

Book Review: *Monte Carlo and Molecular Dynamics of Condensed Matter Systems*

Monte Carlo and Molecular Dynamics of Condensed Matter Systems. K. Binder and G. Ciccotti, eds., Editrice Compositori, Bologna, Italy, 1996.

Computer simulations are nowadays widely used in various branches of statistical and solid-state physics as well as neighboring fields. This book, the proceedings of a Summer School, aims to review recent progress in molecular dynamics and Monte Carlo techniques and to narrow the gap between the practitioners of the two methods.

Indeed, the two School chairmen and book editors, excellent experts themselves, succeeded in attracting a competent group of 35 lecturers from Europe and the United States (among them, without disregarding the others, B. Alder, K. Binder, R. Car, D. M. Ceperley, G. Ciccotti, D. Frenkel, J. E. Gubernatis, J.-P. Hansen, D. W. Heermann, S. Hess, W. Kohn, K. Kremer, D. P. Landau, P. Nielaba, H. De Raedt, E. Tosatti, and A. P. Young). Of course, important simulational work is performed on other continents, as well; many of the findings resulting from that research are included in the book. The talks are documented in the voluminous proceedings of about 1000 pages, ranging from introductory presentations to reports on the state of the art of special topics such as proteins, polymers, lipid bilayers, surface phenomena, fluids under shear, and phase transitions in random systems.

The book contains seven main parts, with 37 chapters: statistical mechanics and simulations; phase transitions; quantum theory and simulation; density functional approach; biophysics; dynamical and nonequilibrium phenomena; and miscellaneous topics (for instance, parallelization and computational implementation). The last, eighth part consists of short contributed papers, some of which, however, might have been omitted without much regret.

I have to confess that I did not read each page of the proceedings, but I much enjoyed browsing through the book, getting quite often caught by clear reasoning and/or novel results or being amused by one or the other

remark (e.g., "Except for the speaker, everybody gets old," D. Stauffer in his chapter on aging and immunology).

A simple reflection on the computing powers of today shows that computational physics and chemistry still have to go a very long way to reproduce, from first principles, quantitatively the properties of systems of even rather few interacting particles. Meanwhile, computer simulations, based on approximate descriptions or somewhat simplified models, will be most helpful in interpreting and motivating experiments and in testing and motivating analytic work. They will lead to intriguing challenges for researchers trying, for instance, to cope with more and more realistic models and dynamics.

For those who would like to join the "simulators," the book provides a solid foundation for various modern simulational techniques, including path-integral Monte Carlo methods and the density functional approach combined with molecular dynamics (the beginner may find textbooks, with concrete programming examples, to be very useful, too). For curious scientists, in general, the book presents a nearly overwhelming wealth of up-to-date information, covering a broad range of selected applications of current interest. For specialists in simulations, the proceedings offers the opportunity to see what their colleagues are doing at the frontier of research, concerning both technical aspects and the choice of the topics. The only persons who may be disappointed by the book are the friends of good photography. Most pictures, of the lecturers and participants, are reproduced rather poorly. Improvements with the help of simulational tools for pattern recognition would be possible, in principle, but they would be too cumbersome.

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