Journal of Statistical Physics, Vol. 53, Nos. 5/6, 1988

Book Review: *An Introduction to Computer Simulation Methods*

An Introduction to Computer Simulation Methods, Parts 1 and 2. H. Gould and J. Tobochnik. Addison-Wesley, 1988.

The pair of volumes under review address two very distinct aspects of the role of computer simulation in physics. The first is the use of numerical methods in studying a range of problems that typically arise fairly early in the undergraduate physics curriculum. The second is the application of Monte Carlo (statistical sampling) methods to research-oriented problems in statistical physics—the field of interest of the authors. The two distinct themes are also reflected in the subdivision of material between the volumes.

Both volumes adopt the same format, with each chapter being devoted to a single general theme and focusing on a number of case studies. Each begins with a certain amount of background material and is followed by a computer program designed to "solve" the particular problem by simulation. Simple numerical techniques are introduced as required. A series of exercises then follow which begin by using the program to answer particular questions, and then call for the program to be modified in order to study other aspects of the problem, or, after more substantial changes, to explore related problems. A set of references to physics texts, as well as to both popular and technical journals, brings each chapter to a close.

The first volume begins with a brief general introduction to computers and programming. This is followed by some of the rudiments of numerical differential equation solving with application to gravitational motion; then oscillations, both mechanical and electrical. The two chapters which follow jump to more advanced material: there is an introduction to the molecular dynamics method for liquids and gases, including a discussion of transport, and this is followed by a chapter on non-linear maps, period doubling and chaos. The material then drops back to the more familiar undergraduate level: waves, interference, polarization, and a minimal amount of geometrical optics. A chapter on static electric and magnetic fields, including a numerical solution of the Laplace equation, brings the first part

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to a close. While a broad range of subjects are addressed, several important topics are conspicuous by their absence.

The second volume deals with subjects closer to the hearts of the present readership. The general Monte Carlo approach for evaluating integrals is described in the opening chapter. Then comes a chapter on random walks of various kinds, polymers, and random number generation. Percolation is discussed both as a topic in its own right and as a vehicle for introducing critical phenomena, with critical exponents, finite-size scaling and real-space renormalization all receiving mention. A chapter is devoted to growth processes; fractals are introduced, and DLA and "ant" problems discussed, as are cellular automata (normally a deterministic rather than a stochastic process). The way in which Monte Carlo allows systems to equilibrate and the notion of entropy are treated, and this is followed by chapters in which Ising and related models are studied in both the microcanonical and canonical ensembles. There is a chapter on quantum systems where diffusion and Monte Carlo variational approaches are demonstrated. The final chapter attempts to convey that very different methods can be used to study a particular problem (here differential equations and cellular automata), while a given method can sometimes be used in surprising contexts (percolation applied to galaxy formation).

The programs included in the body of the text are written in a language known as True Basic, a descendant of the original Basic language familiar to microcomputer users. The language is an improvement in that it allows more by way of structured programming than its predecessor (a necessary ingredient in writing coherent software), and it also incorporates the basic necessities for graphics. It does not look a great deal different from some recent versions of Fortran, the familiar workhorse of scientific computing. The alternative to using this language (which requires its own interpreter) is to translate the programs and substitute alternative graphics functions; some 15% of the page count is devoted to appendices in which Fortran and Pascal versions of the programs are listed, something of a waste, since all but the complete tyro should be able to convert the software to his/her favorite language with little effort (almost all the algorithms are very simple).

The authors are to be complimented on their initiative—there is a conspicious lack of teaching material that is aimed at integrating computing into physics, and this is one of the goals of these books. One could, however, take issue with the way they have chosen a combination of introductory physics and statistical mechanics as the focal point of their efforts; far better a pair of unconnected books (even with different titles), one for the beginner the other for the statistical mechanician—there are many other branches of simulational/numerical physics at the level of the latter.

There is little mention of analytical theory; it is often the case that the simplest of simulations can be validated by comparison with analytic results (at least in certain limiting cases), not to mention the fact that the analytic approach can actually be used to solve problems. References are made to texts and journal articles where more details are to be gound, but in an introductory textbook less reliance should be placed on such sources.

A more significant issue is the absence of solutions to the exercises. The approach taken is one of learning by doing, but it is very difficult to measure success. There are many suggestive questions attached to the exercises, but no way for a person doing the work to determine whether the results that emerge are correct. Since error-free programming remains a utopian vision, an appendix containing solutions to all exercises ought to be incorporated in a subsequent edition—hopefully the authors have the material available.

A couple of remarks on the statistical mechanics part of the work. Critical exponents (omitted from the subject index!) are literally pulled out of thin air, with no mention of their analytical or series-expansion (a subject not mentioned) origins. Random number generation uses only the congruential method; more efficient and reliable shift register methods are not discussed. The longest and most complicated algorithm seems to be that for percolation clusters; the technique used for cluster labeling is an efficient one but rather obscure, and the far simpler direct approach might have been preferable. And the issue of NP-completeness—a matter of some significance in determining whether algorithmic methods can be used at all (as with the traveling salesman) is dismissed in what some might consider an offhand manner.

Where will these books prove of value? (Someone surely deserves credit for bringing them out in paperback form.) Most of Part 1 and some of Part 2 can serve as an undergraduate introduction to the uses of computers in physics, although a little more by way of numerical methods would be required. Alternatively, individual chapters can be used to augment introductory physics courses where the standard texts usually omit to mention that it is the computers that eventually have to solve the problems. Part 2 (which is not independent of Part 1) could be used in a course on numerical statistical mechanics, or as an introduction to Monte Carlo methods for the researcher who wants to acquire a working knowledge of the field. There are certainly enough problems to allow plenty of practice. For those too lazy to actually solve the problems, the reading is pleasant.

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