An Introduction to Computational Physics

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BOOK REVIEWS

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Computational Physics. Rubin H. Landau and Manuel Páez. 520 pp. Wiley, New York, 1997. Price: $69.95 ISBN 0-471-11590-8.

An Introduction to Computational Physics. Tao Pang. 374 pp. Cambridge U.P., New York, 1997. Price: $85.00 (cloth) ISBN 0-521-48143-0; $39.95 (paper) ISBN 0-521-48592-4.

Stochastic Simulation in Physics. P. Kevin MacKeown. 456 pp. Springer, New York, 1998. Price: $59.00 (paper) ISBN 9813083263. (Reviewed by Harvey Gould and Jan Tobochnik.)

The rapidly increasing importance of computers in physics has led to the publication of many books on various aspects of the subject. In the following, we review three new textbooks on computational physics. In addition to these we also note the recently published *Computational Physics* by Nicholas Giordano (Prentice–Hall, 1997) and the second edition of our own *Introduction to Computer Simulation Methods* (Addison–Wesley, 1996).

Landau and Páez's book begins with an excellent introduction to the nature of computational science and how it differs from computer science. Part I introduces various general ideas and methods, such as fixed and floating point numbers, roundoff errors, and methods of integration. We found the discussion of the first two topics particularly useful. Part II of the text emphasizes applications, which include data fitting, random number generators, the numerical solution of differential equations, nonlinear systems, matrix computations, high performance computing, object-oriented programming, simulations of the Ising model, and fractals. Parts III and IV treat linear and nonlinear partial differential equations, respectively.

The discussion of such a wide range of applications illustrates the interdisciplinary nature of computational physics and ensures that readers will find at least several topics which interest them. However, such broad coverage carries with it the danger that some of the discussion will be too brief, and in a few cases might even be misleading. In the discussion of the Ising model (a topic close to our own research interests) we found many statements that could be misinterpreted by students and professors who are not expert in statistical mechanics or simulations. An example is the statement that the measured heat capacity in a simulation of the two-dimensional Ising model ''...should diverge at the transition (you may get only a peak).'' In fact, the heat capacity is divergent only in the limit of an infinite system, and simulations of a finite system *can* only exhibit a peak.

The authors make frequent reference to materials available on their Web site, http://www.physics.orst.edu/~rubin/CPbook/, and to other sites as well. Although the text can be used independently of the Web, we found that the information referenced by the authors enhances the text. We believe that the complementary use of the Web is a harbinger of the way texts will be written and used in the future.

Many program listings are given in FORTRAN and C. Unfortunately, the former are in FORTRAN 77 rather than Fortran 90 or F. Fortran 90 compilers are readily available (though expensive), while F is freely available on Linux and is reasonably priced on other platforms. The programs do not incorporate the use of graphics; the authors acknowledge the importance of graphics, but expect readers to plot their results using separate programs.

The strength of the text is the discussion of numerical and programming methods, rather than simulations. We particularly enjoyed reading the chapters on computing hardware, high-performance computing, parallel computing and parallel virtual machine (PVM), object-oriented programming, solitons and the Korteweg–de Vries and Sine–Gordon equations. An excellent course could easily be based on these topics. Landau and Páez's book would be an excellent choice for a course on computational physics which emphasizes computational methods and programming.

Pang's *An Introduction to Computational Physics* is a clearly written text which covers just about every area of the subject including general comments about computational science, topics in numerical analysis such as numerical methods for matrix operations, computer simulations using both molecular dynamics and Monte Carlo techniques, and a survey of symbolic and high performance (parallel) computing. In the preface Pang states that ''Computational physics, in my view, is the foundation of computational science.'' We agree, and encourage the physics community to participate actively in interdisciplinary programs in computational science and engineering. The text describes wavelet transforms as well as Fourier transforms, finite difference and finite element methods, and discussions of percolation, the renormalization group, quantum Monte Carlo, the Car–Perrinello simulation scheme, random number generators, critical slowing down, Boltzmann lattice gas methods, and even groundwater dynamics. The author has avoided some fashionable topics such as fractals, cellular automata, chaotic maps, and random walks. As is typical of computational physics texts, the large number of topics means that most of them are not covered in depth. We agree with the author's claim that the first six chapters on basic numerical analysis are accessible to well prepared undergraduates. However, many of the more interesting topics in later chapters are treated in a way that is too formal or too advanced for most undergraduates and even many graduate students. Even though the writing is clear, much background would be needed to follow these chapters. However, these advanced chapters offer an excellent start for a graduate student or researcher who wants to learn about a new technique. In most cases additional materials would be needed to write actual programs.

The text was carefully put together and well edited. Typographical and grammatical errors are few. Algorithms are illustrated by subroutines written in FORTRAN 77, and there are some complete program listings. The FORTRAN 77 code appears ancient. However, Fortran 90 and C programs are available at http://www.physics.unlv.edu/~pang/cp.html. Several relatively straightforward exercises are given at the end of each chapter. In the later chapters there is little guidance as to the difficulty of the exercises; a four line problem might actually be material for a term paper or an undergraduate research project.

As with MacKeown's book, there is little or no mention of graphics, interactive computing, or object oriented programming. Our preference would be to use this book in a course where the students already have some programming experience.

Unlike the first two books, the text by MacKeown focuses exclusively on Monte Carlo techniques. He provides a more extensive introduction to basic statistics, random number generators, and sampling, than the other texts, and covers topics such as percolation, genetic algorithms, simulated annealing, random walks, Monte Carlo simulations in thermal physics, and quantum Monte Carlo. In addition, he has a chapter on particle transport, which is not found in the other books.

The text is at the advanced undergraduate level, but like the others it is uneven in level of difficulty. Whereas most of it would be accessible to undergraduates, the chapter on quantum Monte Carlo and subsections of some other chapters would be more appropriate for graduate students. The coverage is also uneven. For example, in the discussion of percolation, a fair amount of time is spent on the Hoshen–Kopelman algorithm for cluster counting, but no mention is made of finite size scaling, which would be the most useful method for analyzing the data. The chapter on Monte Carlo in thermal physics includes discussions of different ensembles, cluster algorithms, histogram analysis, and umbrella sampling, but does not say much about extensions to simulations of off-lattice particle systems.

This book would be difficult to use as a stand-alone text. The number of exercises is too small; some chapters have only two or three, and there are none in the chapter on quantum Monte Carlo. Many of the exercises involve derivations, rather than designing and running simulations. Very few of the exercises encourage much exploration by the student. There are no full program listings and only three FORTRAN subroutines are given in the appendix. There are some step-by-step listings of algorithms, but more would have been helpful. The focus on physics and algorithms is excellent, but some discussion of the actual implementation would be desirable.

The illustrations are crude by today's standards, and the text was not well edited. There are many typographical errors (for example on page 101 it appears that a paragraph was not finished), and some of the grammar is either awkward or incorrect. Also some of the writing is confusing. For example, the author seems to imply that a measure of the temperature for an isolated system is the mean energy per degree of freedom. In general, this statement is not correct.

Overall, MacKeown's book has more coherence than Landau and Páez's, and is less formal than Pang's. If your interests include Monte Carlo methods, it would be a useful supplement.

The fact that all three texts are uneven in level is not surprising, given that the difficulty of the physics and that of the programming are not directly correlated. The same comment could be made as well about other computational physics texts. Unlike many physics texts, the authors convey their enthusiasm for learning physics with computers and give students an entrée to current research.

All three books should be made available to students, and they all belong on the shelf of any computational physicist. We learned something from each of them. Given the eclectic nature of most courses on computational physics and numerical methods, many teachers and students will choose to use more than one text in their courses.

Now that the physics community has many choices of books which introduce the broad range of problems that can be approached using computational methods, our priority should be to incorporate the use of computers into the rest of the curriculum. We need more texts which integrate computational and analytical methods in areas such as electrodynamics, mechanics, quantum mechanics, and thermal physics. As this integration takes place, we expect that the relative importance of the various areas of physics will change.

As computers become better integrated into the physics curriculum, we need to remind ourselves, and especially our students, that our main goal in teaching and learning physics is to understand nature in the simplest possible terms. For this reason our use of computers as physicists will differ in emphasis from the use of computers in everyday life, where they mainly serve to convey information. The use of computers in physics, as exemplified by the texts reviewed here, does not yield the same instant gratification as might be found in some other computer applications. As teachers, we need to provide students with opportunities to learn that computers do not lessen the need for thinking deeply, and that such thinking has its own rewards.

Harvey Gould, hgould@clarku.edu, and Jan Tobochnik, jant@kzoo.edu, are coauthors of an undergraduate text on computer simulations. A listing of most of the available books on computational physics can be found on their Web site at http://sip.clarku.edu/books.html. They have just begun a new NSF-sponsored project to incorporate computers into the statistical and thermal physics curriculum (http://stp.clarku.edu). Gould's main research interests involve supercooled liquids near the glass transition, and Tobochnik's most recent work has been on simulations of phospholipids.

The Mathematics of Projectiles in Sport (Australian Mathematical Society Lecture Series, 6). Neville De Mestre. 175 pp. Cambridge U.P., New York, 1990. Price $30.95 (paper) ISBN 0-521-39857-6. (Reviewed by Rod Cross, School of Physics, University of Sydney, Sydney 2006, Australia, electronic mail: cross@physics.usyd.edu.au)

Mini-review. *From time to time one runs across a little-known book that deserves a wider audience. If you know of one, and would like to call it to the attention of the physics community, please submit a one-paragraph review, such as the one below, and we will be happy to consider it for publication.*

David Griffiths, Book Review Editor.

I recently discovered a small gem hidden away in our math library. It would be excellent reading for anyone interested in the physics or mathematics of sport. It is called **The Mathematics of Projectiles in Sport**, by Neville De Mestre, published in 1990 by Cambridge University Press. It is the right length (175 pp.), and not too mathematical. It is written as a textbook for undergraduates, starting with motion under gravity alone, and works its way through the aerodynamics of linear drag, nonlinear drag, lift, wind effects, and spin. Coriolis, air density, and gravity corrections are also considered. It is full of interesting examples, both analytical and numerical, includes about ten problems at the end of each chapter, and has a list of 65 references, including articles from this journal. The author lectured at the Australian Defence Force Academy at the time of writing, which perhaps accounts for his interest in projectiles and his insights into the practical applications of the subject. It covers most sports involving projectiles, including human projectiles, and describes some phenomena that might perplex North American readers (''Joel Garner from the West Indies cricket team hit a massive six that went up as high as it went forward.''). Frisbees, boomerangs, and dam busting balls are described, along with golf balls, tennis balls, baseballs, basketballs, footballs, cricket balls, seeds, shells, arrows, ski jumpers, and kangaroos, some in more detail than others.

BOOKS RECEIVED

Accretion Processes in Star Formation. Lee Hartmann. 237 pp. Cambridge U.P., New York, 1998. Price: $69.95 ISBN 0-521-43507-2.

Albert Einstein's Special Theory of Relativity: Emergence (1905) and Early Interpretation (1905–1911) (paperback edition). Arthur I. Miller. 446 pp. Springer, New York, 1981, 1998. Price: $39.95 (paper) ISBN 0-387-94870-8. [Reviewed Am. J. Phys. **50**, 476 (1982).]

Basic Notions of Condensed Matter Physics (paperback edition). Philip W. Anderson. 549 pp. Addison-Wesley, Reading, MA, 1984, 1997. Price: $39.00 (paper) ISBN 0-201-32830-5.

Causal Asymmetries. Daniel M. Hausman. 300 pp. Cambridge U.P., New York, 1998. Price: $54.95 ISBN 0-521-62289-1.

Classical Electrodynamics, 3rd ed. John David Jackson. 808 pp. Wiley, New York, 1962, 1999. Price not given; ISBN 0-471-30932-X.

Experimental Techniques in Condensed Matter Physics at Low Temperatures (paperback edition). Edited by Robert C. Richardson and Eric N. Smith. 338 pp. Addison-Wesley, Reading, MA, 1988, 1998. Price: $35.00 (paper) ISBN 0-201-36078-0. [Reviewed Am. J. Phys. **57**, 287 (1989).]

Fundamentals of Ultrasonic Nondestructive Evaluation: A Modeling Approach. Lester W. Schmerr, Jr. 559 pp. Plenum, New York, 1998. Price: $125.00 ISBN 0-306-45752-0.

Galactic Astronomy. James Binney and Michael Merrifield. 796 pp. Princeton U.P., Princeton, NJ, 1998. Price: $99.50 (cloth) ISBN 0-691-00402-1; $35.00 (paper) ISBN 0-691-02565-7.

Gauge Theories of the Strong, Weak, and Electromagnetic Interactions (paperback edition). Chris Quigg. 334 pp. Addison-Wesley, Reading, MA, 1983, 1997. Price: $35.00 (paper) ISBN 0-201-32832-1.

Geometry, Particles, and Fields. Bjørn Felsager. 672 pp. Springer, New York, 1998. Price: $69.95 ISBN 0-387-98267-1.

Handbook of Radioactivity Analysis. Edited by Michael F. L'Annunziata. 771 pp. Academic, San Diego, CA, 1998. Price: $115.00 ISBN 0-12-436255-9.

Intermediate Quantum Mechanics, 3rd ed. (paperback edition). Hans A. Bethe and Roman Jackiw. 396 pp. Addison-Wesley, Reading, MA, 1964, 1997. Price: $39.00 (paper) ISBN 0-201-32831-3.

Kinetic Theory in the Earth Sciences. Antonio C. Lasaga. 811 pp. Princeton U.P., Princeton, NJ, 1998. Price: $99.50 ISBN 0-691-03748-5.

Luminescence of Solids. Edited by D. R. Vij. 427 pp. Plenum, New York, 1998. Price: $115.00 ISBN 0-306-45643-5.

Macroscopic Quantum Tunneling of the Magnetic Moment. Eugene M. Chudnovsky and Javier Tejada. 173 pp. Cambridge U.P., New York, 1998. Price: $54.95 ISBN 0-521-47404-3.

Monte Carlo Simulation in Statistical Physics: An Introduction, 3rd ed. K. Binder and D. W. Heermann. 150 pp. Springer, New York, 1988, 1997. Price: $24.95 (paper) ISBN 3-540-63265-4.

Musical Temperaments. Erich Neuwirth. 70 pp. (plus CD-ROM). Springer, New York, 1997. Price: $49.95 (paper) ISBN 3-211-83040-5.

Nuclear and Particle Astrophysics. Edited by J. G. Hirsch and D. Page. 297 pp. Cambridge U.P., New York, 1998. Price: $69.95 ISBN 0-521-63010-X.

Our Cosmic Origins: From the Big Bang to the Emergence of Life and Intelligence. Armand Delsemme. 322 pp. Cambridge U.P., New York, 1998. Price: $24.95 ISBN 0-521-62038-4.

Pauli and the Spin-Statistics Theorem. Ian Duck and E. C. G. Sudarshan. 512 pp. World Scientific, River Edge, NJ, 1997. Price $56.00 ISBN 981-02-3114-8.

Philosophical Concepts in Physics: The Historical Relation Between Philosophy and Scientific Theories. James T. Cushing, 424 pp. Cambridge U.P., New York, 1998. Price: $74.95 (cloth) ISBN 0-521-57071-9; $29.95 (paper) ISBN 0-521-57823-X.

Photon-Hadron Interactions (paperback edition). Richard P. Feynman. 282 pp. Addison-Wesley, Reading, MA, 1972, 1998. Price: $35.00 (paper) ISBN 0-201-36074-8.

Phthalocyanine Materials: Synthesis, Structure and Function. Neil B. McKeown. 193 pp. Cambridge U.P., New York, 1998. Price: $74.95 ISBN 0-521-49623-3.

Physics by Computer: Programming Physical Problems Using Mathematica and C. W. Kinzel and G. Reents. 289 pp. (plus CD-ROM). Springer, New York, 1998. Price: $49.95 ISBN 3-540-62743-X.

Physics for Computer Science Students, with Emphasis on Atomic and Semiconductor Physics, 2nd ed. Narciso Garcia *et al.* 557 pp. Springer, New York, 1991, 1998. Price: $59.00 ISBN 0-387-94903-8.

Principles of Chemical and Biological Sensors. Edited by Dermot Diamond. 334 pp. Wiley, New York, 1998. Price: $89.95 ISBN 0-471-54619-4.

Quantum Electrodynamics (paperback edition). Richard P. Feynman. 198 pp. Addison-Wesley, Reading, MA, 1961, 1998. Price: $35.00 (paper) ISBN 0-201-36075-6.

Quantum Gravity in 2+1 Dimensions. Steven Carlip. 276 pp. Cambridge U.P., New York, 1998. Price: $80.00 ISBN 0-521-56408-5.

Quantum Mechanics: A Modern Development (reprint). Leslie E. Ballentine. 658 pp. World Scientific, River Edge, NJ, 1990, 1998. Price: $58.00 ISBN 981-02-2707-8. [Reviewed Am. J. Phys. **59**, 1153 (1991).]

Quantum Mechanics: Special Chapters. W. Greiner. 378 pp. Springer, New York, 1998. Price: $59.95 (paper) ISBN 3-540-60073-6.

The Rock Physics Handbook: Tools for Seismic Analysis in Porous Media. Gary Mavko *et al.* 329 pp. Cambridge U.P., New York, 1998. Price: $64.95 ISBN 0-521-62068-6.

Selected Scientific Works of Hans Christian Ørsted. Translated and edited by Karen Jelved *et al.* 647 pp. Princeton U.P., Princeton, NJ, 1998. Price: $89.50 ISBN 0-691-04334-5.

Self-Organized Criticality: Emergent Complex Behavior in Physical and Biological Systems. Henrik Jeldtoft Jensen. 153 pp. Cambridge U.P., New York, 1998. Price: $32.95 (paper) ISBN 0-521-48371-9.

Shock Compression of Condensed Materials. R. F. Trunin. 167 pp. Cambridge U.P., New York, 1996. Price: $49.95 ISBN 0-521-58290-3.

Statistical Data Analysis, with Applications from Particle Physics. Glen Cowan. 197 pp. Oxford U.P., New York, 1998. Price not given; (cloth) ISBN 0-19-850156-0; (paper) ISBN 0-19-850155-2.

Statistical Mechanics: A Set of Lectures (paperback edition). Richard P. Feynman. 354 pp. Addison-Wesley, Reading, MA, 1972, 1998. Price: $35.00 (paper) ISBN 0-201-36076-4.

The Theory of Fundamental Processes (paperback edition). Richard P. Feynman. 172 pp. Addison-Wesley, Reading, MA, 1961, 1998. Price: $35.00 (paper) ISBN 0-201-36077-2.

Theory of Interacting Fermi Systems (paperback edition). Philippe Nozières. 370 pp. Addison-Wesley, Reading, MA, 1964, 1997. Price: $35.00 (paper) ISBN 0-201-32824-0.

Thermodynamics of Crystals (reprint). Duane C. Wallace. 484 pp. Dover, Mineola, NY, 1972, 1998. Price: $16.95 (paper) ISBN 0-486-40212-6.

Tuning, Timbre, Spectrum, Scale. William A. Sethares. 345 pp. (plus CD-ROM). Springer, New York, 1998. Price: $69.95 (paper) ISBN 3-540-76173-X.

Weyl Transforms. M. W. Wong. 158 pp. Springer, New York, 1998. Price: $44.95 ISBN 0-387-98414-3.

Why Things Are the Way They Are. B. S. Chandrasekhar. 254 pp. Cambridge U.P., New York, 1998. Price not given; (paper) ISBN 0-521-45660-6.

X-Ray Diffraction: A Practical Approach. C. Suryanarayana and M. Grant Norton. 273 pp. Plenum, New York, 1998. Price: $49.50 ISBN 0-306-45744-X.