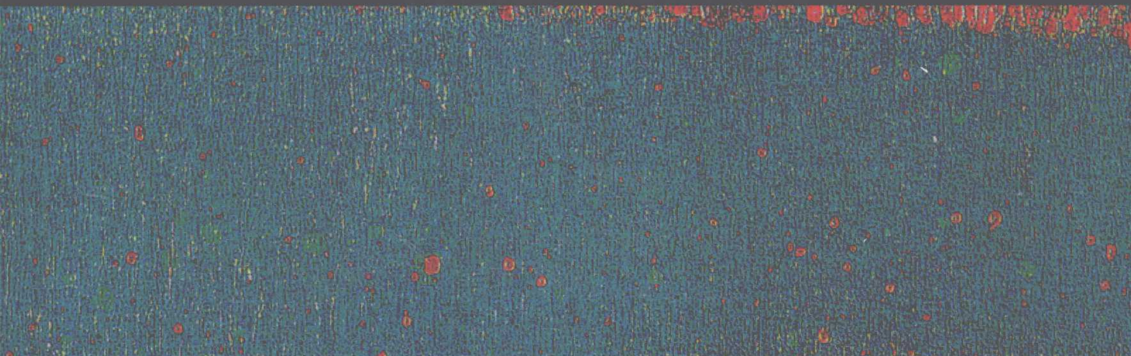
Christoph W. Ueberhuber

Numerical Computation 1

Methods, Software, and Analysis



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NUMERICAL COMPUTATION 1

Methods, Software, and Analysis

With 157 Figures

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Christoph W. Ueberhuber

Technical University of Vienna
Wiedner Hauptstrasse 8–10/115
A-1040 Vienna
Austria

e-mail: cwu@uranus.tuwien.ac.at

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ROBERT LETTNER *created the picture on the cover of this book. He is the person in charge of the central printing and reprography office at the Academy of Applied Arts in Vienna, Austria. In the past few years Robert Lettner, inspired by advancements in digital image processing, has developed new forms of aesthetics.*
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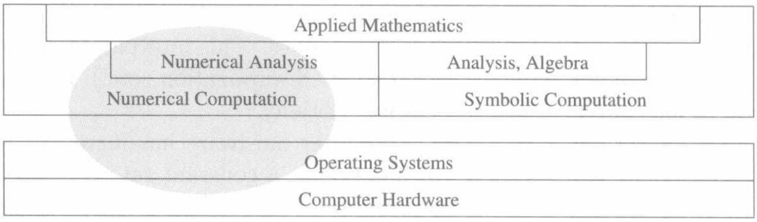
Preface

This book deals with various aspects of scientific numerical computing. No attempt was made to be complete or encyclopedic. The successful solution of a numerical problem has many facets and consequently involves different fields of computer science. Computer numerics—as opposed to computer algebra—is thus based on applied mathematics, numerical analysis and numerical computation as well as on certain areas of computer science such as computer architecture and operating systems.



Each chapter begins with sample situations taken from specific fields of application. Abstract and general formulations of mathematical problems are then presented. Following this abstract level, a general discussion about principles and methods for the numerical solution of mathematical problems is presented. Relevant algorithms are developed and their efficiency and the accuracy of their results is assessed. It is then explained as to how they can be obtained in the form of numerical software. The reader is presented with various ways of applying the general methods and principles to particular classes of problems and approaches to extracting practically useful solutions with appropriately chosen numerical software are developed. Potential difficulties and obstacles are examined, and ways of avoiding them are discussed.

The volume and diversity of all the available numerical software is tremendous. When confronted with all the available software, it is important for the user to have a broad knowledge of numerical software in general and to know where this software can be optimally applied in order for him to be able to choose the most appropriate software for a specific problem. Assistance in this complicated matter is offered in this book.

This book gives a comprehensive survey of the high quality software products available and the methods and algorithms they are based on. Positive properties and inherent weaknesses of specific software products are pointed out. Special subsections in this book, devoted to software, provide relevant information about commercially available software libraries (IMSL, NAG, etc.) as well as public domain software (such as the NETLIB programs) which can be downloaded from the Internet.

This book addresses people interested in the numerical solution of mathematical problems, who wish to make a good selection from the wealth of available software products, and who wish to utilize the functionality and efficiency of modern numerical software. These people may be students, scientists or engineers. Accordingly, this monograph may be used either as a textbook or as a reference book.

The German version *Computer-Numerik* was published in 1995 by Springer-Verlag, Heidelberg. The English version, however, is not merely a translation; the book has also been revised and updated.

Synopsis

Volume I starts with a short introduction into scientific model building, which is the foundation of all numerical methods which rely on finite models that replace infinite mathematical objects and techniques. This unavoidable finitization (found in floating-point numbers, truncation, discretization, etc.) is introduced in Chapter 2 and implications are discussed briefly.

The peak performance of modern computer hardware has increased remarkably in recent years and continues to increase at a constant rate of nearly 100 % every year. On the other hand, there is a steadily increasing gap between the potential performance and the empirical performance values of contemporary computer systems. Reasons for this development are examined and remedial measures are presented in Chapter 3.

Chapter 4 is dedicated to the objects of all numerical methods—numerical data—and to the operations they are used in. The main emphasis of this chapter is on standardized floating-point systems as found on most computers used for numerical data processing. It is explained as to how portable programs can be written to adapt themselves to the features of a specific number system.

Chapter 5 deals with the foundations of algorithm theory, in so far as this knowledge is important for numerical methods. Floating-point operations and arithmetic algorithms, which are the basic elements of all other numerical algorithms, are dealt with extensively.

Chapter 6 presents the most important quality attributes of numerical software. Particular attention is paid to techniques which provide for the efficient utilization of modern computer systems when solving large-scale numerical problems.

Chapter 7 gives an overview of readily available commercial or public domain software products. Numerical programs (published in TOMS or in other journals or books), program packages (LAPACK, QUADPACK etc.), and software libraries are dealt with. Particular emphasis is placed on software available on the Internet (NETLIB, ELIB etc.).

Chapter 8 deals with modeling by approximation, a technique important in many fields of numerical data processing. The applications of these techniques range from data analysis to the modeling processes that take place in numerical programs (such as the process found in numerical integration programs in which the integrand function is replaced by a piecewise polynomial).

The most effective approach to obtaining model functions which approximate given data is interpolation. Chapter 9 gives the theoretical background necessary to understanding particular interpolation methods and programs. In addition, the algorithmic processing of polynomials and various spline functions is presented.

Volume II begins with Chapter 10 which contains best approximation techniques for linear and nonlinear data fitting applications.

Chapter 11 is dedicated to a very important application of approximation: the Fourier transform. In particular, the fast Fourier transform (FFT) and its implementations are dealt with.

The subject of Chapter 12 is numerical integration. Software products which solve univariate integration problems are systematically presented. Topical algorithms (such as lattice rules) are covered in this chapter to enable the user to produce tailor-made integration software for solving multivariate integration problems (which is very useful since there is a paucity of ready made software for these problems).

The solution of systems of linear equations is undoubtedly the most important field of computer numerics. Accordingly, it is the field in which the greatest number of software products is available. However, this book deals primarily with LAPACK programs. Chapter 13 answers many questions relevant to users: How should algorithms and software products appropriate for a given problem be chosen? What properties of the system matrix influence the choice of programs? How can it be ascertained whether or not a program has produced an adequate solution? What has to be done if a program does not produce a useful result?

Chapter 14 deals with nonlinear algebraic equations. The properties of these equations may differ greatly, which makes it difficult to solve them with black box software. Chapter 15 is devoted to a very special type of nonlinear equations: algebraic eigenproblems. There is a multitude of numerical software available for these problems. Again, this book deals primarily with LAPACK programs.

Chapter 16 takes a closer look at the topics found in previous chapters, especially problems with large and sparse matrices. Problems of this type are not covered using black box software; a solution method has to be selected individually for each of them. Accordingly, this chapter gives hints on how to select appropriate algorithms and programs.

Monte Carlo methods, which are important for solving numerical problems as well as for empirical sensitivity studies, are based on random numbers. The last chapter of the book, therefore, gives a short introduction into the world of random numbers and random number generators.

Acknowledgments

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Wolfgang Moser contributed considerably to the process of translating the German version of this book. He organized the technical assistance of many students who produced a rough draft of the English version. He also translated several chapters himself.

Yolanda Goss was a competent and helpful collaborator in linguistic matters. She brought the rough draft of the English manuscript a giant step nearer to the final version. We even managed to squeeze some fun out of the dry business of improving the grammar, style and form of the draft version.

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Christoph Schmid and Thomas Wihan deserve particular appreciation for the appealing text lay out and the design of the diagrams and illustrations. Christoph Schmid created the final LaTeX printout with remarkable dedication.

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