Book Reviews

Statistical Mechanics: Fundamentals and Modern Applications. By Richard E. Wilde and Surjit Singh (Texas Tech University). Wiley-VCH: New York. 1997. $89.95. xv + 400 pp. ISBN 0-471-16165-9.

According to the authors this book is aimed at upperclass undergraduates and beginning graduate students as well as providing those not working in statistical mechanics with an overview of many new developments in the field. While it is terse in its derivations, all essentials are in place though the unsophisticated student might require some guidance between equations given in the text. An unusual feature of the text is the inclusion of fourteen short FORTRAN 77 programs in an appendix at the rear of the text. These are short text-mode programs ranging from Brownian motion and the Ising model to a simple one-dimensional molecular dynamics program using a Lennard-Jones fluid.

One of the features of the text is the inclusion of material unusual in a text at this level. There are three sections in the text. The first, titled Essentials, outlines both classical and quantum statistical mechanics including such topics as the ergodic hypothesis, the H-theorem, and Liouville's theorem as well as ensembles and classical and quantum ideal gases. All of this is done in 80 pages. The second section titled Equilibrium Statistical Mechanics deals with phase transitions, critical phenomena, the liquid state, methods and techniques of molecular dynamics, Monte Carlo methods, and polymers, proteins, and spin-glass models. Again, while the treatments are terse, they do cover most salient points. And, again, much of this material is simply not available in another text at this level. The second section takes up a few less than 100 pages. The third section is titled Nonequilibrium Statistical Mechanics and covers both classical and new material such as the Boltzmann equation, Brownian motion including the Langevin equation and Fick's laws, the Zwanzig−Mori formalism, kinetics in the form of the activated barrier-crossing problem, oscillating chemical reactions, and cellular automata as models of systems. This section takes up about 150 pages. The FORTRAN programs and a few appendices fill the remaining 30 or so pages.

Several things are striking about this book: the first is the broad range of coverage. Some mention can be found here of almost any subject its audience might raise. References are given covering not only the classical papers but significant later contributions up through the early part of this decade. Another striking thing is the fact that the derivations are very concise. As a text in a lecture course this will cause no trouble. The solitary neophyte may have some difficulty. Lastly, the authors are to be complemented for including programs to illustrate, in a general way, modern computations. The programs are easily extended and, with a little ingenuity, can be made graphical to fit most current computer interfaces.

Paul J. Gans, *New York University*

JA9856102

10.1021/ja9856102

Computational Grids, Generation, Adaptation and Solution Strategies. By Graham F. Carey (University of Texas at Austin). Taylor & Francis: Bristol. 1997. xiii + 496 pp. $69.95. ISBN 1-56032-635-2.

This book covers a particularly wide range of methods and ideas in computational techniques. Perhaps some of these methods are outdated and are no longer in common use. However, the inclusion of their detail in the wide span of the methods listed in the book takes the reader to points of reference in the logical and perhaps historical development of computational grids.

The author's focus starts on structured quadrilateral and triangular meshes. Finite difference schemes are significantly simplified when the connectivity of adjacent nodes is uniform throughout the interior domain. The restrictions of structured grids defy the purpose of mesh adaptation to the widest range of applications. This takes the author to the Delaunay idea of optimal trangulation, and to grid smoothing using the Delaunay/Voronoi ideas. The reader is led through the development of trangular techniques in meshing of irregular domains. The Delaunay idea is then expanded with Voronoi polygons, naturally leading to Voronoi polyhedral grids in three-dimensional computations. Data structures as means of efficiently balancing computations and storage strategies are sufficiently elucidated. The inclusion of Sierpinski gaskets and fractal principles enriches the discussion and provides the reader with a little window on fractal geometry.

Readers who are seeking in-depth knowledge and practice in one particular grid technique or direction in meshing may well be advised to consult more specialized literature. However, the book is of a definite value for the reader who is engaged in a scanning process of computational grids and meshing.

For example, the author discusses posteriori error indicators and postprocessing algorithms, introducing norm formulations, adaptive refinement, and a host of error estimates, extrapolation, and residuals. This leads naturally to a lucid account of the Galerkin and Collocation methods. More detail on refinement algorithms is given in chapter four. The purpose of the adaptive refinement strategy is to automate the meshing process using an accurate approximate solution of the problem. Strategies for one-dimensional and two-dimensional refinements lead to a discussion of singularities and data structure. This leads the author to a detailed account of sparse solutions, element-by-element iterative solutions with refinement, as well as nonlinear solutions. Iterative methods including SOR, ADI, Jacobi, and Galerkin are followed by the nonlinear techniques. Data structures are called upon here. Local elliptic projections are described as a refinement strategy, and upwinding is discussed in the context of oscillations and stability of solutions.

The author also touches upon methods of domain decomposition and multigrids. Adaptive and nonlinear multigrids are briefly discussed. The impact of higher-order methods on the degree of element basis in the finite-element method, or on higher-order difference formulas in finite-difference methods, is meshed with adaptive methods.

Optimizing solution strategy by grid point redistribution is presented as an alternative to optimizing solutions through higher level approximations. The author briefly describes optimization algorithms. Finally, in the last chapter the author groups strategies for moving grids. Applications in sciences and engineering provide us more frequently with unsteady state solutions with higher gradients. Wave propagation, material discontinuities and phase interfaces, and problems involving chemical reactions are prime examples. The discussion of moving grids leads naturally to a brief view of the method of characteristics.

The book is not rich in illustrations and graphics. Although each chapter is followed by a good number of conceptual questions, computational examples and references to practical solutions are few. The author however delves frequently into the kind of complex mathematical detail that might be better explained by examples. Some of the concepts used in this detail are probably unfamiliar to the average science or engineering reader. Dr. Carey's book is a useful inventory of computational methods described through the principles of constructing computational grids. There is a definite bias in the book toward finite-element techniques, but the book should be useful to readers whose interest lies in other numerical methods.

M. Nabil Esmail, *Concordia University*

JA975642+

10.1021/ja975642+