Graduate Texts in Physics

Philipp O. J. Scherer

Computational Physics

Simulation of Classical and Quantum Systems

Second Edition

计算物理学 第2版

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To Christine

Preface to the Second Edition

This textbook introduces the main principles of computational physics, which include numerical methods and their application to the simulation of physical systems. The first edition was based on a one-year course in computational physics where I presented a selection of only the most important methods and applications. Approximately one-third of this edition is new. I tried to give a larger overview of the numerical methods, traditional ones as well as more recent developments. In many cases it is not possible to pin down the "best" algorithm, since this may depend on subtle features of a certain application, the general opinion changes from time to time with new methods appearing and computer architectures evolving, and each author is convinced that his method is the best one. Therefore I concentrated on a discussion of the prevalent methods and a comparison for selected examples. For a comprehensive description I would like to refer the reader to specialized textbooks like "Numerical Recipes" or elementary books in the field of the engineering sciences.

The major changes are as follows.

A new chapter is dedicated to the discretization of differential equations and the general treatment of boundary value problems. While finite differences are a natural way to discretize differential operators, finite volume methods are more flexible if material properties like the dielectric constant are discontinuous. Both can be seen as special cases of the finite element methods which are omnipresent in the engineering sciences. The method of weighted residuals is a very general way to find the "best" approximation to the solution within a limited space of trial functions. It is relevant for finite element and finite volume methods but also for spectral methods which use global trial functions like polynomials or Fourier series.

Traditionally, polynomials and splines are very often used for interpolation. I included a section on rational interpolation which is useful to interpolate functions with poles but can also be an alternative to spline interpolation due to the recent development of barycentric rational interpolants without poles.

The chapter on numerical integration now discusses Clenshaw-Curtis and Gaussian methods in much more detail, which are important for practical applications due to their high accuracy.

Besides the elementary root finding methods like bisection and Newton-Raphson, also the combined methods by Dekker and Brent and a recent extension by Chandrupatla are discussed in detail. These methods are recommended in most text books. Function minimization is now discussed also with derivative free methods, including Brent's golden section search method. Quasi-Newton methods for root finding and function minimizing are thoroughly explained.

Eigenvalue problems are ubiquitous in physics. The QL-method, which is very popular for not too large matrices is included as well as analytic expressions for several differentiation matrices.

The discussion of the singular value decomposition was extended and its application to low rank matrix approximation and linear fitting is discussed.

For the integration of equations of motion (i.e. of initial value problems) many methods are available, often specialized for certain applications. For completeness, I included the predictor-corrector methods by Nordsieck and Gear which have been often used for molecular dynamics and the backward differentiation methods for stiff problems.

A new chapter is devoted to molecular mechanics, since this is a very important branch of current computational physics. Typical force field terms are discussed as well as the calculation of gradients which are necessary for molecular dynamics simulations.

The simulation of waves now includes three additional two-variable methods which are often used in the literature and are based on generally applicable schemes (leapfrog, Lax-Wendroff, Crank-Nicolson).

The chapter on simple quantum systems was rewritten. Wave packet simulation has become very important in theoretical physics and theoretical chemistry. Several methods are compared for spatial discretization and time integration of the one-dimensional Schrödinger equation. The dissipative two-level system is used to discuss elementary operations on a qubit.

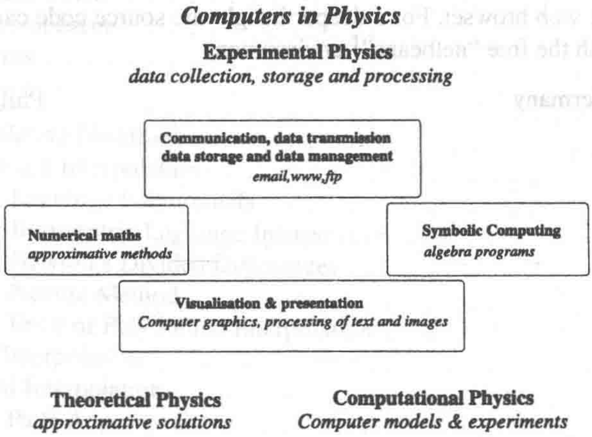
The book is accompanied by many computer experiments. For those readers who are unable to try them out, the essential results are shown by numerous figures.

This book is intended to give the reader a good overview over the fundamental numerical methods and their application to a wide range of physical phenomena. Each chapter now starts with a small abstract, sometimes followed by necessary physical background information. Many references, original work as well as specialized text books, are helpful for more deepened studies.

Garching, Germany Philipp O.J. Scherer
February 2013

Preface to the First Edition

Computers have become an integral part of modern physics. They help to acquire, store and process enormous amounts of experimental data. Algebra programs have become very powerful and give the physician the knowledge of many mathematicians at hand. Traditionally physics has been divided into experimental physics which observes phenomena occurring in the real world and theoretical physics which uses mathematical methods and simplified models to explain the experimental findings and to make predictions for future experiments. But there is also a new part of physics which has an ever growing importance. Computational physics combines the methods of the experimentalist and the theoretician. Computer simulation of physical systems helps to develop models and to investigate their properties.



This book is a compilation of the contents of a two-part course on computational physics which I have given at the TUM (Technische Universität München) for several years on a regular basis. It attempts to give the undergraduate physics students a profound background in numerical methods and in computer simulation methods but is also very welcome by students of mathematics and computational science who want to learn about applications of numerical methods in physics. This book may also support lecturers of computational physics and bio-computing. It tries to bridge between simple examples which can be solved analytically and more complicated but instructive applications which provide insight into the underlying physics by doing computer experiments.

The first part gives an introduction into the essential methods of numerical mathematics which are needed for applications in physics. Basic algorithms are explained in detail together with limitations due to numerical inaccuracies. Mathematical explanations are supplemented by numerous numerical experiments.

The second part of the book shows the application of computer simulation methods for a variety of physical systems with a certain focus on molecular biophysics. The main object is the time evolution of a physical system. Starting from a simple rigid rotor or a mass point in a central field, important concepts of classical molecular dynamics are discussed. Further chapters deal with partial differential equations, especially the Poisson-Boltzmann equation, the diffusion equation, nonlinear dynamic systems and the simulation of waves on a 1-dimensional string. In the last chapters simple quantum systems are studied to understand e.g. exponential decay processes or electronic transitions during an atomic collision. A two-state quantum system is studied in large detail, including relaxation processes and excitation by an external field. Elementary operations on a quantum bit (qubit) are simulated.

Basic equations are derived in detail and efficient implications are discussed together with numerical accuracy and stability of the algorithms. Analytical results are given for simple test cases which serve as a benchmark for the numerical methods. Many computer experiments are provided realized as Java applets which can be run in the web browser. For a deeper insight the source code can be studied and modified with the free "netbeans"[1] environment.

Garching, Germany Philipp O.J. Scherer
April 2010

[1] www.netbeans.org.

Contents