Computer Modeling in Physics

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Contents

Preface

This book is based on the one-term lecture course (about twenty lectures) which has been given by one of the authors in 1988–1992 at Kiev University for forth–year students (that corresponds to last–year undergraduate or first–year graduate students) of the Radiophysical Department. The aim of the course was to explain *in what a way* a computer can be used for solution of physical problems. It is natural, therefore, that special attention in the course is devoted to the main methods of computer simulation, namely the Molecular Dynamics (MD) method and the Monte Carlo (MC) method, and also to the Stochastic Equations (SE) method which may be considered as an intermediate one between the MD and MC methods. Note that these methods were discussed also in other books, for example, in the book of Heerman [1] or in the book of Gould and Tobochnik [2] (see also [191]).

However, besides the answer on the question *in what a way,* the principal aim of this book is an attempt to answer two additional important questions: *when* and *why* we should use computer modeling. Evidently that modeling in a general sense forms a base for development of any field of science from mathematics to philosophy. Indeed, the global aim of science is to find and explain evolution laws of the Universe. But because any phenomenon in the world is extremely complicated, the only way of solution of the problem is the following: we must maximally simplify the given phenomenon (object, process, *etc.*), i.e., to throw out all inessential details and to leave the most significant ones only. That is just what is called *to invent a model.* The invitation of new models is an art. The appearance of a new model is always the outstanding event in science, and the model is called usually by the name of the scientist who invented it. Clearly, it is impossible to teach how to invent models. But it is possible, and namely this is done in the present book, to tell about the most known models used in physics. Then, combining the known models in an appropriate way, one will be able to solve successfully almost any of standard physical problems.

The modeling in a general sense is too wide topic even for a series of many books. In the present book we set up a more modest task: to tell on those models only, for investigation of whose a computer is necessary or very desirable at least. Namely, such a situation corresponds to models from two extremely interesting divisions of physics, the stochastic theory and the solitonic theory, and also from the old (but very interesting as well) division, the statistical physics. We cannot say categorically that most problems from these divisions of physics could not be solved without computers. But it is evident that these solutions would be found much more latter (perhaps, for decades).

List of questions considered in this book can be found in Contents. We would like to mention only the questions which are not included in this book while they could be included in the book with such a title. Excepting few words in Introduction, it is absent a discussion of computers and formalize languages. We do not discuss numerical methods and do not give texts of computer programs. All these questions may be found in other textbooks, the references are given in the corresponding sections. The presentation is accompanied by a large number of examples taken, as a rule, from original papers published last time. An essential number of examples is taken from surface physics, where one of the authors of this book worked for a while. But all the examples are of a general character and may be successfully used in other divisions of physics as well.

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Chapter 1

Introduction

1.1 Stages of modeling

The global aim of modeling is to explain or predict some phenomenon or process, i.e., to develop a corresponding theory. In order to achieve this aim we have, first of all, to invent a model or to select a suitable one, then to work out a method for its solution, then to carry out an investigation of the solution and, finally, to reveal laws or regular trends of the phenomenon under investigation. Let us consider these stages in more detail.

A. Setting of the problem. The first stage of modeling is to invent a corresponding model. The very limited number of scientists is a success to contrive a new model. As a rule, in such case the model takes the name of the scientist who contrived it. Recall, for example, the widely known Ising model, Baxter model, Anderson model, Frenkel-Kontorova model which became the classical ones. Clearly that to teach somebody to invent new models is impracticable task. However, we will try to acquaint a reader of this book with the main models used most often, so she/he could use them after some modifications in own investigations.

Let us set out basic requirements that must be imposed upon a physical model.

(a) *The model must be maximally simple.* Beginner investigators always try to set the problem in the most general form taking into account as many as possible factors from the very beginning. This is completely mistaken way, and it *never* leads to a success. The model must be maximally simplified, all factors of secondary importance should be omitted, and only the relevant factors, i.e. the ones which are representative of the main qualitative points of the phenomenon under investigation, have to be kept. And only at the last stage of modeling, additional factors which help to describe the phenomenon in more detail, may be included one by one.

(b) *The model has to have a solution,* or, in other words, the problem should be set *correctly.* Moreover, from the very beginning we should intuitively know or, at least, should be clear in mind the final as well as all intermediate results, whereas the purpose of modeling is to prove that the intuition was right. Of course, sometimes results of modeling may occur to be far from those being expected. But in this case we will stay to win and to make a discovery.

(c) *The model should be elegant.* Being trivial, this requirement is the necessary one for the modeling to be a success.

(d) *Variables of the model should be dimensionless,* i.e., the used system of units has to be natural for the given problem. As a rule, we can introduce three dimensionless variables. These variables may be chosen more or less arbitrary, but usually the units of time, distance, and energy (or charge, or mass) are made dimensionless. Often beginners try to use seconds for time, centimeters for distance, ergs or joules for energy, *etc.* In a result, the calculations are "overloaded" by redundant numbers. To avoid this inconvenience, the units should be related to values which are inherent for the given system. For example, the period of intrinsic oscillations of the system has to be taken as the unit of time, the Bohr radius or the mean interparticle distance, as the unit of distance, the electron charge, as the unit of charge, *etc.*

B. Developing of a computer program for the solution of the settled problem. In this book we will consider only the models where the computer plays a central role in the investigation. Moreover, the computer is used not as a great calculator for an approximate solution of complicated equations, but as an "experimental device", i.e., the computer with the program appears as the instrument and, at the same time, as the system under investigation. For computer modeling in physics two methods are mainly used, the Molecular Dynamics (MD) method and the Monte Carlo (MC) method. It is interesting that both methods have been sampled for the first time in 1950-th when the first, very unsophisticated computers appeared. The MD and MC methods are considered in Chapters 3 and 5 correspondingly. Below we also give some practical advices on the choice of numerical methods and the computer as well as on the organization of the computer program and its de-bugging.

C. Investigation of the solution, or the computer simulation itself. This stage is the analog of the carrying out of a laboratory physical experiment. Namely, we vary the input program parameters acting on the state of the physical system, and study the resulting system behavior, i.e., its response to these variations. When a sufficient number of dependences have been obtained, we can proceed to the final (and the main) stage of modeling.

D. Reveal of the theory. This stage has no difference from the corresponding stage in experimental or theoretical physics. Note only that namely at this stage we may and must complicate and generalize the model in order to clear up a role of the factors which were assumed to be of secondary importance at the first stage.

1.2 Numerical methods

A computer can carry out only a finite number of the before-handed deterministic operations with a finite (discrete) set of rational numbers. Infinities, continuum variables, real or random numbers, *etc.* do not exist in numerical methods. These points must be clearly understood at the first stage of modeling when the model is chosen. For example, in the theoretical investigation of problems of the solid state physics, the continuum approximation is often used, where a discrete variable $l = 0, \pm 1, \ldots$ which numerates the atoms, is replaced by the continuum variable x: $l \to x_l = la \to x$, where a is the lattice constant. The resulting model is described by differential equations. However, at numerical investigation of these equations we must discretize them, i.e., we have to replace the continuum variable x by the discrete variable j: $x \to x_j = j\Delta x \to j$, where Δx is the integration step. Of course, for this problem the investigation of the discrete model from the very beginning will be more natural as well as more correct.

In modeling of physical problems we usually need the following numerical methods:

(a) Practically always a matrix algebra, e.g., addition and multiplication of matrices is used. More rarely we need to calculate determinants or to inverse a matrix. Often physical problems lead to eigenvalue matrix equations. All these methods are developed quite well, and some of them are even included into syntax of the standard FORTRAN or other formalize languages; besides, there are several well-developed libraries.

(b) The solution of an algebraic equation $f(x) = 0$ is carried out by well-developed methods such as the method of cutting the interval as well as various iteration methods, for example, the method of sections, the Newton-Raphson method, *etc.*

(c) The numerical integration is well developed too (recall the method of rectangulars, the method of trapezoidals, the Simpson method, the Gauss method, *etc.*).

(d) The numerical differentiation is a more complicated operation which should be avoided if possible. Sometimes it would be necessary to smooth the function before its differentiation.

(e) For the solution of differential equations, usually the Verlet algorithm or different variants of the Runge-Kutta (RK) method are used. The most popular ones are the forth-order RK method and the fifth-order predictor-corrector RK method with the automatic choice of the integration step. Note that for some problems (for example, for solution of the Langevin equation, see Sec. 4.2) the step of integration must be kept fixed.

(f) Partial differential equations appear in theoretical physics quite often, but their solution requires special methods, typically rather complicated ones [192, 120]. An example is presented in Sec. 4.5.2, although this topic is too wide to be discussed in the present course.

(g) A need to solve an integral equation occurs not too often. Usually the integral equation is reduced to the matrix one, the latter being solved by the method of consecutive iterations.

(h) In physical modeling we often meet with the necessity to find an extremum (usually minimum) of a many-variable function. As a classical example we recall that the thermodynamically equilibrium state must correspond to the minimum of the system free energy. The standard method of solution of this problem, the so-called steepest-descent method, consists in a search (usually by the MC method) of the direction along which the function decreases most steeply.

(i) Often one arises the necessity to use a generator of pseudo-random numbers. This problem is briefly discussed in Chapter 5.

(j) Finally, let us say a few words about computer arithmetics. The numbers in computer may be integer ("fixed point") and real ("floating point"). Arithmetics between integers is exact, provided the answer is not outside of the available range (which typically is $\sim 2^{15} \approx 3.28 \times 10^4$ or $\sim 2^{31} \approx 2.15 \times 10^9$ if the integer is declared as "long"); also recall that division produces an integer too (e.g., 5/2 gives 2). Arithmetics among real umbers is not exact, it is determined by the "machine accuracy" ϵ (defined as the smallest number which, when added to 1.0, produces a result different from 1.0; for the 32-bit computer $\epsilon \sim 3 \times 10^{-8}$). A nonzero machine accuracy leads to the so-called "roundoff errors" which accumulate during calculation — if an operation is performed n times, the total error will be $\sim \epsilon\sqrt{n}$ is the best case and $\sim \epsilon n$ in the most unfavorable case.

A detailed discussion of numerical methods may be found in the handbook of Korn and Korn [3] as well as in a number of textbooks and monographs [4, 5, 6, 7]. In choosing the numerical method it is to be taken into account that usually the more simple is the method, the more reliable is it; at the same time a more simple method requires the more processor time in order to achieve the same accuracy. Besides, the priority should be given to those methods which are realized by the reliable standard subroutines (e.g., see [8]); the best set of numerical methods is collected, of course, in the famous "Numerical Recipes" [9].

1.3 Choice of a computer

Naturally that the choice of the computer is an important stage of modeling because the computer should be suitable for the given problem. In this choice we have to take into account such computer parameters as the speed of calculation, the word length, the active storage, the availability of a convenient and reliable software (standard libraries, translators, editors) and external devices (first of all for computer graphics).

Modern computers, even personal laptops, already have the active storage (i.e., the memory which could be directly accessed from the central processor) of a few gigabites (1 Gb = 10^9 bites), which could be enough for physical simulation. Much more worse is the situation with the speed of calculation, which now is of the order of 2 gigahertz (1 GHz = 10^9 operations per second) and already approaches to the maximally achievable limit. Parallel (vector, array) computers, or supercomputers, may be one-two orders of magnitude faster, but the acceleration may be achieved only for programs that can be split into parallel independent parts, and they need special methods of programming.

The calculation speed is closely connected with another important parameter of the computer, the word length. The 16-bit cell used ten years ago, is sufficient for bookkeeping calculations, but typically is insufficient for mathematical modeling, because in the latter case we have to use the double precision (i.e., two cells for storage of one number), and in a result the calculation speed may be decreased in up to ten times. For modeling problems one should prefer a computer with the 32-bit cell or better with the 64-bit cell. Note that the two parameters, the calculation speed and the available memory, are coupled, and that the chosen method of calculation should depend on these characteristics of the computer. For example, each program has a set of values (sometimes, arrays) that are used many times. If the computer storage is large

but computation speed is small, these values can be calculated one time and then they have to be stored; otherwise, for small storage and high computation speed, it will be better to calculate these values each time when they are needed.

Thus, the computer must correspond to the setting problem. Sometimes successful results may be obtained with the help of a small computer, up to a simple pocket calculator (as, for example, it occurs in developing of the Feigenbaun theory, see below Sec. 2.4). As a rule, however, we meet with the opposite situation, when the computer should be as powerful as possible. Let us present some typical examples. For sufficiently simple models such as one-dimensional systems studied by the MD method or the percolation two-dimensional lattices studied by the MC method, it is enough to have a modern laptop. For MD modeling of two-dimensional systems, it would be better to use a cluster. For MD investigation of three-dimensional systems as well as for MC studying of thermodynamical properties, a supercomputer is to be preferable.

Unfortunately, it is not so simple to find the necessary computer for the given problem, because, in particular, there is a number of physical problems which are in need of so powerful computer that simply does not exist at all. Therefore we have to choose the problem under consideration appropriately for the accessible computer, or to refuse the modeling from the very beginning. Indeed, let us assume that we start the investigation of the thermodynamics of a system by the MC-Metropolis method with a personal computer. At the first stage we, may be, will get some realistic results. But as soon as we will try to carry out the calculations with a higher accuracy, or with a more complicated program, we will immediately meet with the fact that a single calculation step will take, e.g., one hour, the calculation of a single point will need one day, and a single dependence, one month, *etc.* Clearly that in this case the chosen computer is inappropriate for the setting problem, and it will be much better to throw out such a problem as early as possible.

1.4 Some practical advices

In writing and de-bugging of computer programs, we may recommend to hold on the following rules.

(1) The program has to be written as simple as possible. Complex constructions, especially with control passings, and nonstandard peculiarities of a given formalize language which can be used for the given translator only, must be avoided.

(2) The text of the program has to be followed by detailed comments, and also all used variables are to be declared explicitly (even when the implicit declaration of variable types is available).

(3) Because the program will usually run many times during simulation, the sufficient attention should be spared to input and output of information, preferably by writing this blocks as separated subroutines. Accessing to the program should be simple, the input parameters should include only "external", i.e. physical variables (such as, e.g., temperature, concentration, *etc.*) and, may be, a "key" which determines the regime of program operation (for example, the body of information which is displayed or printed). The output information must be followed by comments (the title and date of the simulation, the name of the printed variable, units, *etc.*). Besides, the results have to be easy-to-interpreted, so the graphical presentation is preferable.

(4) The program should be split into more or less independent units (blocks) and written in the form of subroutines. Often it is very convenient to show the interplay between the units by a block-scheme.

(5) De-bugging of the program has to be started from de-bugging of each subroutine (unit, block); for this purpose special control examples should be written for each subroutine. When a standard subroutine or the subroutine taken from a library is used, it must be checked with the help of a control example written specially for this case.

(6) When we are sure that all subroutines proceed without errors, we can link them together into the whole program. Usual errors at this stage are that the types of variables, or array dimensions, or sizes of common blocks (global variables) do not match one another. Recall that in the main FORTRAN program the common blocks and arrays must be declared with the maximal lengthes and dimensions.

(7) Next, the "training" of the program should be done. The program operation should be checked for an essentially wider range of intrinsic and external parameters comparing with those that will be used. In particular, simulation results must remain to be practically unchanged when the intrinsic parameters (such as, e.g., the integration step) are increased as well as decreased in two-three times.

(8) The last very important advise is the following: files have a "property" to be damaged, rubbed out, lost, *etc.* Therefore, after each stage of de-bugging, the text of the program together with the example of its proceeding has to be saved on external disks, better in two-three copies.

Experience shows that de-bugging usually takes more than 50% of the whole simulation time.

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