Basic Concepts in Computational Physics

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Second Edition

Springer

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Supplementary material and data can be found on extras.springer.com

ISBN 978-3-319-27263-4 ISBN 978-3-319-27265-8 (eBook)
DOI 10.1007/978-3-319-27265-8

Library of Congress Control Number: 2015959954

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG Switzerland

Preface

Traditionally physics is divided into two fields of activities: theoretical and experimental. As a consequence of the stunning increase in computer power and of the development of more powerful numerical techniques, a new branch of physics was established over the last decades: Computational Physics. This new branch was introduced as a spin-off of what nowadays is commonly called *computer simulations*. They play an increasingly important role in physics and in related sciences as well as in industrial applications and serve two purposes, namely:

- Direct simulation of physical processes such as
  - Molecular dynamics or
  - Monte Carlo simulation of physical processes
- Solution of complex mathematical problems such as
  - Differential equations
  - Minimization problems
  - High-dimensional integrals or sums

This book addresses all these scenarios on a very basic level. It is addressed to lecturers who will have to teach a basic course/basic courses in Computational Physics or numerical methods and to students as a companion in their first steps into the realm of this fascinating field of modern research. Following these intentions this book was divided into two parts. Part I deals with deterministic methods in Computational Physics. We discuss, in particular, numerical differentiation and integration, the treatment of ordinary differential equations, and we present some notes on the numerics of partial differential equations. Each section within this part of the book is complemented by numerous applications. Part II of this book provides an introduction to stochastic methods in Computational Physics. In particular, we will examine how to generate random numbers following a given distribution, summarize the basics of stochastics in order to establish the necessary background to understand techniques like MARKOV-Chain Monte Carlo. Finally, algorithms of stochastic optimization are discussed. Again, numerous examples out of physics like diffusion processes or the POTTS model are investigated exhaustively. Finally, this book contains an appendix that augments the main parts of the book with a detailed discussion of supplementary topics.

This book is not meant to be just a collection of algorithms which can immediately be applied to various problems which may arise in Computational Physics. On the contrary, the scope of this book is to provide the reader with a mathematically well-founded glance behind the scene of Computational Physics. Thus, particular emphasis is on a clear analysis of the various topics and to even provide in some cases the necessary means to understand the very background of these methods. Although there is a barely comprehensible amount of excellent literature on Computational Physics, most of these books seem to concentrate either on deterministic methods or on stochastic methods. It is not our goal to compete with these rather specific works. On the contrary, it is the particular focus of this book to discuss deterministic methods on par with stochastic methods and to motivate these methods by concrete examples out of physics and/or engineering.

Nevertheless, a certain overlap with existing literature was unavoidable and we apologize if we were not able to cite appropriately all existing works which are of importance and which influenced this book. However, we believe that by putting the emphasis on an exact mathematical analysis of both, deterministic and stochastic methods, we created a stimulating presentation of the basic concepts applied in Computational Physics.

If we assume two basic courses in Computational Physics to be part of the curriculum, nicknamed here *Computational Physics 101* and *Computational Physics 102*, then we would like to suggest to present/study the various topics of this book according to the following syllabus:

- Computational Physics 101:
  - Chapter 1: Some Basic Remarks
  - Chapter 2: Numerical Differentiation
  - Chapter 3: Numerical Integration
  - Chapter 4: The KEPLER Problem
  - Chapter 5: Ordinary Differential Equations: Initial Value Problems
  - Chapter 6: The Double Pendulum
  - Chapter 7: Molecular Dynamics
  - Chapter 8: Numerics of Ordinary Differential Equations: Boundary Value Problems
  - Chapter 9: The One-Dimensional Stationary Heat Equation
  - Chapter 10: The One-Dimensional Stationary SCHRÖDINGER Equation
  - Chapter 12: Pseudo-random Number Generators
- Computational Physics 102:
  - Chapter 11: Partial Differential Equations
  - Chapter 13: Random Sampling Methods
  - Chapter 14: A Brief Introduction to Monte Carlo Methods
  - Chapter 15: The ISING Model

– Chapter 16: Some Basics of Stochastic Processes
– Chapter 17: The Random Walk and Diffusion Theory
– Chapter 18: MARKOV-Chain Monte Carlo and the POTTS Model
– Chapter 19: Data Analysis
– Chapter 20: Stochastic Optimization

The various chapters are augmented by problems of medium complexity which help to understand better the numerical part of the topics discussed within this book.

Although the manuscript has been carefully checked several times, we cannot exclude that some errors escaped our scrutiny. We apologize in advance and would highly appreciate reports of potential mistakes or typos.

Throughout the book SI-units are used except stated otherwise.

Graz, Austria
July 2015

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Acknowledgments

The authors are grateful to Profs. Dr. C. Lang and Dr. C. Gattringer (Karl-Franzens Universität, Graz, Austria) and to Profs. Dr. W. von der Linden, Dr. H.-G. Evertz, and Dr. H. Sormann (Graz University of Technology, Austria). They inspired this book with their lectures on various topics of Computational Physics, computer simulation, and numerical analysis. Last but not least, the authors thank Dr. Chris Theis (CERN) for meticulously reading the manuscript, for pointing out inconsistencies, and for suggestions to improve the text.

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