## Books Received

### Simulations for Solid State Physics
Robert H. Silsbee and Jorg Drager
Cambridge University Press, New York, 1997; ISBN 1-521-59094-9; 348 pp., cloth plus CD-ROM, $59.95 (also available in a student edition without CD-ROM: ISBN 1-521-59911-3, 384 pp., paper, $24.95).

### Web-Teaching
David W. Brooks
Plenum, New York, 1997; ISBN 0-306-45552-8; 213 pp., paper, $25.00.

### The Art of Molecular Dynamics Simulation
Dennis C. Rapaport
Cambridge University Press, New York, 1997; ISBN 0-521-59942-3; 400 pp., paper, $39.95.

### Quantum Communication, Computing, and Measurement
O. Hirota, A.S. Holevo, and C.M. Caves, editors
Plenum, New York, 1997; ISBN 0-306-45685-0; 546 pp., cloth, $139.00.

### Numerica: A Modeling Language for Global Optimization
Pascal Van Hentenryck, Laurent Michel, and Yves Deville
MIT Press, Cambridge, MA, 1997; ISBN 0-262-72027-2; 210 pp., paper, $25.00.

### Mathematica for Scientists and Engineers
Richard Gass
Prentice Hall, Upper Saddle River, NJ, 1997; ISBN 0-13-227612-7; 498 pp., paper plus CD-ROM, $42.00.

### Scientific Computing: An Introductory Survey
Michael T. Heath
McGraw-Hill, New York, 1997; ISBN 0-07-027684-6; 408 pp., cloth, $62.50.

### Using PLAPACK
Robert A. van de Geijn
MIT Press, Cambridge, MA, 1997; ISBN 0-262-72026-4; 194 pp., paper, $27.50.

tions include the finite square well. The list goes on, and in every case Tam is careful to provide a precise statement of the problem and the associated physical principles. The code is well documented and clever, but right in line with the principles discussed in Part I. Armed by the information presented here, students (and professors!) will be able to apply elegant symbolic programming to most any subject area.

There are a few areas in which the book could be improved. For example, common pitfalls could be emphasized more, especially those likely to be encountered by nonmathematicians. One such pitfall involves the physicist's Unwritten Rule that all constants are real unless declared complex. Adherence to this convention often presents physics students with difficulties when they try to use Mathematica to solve homework problems that involve complex numbers. Tam provides at least two antidotes, but these appear almost parenthetically within discussions of fairly advanced programming topics, and may not come soon enough to help the unsuspecting quantum-mechanics student. I would also like to see a discussion of issues relating to data analysis, such as reading and writing data files, nonlinear fitting, and data-smoothing techniques.

Tam suggests using the text for a one-semester introduction to programming and numerical analysis, or as a supplement in upper-level core physics courses. There are a number of good problems at the end of each chapter, and solutions to the odd-numbered ones are provided in an appendix. Regardless of whether it is used formally in a course or for a self-paced tutorial, this book provides a clear and effective learning resource that is also an outstanding reference.

### References

1. Stephen Wolfram, *Mathematica*, 2nd ed. (Addison-Wesley, Reading, MA, 1991). The subtitle has (thankfully) been removed from the third edition.
2. Roman Maeder, *The Mathematica Programmer* (Academic Press, New York, NY, 1993). ◆


## Molecular Modeling, Basic Principles and Applications

H. D. Holtje and G. Folkers
Methods and Principles in Medicinal Chemistry, edited by R. Mannhold, H. Kubinyi, and H. Timmerman, Vol. 5 Wiley/VCH, Weinheim, New York, Basel, Cambridge, and Tokyo, 1997; ISBN 3-527-29384-1; 194 pp., cloth, $140.00.

Reviewed by Alenka Luzar

An important feature of advanced molecular biophysics at the end of the twentieth century, particularly in the arena of pharmaceuticals and biotechnology, is the use of computational molecular modeling for de novo ligand and protein design.[1,2] A big success story in structure-based design is the HIV-1 protease inhibitor.[3] This enzyme is crucial to the replication of the HIV virus, and so inhibitors may have therapeutic value as anti-AIDS treatments. This success was made possible in part by developing tools to predict the three-dimensional structures of drug and receptor molecules, and to enable the visualization of their molecular surface properties and the optimization of drug-receptor interactions.

Holtje and Folkers's book offers a practical introduction to this important field of molecular modeling. The book

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