中国科学院研究生教学丛书

计算物理学

COMPUTATIONAL PHYSICS

K.H.Hoffmann
M.Schreiber
编

科学出版社 Springer

影印版

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内 容 简 介

本书属于中国科学院推荐的研究生用原版教材。本书的主要内容为蒙特卡洛方法和分子动力学方法在固体、纳米材料、分形、化学反应及生物中的应用。书中介绍了目前常用的模型，并给出了简单的练习。

本书可供物理、化学、力学、生物相关专业的研究生阅读，亦可供相关领域的科技人员参考。

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《中国科学院研究生教学丛书》序

在21世纪曙光初露，中国科技、教育面临重大改革和蓬勃发展之际，《中国科学院研究生教学丛书》——这套凝聚了中国科学院新老科学家、研究生导师们多年心血的研究生教材面世了。相信这套丛书的出版，会在一定程度上缓解研究生教材不足的困难，对提高研究生教育质量起着积极的推动作用。

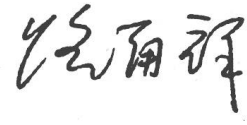
21世纪将是科学技术日新月异，迅猛发展的新世纪，科学技术将成为经济发展的最重要的资源和不竭的动力，成为经济和社会发展的首要推动力量。世界各国之间综合国力的竞争，实质上是科技实力的竞争。而一个国家科技实力的决定因素是它所拥有的科技人才的数量和质量。我国要想在21世纪顺利地实施“科教兴国”和“可持续发展”战略，实现邓小平同志规划的第三步战略目标——把我国建设成中等发达国家，关键在于培养造就一支数量宏大、素质优良、结构合理、有能力参与国际竞争与合作的科技大军。这是摆在我国高等教育面前的一项十分繁重而光荣的战略任务。

中国科学院作为我国自然科学与高新技术的综合研究与发展中心，在建院之初就明确了出成果出人才并举的办院宗旨，长期坚持走科研与教育相结合的道路，发挥了高级科技专家多、科研条件好、科研水平高的优势，结合科研工作，积极培养研究生；在出成果的同时，为国家培养了数以万计的研究生。当前，中国科学院正在按照江泽民同志关于中国科学院要努力建设好“三个基地”的指示，在建设具有国际先进水平的科学研究基地和促进高新技术产业发展基地的同时，加强研究生教育，努力建设好高级人

才培养基地，在肩负起发展我国科学技术及促进高新技术产业发展重任的同时，为国家源源不断地培养输送大批高级科技人才。

质量是研究生教育的生命，全面提高研究生培养质量是当前我国研究生教育的首要任务。研究生教材建设是提高研究生培养质量的一项重要的基础性工作。由于各种原因，目前我国研究生教材的建设滞后于研究生教育的发展。为了改变这种情况，中国科学院组织了一批在科学前沿工作，同时又具有相当教学经验的科学家撰写研究生教材，并以专项资金资助优秀的研究生教材的出版。希望通过数年努力，出版一套面向21世纪科技发展、体现中国科学院特色的高水平的研究生教学丛书。本丛书内容力求具有科学性、系统性和基础性，同时也兼顾前沿性，使阅读者不仅能获得相关学科的比较系统的科学基础知识，也能被引导进入当代科学研究的前沿。这套研究生教学丛书，不仅适合于在校研究生学习使用，也可釉作为高校教师和专业研究人员工作和学习的参考书。

“桃李不言，下自成蹊。”我相信，通过中国科学院一批科学家的辛勤耕耘，《中国科学院研究生教学丛书》将成为我国研究生教育园地的一丛鲜花，也将似润物春雨，滋养莘莘学子的心田，把他们引向科学的殿堂，不仅为科学院，也为全国研究生教育的发展作出重要贡献。



Preface

Computational physics is the field in physics that has experienced probably the most rapid growth in the last decade. With the advent of computers, a new way of studying the properties of physical models became available. One no longer has to make approximations in the analytical solutions of models to obtain closed forms, and interesting but intractable terms no longer have to be omitted from models right from the beginning of the modeling phase. Now, by employing methods of computational physics, complicated equations can be solved numerically, simulations allow the solution of hitherto untractable problems, and visualization techniques reveal the beauty of complex as well as simple models. Many new and exciting results have been obtained by numerical calculations and simulations of old and new models.

This book presents samples of many of the facets that constitute computational physics. Our aim is to cover a broad spectrum of topics, and we want to present a mixture ranging from simple introductory material including simple exercises to reports of serious applications. This is not meant to be an introductory textbook on computational physics, nor is it a proceedings volume of a research conference. This book instead provides the reader with an overview of computational physics, its basic methods, and its many areas of application. Our coauthors lead the reader into new and "hot" topics of research, but the presentation does not require any specific knowledge of the topics and methods. We hope that a reader who has gone through the book can appreciate the wealth of computational physics and is motivated to proceed with further reading.

The topics covered in this book cover a wide spectrum, with a coarse division into "Monte Carlo" type and "molecular dynamics" type chapters. We start with discussing random numbers and their generation on computers. Then these random numbers are used in a variety of applications, which center around "Monte Carlo methods". In these applications the focus is first on classical systems in physics, chemistry, biology, material science, and optimization. Then quantum-mechanical problems are investigated by Monte Carlo procedures. On our way we also encounter quantum chaos and fractal concepts, which are of increasing importance nowadays. The transition from "Monte Carlo" to "molecular dynamics" occurs in the chapter on hybrid methods, which combine elements of both. Then "molecular dynamics" methods are presented, with fluids and solids covered. A chapter on finite-element methods follows, and the two final chapters present principles of parallel computers and associated programming models.

As usual in physics, only active interaction with the matter at hand provides

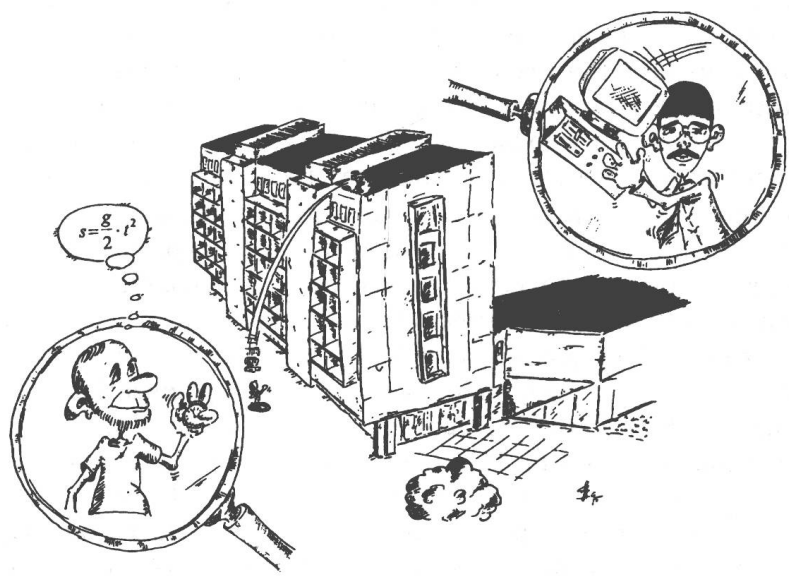
deep insight, and thus we include a diskette that contains sample programs and demonstrations to support the interaction of the reader with the text. The sample programs and demonstrations are selected to provide a glimpse of current research activities, even though the limitations of the available hardware and/or the limited patience of some readers might require a reduction in the dimensionality or size of the application. Also some exercises are included to further foster an active use of this book.

The material in this book is born out of lectures the authors gave at a Heraeus Summer School on computational physics at the Technical University in Chemnitz. The aim of the summer school was the same as the aim of this book: to give a sampler of the field. Due to the gracious funding by the Dr. Wilhelm Heinrich Heraeus and Else Heraeus Foundation the editors (see figure) were able to present two weeks of intense lecturing and "learning by doing" to more than 80 students. We would like to use this opportunity to thank the Heraeus Foundation for making the summer school and this book possible.

But most important we like to thank our coauthors for their contributions to this volume (as well as for their lectures at the summer school). We very much appreciate their willingness to contribute even under the severe limitations that their everyday teaching and research activities (and administrative duties) put on their time. And finally we thank Jörg Arndt, Peter Blaudeck, Andre Fachat, Göran Hanke, Karin Kumm, Sven Schubert, and Peter Späht for their technical help and Springer-Verlag for making this volume a reality.

Chemnitz, December 1995

Karl Heinz Hoffmann and *Michael Schreiber*



With this original answer to the question "How to measure the height of the building of the Institut für Physik in Chemnitz with a computer and a stop watch only?" the editors give a peculiar interpretation of the topic "Physics with a computer".

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Random Number Generation*

Dietrich Stauffer

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Abstract. The sad situation of random number generation is reviewed: there are no good random numbers. But life has to go on anyhow, and thus we explain how to produce reasonable random numbers efficiently, emphasizing multiplication with 16807 and the Kirkpatrick–Stoll R250 generator.

1 Introduction

Molecular Dynamics and Monte Carlo are the two standard simulation methods of the last decades. Monte Carlo simulations use random numbers to produce random fluctuations. Today, they are no longer made at the roulette tables in Monaco, but on computers. In the good old days, people printed tables of random numbers from which the user could read them off. This, of course, is somewhat tedious when simulating a square lattice of size one million times one million, today's world record [1]. About a decade ago, computer chips became available which produced random numbers through the thermal noise of the electrons, about one number per microsecond. This is not fast enough for many quality applications. Besides, for testing purposes we would like to have *reproducible* random numbers: when we have made a program more efficient without changing the results, we want to run it again and indeed get exactly the same results, and not just roughly the same, within the statistical errors of the Monte Carlo simulations. Moreover, when we switch from one computer to another, we would like again to get the same results: portability is important. Thus special chips using thermal noise are not suitable for this purpose.

Also, the random numbers should be produced quickly since Monte Carlo simulations consume lots of time and we never have enough of it. Thus we need efficient methods, and on many computers it is very slow to call a function or subroutine to produce one random number. Thus a good random number generator should be:

(1) random
(2) reproducible
(3) portable
(4) efficient

Using the built-in random number generator of your computer can make your program inefficient and nonportable. (Seymour Cray knew what he was doing:

* Software included on the accompanying diskette.