Computational Statistical Physics

Providing a detailed and pedagogical account of the rapidly growing field of computational statistical physics, this book covers both the theoretical foundations of equilibrium and nonequilibrium statistical physics and modern, computational applications such as percolation, random walks, magnetic systems, machine learning dynamics, and spreading processes on complex networks. A detailed discussion of molecular dynamics simulations, a topic of great importance in biophysics and physical chemistry, is also included. The accessible and self-contained approach adopted by the authors makes this book suitable for teaching courses at the graduate level, and numerous worked examples and end-of-chapter problems allow students to test their progress and understanding.

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CAMBRIDGE
UNIVERSITY PRESS

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University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning, and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781108841429
DOI: 10.1017/9781108882316

First published 2021

Printed in the United Kingdom by TJ Books Limited, Padstow Cornwall

A catalogue record for this publication is available from the British Library.

ISBN 978-1-108-84142-9 Hardback

Dedicated to all students who attended our lectures on Computational Physics.
— Lucas Böttcher and Hans J. Herrmann
I also dedicate this book to my great-grandparents Doris and Gerhard.
— Lucas Böttcher

Contents

Preface

This textbook was born from the lecture notes of a course given first at the University of Stuttgart (1999–2006) as a core subject of the bachelor curriculum in computational physics and then at ETH Zurich as part of the bachelor and master curriculum in physics and computational science and engineering. Over the years, the course was continuously modified according to current scientific findings and breakthroughs in the fields of statistical physics and complex systems science.

The book is divided into two parts: Stochastic Methods (Part I) and Molecular Dynamics (Part II). In Part I, we cover computational approaches to studying percolation, random walks, spin systems, and complex networks. We include examples and exercises to illustrate that computational methods are invaluable in obtaining further insights into certain systems when analytical approaches are not feasible. In the context of Boltzmann machines, we also describe recent developments in connecting statistical physics concepts to machine learning. We conclude Part I with a discussion of computational methods to study nonequilibrium systems and highlight applications in modeling epidemic spreading, opinion dynamics, and irreversible growth.

In Part II, we focus on molecular dynamics and establish a connection between the study of microscopic particle interactions and their emerging macroscopic properties that can be analyzed statistically. We provide an overview of different simulation techniques that enable the reader to computationally study a broad range of interaction potentials and particle shapes. We discuss thermostat and barostat methods to simulate molecular interactions in canonical temperature and pressure ensembles. For the simulation of rigid particles, we cover the method of contact dynamics. To account for quantum-mechanical effects in molecular-dynamics simulations, we conclude with outlining the basic concepts of density functional theory and the Car–Parrinello method.

Throughout the book, we point to applications of the discussed mathematical and computational methods in different fields besides physics, including engineering, social sciences, and biology. In addition to providing a solid theoretical background in computational statistical physics, the aim of the book is to inspire the reader to develop their own simulation codes and computational experiments. We therefore include a carefully chosen selection of detailed exercises, which will enable the reader to implement and better understand the discussed theory and algorithms. For the interested reader, we also include side notes and information boxes that explore certain topics in greater depth.

We assume that the reader is familiar with at least one programming language and has some basic knowledge in classical mechanics, electrodynamics, statistical physics, and numerical mathematics.

This book benefited from the comments of many colleagues. In particular, we thank Stefan Luding, Malte Henkel, Dirk Kadau, Lorenz Müller, Marco-Andrea Buchmann, Nicola Offeddu, Marcel Thielmann, Madis Ollikainen, Alisha Föry, Josh LeClair, Fernando Alonso-Marroquin, Yupeng Jiang, and Thomas Asikis for their feedback. We also thank Giovanni Balduzzi for his support with performing different simulations. Moreover, we are grateful to the numerous scientists in the fields of computational and statistical physics for contributing photos that we included in biographical panels to highlight their work. Historically, a gender imbalance has been very much ingrained in computational physics, but fortunately the situation is starting to change.

What is Computational Physics?

Computational physics is the study and implementation of numerical algorithms to solve problems in physics by means of computers. As we will see throughout the book, finding numerical solutions to a given problem is useful because there are only very few systems that can be solved analytically. In particular, computational physics methods are used to simulate many-body particle systems. The simulated "virtual reality" is sometimes referred to as the third branch of physics (between experiment and theory) [1].

The analysis and visualization of large data sets that are generated numerically and experimentally is also part of computational physics but will not be treated in the present book.

Computational physics plays an important role in the following fields:

- Computational fluid dynamics (CFD): solving and analyzing problems that involve fluid flows
- Classical phase transitions: percolation, critical phenomena
- Solid state physics (quantum mechanics)
- High-energy physics/particle physics: in particular, lattice quantum chromodynamics ("lattice QCD")
- Astrophysics: many-body simulations of stars, galaxies, etc.
- Geophysics and solid mechanics: earthquake simulations, fracture, rupture, crack propagation, etc.
- Agent-based modeling (and interdisciplinary applications): complex networks in biology, economy, social sciences, and other disciplines