Computer simulation studies in condensed matter physics

B. M. Smirnov
Usp. Fiz. Nauk **158**, 545–546 (July 1989)

Computer Simulation Studies in Condensed Matter Physics/Eds. **D. P. Landau, K. K. Mon and H. B. Schüttler**: Proceedings of Workshop. Athens, USA, February 1988. Springer-Verlag, Berlin; Heidelberg; New York; Paris; London; Tokyo, 1988. 240 pp. (Springer Proceedings in Physics, V.33).

During the last decade computer experimentation has occupied a noticeable place in physics research. Computer simulation of physics systems enables one to obtain numerical information concerning them, and also on the basis of graphic imaging provides a possibility of getting an idea of an object with the aid of which one might develop optimal methods of investigating the object. Among the mathematical methods of describing physical systems and phenomena and of numerical analysis of them, the simulation of such objects and processes on the basis of the Monte Carlo Method is becoming one of the basic ones. This method is particularly useful for complex physical systems with a complicated mathematical description.

Serious progress in the utilization of the Monte Carlo method is connected to a great extent with new possibilities of modern computational technique. While twenty years ago at the initial stages of simulation the object under investigation could be divided in one dimension approximately into a hundred Monte Carlo steps, now in the simple models the one-dimensional scale consists of millions of Monte Carlo steps. Also the speed of obtaining information has significantly increased. As a result of this we now have the possibility of investigating properties of physics systems using realistic models. At present the possibilities of computer simulation in solving a number of problems significantly exceed the possibilities of experiment both in regard to the speed of obtaining information and also in regard to its cost. This increased the role played by computer experimentation in modern physics and in a number of the directions of physics our modern concepts are based largely on information obtained using computer simulation.

It is clear that for progress in the field under discussion it is necessary along with a perfected computational technique to have algorithms and approaches which enable one to utilize it effectively. These problems together with analysis of the corresponding physical systems constitute the modern content of computer simulation by the Monte Carlo method. The problems of this direction and its achievements have been reflected in recently published collections of articles.[1,2] The collection of articles under review contains materials of a workshop devoted to computer simulation of condensed systems which took place in February 1988 in Athens, USA.

The collection of articles consists of four parts. The first three (classical systems; quantum systems; computer graphics) include short review articles representing narrow problems, to the development of which the authors made a significant contribution. The last part contains original papers devoted to individual problems of computer simulation by the Monte Carlo method.

Approximately one-half of the book is its first part devoted to complicated classical systems. The proportion between methodological elements and the physical results in each of the articles is different and depends on the taste of the author, but both these elements are present in each article. We enumerate the main problems discussed in this part. They include an analysis of critical phenomena, the dynamics of classical systems of interacting spins, the properties and processes of the growth of fractal aggregates, the dynamics of dense polymers, the problems of gas dynamics. This list is a testimony to the timeliness of the collection of articles. It is significant that these problems are described on the basis of realistic models which frequently provide the basic information on the subject of investigation.

The second part of the collection investigates quantum systems. In contrast to the problems of the first part of the collection which are described on the basis of realistic models, in the case of quantum systems "range-finding" is taking place: the possibility is being tested of applying simulation on the basis of the Monte Carlo method, and its possibilities are being demonstrated. In the future the Monte Carlo method promises to find its place in simulating quantum systems.

The third part of the book consists of a single article by Follin, devoted to computer graphics in science and technology. This is an interesting modern direction. The final result is obtaining graphs and diagrams of models (for example, aircraft, rockets, automobiles, etc.), which are calculated under prescribed conditions and optimized with respect to definite parameters. Such approaches occupy solid positions in modern design, and in the future their role will increase.

The fourth and final part of the book includes short original papers which are not interrelated. For example, in one of them there is proposed and calculated a new model of a percolation cluster, in another, calculations are made concerning the distribution of rubidium of the surface of graphite in the liquid and solid phase.

On the whole the book reflects the present-day stage in the development of computer simulation and will be useful both for specialists creating and utilizing these models, and also for a wide circle of physicists for whom new physical results and concepts concerning complex physical objects obtained by these methods are important.

[1]Monte-Carlo Methods in Statistical Physics. (Ed.) K. Binder, Springer-Verlag, Heidelberg, Berlin, 1979.
[2]Monte-Carlo Methods in Statistical Physics. (Ed.) K. Binder, 2nd ed. Springer-Verlag, Heidelberg, Berlin, 1986.

Translated by G. M. Volkoff