

PROBLEMS AND TRENDS IN MATHEMATICAL MODELING

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Main problems and trends in mathematical modeling — a new line of research into various processes and phenomena — are formulated. The status and future prospects are analyzed using as an example the mechanics of continuous media. Emphasis is on two stages of modeling — the selection of physicomathematical models of the mechanics of continuous media and numerical algorithms of solution.

Introduction. Mathematical modeling as a new method for investigating and obtaining new knowledge emerged in the 1970s based on wide application of mathematical methods to the solution of theoretical and practical problems in natural science. Its emergence and evolution was due to the design of powerful computers capable of extremely rapid arithmetic and logical calculations. The increasing complication of problems in science, technology, engineering, and national economy has required the development and justification of mathematical models reflecting the main features of the phenomena studied and efficient numerical algorithms of solution. In turn, efficient implementation of those algorithms not only has led to the emergence of new computers but has also given impetus to the design of new programming languages, operating systems, and software support systems and the development of new approaches to programming and informational technologies. This has made it possible to convert from the use of a computer as a high-speed calculator to a modeling system that includes the entire process, starting from the construction of mathematical models and numerical algorithms and programming to the development of program systems and packages for solution of special classes of problems and analysis, output, and storage of results, which constitutes a new scientific discipline — mathematical modeling [1–11].

The emergence of this new line of research has given rise to new problems, whose solution determines further progress in this direction. Mathematical models and algorithms, program systems and software packages, computers and support systems for problem solution are elements of modeling. Their role can be properly assessed only considering the entire modeling chain, which will further be referred to as the technological chain (see [11]). By the technological chain of modeling we understand a set of elements implemented in a definite order and constituting a complete cycle. Clearly, for different research areas, those elements can be different, and, therefore, the basis of the technological chain must contain elements that are common for all fields of modeling. In accordance with modern views, the modeling process can be represented as the following sequence: the phenomenon under study → mathematical models → numerical algorithms → programming → computer → calculations and analysis → processing and storage of results, which complements the well-known triad of mathematical modeling “model–algorithm–program” [2, 4, 11]. Obviously, all elements of the technological chain are interrelated, this relation is nonlinear, and a change of one of the elements can modify not only the subsequent but also the preceding elements. Prior to modeling, a researcher performs an explicit or implicit analysis of the entire modeling chain proceeding from the present-day views on the examined phenomenon or process, the available computer resources, numerical algorithms, etc. Of course, for certain phenomena and classes of problems, some chain elements can evidently be omitted. As an example, we give N. N. Yanenko’s idea of a difference scheme (numerical algorithm) as a mathematical model for describing a physical phenomenon. The construction of more complete mathematical models adequate for describing more complicated processes and the development of more accurate and efficient numerical algorithms have required more powerful computers. This can be attained not only through the improvement of

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the element basis but also by the development of new computer architectures using the principles of multiprocessor systems and parallel computations. These architectures in turn, impose certain requirements on numerical algorithms, most of which were developed in the era of uniprocessor computers, in which computations were carried out successively. New computer architectures require the design of new numerical algorithms and revision of existing numerical methods aimed at adapting them to those architectures.

At present, we can state that along with physical and full-scale experiments, mathematical modeling is one of the basic methods for investigating and obtaining new knowledge in various fields of natural science. Its significance can be expected to further increase in the nearest years but it will never replace physical or full-scale experiments, because experience will necessarily remain the primary basis of any study. It should be expected that various methods of investigation complementing each other will become closer. Extensive use of mathematical modeling in various fields of natural sciences and human activity is due to many factors, mainly the following:

- the increasing sophistication of the class of research problems, whose solution requires expensive new experimental setups or model objects (in some cases, numerical modeling of these problems involves much lower expenses);
- high costs and power consumption required for the operation of experimental setups and objects;
- a demand for solving environmental, social, and other problems;
- impossibility of carrying out physical (chemical, economic etc.) or full-scale experiments in some fields of investigation (where mathematical modeling is the only way out).

To the indicated factors we should add potential reduction in the time of investigation and obtaining results and the possibility of multiple repetition of studies, refinement of results, storage, etc. The development of mathematical modeling results in automatic control systems, which can drastically increase labor productivity and eliminate the negative effect of the so-called “human element” on decision making. Thus, mathematical modeling has become a major method of investigation and obtaining new knowledge. At the same time, results of mathematical modeling have been extensively used in industry and other human activities (e.g., in developing automatic design systems, expert systems, etc., [12]). The present paper considers some trends in mathematical modeling. Since the scope of this paper does not allow us to cover all spheres of its application, we focus on problems of the mechanics of continuous media. In this area, mathematical modeling has been widely used because other approaches are often inapplicable and because this class of problems is of great significance for industrial development (see, e.g., [1–12]). As was noted above, the efficiency of mathematical modeling can be adequately assessed when the entire technological chain is considered. Therefore, we will concentrate on the status and development of individual elements of this chain and their interrelation. Focus is on the selection of models and numerical algorithms.

1. Physicomathematical Models. For problems of the mechanics of continuous media in full formulations, physicomathematical models can be described by the integral laws of conservation

$$\frac{\partial}{\partial t} \int_V W_0 dV + \oint_S W ds = \int_V F dV, \quad (1.1)$$

which express the relationship between time variations of some quantities in a closed volume V (fluxes and their change with passage through the boundary S , and the interaction of the fluxes with external sources or sinks. The integral laws of conservation (e.g., of mass, momentum, and energy for models of continuous media) describe motion in the most general form and are valid both for both continuous and discontinuous solutions. In addition to the integral form, it is common to use their differential representation

$$\frac{\partial W_0}{\partial t} + \operatorname{div} W = F,$$

which is obtained from (1.1) but valid only for continuous solutions.

The variety and multiparameter nature of the problems studied and the nonuniform scales of the processes lead to a sequence of physicomathematical models, each of which is obtained under certain assumptions on the nature of the examined phenomenon and describes its main regularities. Another characteristic feature of this approach is the variety of equations describing the models used. The obtained equations can be of different types (hyperbolic, parabolic, or equations of a variable type), which leads to different formulations of initial and boundary problems. Moreover, in studies of the same class of problems, the type of equations can change, depending on the type of solution. For instance, the steady equations of gas dynamics are elliptic equations for subsonic velocities and hyperbolic equations for supersonic velocities, i.e., in individual calculation subdomains, it is necessary to solve equations of different types, which imposes additional requirements on the applied numerical methods.

Most processes in fluid mechanics are nonlinear and evolutionary, and, as a consequence, the same properties are inherent in the systems of equations describing these processes. The properties of such equations have been studied inadequately. For most problems, the existence and uniqueness theorems have not yet been proved, and, moreover, their solutions can be nonunique and discontinuous even for smooth initial data (see [10]). Conversion to multidimensional problems and more complex calculation domains (consideration of real geometries) makes their formulation even more difficult. In the absence of rigorous proofs of the existence and uniqueness of solutions, the question arises of whether the employed physicomathematical model is adequate to the phenomenon investigated. When there is no sufficient information on the phenomenon under study, it is necessary to consider different models taking into account the major regularities of the phenomena investigated for various ranges of the main parameters. Therefore, the choice and formulation of physicomathematical models becomes a multiparameter problem, whose solution requires an analysis of the entire set of models. Prior to modeling, a researcher needs to answer a number of questions. For example, what is the ultimate goal of the research and what results are expected from the solution of the problem? How important is the problem at hand and what is its significance for the general problem? What is the accuracy of the model and what accuracy of the solution is required? What resources need to be employed in the solution and what mathematical and engineering resources are available to the researcher? Actually, the researcher analyzes the entire technological chain of modeling and draws an inference about the feasibility of solving the problem by employing the existing models, numerical algorithms, and hardware (computers) or formulates the conditions and requirements necessary for its solution (e.g., the necessity of developing additional models, numerical methods, new computer designs, etc.).

The development of models describing adequately the phenomenon or process under study includes their mathematical justification and correct formulation of initial boundary-value problems. According to present-day views, all classes of models for problems of mechanics can be divided into four groups (levels):

- 1) analytical approximations and linearized equations;
- 2) nonlinear equations ignoring dissipation processes;
- 3) nonlinear equations allowing for dissipation processes
- 4) full unsteady models described by equations taking into account real effects (such as Navier–Stokes equations allowing for compressibility, thermal conductivity, turbulence, etc.), the equations of multicomponent and multiphase media, magnetohydrodynamic models of various levels, etc.

Nowadays, all groups of models are used (depending on the purpose of investigation, classes of the problems studied, their general significance, required accuracy of solution, available software and hardware, and other factors) starting from the simplest ones (first level) and up to the most sophisticated models (third and fourth levels). Let us consider some examples from computational aerodynamics. In the approximation of potential flow (first level), the panel method is appropriate for solving problems of flows past aircraft of real configurations (e.g., F4F aircraft with weapon loading) and obtaining distributions of flow parameters over the aircraft surface [13]. First calculations of this type were carried out in the 1970s on low-power computers. This model, however, does not allow for real effects in gas, such as compressibility, viscosity, and thermal conductivity, and does not yield the distribution of gas-dynamic flows in the vicinity of the body. Conversion to high velocities necessitates the use of nonlinear models described by gas-dynamic equations (second level). Their solutions can contain discontinuities of gas-dynamic parameters, which requires the use of special calculation methods and high-capacity computers (10^9 FLOP) (FLOP is the number of floating-point operations per second). The emergence of high-speed computers in the 1980s, has made it possible to calculate flows past a supersonic airplane (e.g., F16) in the approximation of Euler equations over time comparable to flight time. Even at present, however, the problem of unsteady flow past a body taking into account real gas properties, such as turbulent viscosity and thermal conductivity (third and fourth levels) can be solved only for model aircraft even using giant-powered computers. These difficulties are associated not only with the multiparameter nature of the problem (various Mach's and Reynolds numbers, geometry of aerodynamic bodies etc.) but also with the insufficient justification of mathematical models and their closing relations, for example, insufficient justification of turbulence models and their applicability. Similar difficulties also arise in hypersonic aerodynamics, in which besides solving the above-mentioned problems, it is necessary to assess the effect of the chemical reactions proceeding in the gas near the aerodynamic body and on its surface at high temperatures, estimate the surface failure, and allow for strength and other characteristics.

Naturally, the solution of other problems using various approximations involves other difficulties, whose resolution determines progress in mathematical modeling. The variety of parameters of the problems investigated and the fact that the processes studied are nonuniformly scaled, nonlinear, and multidimensional makes it impossible

to develop general approaches to formulating problems and obtaining solutions. We can only discuss some directions of research and general trends, which include:

- using models of different levels depending on the purpose of investigation;
- using increasingly sophisticated models in order to allow for more real physical effects of phenomena under study;
- analysis and systematization of models and identification of certain classes of general models applicable to the description of a wide variety of problems;
- further mathematical justification of physicomathematical models and correct formulations of initial boundary-value problems.

It must be noted that simplified models are usually obtained from models of higher levels under various assumptions on the nature of the phenomenon investigated. Therefore, based on a fuller model, it is possible to obtain a set of simplified models. Full models from which their simplified approximations can be derived will be referred to as covering models. An example of such models is the model described by Navier–Stokes equations for a compressible heat-conducting gas (fourth-level model). Ignoring the effects of viscosity and thermal conductivity, we obtain a gas-dynamic model suitable for description of many physical problems. For high-viscosity flows, it is possible to use the boundary-layer approximation obtained from the Navier–Stokes equation by retaining terms of order $O(1/\sqrt{\text{Re}})$ and neglecting terms of higher-order smallness. Within the same approach, models of viscous shock layer, models of “parabolized” Navier–Stokes equations, etc., can be obtained (see, e.g., [14]). Obviously, for other classes of problems, chains of simplified models can be constructed on the basis of a basic covering model. This approach allows one to reduce the number of models considered and focus on the study of basic models describing general classes of problems.

It should be noted that the present-day level of mathematical modeling (at least, in the mechanics of continuous media) is based on the extensive previous research in theoretical mathematics, mechanics and physics. New achievements in mathematical modeling will be based on new theoretical results in those fields and their use by computational mathematics. The drastic qualitative improvement in computer speed of up to 10^{12} – 10^{14} FLOP attained over the past decade has made it possible to proceed to numerical modeling of fourth-level problems, for example, modeling of real processes in metallurgy and chemistry, in aerodynamics for the optimization of the design of real aircraft over a wide range of incident-flow parameters, modeling for hypersonic, air-breathing and rocket engines, simulation of the transfer from laminar to a turbulent flow and back, etc.

2. Numerical Algorithms. As was already noted, the nonlinearity of most problems under study and corresponding systems of differential equations hinders obtaining their exact solutions, except in some particular cases. Moreover, such solutions are sometimes nonexistent, and, therefore, the main methods for obtaining them are approximate and numerical methods. Approximate methods are based on a certain representation of a solution using known assumptions on the nature of the solution. For example, in asymptotic methods of aerodynamics, a solution is represented as an expansion in a small parameter (in inverse Reynolds numbers for large Re numbers or in Mach numbers M for hypersonic velocities, etc.). Although such solutions can be readily obtained, these approaches can be used only for comparatively simple problems in which just one flow type is predominant. The question of the applicability and validation of these approaches remains to be solved. Asymptotic methods were extensively used in the initial stage of modeling. The conversion to more complex models has required the development and application of numerical algorithms for solution of multidimensional problems using various physicomathematical models.

In the current stage of development of mathematical modeling, various numerical methods, such as the finite-difference method (FDM), the finite-volume method (FDV), the method of finite elements, and the method of boundary elements, and special methods, such as particle-in-cell method, the statistical Monte Carlo method, etc. We analyze the development of the FDM and FDV, which have been extensively used to solve problems of the mechanics of continuous media because of their universality. The fundamentals of the FDM and FDV are presented in numerous publications (see, e.g., [15–22]). Let us recall the main notions. In a domain $\Omega = \Omega(\mathbf{x})$ with boundary γ , let it be required to find a solution of the boundary-value problem

$$L\mathbf{u} = \mathbf{f}, \quad l\mathbf{u}_\gamma = \boldsymbol{\varphi}, \quad (2.1)$$

where L and l are differential, integral or algebraic operators, $\mathbf{u} = u(\mathbf{x})$ is the vector of the sought functions, $\mathbf{x} = (t, x_1, \dots, x_N)$ and \mathbf{f} and $\boldsymbol{\varphi}$ are vectors of the right sides. Let us assume that problem (2.1) is well posed. Change-over from mathematical formulation of the problem to numerical solution includes the following stages:

- replacement of the domain Ω of the continuous argument \mathbf{x} by its discrete analogue Ω_h ;
 - replacement (approximation) of the functions \mathbf{u} , \mathbf{f} , and φ of the continuous argument \mathbf{x} by discrete functions \mathbf{u}_h , \mathbf{f}_h , and φ_h ;
 - approximation of the initial operators L and l by their discrete analogues L_h and l_h .
- The above-mentioned operations result in the system of discrete equations

$$L_h \mathbf{u}_h = \mathbf{f}_h, \quad l_h \mathbf{u}_h|_{\gamma_h} = \varphi_h, \quad (2.2)$$

which is referred to as a difference scheme. As a consequence, the question arises of the relationship (similarity) between the solutions of the initial differential problem (2.1) and the discrete problem (2.2). Since every stage of formulation of the discrete problem can be performed by various methods, for the solution of problem (2.1) a family of discrete formulations (2.2) can be obtained, which, generally speaking, can have different properties. The requirements to numerical algorithms can also differ. Let us formulate the most important of them:

- convergence of the solution of the discrete problem (2.2) to the solution of the initial problem (2.1);
- sufficient calculation accuracy;
- economic efficiency of the algorithm;
- universality of the algorithm, i.e., its adaptability to various physicomathematical models;
- adaptability of the algorithm to various computer designs and architectures.

Obviously, the above requirements, as was noted above, must be supplemented by the requirement that the properties of the difference schemes must be adequate or close to the properties of the initial problem (see [21]), by the conditions of scheme conservatism, algorithm homogeneity, etc. The modeling efficiency at this stage can be accurately estimated only over the entire processing (technological) chain. It must be noted that the requirements to numerical algorithms are somewhat contradictory, and depending on the purpose of investigation, some of them can be omitted. For example, if it is important to obtain a high-accuracy solution, the economic efficiency or universality of the algorithm can prove to be of less significance. Thus, satisfaction of all requirements leads to the optimization problem of optimization. As any other optimization problem, this one can have one or several solutions (or have no solutions at all). An obvious consequence of the aforesaid is that it is impossible to design a universal algorithm for solving different classes of problems and that it is necessary to work out various algorithms intended for different purposes of investigation.

Let us analyze the main requirements to numerical algorithms. In order to guarantee the *convergence* of a numerical solution to the solution of the initial problem, the conditions of approximation and stability (correctness) of the difference solution must be satisfied (as follows from the theory of difference schemes [16, 17]). The proof of these statements is rather complicated, especially for the case of nonlinear equations, and is an important problem of the theory of difference schemes.

Requirements to calculation *accuracy* for various physicomathematical problems vary depending on the aim of modeling. Doubtlessly, calculation accuracy must agree with the accuracy of the selected physicomathematical model. Improvement in calculation accuracy as one of the most significant characteristics can be attained by refining the grid steps or calculation cells, using nonuniform and moving grids, constructing higher-order schemes. In recent years, calculation accuracy was also improved by different methods, such as: extrapolation of numerical solutions obtained on a succession of grids [23], employing information on the solution smoothness (algorithms without saturation [24]), using exact solutions (in a grid cell with piecewise constant or piecewise linear initial data), as in the Godunov scheme, used as the basis for construction of new classes of difference schemes [25], identification of the main singularities of a solution, for example, a bow shock wave in supersonic flow problems, etc., The uniform refinement of grid steps (or calculation cells) is not an efficient method for improving the accuracy in solving multidimensional problems because of the power-law increase in the number of grid nodes in the calculation domain and the respective increase in the number of arithmetic operations. Although this approach does not require alterations in the algorithm and programs, it is used comparatively seldom. For problem solution, non-uniform grids are most frequently used, including grids condensed in the regions of high gradients. If information on the behavior of a solution is available, the coordinates are converted so as to condense cells in the regions containing singularities of the solution (boundary layers, shock waves, etc.). This approach proves to be highly efficient, because it results in a notable improvement in accuracy without a considerable increase in the number of calculation cells. However, for most problems, regions of high gradients or other singularities are usually unknown *a priori* and can be obtained only in the course of solution.

An even more complicated situation arises for unsteady problems, whose solution varies in time and calculation grids are time-dependent. In order to solve such problems, the initial equations must be supplemented by unsteady equations to determine the laws of motion for the grid [25–28]. Complication of calculation domains and transfer to the solution of multidimensional problems necessitated the development of special methods for constructing or generating grids satisfying particular requirements. At the present stage of modeling, the problem of constructing efficient grids becomes crucial, and, according to expert evaluation, most of computational burdens fall on the solution of this problem. Some approaches to solving such problems are presented in [25–29]. Let us indicate one more method for improving calculation accuracy, namely, the construction of a solution on nested or adaptively nested grids. Although this approach has not been sufficiently developed, it can serve as the basis of preliminary solution, after which the solution process can be repeated until the desired accuracy of solution is attained. Some methods for solving equations on non-structured grids are discussed in [29].

In recent decades, in addition to nonuniform grids, higher-order schemes have been widely used, mostly of two types: schemes using an extended pattern (see [20, 22]) and so-called high-order compact schemes using a three-point pattern [30, 31]. In the first case, in constructing continuous computation schemes for problems with discontinuous data, oscillations of numerical solutions are reduced using various methods of monotization; to the initial equations of the difference scheme dissipative terms are added, which reduce oscillations and smooth the solution. In TVD-type schemes based on the principle of minimum derivatives, solution monotonicity is attained by introducing nonlinear numerical dissipation, which provides for feedback between the numerical scheme and the solution [32–34]. As a rule, such schemes fit the entropy inequality and have second or higher orders of approximation. The solution is smoothed on a limited number of grid cells. There are numerous modifications of the scheme (ENO-schemes, correlation schemes, schemes with limited antidiffusion, etc. [34]), which retain monotonicity, higher order on discontinuities, conservatism, etc. It must be noted that the use of expanded patterns in these schemes necessitates the specification of fictitious layers and additional boundary conditions absent in the initial formulation of problems or changing the approximation in near-boundary nodes, which disturbs the scheme uniformity.

In the case of compact schemes, higher-order approximation is attained on a three-point pattern through a special choice of an equation approximation that eliminates lower-order errors (see [20, 22, 30, 31]). A disadvantage of these schemes is that the approximation is considerably complicated, especially for multidimensional cases. At the same time, the use of higher-order schemes is the only method for solving multidimensional problems with reasonably high accuracy.

A modification of the FDM is the FDV, which is based on the approximation of initial equations in integral form (see, e.g., [16–20]). The possibility of choosing various forms of calculation cells in approximating calculation domains has made the FDV rather popular in solving problems with complex geometry, including multiply connected domains. Initial equations are approximated for every initial cell, i.e., the obtained schemes are conservative. The order of approximation depends on the approximation accuracy for volume and surface integrals, which facilitates the construction of higher-order schemes.

The *economic efficiency* of an algorithm has always been one of the most significant requirements and it is understood as the minimization of the number of arithmetic operations required to solve the problem. We estimate computer resources required to solve multidimensional unsteady problems (see [11]). Let M be the space dimensionality of a problem, m the number of equations (unknown functions), I_j the number of grid nodes in the direction x_j , q the average number of arithmetic operations per grid node, and N the number of time steps. Then, the total number of operations required to solve the problem is

$$Q = mqNI, \quad (2.3)$$

where $I = I_1 \times I_2 \times \dots \times I_M$. This formula does not allow for some factors that influence the consumption of computer resources, such as the number of internal iterations, specified computation accuracy, initial approximation, etc. We assume that they were allowed for *a priori* in the coefficient q . As an example, let us choose average values of parameters in solving problems by existing methods: $I_j = I = 10^2$ – 10^3 , $m = 10$ – 10^2 , $N = 10^3$ – 10^4 , and $q = 10^2$ – 10^4 . For $M = 3$ (three-dimensional case), $Q = 10^{12}$ – 10^{19} FLOP. Let R denote the number of computer operations per second. Then,

$$T = Q/R \quad (2.4)$$

is the time of problem solution. Correspondingly, the RAM consumption can be calculated from the formula

$$L = mLI,$$

where l is the number of time layers required for storage in RAM (normally, $l = 2$). Expert appraisal shows that a design using the results of mathematical modeling is optimal when the calculation of a single version does not exceed 15 min (about 10^3 sec). In order to satisfy this condition, the computer speed and RAM size for the solution of a three-dimensional problem must be $R = Q/T = 10^9\text{--}10^{16}$ FLOP, $L = 2 \cdot 10^7\text{--}2 \cdot 10^{11}$ bytes. We note that in the U.S. national aerospace modeling project (see [6]), worked out in the 1980s and intended for the solution of aerodynamic problems, the computer characteristics were as follows: $R = 10^9\text{--}10^{10}$ FLOP and $L \approx 2.5 \cdot 10^8$ bytes, i.e., it was planned to design a computational system for the solution of 3D aerodynamic problems in the approximation of gas-dynamic equations and simplified Navier–Stokes equations (models of second and third levels).

The above definition of the speed R did not specify whether a uniprocessor or multiprocessor computational system was employed. The speed R was assumed not to be dependent on the type of algorithms, problem dimensionality, memory consumption, and other factors. Actually, the processing speed depends on many factors. For approximate allowance of the latter, the processing speed can be written as

$$R' = sR,$$

where R is the peak performance of the system, s is the average loading factor for processors ($s < 1$), whose value can vary significantly for different multiprocessor systems. According to (2.4), the cost of problem solution can be reduced by decreasing Q or improving the processing speed R . The number of arithmetic operations Q determines the economic efficiency of an algorithm. A numerical algorithm can be called *economic* if Q in (2.3) is a linear function of the number of grid nodes in time and space. As is known, the difference schemes are divided into explicit and implicit classes. As a rule, explicit schemes are conditionally stable, i.e., a difference problem is correct under a certain relationship between the time (iterational), τ , and space, h_j , steps of the grid. For implicit schemes, there are no such constraints or those are weaker than for the explicit schemes. In accordance with the above-mentioned definition, explicit schemes are not economic. Let us consider a very simple example. Let (2.2) be an explicit difference scheme, which approximates an unsteady heat-conduction equation in region $\Omega = \{0 \leq t \leq 1, 0 \leq x \leq 1\}$. We introduce difference grid steps $\tau = 1/N$ and $h = 1/I$, where N and I are the numbers of grid nodes in the t and x directions. The explicit scheme is stable when the condition $\tau \leq h^2/2 = KI^{-2}$ is satisfied. Then, the number of arithmetic operations required to solve the problem is $Q = qNI \approx KqI^3$. When the grid step is changed h , i.e., when the number of nodes (I) increases, the number of operations increases by a factor of p^3 . A similar situation arises when explicit schemes are used to solve hyperbolic equations for which the number of operations increases according to the square law under a linear increase in the number of grid steps.

We now consider the questions of algorithm *universality*. For explicit schemes, extension of algorithms to the multidimensional case does not involve serious difficulties but economic efficiency becomes a major problem because an increase in problem dimensionality leads to more rigid constraints on stability. Even for linear systems for multidimensional problems, the implementation of implicit schemes becomes much more complicated. For instance, for $\alpha \geq 0.5$, a difference scheme with weights for numerical solution of the linear heat-conduction equation (see [20]) is unconditionally stable and approximates the heat-conduction equation with order $O(\tau^2 + h^2)$ at $\alpha = 0.5$. In the one-dimensional case, it is implemented by scalar triple-point marching and requires eight arithmetic operations per grid node. For the two-dimensional case, its solution can be obtained by matrix sweep, which requires inversion of $I \times I$ matrices at each grid node. Obviously, for a great number of nodes, this scheme becomes economically inefficient. Such a situation is also characteristic of hyperbolic equations. Therefore, extension of efficient implicit schemes for solving one-dimensional problems to the multidimensional case usually complicates their realization or leads to lower economic efficiency. The conversion from the solution of one-dimensional equation to the solution of multidimensional problems required the development of new numerical algorithms that can be effectively used to solve problems of any dimensionality. Such algorithms were developed in the 1970s–1980s on the basis of factorization and splitting methods (see, e.g., [1, 3, 14–22]). They reduce the initial multidimensional problem to a succession of its one-dimensional analogues or simpler problems. In factorization method, basic schemes are represented as an approximate product of one-dimensional or simpler difference analogues, and in the splitting method, the initial problem is represented as a set (weak approximation) of simpler one-dimensional problems, which are then approximated by explicit and implicit difference schemes (see [3, 15, 18]). It must be noted that the introduction of splitting or factorization into difference schemes leads to the appearance of additional terms of order $O(\tau^2)$, absent in the initial equations, which can deteriorate the solution accuracy or increase the number of iterations required to obtain a steady-state solution by the relaxation method.

The last but not less important requirement to numerical algorithms is their *adaptation* to different architectures of computer systems. The basic numerical algorithms used to solve problems of different classes were developed at the time of uniprocessor computers and imply successive arithmetic operations. The emergence of various multiprocessor computing systems has made it necessary to revise the developed numerical algorithms and to assess their efficiency and adaptability to new architectures. This problem is especially difficult because there are various approaches to designing computer architectures. Therefore, at present, the adaptability of most existing methods to various types of computing systems has not been sufficiently studied. It is much easier to parallel explicit schemes. For example, in explicit computation in a new step, an original problem can be divided into separate segments or modules, each of which can be solved independently (with accuracy up to calculations on segments boundary and data transfer from one segment to the others). Therefore, the emergence of new computing facilities resulted in the appearance of a new trend in computational mathematics — the development of parallel algorithms for solving multidimensional problems.

Let us formulate the main problems that arise in the design of numerical algorithms:

- development of mathematical apparatus and its application to the justification of numerical algorithms;
- generation of calculation grids with specified characteristics (e.g., those adapting to solution) for the solution of multidimensional problems in complex, multiply connected geometries;
- adaptation of existing and development of new, economically efficient, numerical algorithms using various physicomathematical models and computers with various architectures.

It should be noted that significant advances have been attained in the development of the other elements of the technological chain “programming–computer.” The state of the art of programming languages and the prospects of their development are discussed in [35]. The speed of computers and computing systems increases exponentially both due to the refinement of the element base and the design of fundamentally new architectures of computing structures and modeling systems. In addition to the emergence of supercomputers with a peak power up to 10^{12} – 10^{15} FLOP, computational facilities of the cluster type are being developed, which network computers of different level: PC, workstations, etc. One should expect the emergence of new computer facilities, their increasing influence on the development of numerical algorithms and models, and the design of expert systems and modeling systems for various spheres of human activity.

REFERENCES

1. N. N. Yanenko, *Selected Papers. Mathematics. Mechanics* [in Russian], Nauka, Moscow (1991).
2. A. A. Samarskii, “Mathematical modeling and computational experiment,” *Vestn. Akad. Nauk SSSR*, **5**, 38–49 (1979).
3. O. M. Belotserkovskii, *Numerical Modeling in the Mechanics of Continuous Media* [in Russian], Nauka, Moscow (1984).
4. N. N. Yanenko and A. N. Konovalov, “Modular approach to constructing programs as the basis for development of an application software package for solving of problems of continuum mechanics,” in: *Application Software of Mathematical Physics* [in Russian], Comput. Center, Acad. of Sci. of the USSR, Novosibirsk (1972), pp. 46–54.
5. A. Jamesson, “The evaluation of computational methods in aerodynamics,” *Trans ASME, J. Appl. Mech.*, **50**, 1051–1070 (1983).
6. F. R. Balley, “Status and projections of the NAS program,” Technishe Memorandum Report No. 88339, NASA, Amer. Res. Center, CA (1986).
7. P. Kutler, “A perspective of theoretical and applied computational fluid dynamics,” *AIAA J.*, **23**, No. 23, 328–341 (1985).
8. *Comput. Fluid Dyn. J.*, **9**, No. 1: *Proc. of Int. Symp. on CFD* (1999).
9. *Comput. Fluid Dyn. J.*, **9**, No. 4: *Advanced Method for Computational Fluid Dynamics* (Special issue) (2001).
10. B. L. Rozhdestvenskii and N. N. Yanenko, *Systems of Quasilinear Equations* [in Russian], Nauka, Moscow (1968).
11. V. M. Kovenya, *Computational Methods (Supplementary Chapters)* [in Russian], Novosibirsk State University, Novosibirsk (1995).
12. O. M. Belotserkovskii, “Mathematical modeling using supercomputers (experience and trends),” *Zh. Vychisl. Mat. Mat. Fiz.*, **40**, No. 8, 1221–1236 (2000).
13. *Numerical Methods in Fluid Dynamics*, Hemisphere, Washington–London (1979).

14. V. M. Kovenya and N. N. Yanenko, *Splitting Method in Problems of Gas Dynamics* [in Russian], Nauka, Novosibirsk (1981).
15. N. N. Yanenko, *Splitting Method for Solving Multidimensional Problems of Mathematical Physics* [in Russian], Nauka, Novosibirsk (1967).
16. A. A. Samarskii, *Theory of Difference Schemes* [in Russian], Nauka, Moscow (1989).
17. S. K. Godunov and V. S. Ryaben'kii, "Difference schemes. An introduction to the underlying theory," in: *Studies in Mathematics and Its Applications*, Vol. 19, North-Holland, Amsterdam (1987).
18. G. I. Marchuk, *Methods of Computational Mathematics* [in Russian], Nauka, Moscow (1980).
19. S. A. Fletcher, *Computational Techniques for Fluid Dynamics*, Vols. 1 and 2, Springer Verlag, New York (1988).
20. A. A. Samarskii and E. S. Nikolayev, *Methods for Solving Grid Equations* [in Russian], Nauka, Moscow (1978).
21. Yu. I. Shokin and N. N. Yanenko, *Method of Differential Approximation* [in Russian], Nauka, Novosibirsk (1985).
22. N. S. Bakhvalov, N. P. Zhidkov, and G. M. Kobel'kov, *Numerical Methods* [in Russian], Nauka, Moscow (1987).
23. G. I. Marchuk and V. V. Shaidurov, *Improving Solution Accuracy of Difference Schemes* [in Russian], Nauka, Moscow (1979).
24. K. I. Babenko, *Fundamentals of Numerical Analysis* [in Russian], Nauka, Moscow (1986).
25. S. K. Godunov, A. V. Zabrodin, M. Ya. Ivanov, et al., *Numerical Methods for Solving Multidimensional Problems in Gas Dynamics* [in Russian], Nauka, Moscow (1989).
26. V. D. Liseikin, *Grid Generation Method* [in Russian], Springer Verlag, Berlin (1999).
27. V. D. Liseikin, "Overview of methods for constructing structured adaptive grids," *Zh. Vychisl. Mat. Mat. Fiz.*, **36**, No. 1, 3–41 (2000).
28. A. N. Gil'manov, *Adaptive Grid Methods in Problems of Gas Dynamics* [in Russian], Nauka, Moscow (2000).
29. A. A. Samarskii, A. V. Koldoba, Yu. A. Poveschenko, et al., *Difference Schemes on Irregular Grids* [in Russian], Kriterii, Minsk (1996).
30. A. I. Tolstykh, *Compact Difference Schemes and Their Application to Problems of Hydrodynamics* [in Russian], Nauka, Moscow (1996).
31. V. I. Paasonen, "Scheme of third-order approximation on a nonuniform grid for Navier–Stokes equations," *Vychisl. Technol.*, **5**, No. 5, 78–85 (2000).
32. A. Harten, "A high resolution scheme for the computation of weak solution of hyperbolic conservation laws," *J. Comput. Phys.*, **49**, No. 3, 357–393 (1983).
33. V. B. Karamyshev, *Monotonic schemes and their application to gas dynamics* [in Russian], Izd. Novosib. Univ., Novosibirsk (1994).
34. V. I. Pinchukov and Ch. V. Shu, *Higher-Order Numerical Methods for Problems of Aerohydrodynamics* [in Russian], Izd. Sib. Otd. Akad. Nauk, Novosibirsk (2000).
35. V. Sh. Kaufmann, *Programming Languages: Concepts and Principles* [in Russian], Radio Svyaz', Moscow (1993).