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Large Scale Scientific Computing

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PREFACE

In this book, the new and rapidly expanding field of *scientific computing* is understood in a double sense: as computing for scientific and engineering problems and as the science of doing such computations. Thus scientific computing touches at one side mathematical modelling (in the various fields of applications) and at the other side computer science. As soon as the mathematical models describe the features of real life processes in sufficient detail, the associated computations tend to be *large scale*. As a consequence, interest more and more focusses on such numerical methods that can be expected to cope with large scale computational problems. Moreover, given the algorithms which are known to be efficient on a traditional computer, the question of implementation on modern supercomputers may get crucial.

The present book is the proceedings of a meeting on "Large Scale Scientific Computing", that was held at the Oberwolfach Mathematical Institute (July 14-19, 1985) under the auspices of the Sonderforschungsbereich 123 of the University of Heidelberg. Participants included applied scientists with computational interests, numerical analysts, and experts on modern parallel computers. The purpose of the meeting was to establish a common understanding of recent issues in scientific computing, especially in view of large scale problems. Fields of applications, which have been covered, included

semi-conductor design,
chemical combustion,
flow through porous media,
climatology,
seismology,
fluid dynamics,
tomography,
rheology,
hydro power plant optimization,
subway control,
space technology.

The associated mathematical models included ordinary (ODE) and partial (PDE) differential equations, integral equations (IE) and mixed integer-real optimization problems.

The present book comprises 6 parts to be described here from an introductory point of view. For all chapters, *nonlinearity* plays a dominant role. Moreover, the book reflects an interesting issue of present research: ODE techniques of a rather high degree of sophistication gradually intrude into the PDE region. For this reason, the first two parts jointly cover ODE and PDE problems and techniques.

Part I covers initial value problems (IVP) for ODE's and initial boundary value problems (IBVP) for parabolic PDE's - recall that a method of lines approach to such IBVP's anyway leads to large scale stiff IVP's of a special structure. Chapter 1 (Bank, Fichtner, Rose, Smith) deals with computational techniques for semiconductor device modelling, which plays an important role in chip fabrication. Mathematically speaking, the models represent 3-D nonlinear PDE's. At present, the 2-D case is regarded as tractable (multigrid techniques, moderate size models), whereas the 3-D case is still in its infancy. In chapter 2 (Yserentant) the new and fascinating "hierarchical" finite element (FE) approach, which has been developed for 2-D elliptic PDE's, is transferred to the time-dependent case. The new approach seems to be rather promising especially for essentially parabolic PDE systems that are strongly coupled. After spatial discretization, where typically nonlinearity requires moving grid points, implicit ODE's or differential algebraic equations (DAE's) arise - which are treated in chapter 3 (Deuflhard, Nowak). In this chapter rather recent, highly sophisticated extrapolation techniques are described including order and stepsize control and index monitoring (recall that index >1 DAE's require further analytical preprocessing). The only illustrative example of this chapter stems from combustion. The next chapter (Warnatz), written by a combustion expert, gives a general survey of the demands arising from computational combustion. These include the numerical solution of auto-ignition problems (0-D), stationary flame problems (1-D), and instationary ignition/quenching problems (1-D). Both the above extrapolation techniques and recent multistep techniques play a role in that field. In chapter 5 (Fu, Chen) physical considerations led to the suggestion of a numerical scheme valid for large time scales. The method represents an asymptotic expansion around the equilibrium points of the physical systems under consideration. Finally, the last chapter (Knabner) could as well be subsumed into part II of the book: this chapter deals with both saturated and unsaturated see page flow through porous media, which mathematically leads to a mixed parabolic-elliptic free boundary value problem. As the paper focusses slightly on the question of time discretization and time step control, the editors decided to put it into part I.

Part II covers boundary value problems (BVP's) for both ODE's and elliptic PDE's. Unless the elliptic problems are embedded into parabolic problems (see part I), the typical nonlinearities of real life models strongly suggest the use of *numerical continuation techniques* - which are described in the first 3 chapters of this part. In chapter 7 (Deuflhard, Fiedler, Kunkel) a rather efficient numerical pathfollowing technique, known from bifurcation diagram computations in algebraic equations, is transferred to the case of ODE-BVP's. The method described carries over to PDE problems, wherein the arising large linear systems can be solved by a direct sparse solver (compare e.g. chapter 20). Illustrative numerical comparisons with competing techniques are included. In chapter 8 (Jarausch, Mackens) 2-D nonlinear elliptic PDE problems are treated. The treatment applies the hierarchical basis techniques (cf. chapter 2). The main idea of the chapter is to condense the effect of the nonlinearity numerically in a small system - which is then treated using a variant of the continuation techniques of chapter 7. The following chapter 9 (Giovangigli, Smooke) suggests a special ODE/PDE version of the so-called pseudo-arclength continuation method. In order to preserve the block structure of the arising linear systems, the embedding parameter is added as a trivial ODE - thus leading to continuation only in a selected boundary value. The method is illustrated by impressive combustion problems including extensive chemical mechanisms. The last two chapters of this part deal with *hybrid algorithms*. In chapter 10 (Ascher, Spudich), which is joint work of a numerical analyst and a seismologist, roughly 10^4 BVP's are to be solved in order to evaluate seismograms. Analytical preprocessing techniques include Hankel and Fourier-Bessel transforms. For actual computation a well-designed mixture of the known approaches is applied: collocation, orthogonal function expansion, multiple shooting (via transfer matrices). The last chapter (Hebeker) of this part aims at special 3-D Stokes problems. The hybrid nature of the advocated approach shows up in the mixed use of fundamental solutions, boundary element method and spectral method. One of the illustrative examples is parabolic, so that part I might also have been a place for presentation. At the same time, this chapter also touches the next part of the book.

Part III deals with hyperbolic fluid dynamics, a traditionally central part of scientific computing that is well represented in the literature. For this reason, only two state-of-the-art papers are included here. The first chapter (Engquist, Harten, Osher) derives new, rather general shock-capturing schemes of high order. The schemes automatically adjust the locally used computational stencil without making use of limiters - a distinguishing feature of this approach. The given treatment covers 1-D shocks and uniform grids. The efficiency of the smoothing around shocks is demonstrated by the illustrative example of Euler equations for the polytropic gas. In the next chapter (Rizzi) sophisticated 3-D computations for the compressible or incompressible Euler equations are presented using a finite volume method with up to 6.10^5 grid cells! The question studied is whether vorticity in the Euler equations is created by discretization errors or is a phenomenon depending on nonlinearity - a question, which seems to be far beyond elucidation by analytical techniques. In the examples included (traverse circular cylinder, two delta wings, prolate spheroid) both situations occur. In addition, one of the examples seems to exhibit a spiral singularity - an observation that will certainly stimulate further investigations (both numerical and analytical).

The following *part IV* shortly surveys some recent results for inverse problems. The first two chapters deal with two alternative ways of treating the inverse Radon transform problem arising in *computer tomography*. In chapter 14 (Louis, Lewitt) certain optimal filtering techniques are proposed and worked out to solve the 3-D discrete inversion problem on a minimal set of data. In chapter 15 (Kruse, Natterer) the ill-posed first-kind Fredholm problem (2-D case) is directly attacked leading to some Toeplitz matrix problem that can be solved in a fast way including Tikhonov regularization. Finally, chapter 16 (Friedrich, Hofmann) presents numerical techniques for identification and optimal control in parabolic PDE's in a common theoretical framework - thus also leading over to the next part of the book. The paper advocates to regularize the inverse problem in close connection with discretization of the PDE. An illustrative example from rheology is sketched.

Part V concentrates on large scale optimization and optimal control problems. In chapter 17 (Spielberg, Suhl), production software for mixed integer-real optimization is described. The mixing in the problem induces a mixing of methods: a fast linear programming solver (utilizing deep hardware structure of a special computer) is combined with branch and bound techniques. As it turns out, a crucial part in the whole computational speed-up is played by preprocessing of the model, e.g. separation of reducible graphs to irreducible subgraphs or increase of constraints, which are then more easily handled. In chapter 18 (Krämer-Eis, Bock) feedback control techniques for control and state constrained problems are worked out in the setting of the multiple shooting method for ODE-BVP's. Two interesting applications are given: energy minimization on a subway car ride and a space shuttle re-entry flight. Techniques of the preceding two chapters should, in principle, also apply to the problem of chapter 19 (Wacker). This chapter describes both the modelling and the computations necessary for optimizing the production scheme of a real life hydro power plant system in Austria. The results of these computations helped to drastically improve the actual performance of this plant system.

Last not least, adaptations of various algorithms to supercomputers are arranged within *part VI*. In chapter 20 (Duff), the performance of well-known sparse linear equation solvers on different supercomputers is compared. The insight coming from the detailed studies is: frontal methods are highly efficient on vector machines, but cannot take advantage of parallelism, whereas multi-frontal methods can, but are not as efficient on pure vector machines; general sparse codes, however, are generally not very efficient on present day supercomputers. The next chapter (Gropp) presents a modification of adaptive gridding that was especially developed in view of supercomputers: the basic idea is to work with a global uniform coarse grid and a local uniform fine grid simultaneously. Experience from the actual implementation of this concept is reported. Finally, chapter 22 (Hayes) presents a study of a special iterative method, which has been developed for FE methods on rather irregular 3-D domains. The field of application of this method includes cryopreservation of tissues, design of suits for deep space or deep sea exploration, or whole body cooling for premature infants (a basis for surgery in extreme cases). As is typical also for other scientific computing applications, the simulations have a pilot function before the explicit real life test.

Summarizing, the book presents the main recent issues of large scale scientific computing, such as adaptive time stepping and space gridding, treatment of strong nonlinearities, algorithm implementation for large scale problems subject to computing time and storage restrictions. As many of the described problems are near the border of tractability, all of the different issues are typically connected in the treatment of a particular problem. A basic knowledge of all of the different aspects described herein seems to be extremely helpful when attacking any realistic computational problem.

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(* indicates speaker among several authors)