purposes into a sequence of three elementary random events. A Monte Carlo calculation might or might not make that distinction, depending on its intent. On the other hand, ''simple elastic scattering'' is most likely an elementary event; that is, it is not possible to distinguish more basic stages.

Given an elementary event with a countable set of discrete random outcomes, $E_1, E_2, \ldots, E_n, \ldots$, there is associated with each possible outcome E_k a number called a *probability*, p_k, which can lie between 0 and 1,

$$0 \leq p_k \leq 1.$$

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ISBN: 978-3-527-40760-6