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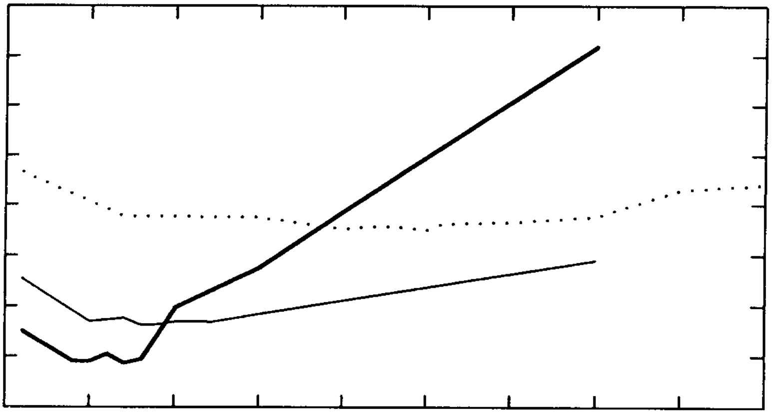
Numerical Integration

on Advanced Computer Systems



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Preface

Numerical integration is an important technique in many fields of scientific computation ranging from computational statistics to finite element methods. Since numerical integration methods are often very time consuming, substantial efforts have been made to find ways of exploiting the computing power offered by advanced computer systems, like vector or parallel computers. Even network-based distributed computing has been used recently.

When trying to solve numerical integration problems, one is faced with a vast amount of relevant literature consisting of well over a thousand articles in mathematical journals, a number of books (Braß [35], Davis, Rabinowitz [59], Engels [80], Evans [84], Krylov [145], Stroud [216] [217]), dozens of published algorithms and programs, a special software package (QUADPACK [191]), and extensive sections of numerical program libraries (IMSL [229],[230], NAG [173], etc.).

Scope

This monograph has been written with three major goals in mind. First, it is meant to cover many recent developments in numerical integration that have not yet been presented by any other textbook in a uniform style. Thus it gives the reader an up-to-date overview of the theoretical and computational aspects of numerical integration. Then, this book is aimed at giving a prototypical coverage of ways to determine the potential parallelism in problem adaptive numerical solution processes and to utilize this potential parallelism by means of dynamic load distribution techniques. In contrast, most existing books on parallel numerical algorithms, for instance, those on parallel linear algebra algorithms, deal mainly with static load distribution. Finally, this book discusses the basics of producing efficient and reliable software for numerical integration on parallel systems. It provides concepts and introduces methodologies for solving the problems that have so far prevented the development of such high-quality software.

The authors anticipate that there will be three categories of readers interested in this monograph. The first group are graduate students (and their instructors) who may use it as a textbook for advanced courses on current techniques in scientific computing and numerical analysis. The second group are computational scientists and engineers working on problems for which highly efficient methods for calculating integrals are required. They may use this volume as a reference book. The third group are researchers in applied numerical analysis and mathematical software development who will find a well organized representation of relevant material along with an extensive bibliography that covers many pertinent articles published in the last 10 years.

Synopsis

Part I introduces the topic of numerical integration. Chapter 1 describes several prototypical areas of scientific computing in which numerical integration plays an important role. The importance of numerical integration as a fundamental computational technique is demonstrated. Additionally, this chapter clarifies the requirements which numerical integration software has to meet in order to be of real value to potential users. The fundamentals of numerical integration are outlined in Chapter 2. In particular, the basic problem in numerical integration is precisely stated and the pros and cons of numerical and *symbolic* integration are discussed.

Part II describes the mathematical concepts underlying numerical integration. Chapter 3 discusses the various practically relevant types of integrals and provides the most frequently occurring integration regions and weight functions. Additionally, ways of preprocessing integrals so that their numerical computation becomes easier are described. Most of the material in this part of the book, however, deals with *integration formulas.* Integration formulas are the central part of any numerical method for discretizing and approximating integral operators. It becomes apparent that the construction of one-dimensional – *quadrature* – formulas is by far easier than the the construction of multi-dimensional – *cubature* – formulas. Quadrature formulas are considered in Chapter 4, cubature formulas in Chapter 5.

Part III deals with algorithmic and computational aspects of numerical integration. Chapter 6 considers the construction of numerical integration algorithms. It describes different algorithmic sections – those implementing, for instance, integration formulas, error estimation procedures, or extrapolation algorithms – and their incorporation into integration programs.

Chapter 7 discusses the important topic of load distribution on parallel and distributed systems and is mainly concerned with *dynamic* load balancing. Dynamic load balancing reacts to the current state of the underlying computer system during the execution of parallel programs. By dynamically redistributing work, dynamic load balancing can improve the utilization and thus the performance of parallel systems when there is unpredictable workload behavior. Such unpredictable workload behavior is a salient feature of *adaptive* numerical integration algorithms.

A classification of the level and degree of parallelism involved in numerical integration programs is given in Chapter 8. Different parallel integration programs may exploit the available parallelism in totally different ways. Chapter 9 introduces a notation for describing how various sections of numerical integration algorithms are actually parallelized in a particular program. Additionally, there is a general discussion of the relevant task characteristics in parallel numerical integration. Chapter 10 describes those parallelization schemes that have already received attention in literature, and relevant papers in the bibliography are classified and referenced in *Bibliographical Notes*, in which the salient features of each paper are given.

Special data structures are used for storing subregions in adaptive numerical integration programs. The need to distribute work dynamically at run-time may have an impact on the management of data in parallel adaptive numerical integration programs. This issue is discussed in detail in Chapter 11.

Part IV provides material concerning the development of numerical integration software for advanced computer systems. Chapter 12 discusses criteria, like robustness, efficiency, etc., for assessing the quality of numerical integration programs. Additionally, evaluation techniques for these quality indices are dealt with. In Chapter 13, the Architecture Adaptive Algorithms (AAA) concept is introduced. The AAA methodology is an attempt to provide concepts and tools for writing *portable* parallel programs that run *efficiently* on a broad range of target machines.

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