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An Introduction to Computational Physics

Numerical simulation is now an integrated part of science and technology. Now in its second edition, this comprehensive textbook provides an introduction to the basic methods of computational physics, as well as an overview of recent progress in several areas of scientific computing. The author presents many step-by-step examples, including program listings in Java™, of practical numerical methods from modern physics and areas in which computational physics has made significant progress in the last decade.

The first half of the book deals with basic computational tools and routines, covering approximation and optimization of a function, differential equations, spectral analysis, and matrix operations. Important concepts are illustrated by relevant examples at each stage. The author also discusses more advanced topics, such as molecular dynamics, modeling continuous systems, Monte Carlo methods, the genetic algorithm and programming, and numerical renormalization.

This new edition has been thoroughly revised and includes many more examples and exercises. It can be used as a textbook for either undergraduate or first-year graduate courses on computational physics or scientific computation. It will also be a useful reference for anyone involved in computational research.

Tao Pang is Professor of Physics at the University of Nevada, Las Vegas. Following his higher education at Fudan University, one of the most prestigious institutions in China, he obtained his Ph.D. in condensed matter theory from the University of Minnesota in 1989. He then spent two years as a Miller Research Fellow at the University of California, Berkeley, before joining the physics faculty at the University of Nevada, Las Vegas in the fall of 1991. He has been Professor of Physics at UNLV since 2002. His main areas of research include condensed matter theory and computational physics.

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Second Edition

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CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 2RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521825696

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First published 1997
Second edition 2006

Printed in the United Kingdom at the University Press, Cambridge

A catalog record for this publication is available from the British Library

Library of Congress Cataloging in Publication data available

ISBN-13 978-0-521-82569-6 hardback
ISBN-10 0-521-82569-5 hardback

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To Yunhua, for enduring love

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Preface to first edition

The beauty of Nature is in its detail. If we are to understand different layers of scientific phenomena, tedious computations are inevitable. In the last half-century, computational approaches to many problems in science and engineering have clearly evolved into a new branch of science, *computational science*. With the increasing computing power of modern computers and the availability of new numerical techniques, scientists in different disciplines have started to unfold the mysteries of the so-called *grand challenges*, which are identified as scientific problems that will remain significant for years to come and may require teraflop computing power. These problems include, but are not limited to, global environmental modeling, virus vaccine design, and new electronic materials simulation.

Computational physics, in my view, is the foundation of computational science. It deals with basic computational problems in physics, which are closely related to the equations and computational problems in other scientific and engineering fields. For example, numerical schemes for Newton's equation can be implemented in the study of the dynamics of large molecules in chemistry and biology; algorithms for solving the Schrödinger equation are necessary in the study of electronic structures in materials science; the techniques used to solve the diffusion equation can be applied to air pollution control problems; and numerical simulations of hydrodynamic equations are needed in weather prediction and oceanic dynamics.

Important as computational physics is, it has not yet become a standard course in the curricula of many universities. But clearly its importance will increase with the further development of computational science. Almost every college or university now has some networked workstations available to students. Probably many of them will have some closely linked parallel or distributed computing systems in the near future. Students from many disciplines within science and engineering now demand the basic knowledge of scientific computing, which will certainly be important in their future careers. This book is written to fulfill this need.

Some of the materials in this book come from my lecture notes for a computational physics course I have been teaching at the University of Nevada, Las Vegas. I usually have a combination of graduate and undergraduate students from physics, engineering, and other majors. All of them have some access to the workstations or supercomputers on campus. The purpose of my lectures is to provide

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the students with some basic materials and necessary guidance so they can work out the assigned problems and selected projects on the computers available to them and in a programming language of their choice.

This book is made up of two parts. The first part (Chapter 1 through Chapter 6) deals with the basics of computational physics. Enough detail is provided so that a well-prepared upper division undergraduate student in science or engineering will have no difficulty in following the material. The second part of the book (Chapter 7 through Chapter 12) introduces some currently used simulation techniques and some of the newest developments in the field. The choice of subjects in the second part is based on my judgment of the importance of the subjects in the future. This part is specifically written for students or beginning researchers who want to know the new directions in computational physics or plan to enter the research areas of scientific computing. Many references are given there to help in further studies.

In order to make the course easy to digest and also to show some practical aspects of the materials introduced in the text, I have selected quite a few exercises. The exercises have different levels of difficulty and can be grouped into three categories. Those in the first category are simple, short problems; a student with little preparation can still work them out with some effort at filling in the gaps they have in both physics and numerical analysis. The exercises in the second category are more involved and aimed at well-prepared students. Those in the third category are mostly selected from current research topics, which will certainly benefit those students who are going to do research in computational science.

Programs for the examples discussed in the text are all written in standard Fortran 77, with a few exceptions that are available on almost all Fortran compilers. Some more advanced programming languages for data parallel or distributed computing are also discussed in Chapter 12. I have tried to keep all programs in the book structured and transparent, and I hope that anyone with knowledge of any programming language will be able to understand the content without extra effort. As a convention, all statements are written in upper case and all comments are given in lower case. From my experience, this is the best way of presenting a clear and concise Fortran program. Many sample programs in the text are explained in sufficient detail with commentary statements. I find that the most efficient approach to learning computational physics is to study well-prepared programs. Related programs used in the book can be accessed via the World Wide Web at the URL `http://www.physics.unlv.edu/~pang/cp.html`. Corresponding programs in C and Fortran 90 and other related materials will also be available at this site in the future.

This book can be used as a textbook for a computational physics course. If it is a one-semester course, my recommendation is to select materials from Chapters 1 through 7 and Chapter 11. Some sections, such as 4.6 through 4.8, 5.6, and 7.8, are good for graduate students or beginning researchers but may pose some challenges to most undergraduate students.

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Preface

Since the publication of the first edition of the book, I have received numerous comments and suggestions on the book from all over the world and from a far wider range of readers than anticipated. This is a firm testament of what I claimed in the Preface to the first edition that computational physics is truly the foundation of computational science.

The Internet, which connects all computerized parts of the world, has made it possible to communicate with students who are striving to learn modern science in distant places that I have never even heard of. The main drive for having a second edition of the book is to provide a new generation of science and engineering students with an up-to-date presentation to the subject.

In the last decade, we have witnessed steady progress in computational studies of scientific problems. Many complex issues are now analyzed and solved on computers. New paradigms of global-scale computing have emerged, such as the Grid and web computing. Computers are faster and come with more functions and capacity. There has never been a better time to study computational physics.

For this new edition, I have revised each chapter in the book thoroughly, incorporating many suggestions made by the readers of the first edition. There are more examples given with more sample programs and figures to make the explanation of the material easier to follow. More exercises are given to help students digest the material. Each sample program has been completely rewritten to reflect what I have learned in the last few years of teaching the subject. A lot of new material has been added to this edition mainly in the areas in which computational physics has made significant progress and a difference in the last decade, including one chapter on genetic algorithm and programming. Some material in the first edition has been removed mainly because there are more detailed books on those subjects available or they appear to be out of date. The website for this new edition is at `http://www.physics.unlv.edu/~pang/cp2.html`.

References are cited for the sole purpose of providing more information for further study on the relevant subjects. Therefore they may not be the most authoritative or defining work. Most of them are given because of my familiarity with, or my easy access to, the cited materials. I have also tried to limit the number of references so the reader will not find them overwhelming. When I have had to choose, I have always picked the ones that I think will benefit the readers most.

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Java is adopted as the instructional programming language in the book. The source codes are made available at the website. Java, an object-oriented and interpreted language, is the newest programming language that has made a major impact in the last few years. The strength of Java is in its ability to work with web browsers, its comprehensive API (application programming interface), and its built-in security and network support. Both the source code and bytecode can run on any computer that has Java with exactly the same result. There are many advantages in Java, and its speed in scientific programming has steadily increased over the last few years. At the moment, a carefully written Java program, combined with static analysis, just-in-time compiling, and instruction-level optimization, can deliver nearly the same raw speed as C or Fortran. More scientists, especially those who are still in colleges or graduate schools, are expected to use Java as their primary programming language. This is why Java is used as the instructional language in this edition. Currently, many new applications in science and engineering are being developed in Java worldwide to facilitate collaboration and to reduce programming time. This book will do its part in teaching students how to build their own programs appropriate for scientific computing. We do not know what will be the dominant programming language for scientific computing in the future, but we do know that scientific computing will continue playing a major role in fundamental research, knowledge development, and emerging technology.

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Acknowledgments

Most of the material presented in this book has been strongly influenced by my research work in the last 20 years, and I am extremely grateful to the University of Minnesota, the Miller Institute for Basic Research in Science at the University of California, Berkeley, the National Science Foundation, the Department of Energy, and the W. M. Keck Foundation for their generous support of my research work.

Numerous colleagues from all over the world have made contributions to this edition while using the first edition of the book. My deepest gratitude goes to those who have communicated with me over the years regarding the topics covered in the book, especially those inspired young scholars who have constantly reminded me that the effort of writing this book is worthwhile, and the students who have taken the course from me.

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