REVIEWS AND DESCRIPTIONS OF TABLES AND BOOKS

The numbers in brackets are assigned according to the American Mathematical Society classification scheme. The 1980 Mathematics Subject Classification (1985 Revision) can be found in the December index volumes of Mathematical Reviews.

29[65–02, 65Mxx, 65Nxx].—STEPHEN F. MCCORMICK (Editor), *Multigrid Methods*, Frontiers in Applied Mathematics, Vol. 3, SIAM, Philadelphia, PA, 1987, xvii + 282 pp., 24 cm. Price $38.50.

There has been a great deal of research activity in the study of multigrid methods during the past two decades. The literature in this area is growing rapidly. However, very few books exist that give an overview of the method. This book, which consists of chapters written by experts in the field, is intended to meet such a need.

The book begins with an introductory chapter written by W. Briggs and S. McCormick. This chapter stands alone as a basic introduction to some of the essential principles of multigrid methods. Another purpose of this chapter is to lay the groundwork for the chapters that follow and, in particular, most of the notational conventions for the book are explained.

The second chapter, written by P. Wesseling, is devoted to multigrid methods designed for linear partial differential equations, with a focus on finite difference and finite volume discretization. The presentation concentrates mainly on the practicalities of the method. By considering model equations such as those arising from second-order elliptic boundary value problems, the major components of the multigrid method, namely prolongation, restriction and smoothers, are discussed. Some numerical experiments are presented. This chapter also contains a description and comparison of some multigrid software that existed up to the date of publication.

The subject of Chapter 3 (written by P. Hemker and G. Johnson) is multigrid approaches to the Euler equations. Facing the fact that a thorough mathematical basis is still missing, the authors adopt the point of view that practical developments and results obtained by multigrid Euler solvers have great potential in this branch of multigrid research. A number of algorithms that have proven to be efficient numerically are discussed in the two-dimensional case.

In Chapter 4, an introduction of the so-called algebraic multigrid (AMG) method is given by J. Ruge and K. Stüben. The authors demonstrate how to use the principles of the usual multigrid method to solve a matrix equation that

0025-5718/91 $1.00 + $.25 per page

does not have a natural multilevel structure. Discussions are presented on the setup of the multilevel structure, construction of multilevel components and the relationship with the usual multigrid method. Some theoretical analysis is also given. Many applications of the method and some directions of present and future research are discussed.

In contrast to the first four chapters of the book, Chapter 5, by J. Mandel, S. McCormick and R. Bank, is solely devoted to the theoretical aspects of the multigrid method. Based on the features of the method with respect to second-order elliptic boundary value problems discretized by finite elements, an abstract framework is presented for the convergence theory of multigrid methods. The theory is built upon a number of abstract algebraic assumptions, and both symmetric and nonsymmetric problems are discussed. This chapter includes a number of exercises and some research problems that a beginning multigrid researcher may find inspiring.

In addition to the five chapters described above, the book includes a list of over six hundred papers, a rather complete survey of the multigrid literature up to the year of 1986. Furthermore, the KWIC reference guide (at the end of the book) that groups the papers by key words, is extremely convenient to use. There is no doubt that this book is a very helpful and convenient reference for any researcher or practical user of multigrid methods.

Since multigrid is still a very young and rapidly changing field, some material in the book may be better presented today by using the latest developments. For example, the theory in Chapter 5 can be extended and some of the problems, open at the time, now have solutions. Nevertheless, this does not diminish the value of the book.

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30[70–01, 82–01, 82A50, 70–04, 82–04].—M. P. ALLEN & D. J. TILDESLEY, *Computer Simulation of Liquids*, Oxford Science Publications, Clarendon Press, Oxford, 1987, xix + 385 pp., 24 cm. Price $95.00.

This book was first published in 1987, but a paperback edition (with corrections) appeared in 1989. Its primary objective is to be a primer for the physical scientist who wants to do computational simulations (see the review by Banavar [1]). However, it can also provide the computational mathematician an introduction to some aspects of computational chemistry.

Computational chemistry is a broad subject with numerous subspecialties. Two of these, molecular dynamics simulations and Monte Carlo methods, are the primary subjects of the book. Quantum mechanical effects are excluded from most of the models discussed in the book, but they are discussed extensively in one chapter and briefly elsewhere.

Computational chemistry has received less attention historically from the computational mathematics community than, say, computational problems in continuum mechanics. There is a rich set of mathematically oriented research problems arising from computational chemistry, and this book provides a good starting place for understanding them. One should not assume, however, that the computational techniques discussed represent the latest developments, as this subject is developing rapidly. We will illustrate this by focusing on molecular dynamics and describing some recent advances.

The basic models of molecular dynamics will be easily grasped by most computational mathematicians. They involve classical mechanics, although the forces, F, between atoms may be more complicated than the gravitational or electrostatic forces encountered in basic mechanics. The most computationally intense parts of the simulation are the evaluation of the forces between atoms (on the face of it, a computation involving $\mathcal{O}(N^2)$ operations for N atoms) and the solution of the resulting ordinary differential equations for the positions, x, of the atoms which express essentially that

$$F = m\frac{d^2x}{dt^2}.$$

The book under review presents complete details regarding the coding of algorithms at a level comparable to what is found in Forsythe, Malcolm, and Moler [5]. Elementary tricks for avoiding unnecessary operations (e.g., square root) are described and complete codes are given in Fortran. However, some more advanced applications of computational science to chemical simulations must be sought elsewhere. For example, there is no discussion of algorithms appropriate for parallel computers, a subject still in its infancy at the time of the writing of the book. Moreover, efficient algorithms for evaluating the forces among atoms have been introduced recently using diverse techniques not described in the book. The evaluation of Coulombic forces has been considered by Greengard and Rokhlin [7] using multipole expansions. The general problem of computing the interaction forces (Coulombic or otherwise) between so-called nonbonded atoms has been attacked by Boris et al. ([2, 3, 8]) using specialized data structures.

Researchers interested in the numerical time-integration of ordinary differential equations may be intrigued by the techniques discussed in this book. Molecular dynamics requires long-time integration, and the ordinary differential equations are stiff. The technique advocated most strongly in the book is a simple, implicit 2nd-order method, and it is said that more sophisticated methods, such as the Gear methods, are less efficient. This stems perhaps from the fact that the stiffness is associated with highly oscillatory modes as opposed to rapidly decaying ones. More recently, work has been done on more complicated time-stepping schemes [6, 10, 11, 12]. Other methods that have been used for molecular dynamics are described in Appendix 1 of [9].

Computational chemistry poses distinct and challenging problems for computational mathematics. The book by Allen and Tildesley is the right place to start for someone interested in entering the subject. For additional material regarding molecular dynamics simulations and Monte Carlo methods, with an emphasis on some applications, one could continue studying the subject with [4] and [9].

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1. J. R. Banavar, Physics Today, March, 1989, pp. 105–106.
2. J. P. Boris, *A vectorized "near neighbors" algorithm of order N using a monotonic logical grid*, J. Comput. Phys. **66** (1986), 1–20.
3. ——, *New directions in computational fluid dynamics*, Ann. Rev. Fluid Dynamics **21** (1989), 345–385.
4. C. L. Brooks III, M. Karplus, and B. M. Pettitt, *Proteins: A theoretical perspective of dynamics, structure, and thermodynamics*, Wiley, New York, 1988.
5. G. E. Forsythe, M. A. Malcolm, and C. B. Moler, *Computer methods for mathematical computations*, Prentice-Hall, Englewood Cliffs, N.J., 1977.
6. R. Friesner, private communication.
7. L. Greengard and V. Rokhlin, *On the evaluation of electrostatic interactions in molecular modeling*, Chemica Scripta **29A** (1989), 139–144.
8. S. G. Lambrakos, J. P. Boris, et al., *Molecular dynamics simulation of $(N_2)_2$ formation using the monotonic Lagrangian grid*, J. Chem. Phys. **90** (1989), 4473–4481.
9. J. A. McCammon and S. Harvey, *Dynamics of proteins and nucleic acids*, Cambridge Univ. Press, 1987.
10. C. S. Peskin and T. Schlick, *Molecular dynamics by the backward-Euler method*, Comm. Pure Appl. Math. **42** (1989), 1011–1031.
11. T. Schlick and C. S. Peskin, *Can classical equations simulate quantum-mechanical behavior? A molecular dynamics investigation of a diatomic molecule with a Morse potential*, Comm. Pure Appl. Math. **42** (1989), 1141–1163.
12. C. S. Peskin, *Analysis of the backward-Euler/Langevin method for molecular dynamics*, Comm. Pure Appl. Math. **43** (1990), 599–645.

31[65–02, 65D07, 65D10, 62–07].—GRACE WAHBA, *Spline Models for Observational Data*, CBMS-NSF Regional Conference Series in Applied Mathematics, Vol. 59, SIAM, Philadelphia, PA, 1990, xii + 169 pp., 25 cm. Price: Softcover $24.75.

This book deals with the problem of fitting noisy data in one or several variables using various types of *smoothing splines*. Such splines arise as the solution of minimization problems where the quantity to be minimized is some combination of *goodness of fit* such as the sum of squares of the deviations and *smoothness* such as integrals involving derivatives of the fitting function.

On one level, the book can be regarded as a rather complete unified treatment of smoothing splines, starting with the classical polynomial smoothing spline, and including discussions of the periodic case on a circle, both scalar- and vector-valued splines on the sphere, and thin-plate splines in the plane (or in higher-dimensional Euclidean space). In addition, two special kinds of

smoothing splines, called partial splines and additive splines, are treated. All of these splines are studied from the standpoint of *reproducing kernel Hilbert spaces*, and for each of the cases treated, the associated reproducing kernel is given explicitly. These fitting methods have numerous applications. As examples, the author mentions or discusses the fitting of economical, medical, meteorological, and radiation data. She also treats the use of smoothing spline methods for solving Fredholm integral equations of the first kind, for solving fluid flow problems in porous media, and for solving inverse problems. The book develops various methods of computing the smoothing parameter, including ordinary cross-validation, generalized cross-validation, and others. Finally, numerical methods for computing smoothing splines are also discussed in depth.

On another level, the book is something quite different: it is a detailed explanation of the role of splines in statistical modelling, and in particular the link to Bayesian estimation. At this level, the cast of characters changes from Sobolev spaces and linear functionals to a plethora of statistical objects, ranging from minimum variance linear unbiased Bayes estimates to design of experiments. Statisticians will delight in the appearance of Butterworth filters, variograms, kriging, degree of freedom of signal, unbiased risk estimates, generalized maximum likelihood estimates, confidence intervals, bootstrapping, projection pursuit, loss functions, log likelihood ratios, components of variance, null hypotheses, random effects models, locally most powerful invariant tests, hazard models, etc.

This very readable book should appeal to both audiences; i.e., to approximation theorists and numerical analysts and their clients, as well as to statisticians and model builders, and it is to be hoped that it will help build bridges between these areas. The material is drawn from a series of lectures presented at a CBMS conference held in 1987, and is designed to be read by anyone with a basic knowledge of Hilbert spaces. To insure a smooth start, the author devotes the first chapter to reproducing kernels and their properties. The remaining material is divided into an additional eleven chapters. A list of approximately 300 references is included.

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32[20–02, 20D05, 20E99].—DEREK F. HOLT & W. PLESKEN, *Perfect Groups*, Oxford Mathematical Monographs, Oxford University Press, New York, 1989, xii + 364 pp., 2 microfiche supplements, 24 cm. Price $70.00.

Since the completion of the classification of finite simple groups, the question arises as to what further collections of finite groups to classify. The authors of this book begin work on the perfect groups, i.e., ones which equal their own commutator subgroup.

Their main tool is the computer, which, supplemented by a lot of modular representation theory and group cohomology, enables them to produce numerous perfect extensions of p-groups by known perfect groups. Their aim was to

classify all perfect groups of order less than a million. They do not quite make it (but see summary, pp. 260–264), there being too many extensions of large 2-groups by the simple groups of order 60 and 168. However, they do an incredible amount of work, both theoretical and computational, vastly extending Sandlöbes' classification of perfect groups of order less than 10^4 [2].

This is a great book for group theorists to dip into, since it brings together all kinds of interesting theorems hidden in the literature. Someone interested, for example, in universal Frattini extensions can find a thorough discussion here. The authors' claim that the book is self-contained, however, might be questioned. They have included accelerated introductions to, e.g., modular representation theory, but for many of the theorems they still have to quote results. That said, it is great to see these theories in action. There are many examples worked out in detail, supplemented by interesting exercises for the reader.

The tables of perfect groups occupy most of the book, extending for hundreds of pages. They are similar to the Atlas [1]. They lack discussion of subgroups, but go on extensively about the cohomology of the groups. Character tables of certain perfect groups are included in a microfiche appendix by W. Hanrath. These are quotients of space groups, which are extensions of lattices by finite groups acting faithfully. One of the best ways to produce finite perfect groups was to find such quotients, and so the book contains theory and tables of perfect space groups.

All in all, an impressive book that makes some very complicated material easily readable.

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1. J. H. Conway, R. T. Curtis, S. P. Norton, R. A. Parker, and R. A. Wilson, *Atlas of finite groups—Maximal subgroups and ordinary characters for simple groups*, Clarendon Press, Oxford, 1985.

2. G. Sandlöbes, *Perfect groups of order less than* 10^4, Comm. Algebra **9** (1981), 477–490.

33[65–06, 65N20, 65N30].—TONY F. CHAN, ROLAND GLOWINSKI, JACQUES PERIAUX & OLOF B. WIDLUND (Editors), *Domain Decomposition Methods for Partial Differential Equations*, Proceedings in Applied Mathematics, Vol. 43, SIAM, Philadelphia, PA, 1990, xx + 491 pp., $25\frac{1}{2}$ cm. Price: Softcover $58.50.

This book is the proceedings of the Third (annual) International Symposium on Domain Decomposition Methods for Partial Differential Equations held in Houston in March, 1989. The fourth of this series has already occurred in Moscow, and the proceedings from it will also be published by SIAM.

The rubric "domain decomposition" embraces a broad set of research interests, from the theory of partial differential equations to numerical algorithms for their solution. The book includes an excellent historical introduction which first appeared in SIAM News [1] and which describes the subject's origins in the theory of partial differential equations and subsequent development. The introduction [1] also includes some comments on the highlights of the Houston meeting, some of which (unfortunately) are not represented in the published proceedings.

It is noted in the introduction [1] that most commercial codes for solving partial differential equations utilize Gaussian elimination in one form or other. More sophisticated methods as discussed in this book obviously offer some possibility of improved efficiency for solution of the linear equations resulting from discretizing partial differential equations. However, missing from the symposium was a critical evaluation of the relative efficiency of the serious competitors for rapid solution of the linear equations resulting from discretizing partial differential equations. In addition to domain decomposition, one would also want to consider some form of multilevel iterative technique ("multigrid") and efficient node numbering schemes for Gaussian elimination (e.g., minimum degree or nested dissection) as well as possibly others. The question of computational complexity of the competing algorithms becomes even more difficult when parallel computers are to be used, as indicated by Part III of the book.

This book represents the state of the art of domain decomposition methods for partial differential equations as of March, 1989. As such it is clearly a must for anyone working in the field or related ones.

R. SCOTT

1. O. Widlund, *Domain decomposition algorithms and the bicentennial of the French Revolution*, SIAM News **22**, July/August, 1989.

34[65–06].—J. C. DÍAZ (Editor), *Mathematics for Large Scale Computing*, Lecture Notes in Pure and Appl. Math., Vol. 120, Dekker, New York and Basel, 1989, xi + 345 pp., 25 cm. Price $85.00.

This book is based on the proceedings of a regional meeting of the American Mathematical Society held in Denton, Texas in 1986. However, it was not published until 1989 due to a lengthy refereeing process. The focus of the book is quite broad, although no more so than the title suggests. It contains both survey articles and original research papers. The principal unifying aspect of the book is the regional location of many of the authors.

The book represents well the breadth of subjects integral to scientific computing. If the individual papers that make up the book had been published in journals, they would have been dispersed among several having distinct objectives. Thus the book can serve as a good indicator of the variety of topics of current research in scientific computing for someone new to the field.

The contents of the book are as follows: On the Gauss-Broyden Method for Nonlinear Least-Squares *by A. Griewank and L. Sheng*; Parallel Adaptive Algorithms for Multiple Integrals *by A. Genz*; A Comparison of Hypercube Implementations of Parallel Shooting *by H. B. Keller and P. Nelson*; An Asymptotic Induced Numerical Method for the Convection-Diffusion-Reaction Equation *by J. S. Scroggs and D. C. Sorensen*; The Rate of Convergence of the Modified Method of Characteristics for Linear Advection Equations in One Dimension *by C. N. Dawson, T. F. Dupont, and M. F. Wheeler*; A Time-Discretization Procedure for a Mixed Finite Element Approximation of Contamination by Incompressible Nuclear Waste in Porous Media by *R. E. Ewing, Y. Yuan, and G. Li*; Implementation of Finite Element Alternating-Direction Methods for Vector Computers *by S. V. Krishnamachari and L. J. Hayes*; Performance of Advanced Scientific Computers for the Efficient Solution of an Elastic Wave Code for Seismic Modeling *by K. E. Jordan*; Generalized Gray Codes and Their Properties *by L. S. Barasch, S. Lakshmivarahan, and S. K. Dhall*; Nested Block Factorization Preconditioners for Convective-Diffusion Problems in Three Dimensions *by G. K. Leaf, M. Minkoff, and J. C. Díaz*; Performance of the Chebyshev Iterative Method, GMRES and ORTHOMIN on a Set of Oil-Reservoir Simulation Problems *by S. Gómes and J. L. Morales*; A Survey of Spline Collocation Methods for the Numerical Solution of Differential Equations *by G. Fairweather and D. Meade.*

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35[93-06, 93B40, 65-06].—K. BOWERS & J. LUND (Editors), *Computation and Control*, Progress in Systems and Control Theory, Vol. 1, Birkhäuser, Boston, 1989, xi + 410 pp., 23 $\frac{1}{2}$ cm. Price $49.00.

The proceedings of the 1988 Bozeman, Montana conference organized by Bowers and Lund reveal the symbiotic relationship of approximation and computation theory with control theory. These thirty published papers cover a broad spectrum of pure and applied mathematics. An indication of the contents is given by listing the titles of the works presented by the organizers and their four plenary speakers C. I. Byrnes, W. Gautschi, C. F. Martin, and F. Stenger:

"Efficient Numerical Solution of Fourth-Order Problems in the Modeling of Flexible Structures" by R. C. Smith, Bowers, and Lund;

"Accuracy and Conditioning in the Inversion of the Heat Equation" by Lund;

"Feedback Design from the Zero Dynamics Point of View" by Byrnes and A. Isidori.

"Orthogonality—Conventional and Unconventional—in Numerical Analysis" by Gautschi;

"Observability, Interpolation and Related Topics" by Martin.

"Explicit Approximate Methods for Computational Control Theory" by Stenger.

The book is printed directly from manuscripts presented in camera-ready form and is remarkably easy to read. It should be a valuable reference work and it augurs well for the success of the series.

E. I.

36[68–02, 65–02, 70–04, 68Q40, 65C99].—ROBERT GROSSMAN (Editor), *Symbolic Computation: Applications to Scientific Computing*, Frontiers in Applied Mathematics, Vol. 5, SIAM, Philadelphia, PA, 1989, x + 185 pp., 23 cm. Price $24.50 paperback.

These collected papers provide a timely summary of the state of symbolic/numerical algorithms and software for dynamical systems, Lie brackets and vector fields, finite difference operators and domains, and perturbation theory. Their particular interest lies in the diversity of approaches represented. The paper "Dynamicist's Workbench" by Abelson and Sussman describes an "automatic programming" technique that symbolically generates a "complete set" of numerical simulation programs to enumerate all "qualitatively different" behaviors of a physical system. At a different point on the spectrum, the papers "Multibody Simulation" by Sreenath and Krishnaprasad and "Symbolic Computations in Differential Geometry" by Akhrif and Blankenship present high-level user interfaces for the instantiation simulation, and visualization of physical systems under human control. The paper "FIDIL: A Language for Scientific Programming" by Hilfinger and Colella presents a *C*-like programming language that supports manipulation of domains and maps for finite difference schemes as first-class objects. The paper "Perturbation Methods and Computer Algebra" by Rand describes the use of computer algebra to automate the solution of nonlinear differential equations by perturbation methods. In the paper "Vector Fields and Nilpotent Lie Algebras" by Grayson and Grossman, the efficient symbolic computation of flows of ordinary differential equations is described. An introductory chapter by Fateman and Grossman sets the stage with a discussion of algebraic manipulation for operator algebras and operator actions.

The material in this volume offers the reader a broad yet detailed view of current progress towards a compelling goal: the combination of symbolic, numerical, and graphical computation for "user-friendly" modeling, visualization and analysis of physical systems. It is warmly recommended to all who share an interest in this goal.

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37[11-06, 11B37, 11B39].—G. E. BERGUM, A. N. PHILIPPOU & A. F. HORADAM (Editors), *Applications of Fibonacci Numbers*, Vol. 3, Kluwer, Dordrecht, 1990, xxiv + 357 pp., 24 $\frac{1}{2}$ cm. Price $99.00/Dfl.195.00.

This volume is made up of 36 of the 45 papers presented at the Third International Conference on Fibonacci Numbers and their Applications held in Pisa, Italy, from July 25 to July 29, 1988. These papers discuss applications of the Fibonacci numbers to such areas as: numerical analysis, elementary number theory, group theory, combinatorics, graph theory, cryptography, and many others.

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