Exploring Computational Physics

From Physical Concepts to
Scientific Simulations, Implementation,
and Mathematical Theory

Richard Olsen



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Preface

The computer has become one of the central tools of modern science and engineering. Computational methods allow researchers to study systems that are difficult, expensive, or even impossible to investigate through analytical calculations or experiments alone. In the early days of computational physics, computers that filled entire rooms were required to perform calculations capable of providing meaningful physical insight. While some of the world's most powerful computers still occupy large facilities today, advances in computing technology have made sophisticated simulations and calculations accessible to virtually anyone. Modern personal computers are powerful enough to explore many advanced problems in physics, and the emergence of graphics processing units (GPUs), containing thousands of computational cores, has further increased the computational power available to individual users. As a result, it is now possible to perform scientifically meaningful simulations and gain genuine physical insight using little more than a standard desktop or gaming computer together with freely available open-source software.

This book was written with the goal of making computational physics accessible to a broad audience, including hobbyists, students, researchers, engineers, programmers, and anyone with an interest in understanding how computers are used to model, simulate, and investigate physical systems. Rather than beginning with heavy mathematics, the chapters first aim to build physical intuition and conceptual understanding. Practical examples and hands-on simulations are then used to connect the theory to real computational workflows, before later chapters develop the underlying mathematical foundations. Scripts, code listings, input files, and other supplementary resources used throughout the book are available on the companion resources page found at

http://scienceperspectivesbooks.com/ecp

The book explores four areas of computational physics: computational fluid dynamics, molecular dynamics, quantum chemistry, and tractography using magnetic resonance imaging. Throughout the text, emphasis is placed on understanding both the physical principles and the computational methods that allow complex systems to be simulated on modern computers.

While the book can be read without performing any of the included tutorials, readers who wish to reproduce the examples may find it useful to set up a Linux environment. Throughout the preparation of this book, the examples were tested using Ubuntu 24.04 LTS running in a virtual machine. Similar Linux distributions and newer Ubuntu releases are expected to work as well, although minor differences in installation procedures may occur.

Over time, it has become clear that many areas of computational physics are built upon a common set of underlying principles. Likewise, exposure to a variety of open-source software packages used across different branches of physics reveals that their workflows often follow similar patterns. These observations motivated the development of the present book, which originated from a collection of material developed over several years while working within different areas of computational physics. Parts of the introductory material on quantum chemistry and molecular dynamics were initially written as part of the author's PhD work [1], while additional background material on computational fluid dynamics, magnetic resonance imaging, and tractography was later developed independently for educational purposes. This material has been reorganized, expanded, and adapted into a unified exploration of the field of computational physics.

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I acknowledge the many researchers, educators, software developers, and open-source communities whose work and contributions have made modern computational physics accessible to students, researchers, engineers, and enthusiasts around the world. The software, educational resources, and scientific literature developed by these communities have played an important role in shaping both the field and the material presented in this book.

I also acknowledge the use of OpenAI's ChatGPT for editorial assistance, language refinement, structural feedback, and general manuscript development support during the preparation of this book. All scientific content, interpretations, implementations, and final editorial decisions remain the responsibility of the author.

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2026

About the Author

Richard Olsen is a physicist and scientific software developer working with scientific and engineering software solutions. He holds master's degrees in particle physics from the University of Bergen and in theoretical physics from University of Utrecht, and received his PhD in physics from the University of Bergen in 2022. His academic and professional work has focused on using and implementing computational methods within molecular dynamics, quantum chemistry, medical imaging analysis, and scientific visualization.

Alongside his doctoral research, he worked in the medical imaging industry developing software for magnetic resonance imaging analysis, including diffusion tensor imaging, tractography, dynamic contrast-enhanced imaging, and perfusion imaging. Since completing his PhD, he has worked as a scientific software developer developing computationally intensive software solutions and optimization methods for computer visualization.

His background combines physics, numerical methods, and practical scientific software engineering across both academia and industry.



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