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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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