Computational Physics
Second Edition

This Second Edition has been fully updated. The wide range of topics covered in the First Edition has been extended with new chapters on finite element methods and lattice Boltzmann simulation. New sections have been added to the chapters on density functional theory, quantum molecular dynamics, Monte Carlo simulation and diagonalisation of one-dimensional quantum systems.

The book covers many different areas of physics research and different computational methodologies, with an emphasis on condensed matter physics and physical chemistry. It includes computational methods such as Monte Carlo and molecular dynamics, various electronic structure methodologies, methods for solving partial differential equations, and lattice gauge theory. Throughout the book, the relations between the methods used in different fields of physics are emphasised. Several new programs are described and these can be downloaded from www.cambridge.org/9780521833462

The book requires a background in elementary programming, numerical analysis and field theory, as well as undergraduate knowledge of condensed matter theory and statistical physics. It will be of interest to graduate students and researchers in theoretical, computational and experimental physics.

JOS THIJSSEN is a lecturer at the Kavli Institute of Nanoscience at Delft University of Technology.

COMPUTATIONAL PHYSICS

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JOS THIJSSEN
Kavli Institute of Nanoscience, Delft University of Technology

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Preface to the first edition

This is a book on computational methods used in theoretical physics research, with an emphasis on condensed matter applications.

Computational physics is concerned with performing computer calculations and simulations for solving physical problems. Although computer memory and processor performance have increased dramatically over the last two decades, most physical problems are too complicated to be solved without approximations to the physics, quite apart from the approximations inherent in any numerical method. Therefore, most calculations done in computational physics involve some degree of approximation. In this book, emphasis is on the derivation of algorithms and the implementation of these: it is a book which tells you how methods work, why they work, and what the approximations are. It does not contain extensive discussions on results obtained for large classes of different physical systems.

This book is not elementary: the reader should have a background in basic undergraduate physics and in computing. Some background in numerical analysis is also helpful. On the other hand, the topics discussed are not treated in a comprehensive way; rather, this book hopefully bridges the gap between more elementary texts by Koonin, Gould and Giordano, and specialised monographs and review papers on the applications described. The fact that a wide range of topics is included has the advantage that the many similarities in the methods used in seemingly very different fields could be highlighted. Many important topics and applications are however not considered in this book – the material presented obviously reflects my own expertise and interest.

I hope that this book will be useful as a source for intermediate and advanced courses on the subject. I furthermore hope that it will be helpful for graduates and researchers who want to increase their knowledge of the field.

Some variation in the degree of difficulty is inherent to the topics addressed in this book. For example, in molecular dynamics, the equations of motion of a collection of particles are solved numerically, and as such it is a rather elementary subject. However, a careful analysis of the integration algorithms used, the problem of performing these simulations in different statistical ensembles, and the problem of

treating long range forces with periodic boundary conditions, are much more difficult. Therefore, sections addressing advanced material are marked with an asterisk (*) – they can be skipped at first reading. Also, extensive theoretical derivations are sometimes moved to sections with asterisks, so that the reader who wants to write programs rather than go into the theory may use the results, taking the derivations for granted.

Aside from theoretical sections, implementations of algorithms are discussed, often in a step-by-step fashion, so that the reader can program the algorithms him- or herself. Suggestions for checking the program are included. In the exercises after each chapter, additional suggestions for programs are given, but there are also exercises in which the computer is not used. The computer exercises are marked by the symbol [**C**]; if the exercise is divided up into parts, this sign occurs before the parts in which a computer program is to be written (a problem marked with [**C**] may contain major parts which are to be done analytically). The programs are not easy to write – most of them took me a long time to complete! Some data-files and numerical routines can be found on www.cambridge.org/9780521833469.

The first person who suggested that I should write this book was Aloysio Janner. Thanks to the support and enthusiasm of my colleague and friend John Inglesfield in Nijmegen, I then started writing a proposal containing a draft of the first hundred pages. After we both moved to the University of Cardiff (UK), he also checked many chapters with painstaking precision, correcting the numerous errors, both in the physics and in the English; without his support, this book would probably never have been completed.

Bill Smith, from Daresbury Laboratories (UK), has checked the chapters on classical many-particle systems and Professor Konrad Singer those on quantum simulation methods. Simon Hands from the University of Swansea (UK) has read the chapter on lattice field theories, and Hubert Knops (University of Nijmegen, The Netherlands) those on statistical mechanics and transfer matrix calculations. Maziar Nekovee (Imperial College, London, UK) commented on the chapter on quantum Monte Carlo methods. I am very grateful for the numerous suggestions and corrections from them all. I am also indebted to Paul Hayman for helping me correcting the final version of the manuscript. Many errors in the book have been pointed out to me by colleagues and students. I thank Professor Ron Cohen in particular for spotting many mistakes and discussing several issues via email.

In writing this book, I have discovered that the acknowledgements to the author's family, often expressed in an apologetic tone as a result of the disruption caused by the writing process to family life, are too real to be disqualified as a cliché. My sons Maurice, Boudewijn and Arthur have in turn disrupted the process of writing in the most pleasant way possible, regularly asking me to show growing trees or fireworks on the screen of my PC, instead of the dull black-on-white text

windows. Boudewijn and Maurice's professional imitation of their dad, tapping on the keyboard, and sideways reading formulae, is promising for the future.

It is to my wife Ellen that I dedicate this book, with gratitude for her patience, strength and everlasting support during the long, and sometimes difficult time in which the book came into being.

Preface to the second edition

Six years have passed since the first edition of this book appeared. In these years I have learned a lot more about computational physics – a process which will hopefully never stop. I learned from books and papers, but also from the excellent colleagues with whom I worked on teaching and research during this period. Some of this knowledge has found its place in this edition, which is a substantial extension of the first.

New topics include finite elements, lattice Boltzmann simulation and density matrix renormalisation group, and there are quite a few sections here and there in the book which either give a more in-depth treatment of the material than can be found in the first edition, or extensions to widen the view on the subject matter. Moreover I have tried to eliminate as many errors as possible, but I am afraid that it is difficult for me to beat the entropy of possible things which can go wrong in writing a book of over 650 pages.

In Delft, where I have now a position involving a substantial amount of teaching, I worked for several years in the computational physics group of Simon the Leeuw. I participated in an exciting and enjoyable effort: teaching in an international context. Together with Rajiv Kalia, from Louisana State, we let students from Delft collaborate with Louisiana students, having them do projects in the field of computational physics. Both Simon and Rajiv are experts in the field of molecular dynamics, and I learned a lot from them. Moreover, dealing with students and their questions has often forced me to deepen my knowledge in this field. Similar courses with Hiroshi Iyetomi from Niigata University in Japan, and now with Phil Duxbury at Michigan State have followed, and form my most enjoyable teaching experience. Much of the knowledge picked up in these courses has gone into the new material in this edition.

For one of the new parts of the book, the self-consistent pseudopotential and the Car–Parrinello program, I worked closely together with Erwin de Wolff for a few months. I am grateful for his support in this, and not least for his structured, neat way of tackling the problem.

Many students, university lecturers and researchers have shared their corrections on the text with me. I want to thank Ronald Cohen, Dominic Holland, Ari Harju,

John Mauro, Joachim Stolze and all the others whose names may have disappeared from my hard disks when moving to a new machine.

Preparing this edition in addition to the regular duties of a university position has turned out to be a demanding job, which has prevented me now and then from being a good husband and father. I thank Ellen and my sons Maurice, Boudewijn and Arthur for their patience and support, and express the hope that I will have more time for them in the future.