An Introduction to Computer Simulation Methods: Applications to Physical Systems, 2nd Edition

Harvey Gould, Jan Tobochnik, Dawn C. Meredith, et al.

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BOOK REVIEWS:
TWO BOOKS ON COMPUTER SIMULATIONS

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An Introduction to Computer Simulation Methods: Applications to Physical Systems, 2nd Edition

Harvey Gould and Jan Tobochnik
Addison-Wesley, Reading, MA, 1996; ISBN 0-201-50604-1; 721 pp., cloth, $55.95.

Reviewed by Dawn C. Meredith

Computational physics is a mix of analytical work, physics, numerical methods, programming, and visualization; authors combine them in different measures to give uniquely different books. In the second edition of their introductory computational-physics text, Harvey Gould and Jan Tobochnik have chosen to emphasize the physics by writing about computer simulation. "Simulation mode," they tell us, "requires a minimum of analysis and emphasizes the exploratory mode of learning."

The authors encourage this mode in several ways. Many of the systems are simple enough to be understood by students with only freshman-level physics and calculus. These systems, such as coffee cooling, planetary motion, and electrostatics, can be defined by a few simple equations; hence the analytical work is not burdensome. The authors ask intriguing, open-ended questions and emphasize plotting and visualization. To make clear that learning should be a discovery process, they encourage instructors to use the materials in a laboratory-like setting. The authors include an inspiring array of topics (for example, universal period doubling, renormalization group, time-dependent Schrödinger equation), although the large number of topics forces the detail on each topic to be limited. Finally, they provide many references to facilitate further study of the topics presented.

Simulation is an important pedagogical tool. Even when a problem has an analytic solution, we can gain insight by using a simulation to understand why it must be so and to see with our eyes that it is so. Simulations in thermodynamics, for example, allow us to understand the system from a microscopic point of view. Using the molecular-dynamics code from this book, students can see the approach to equilibrium, calculate the self-diffusion coefficient by relating it to a microscopic quantity, and check the validity of the ergodic hypothesis. This kind of investigation allows the students to be active, and active learners are known to be more successful.

While it is the physics that organizes and motivates the book, the other aspects of physics computing are not ignored. The authors do not assume a knowledge of programming and so give attention in the first few chapters to teaching how to program. This includes detailed discussions of truncation versus roundoff error, methods of debugging, structured programming, and integers versus real numbers. Some of the assigned problems are strictly on programming with no applications to physics.

The programming language used in the book is True Basic. Some will, no doubt, criticize this choice. However, I agree with the authors' philosophy that programmers experienced in other languages will be able to use the programs written in Basic as pseudocode, whereas novice programmers will be able to learn this language quickly. To help bridge the gap between languages, Basic-to-Fortran and Basic-to-C appendices are provided.

Numerical methods are introduced, but only as needed to solve the physics. For example, the Euler method and its extensions are used to integrate differential equations, and issues of stability and accuracy are discussed and then explored in examples. While the Euler method is sufficient for the purpose, it is by no means the last word in numerical integrators. Because the emphasis is on the physics, the discussion of numerical methods is not the most complete available. This is not to say that all the methods are the most elementary: for example, the authors use Monte Carlo methods in many contexts, such as integration, simulated annealing, and the demon algorithm.

This book is best used in a standalone course on computer simulation, to teach both physics and how to use computers to do physics. Because many chapters are both interesting and accessible to lower-level physics students and nonmajors, I would be likely to use this book for lower-level or interdisciplinary courses. For higher-level students, however, it would be important to supplement this book with one that treats numerical methods in more detail and to require that students do some research and computing on their own. Students, therefore, must be able to work independently and, as the authors suggest, must learn to think critically about their own work. The book is too long to be covered well in a year-long course. Fortunately the chapters are relatively independent, and so an instructor can skip around without hampering the learning of the students.

One of the unique features of this book is the emphasis on statistical mechanics, thermodynamics, and random processes. The authors introduce algorithms and physics not available in other

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books on computational physics, such as percolation and the Hoshen and Kopelman cluster-labeling algorithm. Given this emphasis, I would also find this ideal as a second text for a statistical-mechanics course at any level.

For this second edition, the overall structure and philosophy have not changed. However, there are more research projects and more pedagogy on good programming and debugging. The authors have significantly expanded some chapters, updated references, included more graphics, and unified the two softcover volumes into one hardcover. These additions have improved upon the previous edition's weaknesses without detracting from its strengths. For more details on the book, check the authors' home pages at http://www.clarku.edu/~sip and http://www.kzoo.edu/~sip. The book's preface, table of contents, codes, corrections, and more are located there.

This excellent book provides students with an opportunity to understand physics through simulation mode, a mode that complements the analytical work typical of most classes. The book excels in its concentration on statistical mechanics, thermodynamics, and other modern topics (fractals, complexity, and chaos), and on the numerical methods to treat these systems. However, it is not meant to be a systematic presentation of numerical methods; other similar texts do this job better. ♦

Books Received

Beyond the Third Dimension
Thomas F. Banchoff, Scientific American Libraary, New York, 1996; 0-7167-6015-0, 211 pp., paper, $19.95.

CGI Programming on the World Wide Web
Shichir Gundavaram, O'Reilly & Associates, Sebastopol, CA, 1996; ISBN 1-56592-168-2, 450 pp., paper, $29.95.

Computational Atomic Physics
Klaus Bartshat, Springer, Berlin, 1996; ISBN 3-540-60179-1, 249 pp., cloth and diskette, $74.95.

Market-Based Control
Scott H. Clearwater, World Scientific, Singapore, 1996; ISBN 981-02-2254-8, 311 pp., cloth, $62.00.

Perl 5 Desktop Reference
Johan Vromans, O'Reilly & Associates, Sebastopol, CA, 1996; ISBN 1-56592-187-9, 40 pp., paper, $6.95.

The Mathematica Book, 3rd Edition
Stephen Wolfram, Cambridge University Press, New York, 1996; ISBN 0-521-58889-8, 1395 pp., cloth, $59.95; or ISBN 0-521-58888-X, paper, $44.95.

Mathematical Algorithms in Visual Basic for Scientists and Engineers
Namir C. Shammas, McGraw-Hill, New York, 1996; ISBN 0-07-912003-2, 251 pp., paper with diskette, $45.00.

Topics in Advanced Scientific Computation
Richard Crandall, Springer, New York, 1996; ISBN 0-387-94473-7, 340 pp., cloth, $39.20.

Computational Analysis of One-Dimensional Cellular Automata
Burton H. Voorhees, World Scientific, Singapore, 1996; ISBN 981-02-2221-1, 275 pp., cloth, $53.00.

Computer Simulations with Mathematica: Explorations in Complex Physical and Biological Systems

Richard J. Gaylord and Paul R. Wellin

Springer-Verlag, New York, 1995; ISBN 0-387-94274-2; 297 pp. plus CD-ROM, cloth, $54.95.

Reviewed by Bill Titus

With new tools come new opportunities. This book by Gaylord and Wellin uses Mathematica's capabilities for rule-based and functional programming to explore computer simulations in the physical, chemical, and biological sciences. Indeed, the authors have written an excellent text whose primary objective is "for the enjoyment as well as the edification of the reader."

The book is divided into two parts, "Probabilistic Systems" and "Cellular Automata." Each part has a number of chapters devoted to single topics such as random walks, Darwinian evolution, avalanches, and forest fires. The book is constructed so that readers do not have to go through it sequentially, thus enabling them to pick and choose the topics they wish to study.

Each chapter has the same structure: an introduction with a brief description of the model and its relevance; then the computer algorithm stated, more or less, in English; and, finally, the algorithm implemented in a step-by-step fashion using explicit numerical examples and code fragments to develop the final code. Some chapters use the algorithm along with graphics and analysis tools to explore consequences of the model; other chapters leave that exploration for some of the "computer simulation" projects that are included with each chapter. At the end of each chapter, the authors list some references for background information and further study.

Although I have used Mathematica for several years, I have always been uncomfortable with functional and rule-based programming. This book, because of its numerous programming examples and interesting topics, certainly has helped me to feel more at ease with this mode of programming.

This is not a book for Mathematica beginners. Even though the authors feel that the "Mathematica language is very simple," in my experience, Mathematica has a rather steep learning curve. This book is not the place where a novice would want to start to learn Mathematica. The authors have included an appendix on Mathematica program-

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