INTRODUCTION TO MATHEMATICAL MODELING

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Summary

The essence of the methodology of mathematical modeling consists in the replacement of the original object by its mathematical model and in the analysis of the mathematical models by the up-to-date computational and numerical means. The work with not the object (phenomenon, process), but with its model enables us easily, relatively fast and without essential expenses to investigate its properties and behavior in any conceivable situation. The numerical (computational, imitation) experiments with the objects' models enable us to study deeply and in detail the objects with sufficient completeness that cannot be reached by purely theoretical approaches. The basis of mathematical modeling (mathematical simulation) is composed by the triad **model – algorithm – program.** The main body of a mathematical model consists of partial differential equations. There are three main types of the computational experiment: *search, optimization and diagnosis*. When we investigate a new process or a phenomenon, the usual approach is to construct some mathematical model and to perform calculations changing parameters of the problem. In this case we have a *search computational experiment.* It is worth nothing that while performing computational investigations, separate exact solutions of nonlinear equations can be used for checking the accuracy of numerical algorithms, for their testing (so called benchmark problems).

If data of natural experiments are treated, the *diagnostic computational experiment* is used. By virtue of additional indirect measurements a conclusion on the internal relationships of a phenomenon or a process is made. If the structure of the investigated mathematical model is known, then the problem of identification of the model is settled. For instance, the coefficients of the equations are defined. The diagnostic computational experiment corresponds usually to an inverse problem of mathematical physics.

We often face a situation, when a mathematical model of an investigated process or phenomenon does not exist, and it is impossible to create it. Such a situation is distinctive, particularly, while processing data of a natural experiment. The processing is conducted then in the mode of a "black box," and we deal with approximating models. In the absence of mathematical models, imitation modeling based on extensive computation is performed.

The investigated object is a large complex consisting of separate elements, which interact with one another in a complicated way. Therefore, in the investigated object as a system, it is possible to select separate subsystems with some relationships among them. At this stage we work in accordance with one of the main principle of cognition-analysis. The investigated object is separated into parts, each of which is considered independently. At the final stage (the synthesis) on the basis of knowledge about the individual component elements the system is treated as a united whole. These are the basic principles of *system analysis.*

1. Introduction

Nowadays the foundations of mathematical modeling and computational experiments are formed to support new methodologies of scientific research. The essence of this methodology consists in the replacement of the original object by its mathematical model and in the analysis of the mathematical models by the up-to-date computational and numerical means. The methodology of mathematical modeling is developing and rapidly enveloping new subjects – from operation large scale technical systems and their control to the analysis of complex economical and social processes.

Extensive use of mathematical methods enables us to raise the general level of theoretical investigations and to conduct them in the close connection with experimental investigations. Mathematical modeling may be considered as a new method of getting knowledge for design, and construction. This method possesses the advantages of both the theory and the experiment.

Working with a model, rather than with the actual object (phenomenon, process), enables us easy, relatively fast and without essential expenses, to investigate its properties and behavior in any conceivable situation (the advantages of the theory). At the same time, the numerical (computer, imitation) experiments with the objects' models enable us, leaning upon the power of modern numerical methods and technical instruments of informatics, to study deeply and in detail the objects with sufficient completeness that cannot be reached by purely theoretical approaches (the advantages of the experiment).

Studies of complex technical, ecological, economic and other systems by modern science elude investigations (in the necessary completeness and accuracy) by usual theoretical methods. The direct natural experiment is long, expensive, it is often either dangerous or just impossible. Numerical experiment allows us to perform research faster and cheaper. Mathematical simulation is nowadays one of the most important components of scientific and technical progress. Without applying this methodology no large-scale technological, ecological, or economic project can be realized in developed countries.

The birth and the formation of the methodology of mathematical simulation can be traced to the end of the 1940s – beginning of the 1950s. They were caused at least by two reasons. The first impelling reason was the advent of computers that saved researchers enormous routine numerical work. The second reason was the unprecedented social order – implementation of the national USSR and USA programs on creating nuclear-rocket shields. These complex scientific and technical problems could not have been solved by traditional methods without the use of the available computational methods and equipment. Nuclear explosions and flights of rockets and satellites were first simulated by computers and only then put into practice.

The basis of mathematical modeling (mathematical simulation) is the triad **model – algorithm – program.** Mathematical models of real processes under investigation are rather complex and include systems of nonlinear functional-differential equations. The main body of a mathematical model consists of partial differential equations.

At the first stage of numerical experiment the model of the object under investigation is chosen (or is constructed) to reflect in mathematical form its most important properties – the governing laws, the connections inherent among its components, etc. Mathematical model (its main fragments) is investigated by the traditional analytical means of applied mathematics to obtain the preliminary knowledge about the object.

The second stage is connected with the choice (or developing) of a numerical algorithm for computer realization of the model. It is necessary to obtain solutions with prescribed accuracy, using a given computing technique. Numerical and computing algorithms should not distort the basic properties of the model and, hence, of the original object; they must be adapted to the features of solving problems and of using computing means. Study of the mathematical models is performed by methods of numerical mathematics which consists of the numerical methods of solving the problems of mathematical physics – the boundary value problems for partial differential equations.

At the third stage the software for computer realization of the model and the algorithm is developed. The program product must take into account the most important feature of mathematical simulation that is connected with the use of a series (a hierarchy) of mathematical models and with multifarious calculations. This feature implies wide usage of complexes and packages of applied programs that are elaborated, particularly, at the basement of the object-oriented programming.

The success of mathematical simulation is determined by equally deep working out all basic links of numerical experiment. Based on the triad '**model – algorithm – program',** the researcher gets a universal, flexible, and non-expensive instrument, which is firstly improved, tested and calibrated on solving a solid collection of test problems. After that the large-scale investigation of the mathematical model to obtain the necessary qualitative and quantitative properties and characteristics of the object under investigation is performed.

A numerical experiment, by nature, has inter-disciplinary character; it is impossible to over-estimate the synthetic role of mathematical simulation in modern scientific and technical works. In joint research the specialists in the applied field, in applied and numerical mathematics, in applied and system software take part. Numerical experiment is carried out with the support and extensive use of different methods and approaches – from qualitative analysis of nonlinear mathematical models to up-to-date programming languages.

Modeling, in one form or other, can be found in almost all types of creative activity. Mathematical simulation enlarges the areas of exact knowledge and the field of applications of rational methods. It is based on a clear formulation of basic notions and assumptions, on the *a posteriori* analysis of the adequacy of used models, on the control over the accuracy of numerical algorithms, and on the skilled treatment and analysis of numerical results.

Scientific assurance of the solution of life support problems at present is based on extensive use of mathematical simulation and numerical experiments. Traditionally, the computational means (computers and numerical methods) are well presented in researches in the natural sciences, first of all in physics and mechanics. The process of mathematization of other research areas such as chemistry, biology, earth sciences, etc is active.

The most impressive successes were reached in mathematical simulation applicationsin engineering and technology. Computer investigations of mathematical models replaced to a large extent the tests of aircraft models in wind tunnels, the explosions of nuclear and thermonuclear devices on proving grounds.

Modern information technologies are used in medicine. The collection and analysis of diagnostic data enable us to conduct timely diagnosis of diseases. For instance, computer tomography is an example of how the usage of mathematical methods of treatment of large masses of data allowed us to get qualitatively new medical tools.

We describe here the basic approaches to construction and analysis of mathematical models, which are general for different areas of knowledge and do not depend on a specific application. The surrounding world is a single whole; it can be seen, particularly, in the universality of mathematical models, in using the same mathematical constructions for description of different phenomena and objects. We point out the general features of computational experiment with theoretical and experimental methods in scientific researches. A short description of different types of computational experiment is presented. The computational experiment is considered as the higher stage of mathematical modeling, which is generated by the prevalent use of computers and numerical methods for studying mathematical models.

2. Physical and Mathematical Models

Modeling is widely used in science researches and in solving applied problems in different areas of technology. This methodology is based on studying the properties and characteristics of objects of different nature by means of investigation of natural or artificial analogues (models). Modeling in such a general plane is a twofold process of creating models and investigating them after construction. Using models is always inevitably connected with simplifying and idealizing the simulated object.

Naturally, a model, as such, does not represent the object in all its completeness for all its features; it reflects only some of its characteristics of interest – it is similar to the real object only in terms of a definite set of properties which are of interest. A model is constructed to reflect only a part of the total properties of the object under consideration and, hence, as a rule, it is simpler than the real object or the original. And, most importantly, a model is more convenient and more reachable for investigation than the simulated object.

For more complete investigation of an object a number of models is drawn, each of them simulates certain characteristics of the object. In an applied investigation even for reflecting the same properties of the object the possibility of drawing different models always exists. The models differ by the qualitative and quantitative correspondence to the analyzed object with respect to chosen characteristics, by the opportunities of their investigation. The success of modeling is in the choice of models and of their collection.

Naturally, that choice is mostly subjective; it is based on all the given experimental and theoretical notions about the object and on all the previous experience of simulation.

Among the different models physical and mathematical models can be regarded as the basic ones. Mathematical models are the most typical ideal (speculative) models in natural sciences. Physical models concern material (subject) models, which, imitating some properties of the investigated object, have the same origin as the simulated object.

During physical modeling an experimental investigation of the physical model is performed instead of the object. Physical models have an important advantage that lies in the fact that among the properties of the model there are such properties, which for different reasons cannot be investigated by mathematical models. For example, such a situation occurs when a mathematical model is absent or it is so complicated that cannot be investigated with the desired completeness. Therefore sometimes physical modeling is a unique way to obtain trustworthy information about the analyzed object.

Similarity theory lies in the background of physical modeling. Besides geometrical similarity (similarity of shape, geometric model), physical similarity between the model and simulated object is also necessary. At corresponding spatial points and time moments the values of physical quantities for the object must be proportional to those in the model. This allows us to re-calculate for the instigated object the experimental results obtained for the model. The key point of such modeling is that both for the model and for the object the crucial dimensionless similarity criteria must be the same.

As an example of physical modeling let us note the scale modeling in aerodynamic tunnels. In wind tunnels experiments are conducted for various purposes: to determine the forces acting on aircraft during their flight, on submarines in diving state, on automobiles etc. to optimize their geometric shape. The main crucial criteria in such investigations are Mach number M and Reynolds number Re. The Mach number is the ratio of the speed of the body v to the speed of sound in medium *c*; it is a measure of influence of the compressibility of the medium in the flow process. At $M \ll 1$ gases (fluids) can be considered as incompressible. The Reynolds number

$$Re = \frac{\varrho v l}{\mu} \qquad (1)$$

characterizes the influence of the medium viscosity. Here ϱ is medium density, l is the typical linear size of streamlined body, and μ is the coefficient of dynamic viscosity of medium.

In order to maintain Reynolds number of the reduced model constant during blowing through a wind tunnel, v or ϱ may be increased, or another modeling medium may be used. In aerodynamical investigations where Mach number has a crucial meaning, the speed cannot be changed. These conflicting demands together with a number of dimensionless criteria lead to serious complexities, and physical modeling in the range of interest of dimensionless parameters may be often impossible.

In mathematical modeling the investigation on properties and characteristics of the original object is replaced by investigation on its mathematical models. Mathematical models are studied by methods of mathematics (applied mathematics). Latest developments in mathematical modeling are characterized by extensive (however, not always appropriate) involvement of computers.

Physical models can portray the properties of an investigated object not only at the background of their physical and geometrical similarity but also through inference by virtue of the similarity of their mathematical models. In such a case we deal with hybrid models (or, as say, with models of direct analogy).

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Biographical Sketches

Alexander A. Samarskii is a professor at the Institute of Mathematical Modelling, Russian Academy of Sciences, Moscow, Russia. He born in 1919 in Donetsk region of Ukraina and graduated from the Department of Physics of MSU. Academician Samarskii received a Ph. D. in mathematics from the M.V. Lomonosov State University in Moscow in 1948, and a D. Sc. from the M.V. Keldysh Institute of Applied

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His long-time career as an educator has resulted in the creation of a world-known scientific school in the field of Computational Mathematics and Mathematical Modeling including not only Russian researches, but also colleagues from Germany, Bulgaria, Hungry and some other countries. There are many highly experienced specialists, professors, associate members and members of the RAS among his students. Academician Samarskii has organized and chaired many international conferences on mathematical physics and difference methods, and served as guest lecturer at many other international forums..

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