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Point of View

How to Reorganize Computational Science and Technologies?

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Abstract—The current era of the fourth industrial revolution is inevitably leading to a widening gap between actively and passively developing countries, and the strategy of scientific and technological breakthrough announced in the Russian Federation is the only way to achieve the status of a world power. Modern progress is based on infinite growth rates of computational and informational capacities of the post-petaflop scales, which provide previously unthinkable opportunities for acquiring new fundamental knowledge and introducing innovations in production, natural resource management, and the economic and social spheres. The key role here is played by predictive mathematical modeling of processes and phenomena, including theoretical and applied research, supercomputation, and large-scale computer experiments, operations with large data, and artificial intelligence. Emerging super problems require huge amounts of new-generation intelligent software, which is impossible without the formulation of concepts and paradigms of activity, architectural solutions, and constructive technologies. Global trends are leading to the development of integrated computing and information environments that form an instrumental environment for automating the construction of models and algorithms, their mapping onto supercomputer platforms, and the creation of comfortable interfaces for users with different professional backgrounds. Such an ecosystem is designed for a long life cycle with the continuous development and coordinated participation of various groups of developers, as well as widespread demand, thereby leading to the formation of a new industry with mass professions with a high level of supercomputer literacy. The listed scientific and technological challenges require competent organizational and infrastructural solutions, including the interdepartmental coordination of academic, educational, and production teams. Mathware and software of supercomputer modeling should permeate all spheres of human activity similarly to the circulatory or nervous system and transmit the value of new productive forces that improve the quality of life and ensure the sustainable development of society to become knowledgeable on intensive technologies.

Keywords: supercomputing, interdisciplinary problems, mathematical modeling, computational methods and technologies, software, artificial intelligence, integrated instrumental environment, supercomputer experiment.

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A famous Chinese proverb says, "May you not live in times of change." However, historical experience shows that a complex dynamic system such as world civilization is not limited to evolution but necessarily passes through periods of revolutionary transformations. Such ambivalence is illustrated by the proverb, "Heaven helps those who help themselves," and in the Bible it states that there is "A time to cast away stones, and a time to gather stones together." As a rule, revolution is associated with the destruction of the old way of life, while the creation of a new way is an evolutionary path that does not tolerate any fuss. Although every rule has exceptions.

A fateful moment for Russia has been announced. It is necessary to build a digital economy, raise labor productivity and GDP, and dramatically strengthen national security in six years [1]. Other leading states are rapidly moving in the same direction, and futurologists predict the era of "technological singularity" for humanity, an era of unlimited energy resources, new materials with fantastic properties that are unthinkable today, and biomedical technologies that grant eternal youth and immortality [2]. While observing the

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unprecedented rates of technological progress resulting from new scientific achievements, it is appropriate to recall the words of the great Leonardo da Vinci, who believed that one who loves practice without theory is like a sailor who sits on a ship without a rudder and a compass and therefore never knows where they can end up.

Despite all the balanced development of various basic directions in the XXI century, the importance of mathematics as the driving force of this development is obvious. Its role has dramatically increased after the mass availability of personal computers and due to the creation of multiprocessor teraflop and petaflop supercomputers (10^{12}–10^{15} operations per second). The rate of increase in computer capacity for more than 50 years is subject to the law of G. Moore, one of the founders of Intel; exponential growth of 1000 times in 11 years. Although saturation should have already occurred according to physical laws, the anomalous dynamics persist. Currently, a record supercomputer has about 200 petaflops, and the emergence of exaflops (10^{18} arithmetic operations per second) is expected around 2020. Such a multiprocessing computing system (MCS) will have hundreds of millions of calculating units, and the generation that is now entering the workforce will have access to supercomputations of fundamentally new scales. The possibility of storing and processing huge amounts of numerical data will lead to shocks comparable in resonance with the consequences of the two previous information explosions, i.e., first, the appearance of the Internet and then mobile phones, which radically changed the professional activities and life of a person. Mass remote access to supercomputer centers with cloud and network technologies in the very near future will make high-performance modeling of complex processes and phenomena in all areas, from basic research to production and social services, a trivial fact. Note that we are talking only about cluster architectures traditional for the past two decades; however, fundamentally new computers based on field-programmable gate arrays (FPGAs), as well as quantum and other physical effects, which will be discussed in the future, are on the way.

New super problems are arising with the advent of supercomputers: our time is characterized by the fantastic progress of all sciences and technologies and dealing with physical and mathematical problems of such complexity that a decade ago their study was possible only with the introduction of significant simplifying assumptions. In a certain sense, a theoretical physicist or applied mathematician now has to overcome the psychological barrier in order to understand the level of problems that can be solved using modern computational and informational methodologies.

We must be aware that the development of computational and informational technologies is an irreversible process like the arrival of a tsunami onshore even if it originated thousands of miles away in the depths of the ocean. Fortunately, the wave of computerization is creative, although some atavistic production and social relations will inevitably disappear. The main thing is to be professionally and ethically prepared for the upcoming changes in order to turn them for the benefit of man and society. Historical lessons show (but not always teach us) that technological breakthroughs are double-edged weapons, and it is no coincidence that cyberterrorism has become one of the main subjects at political summits.

The advanced countries have embarked on the fourth industrial revolution characterized by the wide introduction of the digital economy, additive technologies, 3D printers, virtual reality and digital twins, and other attributes of the post-industrial society. The task of the state striving for modern development is to "jump on the footboard of a departing train" so as not to be left behind forever. Next, we will try to show the problems that domestic science, primarily mathematics, is facing in this respect.

STRUCTURE OF MATHEMATICAL KNOWLEDGE AND THE PLACE OF MATHEMATICAL MODELING IN IT

First, it is necessary to decide on a capacious concept such as *mathematics,* because its content provokes serious discussions. Academician V.I. Arnold, one of the founders of mathematics in the XXI century, identified theoretical mathematics and theoretical physics. Moreover, he fiercely fought for their unity and perceived the growing methodological and educational gap between these sciences as a historical tragedy. At the same time, he did not recognize computational mathematics and computer science and called them "handicraft" in his polemical works [3]. Arnold's principal absentee opponent was Academician and programmer A.P. Ershov, an indisputable world authority at the dawn of computerization in the 1960s–1980s, the creator of the unique Siberian School of Computer Science, the author of common terms such as *computer literacy* and *school computer science,* who proudly proclaimed "I am a mathematician." His merits in the field of mathematics were accordingly recognized by the Chebyshev Prize of the USSR Academy of Sciences for the discovery and development of mixed computations. We can recall the great I. Newton, L. Euler, and K. Gauss, whose names were given to numerical algorithms that are still popular, in order to confirm the inseparability of theoretical and applied mathematics.

We will understand under mathematics *a multifaceted structure*, including theoretical and applied mathematics, computational mathematics, mathematical modeling, theoretical, system, and applied programming, as well as the mathematical foundations of artificial intelligence, data processing, knowledge technology (large data and deep knowledge), and computer architectures. The division into the listed components fully corresponds to the most general definition of mathematics as a science about mathematical objects. Obviously, the concepts of applied mathematics, computational informatics, computational geometry and topology, and the phrase *computer science,* which is common in English literature, but the literal Russian translation of which, *computational sciences,* is struggling to be accepted in Russian professional terminology, have the full right to exist. Moreover, areas such as computational physics, computational chemistry, and computational biology should be classified as an application of mathematical methods and technologies in their respective domains.

Mathematical modeling, which can generally be defined as *the study of processes and phenomena by mathematical methods,* has come to the forefront in recent decades among the designated variety of disciplines. Each of the categories used here requires its own meaningful explanation. The processes and phenomena are primarily understood as real (technical, natural, or social), e.g., the production of metals and new materials, natural or man-made disasters, and demographic dynamics. However, the study of abstract models that describe purely mathematical objects is also relevant. Moreover, this is what actually happens: the physical (or chemical, biological, etc.) model is represented by some mathematical model, in which minor effects are almost always neglected. The task of a modeler, a specialist in modeling in a specific application area, is to construct a model competently.

It is crucial that all the disciplinary areas under consideration constitute a unified mathematics: theoretical studies are the basis for computational algorithms and technologies implemented in the software of supercomputers which perform computational experiments to solve basic and applied problems. Moreover, it is important that this whole pattern changes very quickly and interconnectedly, and the symbiosis of basic research and practice is a two-way road. Fundamental results become a source of applied research; however, at the same time information technologies, including artificial intelligence, are an effective tool for formula transformations, the study of functional properties, and qualitative analysis of abstract objects with their visual representation, which completely changes the nature of the work of the researcher-theorist.

The work of specialists from applied fields is changing even more drastically, be it a chemist, geophysicist, or an engineer engaged in the development or operation of a device. A convenient tool for real-time modeling of the situation can also play the role of a navigator for a driver or an autopilot for a pilot. Evidently, in difficult cases it is possible to place an order for analyzing and predicting a process or phenomenon (outsourcing); however, this does not change the heart of the matter, an expert who is professionally skilled in modeling methodology and practice is always needed.

The mission of modeling is to be the main conductor of fundamental ideas and technologies into natural and technical sciences, production, nature management, and humanitarian spheres. In a certain sense, mathematical research methods play the same role in science as the lymphatic, circulatory, and nervous systems that feed and support all the vital organs of a person. All possible states of matter are described by a finite set of types of differential and/or integral relations. Stress-strain states of solids, hydrogasodynamic flows, electromagnetic fields, including phase transitions, chemical interactions, and relativistic and quantum effects, all of them are subject to the conditions of conservation of mass, momentum, energy, and other substances that give us the keys first to knowledge, and then, if we are lucky, to the management of processes and phenomena.

The slogan "We must not wait for favors from Nature; our task is to wrest them from her" was popular in the 1930s. Although the mathematician and philosopher R. Descartes tried to find an absolute method for comprehending all the laws as far back as in the XVIII century, the problem still persists. We do not even know the structure of the core of our planet, while trying to penetrate the mysteries of the universe. The devil is in the details. We do not always have the necessary information. If we know the initial and boundary conditions that ensure the existence of a single solution for the most complex so-called direct, multidimensional problem, we can apparently find it with the required accuracy by resorting to modern computational methods and technologies. It is much more difficult to solve inverse problems in which some of the source data is either parametrically represented or completely absent. In this case, the solution should be found by some additional indirect measurements that usually contain errors. Speaking in mathematical language, a criterion functional, which should be minimized in the parameter space, is formulated on the desired solution. It is these inverse problems that are of the greatest interest, because they are related to urgent problems of either identification of the model parameters, or optimization of the production process, or the design of a device with the given characteristics. An urgent inverse problem is, e.g., the search for minerals according to the geological exploration data.

A frequent "aggravating" factor is the interdisciplinarity of the problems to be solved, which involves studying the interaction of different types of processes described by systems of equations with a large number of unknown functions, which significantly increases the resource intensity of the problem. It is necessary to take into account the fact that modern requirements also force us to ensure a high degree of accuracy (or resolution) of modeling. All this creates extreme interdisciplinary super problems that were beyond the capacity of the most powerful computers of the last century. A vivid example of such a super problem is the simulation of a nuclear explosion, when a substance undergoes various phase transitions, and it is necessary to calculate electromagnetic fields, fluid dynamics, the stress-strain state of a solid, radiative heat transfer, and many other processes.

The complexity of the current super problems is only one reason for the rapid increase in the capacity of supercomputers. Another reason is the unimaginable diversity of all sorts of modeling problems. Here, a systemic approach comes to the rescue, as it makes it possible to look at the situation from the standpoint of modern classification methodologies. A set of modeling problems can be partitioned by different types of specifications, i.e., in different coordinate directions. By industry applications, we can distinguish, e.g., the energy industry, mechanical engineering, metallurgy, transport, chemical production, agriculture, medicine, and the economy, and each of the segments can be divided into fairly autonomous parts. There are many applications, but at the abstract level all of the listed problems are described by a limited set of types of equations: the Maxwell system for electromagnetism, the Navier–Stokes equation for hydrodynamics, the Lamé equation for elastoplasticity, and the Boltzmann equation for kinetics. Obviously, this list is not exhaustive, and these equations can be classified by the differential-integral characteristics, as well as by using group theory approaches.

If by modeling we mean the solution of problems to a logical end, i.e., to achieve results that are clear to the user, then it is necessary to add a variety of computational methods and computer technologies in the qualification of modeling methods. However, this will be discussed later. Now, we can say that the methodology of modeling is a tool for studying almost all applied problems. Evidently, no ready-made solutions have yet been found for any formulations, but this is the subject of ongoing basic research. More importantly, there are a huge number of real-world applications for which all major scientific questions have been answered but not brought into implementation, i.e., to innovations with a large potential economic effect. In order to dot the *i*s, it is necessary to develop mathematical methodologies to the level of working modeling technology. For example, it is sufficient to imagine the huge economic effect that could be achieved in construction using computer optimization of heat networks and building design taking into account the various regional climatic conditions of Russia.

THREE SOURCES AND THREE COMPONENTS OF MATHEMATICAL MODELING

In order to present the functionality and structure of mathematical modeling in general, it is first necessary to briefly characterize "both sides of the coin," mathematical and computer. The concept of a large-scale *computational experiment* was laid in the scientific schools of G.I. Marchuk, A.A. Samarskii, and N.N. Yanenko. It certainly underwent changes over the following decades, especially due to the advent of cluster multiprocessor computing systems with distributed and hierarchical shared memory, the main features of the architecture of which are now well established. Although, in general, the structure of a computer has been and will consist of three main components, i.e., arithmetic processors, memory devices, and means of communication, their continuous evolution has led to the transition of quantity into quality, and now the computer community is on the verge of changing computational and informational methods and technologies. The large number of computational nodes and cores form the base of the scalable parallelism paradigm. The amount of RAM is increasing simultaneously with the increase in performance (historically, a balance is observed, i.e., a machine with the performance of teraflops or petaflops has a memory of about a terabyte or petabyte), which also has many levels with different access times. To this we add the heterogeneity of supercomputers that have graphic accelerators with ultrafast arithmetics but with more limited logic.

Two main components of mathematical modeling can be clearly seen from the presented sketch of the supercomputer's architecture. The first one is high-performance computations, the speed of which initially characterized the class of the machine. Parallelization of algorithms, which is the cornerstone here, consists of the science, technology, and art (as well as patience) of the computer programmer. Success is measured by the real speed of the executable code versus the peak, or theoretical, performance. A figure of about 20% is usually considered the average achievement; increase it will fulfill the wild dreams of managers to make science more economical.

The second computational part of modeling is the storage, processing, and transmission of data. The resource intensity of large problems is usually balanced not only by the number of arithmetic operations but also by the size of the used numerical arrays. The class of problems, which include high-tech modeling problems, have been called *data intensive computing* (large data, large-scale computing) in the English literature. Note that our case is not specific information problems, such as the big data which arise in seismic exploration, space monitoring, or searching the Web. However, the drive for increasing performance in multidimensional modeling problems is a struggle against communication losses, which not only slow down calculations sharply but also have a negative feature such as huge energy expenditure. The power consumption of a supercomputer is becoming a significant factor in its operating costs.

The third component of modeling, which is not so obvious, because it is actualized at a fairly high level of computational and informational technology, is artificial intelligence. This problem was formulated in the mathematical language by Marchuk in the 1980s: automating the construction of algorithms and their mapping on computer architecture. Analytical formula transformations, set-theoretical, and other operations that are not related to arithmetic operations should be dealt with when solving mathematical problems. The first steps in the computerization of such activities were taken 50 years ago, and then an independent programming direction was formed based on cognitive principles and ontologies. The success of artificial intelligence is evident in the machine translation of texts, computer games, object recognition, and other fields.

If we talk about an effective modeling system for a wide class of problems, then it should have a knowledge base of mathematical formulations and algorithms. Natural languages are required for formulations, means for analyzing them, a cataloged archive of typical examples, tools for selecting appropriate methods, etc. In fact, in this case, we are talking about developing a friendly interface of the new generation with the user-mathematician.

Figure 1 presents a diagram reflecting the structure and logistics of a modeling system in general terms. In fact, its top level, "user applications," includes many interfaces for various categories of modelers. This is the integrated environment, or shell, of modeling systems for the outside world. The lower level is the computer hardware together with its system "platform," which can be implemented as a multiple-access computing center (MACC). Such a computing center includes "cloud" and network technologies that determine the estimated capacity of the entire conglomerate. The software segment is key in the number of man-years that need to be spent on the implementation of the entire project. The principal point is that this product should be developed by professional teams of programmers who interact according to agreed terms of reference. In addition, it is important that this software should have production support and general support, as well as the means for the continuous development and testing of codes on various technical devices. The last segment is the main one and consists of three sources (and at the same time components) of mathematical modeling: computational algorithms, data processing tools, and artificial intelligence tools. In the terminology of A.A. Dorodnitsyn, who headed the Soviet Union delegation on computational mathematics and computer science at international forums for many years, this level can be called brainware, because it actually represents the fundamental core of the entire modeling system.

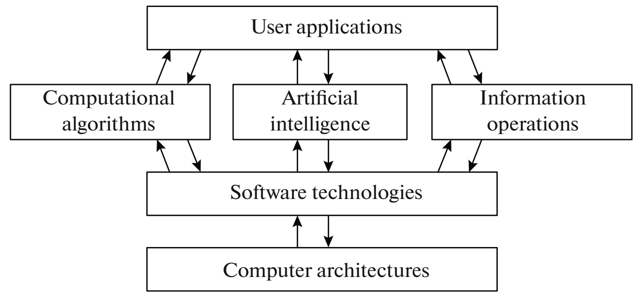

Fig. 1. Modeling system structure.

CONCEPT OF INTEGRATED COMPUTATIONAL ENVIRONMENT

The development of high-tech software for solving problems of mathematical modeling has a long history. A large number of commercial and academic products that represent an invaluable intellectual potential have been accumulated on the world market. However, the entry of advanced countries into the era of post-industrialization associated with the massive emergence of multiprocessor supercomputers and the multiplication of the number of urgent super-large problems has led to a general programming crisis. The situation is aggravated by the fact that the increase in the programmer's labor productivity is dramatically lagging the rapid increase in the productivity of computers. Moreover, the globalization of modeling with the arrival of new users is forcing a switch to a new programming paradigm.

Application software (AS) is divided into open source and commercial softwared from the organizational point of view. Traditional classification according to the functional and methodological characteristics defines three main types of AS.

• *Application software packages* (ASPs) is a problem-oriented software of a specific class (or classes) of practical problems, including instrumental support for the main stages of modeling and relatively weak dependence on external software products. Examples of highly developed and widespread ASPs are NASTRAN, ANSYS, FreeFEM, NGSolve, and FlowVision. It is also called the software application suite (SAS), examples of which are LOGOS and NIMFA developed at the All-Russian Research Institute of Experimental Physics (Sarov).

• *Libraries of algorithms and programs* is a method-based software that contains a fairly representative set of methods for solving a certain mathematical class of problems. Such software includes the "comprehensive" NETLIB library, the library of algebraic methods MKL INTEL, HYPRE, PETSc, EIGEN, SPARSE KIT, etc.

• *Technological tools* in their structure can also be of a library type, but they are associated more with the information support of the corresponding computa-

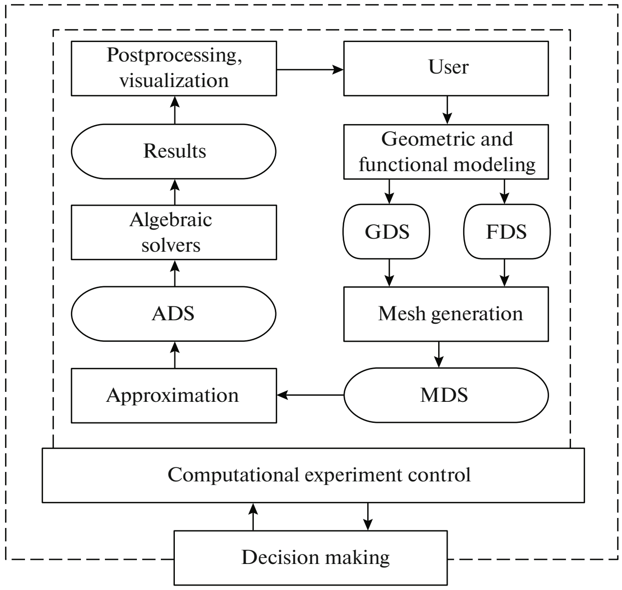

Fig. 2. Structure of functional and informational components of core of base modeling system of geometric, functional, mesh, and algebraic data structures (GDS, FDS, MDS, and ADS, respectively).

tional processes. Examples include mesh generators NETGEN, GMESH, TETGEN, PARAVIEW, VISUAL STUDIO graphics packages, and graph transformation tools METIS, PARMETIS, SCOTCH, etc.

The AS classification does not include general-purpose system software (SS) or self-sufficient products such as the CAD software (CAD, CAM, CAE, and PLM), which have their traditional market but are showing trends of integration with mathematical modeling tools. Examples of domestic (or semi-domestic, i.e., developed using imported components) systems of this kind are TFLEX, COMPAS, and GERBARIA.

The trend of the past decades is the transition to the concept of integrated computing environments (ICE), i.e., to the creation of an open instrumental environment focused on the automated construction of computational models, algorithms, and technologies classified by all the main stages of modeling of a wide range of processes and phenomena. Such projects include OPEN FOAM, DUNE (Distributed Unified Numerical Environment), MATLAB (a commercial product for universities with its own open source version OCTAVE), INMOST (developed by the Institute of Numerical Mathematics of the Russian Academy of Sciences), and the basic modeling system (BMS) developed by the Institute of Computational Mathematics and Mathematical Geophysics of the Siberian Branch of the Russian Academy of Sciences for the comprehensive support of all technological stages of modeling.

BMS is designed for both AS developers and end-users with different professional backgrounds. The ICE concept is dual-purpose: on the one hand, it is a set of tools for qualitatively improving the labor efficiency of developers of mathware and software and, on the other hand, a toolbox for the real-time assembly and operation of high-performance ASP configurations from ready-made BMS functional core blocks for specific applications by analogy with the intelligent LEGO construction set.

Architecturally, BMS is a collection of fairly autonomous method-oriented subsystems, each of which is responsible for its functional stage and is connected with the other blocks only by consistent data structures. Such a scheme implements the formula of N. Wirth, an authoritative specialist in the field of computer science and programming, "program = algorithms + data structures."

All the technological stages of a high-tech machine experiment consist of the following limited set: geometric and functional modeling (description and modification of the computational domain, equations to be solved and additional conditions, identification and analysis of the problem properties), mesh generation (problem discretization, support for parallel domain decomposition algorithms and multigrid approaches), approximation of the initial equations (methods of finite volumes and finite elements of various orders, etc.), solving algebraic problems (the most time-consuming part, because modern systems have up to 10^{10} or more unknowns), post-processing and visualization of numerical results, optimization methods for solving inverse problems, control of the computational process, and the system of decision-making based on calculations.

Figure 2 shows the structure of functional and informational components (rectangles and ovals, respectively) of the core of the BMS. The diagram describes an algorithm for solving direct problems, and the stage of solving inverse problems by optimization methods (by repeatedly solving direct problems) is included for brevity in the "Computational experiment control" stage. Each of the eight blocks is a high-performance implementation of a separate meaningful direction of computational mathematics, and none of the components can be removed from the continuous technological chain of mathematical modeling.

The main architectural principle of the BMS design is that each of its subsystems is not just a certain library of programs but an integrated instrumental environment for the corresponding computational and informational technologies. Consequently, the BMS itself is also an integrated environment.

The principles of the ICE construction (technical requirements) are as follows:

• Flexible expandability of the composition of models of interdisciplinary problems being solved and methods for solving direct and inverse problems without software restrictions on the number of degrees of freedom and on the number of used computing processors and/or cores.

• Adaptability to the evolution of computer architectures involving component technologies to ensure the consistency of internal and external intermodule interfaces.

• Universality and convertibility of data structures that are consistent with the existing common formats and support the effective reuse of external software products.

• Multilingual and cross-platform nature of the software's functional content, openness to the coordinated participation of various groups of developers in the project.

• High performance of the software code with scalable parallelism based on hybrid programming tools on heterogeneous MCSs with distributed and hierarchical shared memory.

• Availability of intelligent user and internal interfaces oriented toward widespread application in various production areas by specialists with different professional backgrounds.

The formulated requirements are intended to ensure a long life cycle and service life of the project, as well as conflicting qualities such as efficiency, versatility, high performance, and producibility of the developed high-tech software. These requirements are made at all stages of the development, maintenance, and use of the products, which can significantly increase the efficiency of developers and the massive demand for their results by end users.

The richness of the underlying functionality of the modeling system and the strict requirements for the performance and quality of programming demand advanced system support for the development of the core of the BMS. The following points can be listed among its components and methodologies:

• Automation tools for verification, validation, and testing of various types of algorithms, also in various external environments.

• Configuration management of multiversion implementations of software modules and the formation of ASPs or their fragments for users. An important subproblem is the development of versions for training.

• Control of the computational process and organization of computational sessions, also in cloud technologies.

• Automation of the development and parallelization of algorithms, their mapping on computer architecture, which requires detailed knowledge of methods and hardware features, as well as the ability to effectively use high-performance high-tech tools, such as Sparse Blas, MAPLE, and METIS.

• Specification and support of programming styles, i.e., modular, assembly, fragmentary, object-oriented, functional, etc.

• Component technologies to support multilingual and cross-platform project, i.e., COM/DCOM, Common Component Architecture (CCA), and language factories: Scientific Interface Definition Language (SIDL) and Domain Specific Languages (DSL).

The ways of organizing teamwork in large software projects are equally important. The SCRUM and AGILE techniques are examples of this. An independent question in corporate development is the remote interaction of various groups, including the outsourcing principle, i.e., management with the distribution of problems to various workers.

The purpose of the listed instrumental approaches is to drastically increase the programming productivity and to develop an integrated mathematical and applied software, comparable to a regular operating system or compiler in terms of serviceability. Project implementation in a certain sense means the manufacture of the tools of production of mass high-tech software products. In the language of the construction industry, we are talking about the transition from the individual technology of building construction to the erection of a plant (or a network of plants) for the production of specific products and other architectural structures. Note that such a strategy for computational and informational components has a significant advantage over material production. For example, while the price of a specific hammered nail includes the price of the metal from which it is made and its transportation, there are practically no similar costs for copying and sending a program module. Continuing this analogy, we can distinguish three production levels related to a nail: its direct use, the production of a nail on a machine, and the creation of the machine itself at the corresponding plant. At the same time, the ICE development refers to the highest level, i.e., to the construction of a machine-tool plant. While describing the integrative role of this project, it should be noted that it is based on a system-forming foundation including three scientific and technological "whales": high-performance computing, large data structures, and artificial intelligence.

WHAT SHOULD BE DONE?

A sacramental question was often asked in our country a few decades ago: Why can India earn billions of dollars from selling its software, and Russia has to spend huge sums to buy it or use "stolen" products? It is necessary to move from purely scientific problems to a discussion of organizational aspects and even touch upon the problems of scientific diplomacy in order to solve this and related problems. First of all, let us formulate a number of provisions which follow from the above.

First, scientific and technical progress in the nearest future will lead to a significant increase in the difference in the economic level of advanced and underdeveloped countries. Today it is being decided which group our country falls into.

Second, mathematical modeling on supercomputers is a powerful catalyst of the fourth industrial revolution.

Third, the phrases "digital economy," "digital twins," "smart houses," and "Internet of things," which are widely used in foreign and domestic media, can be misleading, as if the revolution initiated by supercomputers is associated only with information technologies that are not supported by basic science and mathematical modeling. The propaganda campaign of the automation of the whole country that started in the 1970s throughout the former Soviet Union can be considered as a serious warning (and a lesson). Automation and production management, a matter of great importance, fell victim to bureaucratic incompetence and profanation, when the director of a company simply bought a computer and reported to the regional party committee that he had installed an automated control system.

Fourth, the upcoming fundamental transformations of economic and public life is impossible without the development of huge volumes of the new-generation mathematical computer software, the cost of developing which is not less than the cost of the hardware (the price of a petaflops computer is currently about 1 billion rubles). We should forget about the image of an armchair scientist like G.I. Perelman, who does not need anything for work except a pen and a sheet of paper. Supercomputing and modeling are a serious industry that requires significant investment, but they will certainly pay for themselves many times over.

Fifth, the development of domestic high-tech software is a priority problem for national security, especially considering the current political situation in the world. It is sufficient to imagine a hypothetical situation in which the US State Department prohibits Intel, Microsoft, and others from selling their products to Russia as a form of sanctions. Another point is also important: not every country can create a fully fledged industry of supercomputer mathware and software. However, because of the level of Russian scientific schools, our country can and should do it.

Starting from the formulated five items that reflect the current situation in the field of scientific and technological progress and the inextricably linked position of individual states in the global stage, it is possible to discuss possible plans for reorganizing the management of the development of computational sciences and technologies in our country. It is very useful to critically comprehend the experience of advanced countries that are ahead of us in terms of the level of development of this industry.

The German National Program on supercomputing SPPEXA (Strategic Priority Program 1648 "Software for Exascale Computing" [4], formed in 2013), which is based on a consortium of more than 40 institutions and is now being transformed into two- and three-way interdisciplinary megaprojects with partners from France and Japan, can be noted among the state initiatives in this field. There are similar strategic initiatives in the United States, China, and several other countries.

The International Exascale Software Project (IESP) and the Society for Industrial and Applied Mathematics (SIAM), which publish more than ten of the world's leading journals in all subfields of computer science and organizes major conferences and other events, deserve special attention among nongovernmental initiatives.

In our country, there is a sufficiently large number of state bodies and other organizations de jure involved in the management of the development of science and technology. In addition to the Russian Academy of Sciences, these are the Ministry of Science and Higher Education of the Russian Federation, the Ministry of Digital Development, Communications and Mass Media of the Russian Federation, the Presidential Council for Science and Education, the Russian Foundation for Advanced Research Projects, the Agency for Strategic Studies, the Foundation for the Development of Information Technologies of the Russian Federation, the Skolkovo Foundation, the Russian Venture Company, etc. However, there is no integral national program and unified infrastructure for supercomputer modeling in the country. Obviously, we need a vertical which would unite academic science, educational system of special training, and the organizations-developers of industrial software. The latter should include domestic manufacturers of supercomputer systems (T-platforms, RSK, ELBRUS, ANGARA, etc.) interested in promoting their services to the market. The creation of the infrastructure for maintaining, operating, and supporting the ICE's long life cycle, which includes a huge amount of software, is an important scientific and organizational problem, along with the creation of an integrated computing environment.

International practice shows great benefits from creating associations of software users. Representatives of state and private corporations (Rostec, Rosatom, Roscosmos, RosNano, RosNeft, GazProm, Rusal, etc.), which should be the main customers and interested parties of new scientific and technical initiatives, will take an active part in them.

It seems expedient to create the Russian Foundation of Algorithms and Programs for work activity management as an advanced version of the State Fund of Algorithms and Programs that existed in Soviet times. The tasks of such a structure will include not only the interdepartmental coordination of the development of mathware and software but also the widespread introduction of computer modeling in industry and the organization of mandatory international cooperation.

An analysis of urgent problems indicates the need to form a new state science and technology policy, which implies, in particular, the development and implementation of a strategic basic research program of the Russian Academy of Sciences, which will be implemented in academic institutions, and thematic departments of the Russian Academy of Sciences will coordinate these works. This structure of Russian science has historically justified itself, and an attempt to destroy it during the ongoing reform of the scientific sector violates the universal principle of Hippocrates: "First, do no harm!"

The principal point is that the budget financing of the long-term basic research of the Russian Academy of Sciences should not be less than the grant programs of the Russian Science Foundation and the Russian Foundation for Basic Research. At the same time, the budget should cover expenses for domestic travel, participation in foreign conferences, and the supply of foreign scientific literature. Paraphrasing a well-known maxim, a state that cannot feed its science will feed foreign science. Our country spends huge amounts of money on training qualified personnel, but the best of them then successfully work in foreign universities and industrial companies.

As for the training of young personnel in computational sciences and supercomputer education in general, the situation here is not hopeless, but the revived Ministry of Education and Science of Russia should be concerned about the lack of qualified lecturers and specialists in a number of urgent research areas. Evidently, new forms of attracting foreign scientists should be actively sought.

The main condition for ultimate success is the investment of industries and the wide demand for high-tech developments. At this stage, scientific and organizational activities are faced with the harsh laws of business, but the government should have the last word. Suffice it to recall that in Soviet times the director of each company was obliged to spend at least 5% of the funds for a "new hardware" item, and as a result the USSR Academy of Sciences received more than 50% of the funding from extrabudgetary sources. In the modern world, a powerful incentive for scientific and technological innovation is the tax benefits that we still have in the status of promising, i.e., very distant, ways of stimulating progress.

The coming months and years should truly become crucial for Russian science in general and for the increasing role of mathematization and computational and informational technologies in particular. The implementation of the conceived large-scale projects is a problem that requires mobilizing significant resources in the country, but it is very timely and almost inevitable. The conflicts in world politics that are becoming chronic are convincing evidence that the creation of an "information technology shield" is a problem of national and global security, akin to nuclear and missile projects, the implementation of which has given the world parity and a fairly stable balance.

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