

# Preface to the Third Edition

While the first edition of this textbook was based on a one-year course in computational physics with a rather limited scope, its extent has been increased substantially in the third edition, offering the possibility to select from a broader range of computer experiments and to deepen the understanding of the important numerical methods. The computer experiments have always been a central part of my concepts for this book. Since Java applets, which are very convenient otherwise, have become more or less deprecated and their usage in a browser is no longer recommended for security issues, I decided to use standalone Java programs instead and to rewrite all of the old examples. These can also be edited and compiled with the “netbeans” environment and offer the same possibilities to generate a graphical user interface in short time.

The major changes in the third edition are as follows.

In the first part, a new chapter is devoted to the time-frequency analysis of experimental data. While the classical Fourier transform allows the calculation of the spectrum of a stationary signal, it is not so useful for nonstationary signals with significant variation of the momentaneous frequency distribution. Application of the Fourier transformation to short time windows, a method which is known as short-time Fourier transformation (STFT), allows analyzing the frequency content of a signal as a function of time. Good time resolution, of course, always comes together with a loss in frequency resolution (this is well known as “uncertainty principle”). The STFT method uses the same window for the whole spectrum, therefore the absolute time and frequency resolution is the same for low- and high-frequency components and the time resolution is limited by the period of the lowest frequencies of interest. Analysis of a signal with wavelets, on the other hand, uses shorter windows for the higher frequencies and keeps the relative frequency resolution constant while increasing the time resolution of the high-frequency components. The continuous wavelet transform can be very time consuming since it involves a convolution integral and is highly redundant. The discrete wavelet

transform uses a finite number of orthogonal basis function and can be performed much faster by calculating scalar products. It is closely related to multiresolution analysis which analyzes a signal in terms of a basic approximation and details of increasing resolution. Such methods are very popular in signal processing, especially of audio and image data but also in medical physics and seismology. The principles of the construction of orthogonal wavelet families are explained in detail, but without too many mathematical proofs. Several popular kinds of wavelets are discussed, like those by Haar, Meyer and Daubechies and their application is explored in a series of computer experiments.

In the second part, two new chapters have been added. First I included a discussion of the advection equation. Several methods to solve the one-dimensional problem are discussed from very simple straightforward differencing to quite sophisticated Galerkin-Taylor methods. The properties of these methods are demonstrated in computer experiments, as well by programs in the problems section as by numerous figures in the text. The extension to more dimensions by finite volume methods and dimensional splitting are discussed. A profound understanding of the advection equation and its numerical solution is also the basis for the more complex convection and Navier–Stokes equations.

Another chapter was added to the application of variational methods for quantum systems. The variational principle is very useful to calculate the groundstate energy. Two different types of computer experiments are performed. First we use the variational quantum Monte Carlo method (VQMC) for small atomic and molecular systems like the Helium atom and the Hydrogen molecule. We use trial functions which treat electron correlation explicitly by introducing a Jastrow factor which depends on the electron-electron distances. Such trial functions lead to nonseparable multidimensional integrals which can be efficiently calculated with the VQMC method. A second series of computer experiments studies exciton-phonon coupling in molecular aggregates which are of large interest for energy transfer in artificial and biological systems. The non-Born-Oppenheimer character of the wavefunction makes it necessary to optimize a large number of parameters. Different kinds of trial functions are applied to aggregates of up to 100 molecules to study the localization of the lowest state (so called “self-trapping”).

Apart from these newly added chapters, further improvements have been made throughout the book. The chapter on random numbers now discusses in more detail the principles of modern random number generators, especially the xorshift, multiply with carry (MWC) and complementary multiply with carry (CMWC) methods. Nonstationary iterative Krylov-space methods for systems of linear equations are discussed systematically with a focus on the conjugate gradients (CG) and general minimum residual (GMRES) methods. The QR method for eigenvalue problems is now discussed in much more detail together with its connection to the power iteration method and the Krylov-space methods by Arnoldi and Lanczos.

Finally, I included a computer experiment simulating the transition between two states with wave packet dynamics, which is very helpful to understand the semi-classical approximation, especially the Landau–Zener model, which is the subject of another computer experiment.

Garching, Germany  
March 2017

Philipp O.J. Scherer

# 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 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 Schroedinger 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.

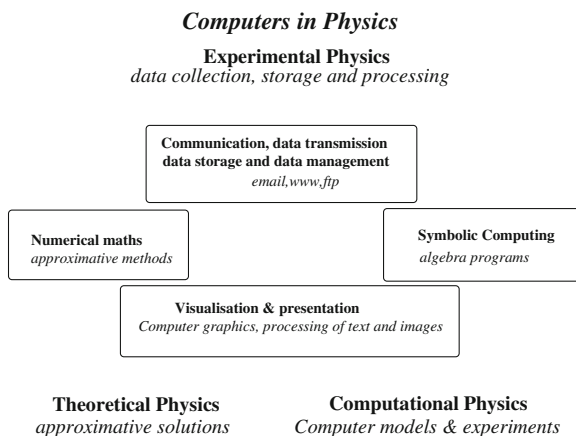
This book is intended to give the reader a good overview over the fundamental numerical methods and their application to a wide range of physical phenomena. Each chapter now starts with a small abstract, sometimes followed by necessary physical background information. Many references, original work as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

Garching, Germany  
February 2013

Philipp O.J. Scherer

# 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”<sup>1</sup> environment.

Garching, Germany  
April 2010

Philipp O.J. Scherer

---

<sup>1</sup>[www.netbeans.org](http://www.netbeans.org).

Computational Physics

Simulation of Classical and Quantum Systems

Scherer, P.O.J.

2017, XXIV, 633 p. 306 illus., 50 illus. in color.,

Hardcover

ISBN: 978-3-319-61087-0