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И МАТЕМАТИЧЕСКОЙ ГЕОФИЗИКИ
СИБИРСКОГО ОТДЕЛЕНИЯ РОССИЙСКОЙ АКАДЕМИИ НАУК**

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PLENARY SESSION

Northern Urbanization under global change: challenges and strategies with respect to weather, climate and air pollution for sustainable development

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Urbanization is accelerating globally, also in Northern high latitudes. This trend causes transformation in the geosphere, biosphere, pedosphere, atmosphere and hydrosphere, affecting the human-environment system over both short- and long-term timescales. Cities represent a complex and highly dynamic interface between Earth components (atmosphere, land, water, etc.) and societal factors (health, social equity, life quality, economy, etc.). At the same time, cities are very sensitive to climate change. This vulnerability is strongly pronounced in the North, especially in the Arctic, a region that is warming at twice the rate as the global average, and has direct and indirect impacts on the local livelihoods, infrastructure, water resources, ecology and air quality.

The World Meteorological Organization (WMO) within the UN Sustainable Development Goals (SDGs) and New Urban Agenda is promoting safe, healthy and resilient cities through the development of science-based Integrated Urban Weather, Environment and Climate Systems and Services (IUS) for sustainable cities under changing climate. The WMO suggested novel concept and methodology for the Urban Integrated Hydro-Meteorological, Climate and Environmental Services (Baklanov et al., 2018; WMO, 2019; Grimmond et al., 2020) to support safe, healthy, sustainable and resilient cities are actively realized for a number of cities around the world. The Guidance on IUS, Volume II: Demonstration Cities (WMO, 2020) uses information gathered from more than 30 demonstration cities to provide examples of the types of IUS and their placement within distinct administrative frameworks. However, among these more than 30 cities, already successfully realizing such approach for sustainable urban development, only a few of winter cities considered (Baklanov et al., 2020) and no Arctic cities involved and analyzed yet. However, northern cities have a strong specific and not always recipes, recommended for other climatic zones, are suitable for them.

Previous studies of urban sensitivity to climate change have mostly focused on lower and mid-latitude cities and rarely considered analysis of Northern/Arctic cities. Due to the specific climatic conditions and societal organization Northern cities embrace many challenges in the advancement of knowledge about physical, chemical, ecological, socio-economic and environmental change, their relationships and implications for the human-environment system. Some of the important issues that require in-depth studies include the effects of urban meteorology such as heat islands and the interactions of stably stratified boundary layers with urban elevated air pollution episodes in a changing climate. In addition, as urbanization progresses and lifestyles globalize, the need for agricultural and industrial products increases. This poses environmental challenges in both cases, local production (unique ecosystems) and transportation to the Arctic (infrastructure development). Moreover, due to the cold weather conditions, high-energy consumption is typical of northern cities. With limited potential for renewable energy generation, adopting sustainable life styles is of particular challenge.

In the Arctic, particularly considering the present status, indigenous communities and population level, the urbanization process involves a large spectrum of settlements of various sizes. In order to understand the social-environmental effects of urbanization under rapid climate change a multiscale approach is necessary in order to be beneficial to the whole Arctic society.

This presentation provides an overview of the current efforts towards future northern IUSs on Arctic urbanization under climate change undertaken by the international initiative Air Pollution in the Arctic: Climate, Environment and Society (PACES) (Arnold et al., 2016; Schmale et al., 2018), the Pan-Eurasian Experiment (PEEX) programme (Kulmala et al., 2015; Lappalainen et al., 2021), the WMO Global Atmospheric Watch Urban Research Meteorology and Environment (GURME) project (WMO, 2019; Sokhi et al, 2021), as well as several ongoing and previous bilateral and international projects, e.g.: FP6 EnviroRISKS (Baklanov and Gordov, 2006; Baklanov et al, 2013); UHIARC (Konstantinov et al, 2018; Varentsov et al, 2018); Belmont Forum's HIARC (Miles and Esau, 2017, 2020) and SERUS (Esau et al., 2020), NordForsk TRAKT-2018 (Mahura et al., 2018; Esau et al., 2021), Kola Arctic studies etc. (Baklanov et al., 2012; Amosov et al., 2014, 2020; Penenko et al., 2015) and Horizon-2020 iCUPE (Petäjä et al. 2020).

The recently organized 4th PACES Open Science meeting (26-28 May 2021) on its Session 2: "Integrated Urban Systems (IUS): Twin cities –GURME initiative" concluded that:

- Complex multidisciplinary approach is needed for building climate and environmentally smart and sustainable Arctic cities;

- Improvements and adaptation of the novel WMO concept of the IUS for Arctic and winter cities are important and require further research;

- It is decided to propose a new GURME project on IUS for Northern Twin Cities. Cities in focus and some initial pairs of twin cities have been identified (e.g., Rovaniemi-Apatity; Tromso-Murmansk/Salekhard; Fairbanks-Norilsk/Nadym).

- Key science focus will be on very stable boundary layers of winter and Arctic cities and their interactions with urban processes, air pollution and climate change.

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On numerical methods for solving direct problems in the mechanics of composite structures

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Solving direct problems of calculating strength of composite structures and analyzing their stress-strain state (SSS) necessitates solving boundary value problems for systems of differential equations. In this report, numerical methods of linear algebra and the least-squares collocation method in combination with modern algorithms of an iterative process acceleration are applied to modelling and simulation of composite beams bending [1]. The quasi-static loading process with repeated solution of systems of nonlinear algebraic equations and boundary value problems for ordinary differential equations is considered to analyze beams SSS [1, 2].

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Conservative-characteristic algorithms for systems of conservation laws of hyperbolic type. Achievements and challenges

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Conservative-characteristic (CH) computational algorithms combine the advantages of conservative difference schemes with automatic trapping of strong discontinuities and the method of characteristics in the domains of solution smoothness. A characteristic feature of these algorithms is the use of two types of unknown quantities - conservative variables related to the centers of the computational cells, and flow variables related to the faces of the computational cells. In this case, flux variables are expressed not only in terms of conservative values in adjacent cells, but also depend on flux variables from the previous time layer.

The conservative-characteristic algorithms are based on the finite volume method, and the flows on the faces of the computational cells are calculated using the characteristic form of the equations. In each computational cell, local Riemann invariants are constructed, the values of which on a new layer in time are calculated by extrapolation or interpolation. Extrapolation algorithms include the CABARET scheme.

Conservative-characteristic algorithms have the second order of approximation on irregular computational grids, which transforms into the first in the vicinity of strong discontinuities. The monotonicity of the solution is achieved by nonlinear correction of fluxes based on the maximum principle, which does not depend on any tuning parameters. As applied to the equations of gas dynamics, CH schemes make it possible to calculate both shock-wave processes of any intensity and turbulent flows with incomplete resolution of the spectrum of turbulent pulsations without tuning parameters, in particular, the generation of sound by turbulent jet and its propagation in the near and middle zones.

The report will provide a brief overview of the use of CH algorithms in the problems of aeroacoustics, hydrogen safety and computational oceanology.

On preconditioning of grid SLAEs using graph transformations

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The general principles and some specific implementations of the construction of graph preconditioners [1, 4] for iterative methods in Krylov subspaces [2] are considered, focused on the fast solution of systems of linear algebraic equations (SLAE) with sparse matrices of large orders that arise when approximating multidimensional boundary value problems of mathematical modeling by the methods of finite differences, finite volumes, finite elements and discontinuous Galerkin [6] algorithms of various orders of accuracy on unstructured grids. Approaches to the construction of spanning trees for multidimensional weighted connected graphs are investigated, a reduction algorithm for fast solution of grid equations on graphs is described, as well as issues of parallelization of the proposed preconditioned iterative processes in Krylov subspaces. Variants of domain decomposition and multigrid methods [3, 5] are considered as special cases of the proposed approach. The results of numerical experiments are discussed that demonstrate the effectiveness of these algorithms on a representative series of typical methodological examples.

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Programmed cell death regulation using rationally designed molecular probes

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There are two types of apoptosis induction: intrinsic-mediated via mitochondria and extrinsic-mediated via death receptor (DR) activation. CD95/Fas is one of the most studied members of the DR family. The induction of apoptosis via CD95 is largely controlled by the Death-Inducing Signaling Complex (DISC), which is formed upon CD95 stimulation. The major components of the DISC complex include CD95, FADD, procaspases-8/10 and c-FLIP (cellular FLICE inhibitory protein) proteins. Deregulation of the CD95 pathway accompanies a variety of tumors and neurodegenerative diseases. Structural modeling of the key components of the DISC complex and in silico screening of compounds targeting them have a great potential towards design of new therapeutics and providing deep insights into molecular mechanisms of the signaling pathway functioning and pathology development.

In the current study we applied structural modeling and virtual screening techniques of large databases of chemical compounds to target the caspase-8/c-FLIPL complex. Designed chemical probe FLIPinBγ was able to target the heterodimerization interface leading to allosteric activation of the pro-apoptotic activity of the complex. Kinetic mathematical model was further developed to analyze the observed effects of FLIPinBγ on DISC activation. Based on the modeling results we could predict that the stabilized FLIPinBγ/caspase-8/c-FLIPL complex plays a major role at the very initial stages of the DISC assembly and procaspase-8 processing. Furthermore, conducted structural analysis of the DISC complex suggests high therapeutic potential of c-FLIP targeting compounds to enhance cell death in cancer cell lines that are characterized by high c-FLIP levels.

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Mesh conservation laws in filtration problems with discontinues solutions

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We proposed new efficient computational algorithms for solving a number of filtration problems for a two-phase fluid in porous and fractured-porous media. Main feature of the considered problems is in the presence of discontinuous solutions which prohibits consideration of the mathematical model in the form of a system of differential equations in the entire computational domain. We have considered a model in the form of integral laws of mass conservation and momentum in arbitrary subdomains. In particular, we formulated Darcy's law in a generalized form for the total velocity, and the phase velocities are given by the product of the total velocity with some functions that are discontinuous in general [1]. The resulting problem formulation naturally leads to a spatial approximation by the mixed finite element method for calculating the total velocity and pressure, and the so-called centered finite volume method for calculating phase saturations. The time approximation of the saturation equation is based on the explicit upwind Euler scheme. We developed this approach both for one-porous and two-porous models describing flow in fractured-porous media using the mass transfer function between pore blocks and fractures. In the case of a two-porous model, we built the upwind scheme both within each medium and for the implementation of mass transfer between the media.

We considered the problem of gravitational segregation of a two-phase fluid in a porous medium [2]. We constructed a new computational scheme for solving the multidimensional problem of gravitational segregation of a two-phase fluid in a porous medium. Unlike the currently well-known IHU (Implicit Hybrid Upwinding) approach proposed in [3], we have developed an explicit version of this approach (EHU) which is not inferior to IHU in accuracy and significantly exceeds IHU in performance. Otherwise, the algorithm with the standard upwind approximation is unable to adequately reproduce the filtration process. For the method we have constructed, we constructed a proof of the weak maximum principle with an explicit indication of the Courant-Friedrichs-Levy condition that ensures the stability and monotonicity of the scheme. In this case, for the Buckley-Leverett model where the saturation dynamics is described by a hyperbolic equation, the obtained conditions are not restrictive in terms of the time step size, and the time step limiting factor is accuracy only. This ensures the competitiveness of the EHU vs. IHU for the specified set of problems.

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A diffusion-convection problem with a fractional derivative along the trajectory of motion

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A new mathematical model of the diffusion-convective process with "memory along the flow path" is proposed. This process is described by a homogeneous one-dimensional Dirichlet problem with a fractional derivative along the characteristic curve of the convection operator, or, in other words, with fractional material derivative. A finite-difference scheme is constructed using an analogue of the well-known L1-approximation of time-fractional derivative for the fractional material derivative and the conventional approximation of the diffusion term.. The unique solvability of the constructed mesh scheme is proved. The stability estimates are derived in the uniform mesh norm, and the accuracy estimates are given under the assumptions of sufficient smoothness of the initial data and the solution of the differential problem. The presented results are based on the article [1].

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Numerically statistical investigation of efficacy of SEIR model

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A comparative analysis of the differential and the corresponding stochastic Poisson SEIR-models [1, 2] was performed for the testing problem of the epidemic COVID-19 in Novosibirsk modeling in the period from the 23rd of March 2020 to the 21th of June 2020, with the initial population $N = 2\ 798\ 170$ [3]. By varying the initial population in the form $N = n \cdot m$ with $m \geq 2$, it was shown that the average values of the sick identified was less (beginning with the 7th of April 2020) the corresponding differential values by the quantity that is statistically not distinguished from $C(t)/m$, with $C \approx 27.3$ on the 21th June. This relationship allows to use the stochastic model for big population N. Practically useful confidential interval “three sigma” for the time interval from the 1th of June 2020 to the 21th of June 2020 is about 110 % (as to the statistical average) and involves the corresponding experimental estimates. The influence on the prognosis of introduction the delay, i. e. the incubation period corresponding to Poisson model, was also investigated.

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One class of relativistic invariant systems of equations of first order

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We consider a new class of partial differential equations of first order (we call them "covariantly equipped systems of equations"), which are invariant with respect to pseudo-orthogonal changes of Cartesian coordinates of pseudo-Euclidian space. We describe a procedure to reduce a Cauchy problem for a system of equation to a Cauchy problem for covariantly equipped system of equations. We prove that such procedure can be apply to the Cauchy problem for Maxwell equations. Covariantly equipped systems of equations give us new point of view on field theory equations.

New correlative randomized algorithms for statistical modeling of radiation transfer in stochastic medium

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For solving the problems of the particle transport through a stochastic medium is often used the method of maximum cross-section (delta Woodcock tracking), in which the random distribution density of the medium is realized only at the end points of the free paths. A simple independent choice of the density at these points leads to the simulation of the transport process in the averaged medium. Therefore, in this talk, new correlation randomized algorithms for modeling the transfer process are presented. In the first of them, at the end of the next free path, the previous value of the density is retained if the free path length does not exceed the correlation length (correlation radius) of the medium. In the second, functional correlated algorithm, the density value is stored with a probability equal to the corresponding value of the correlation function. The second algorithm is more accurate but requires much more information about the density field of the medium. The limits of applicability of the formulated algorithms are studied in detail on the basis of a test problem with extremely anisotropic scattering and using an unbiased double randomization algorithm. It is shown that the new algorithms make it possible to solve problems with small-scale stochasticity, for which the implementation of unbiased transport estimators is practically impossible due to the modeling of the density field as a whole.

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Random walk on spheres based algorithm for transients of exciton transport in semiconductors with near singular behavior of recombination rates around the dislocations

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A Random Walk on Spheres (RWS) based stochastic algorithm is developed in this study to simulate a non-stationary transport of excitons in a semiconductor (SC) with a set of threading dislocations which are randomly distributed in SC. The simulation algorithm is based on the RWS method suggested for solving the transient drift-diffusion-reaction problems in [1]. The excitons are generated in SC uniformly over the x, y coordinates, and exponentially decaying over the z-coordinate. The functions calculated for practical use are the fluxes to the dislocation and substrate plane, and the cathodoluminescence intensity. The cathodoluminescence intensity is computed as a fraction of radiatively recombined excitons. The cathodoluminescence method is employed for the analysis of a material structure. The recent experiments [2] showed that the strain field in the vicinity of dislocations produces a piezoelectric field which affects the exciton life-time close to the dislocation edge and causes a drift of excitons. In our previous model [3] we simulate the threading dislocation as a semi-cylinder whose surface adsorbs excitons. In the present work, the dislocation is simulated with its piezoelectric field around which defines the life-time and the drift of excitons depending on the distance from the dislocation central line. The major challenge encountered in the present study is related to the multiscale character of the problem: the diffusion length of excitons is assumed to be several thousands of nanometers (nm), hence the characteristic size of the simulated semiconductor should be taken at least tens of thousands nanometers while the dislocation diameter is 6 nm, and the piezofield is varying in the cylindrical region of radius 100 nm around the dislocation. This means if a finite-difference method would be applied to solve this problem we would have to introduce a mesh with at least several billions of nodes which is unrealistic. The RWS algorithm developed is meshfree and calculates directly the fluxes and cathodoluminesence intensity in a semiconductor which includes hundreds of dislocations with the piezoelectric fields around them.

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Sensitivity of functionals in variational data assimilation

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The problem of variational data assimilation for a nonlinear evolution model is formulated as an optimal control problem to find the initial state and the unknown parameters of the model. A response function is considered as a functional of the optimal solution after assimilation. The sensitivity of the response function to the observation data is studied. The gradient of the response function with respect to observations is related to the solution of a non-standard problem involving the coupled system of direct and adjoint equations. Based on the Hessian of the original cost function, the solvability of the non-standard problem is studied. Algorithms to compute the gradient of the response function with respect to observation data are formulated and justified. Numerical examples are presented for variational data assimilation problem for the Black Sea thermodynamics model.

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Long-period seismogravitation processes: Analytical analysis

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Recently, a previously unknown experimental fact has been recorded. In the period of formation of focal structures of large seismic events and the moment of the onset of an earthquake (main shock), modern observatory information-measuring systems record an “instantaneous” long-period seismic gravity disturbance. Moreover, it appears earlier than the P-wave at the observation point [1]. It is known that for classical elastic media there can be no signal before longitudinal P-waves. A number of French and American authors explain this paradox by the appearance of gravitational waves propagating with a speed close to the speed of light [1]. Other researchers believe that the physics of the explanation of the seismic-gravitational process proposed in [1] is insufficiently substantiated [2].

A new analytical solution of the Klein-Gordon equation is obtained. The analytical solution showed that in the low-frequency region there is a wave process of two terms. One of them is an “instantaneous” long-period seismic-gravity disturbance. The second is the formed seismic gravity wave P. Thus, the origin of the long-period seism gravity process in the first approximation can be made using the classical Klein – Gordon equation [3]. The analytical modeling results show good agreement with field observations.

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Development of a hybrid parallelization scheme for the numerical solution of the mesoscale meteorological TSUNM3 model equations

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The paper considers a hybrid parallel algorithm for the numerical solution of the forecast meteorological mesoscale TSUNM3 model equations [1]. The TSUNM3 model predicts the components of wind velocity and characteristics of temperature and humidity in the atmospheric boundary layer at 50 vertical levels (up to 10 km) for an area of 200×200 km with a nested area of 50×50 km (grid step is 1 km with the center in the Tomsk city). The initialization of the model is carried out according to the results of a numerical forecast based on the SL-AV operational global model of the Hydrometeorological Center of the Russian Federation [2].

The hybrid algorithm is built as a combination of two parallel programming technologies MPI and OpenMP. The MPI message passing library is used for communication between the computational nodes of the cluster, and the parallelization within one computational node is performed using the OpenMP library for working with the shared memory.

The work was supported by the Russian Science Foundation (project no. 19-71-20042).

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M. V. Keldysh: The Lord of numbers and the formation of applied mathematics. To the 110th anniversary of the birth of M. V. Keldysh in the Year of science and technology

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In the Year of science and technology in Russia, it is important to remember those who laid the fundamental basics of modern civilization. Three Russian GENIUS of worldwide recognition: XVIII century – 310 years since the birth of M. V. Lomonosov (08.11.1701-04.04.1765); XIX century – 200 years since the birth of P. L. Chebyshev (14.05.1821-26.11.1894); XX century – 110 years since the birth of M. V. Keldysh (02.10.1911-24.06.1978) – "Lomonosov of XX century". No one has ever done so much for fundamental and applied science and scientific-technological progress of XX and XXI centuries as Mstislav Vsevolodovich Keldysh. After the elections to academicians in 1946, M. V. Keldysh was responsible for "applied mathematics", and since 1951, as the Chief Mathematician, he was responsible for calculations and computers in strategic projects: "Atomic", "Space", "Nuclear missile shield". As President of the Academy of Sciences of USSR, M.V.Keldysh launched science on a broad front in all areas of knowledge. This is the only scientist named after the "Keldysh Epoch": during his lifetime he realized his "formulas and numbers" in projects for the conquest of aviation, atom, space and the invention of computers, launched the FIRST SPUTNIK and a spacecraft with the FIRST man into space, created manned astronautics, AMS flights to the Moon, Mars, Venus, laid the foundations of modern "informatics" and "digitalization", founded the World's First Institute of Applied Mathematics. The only mathematician – legend – Three Times Hero of Socialist Labor (1956, 1961, 1971).

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Earth Future": radiation field – a immaterial component of climate system, space research and applied mathematics. To the 60th anniversary of cosmic flights of Yu. Gagarin and G. Titov in Year of science and technology

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The twenty-first year of the twenty-first century (2021) is the year of the 60th anniversary of the FIRST space flights of earthlings. The era of the conquest of space by man and the greatness of the Soviet people, the unique mobilization of intelligence and skill has come! 12.04.1961 FIRST cosmonaut Yu.Gagarin saw the Earth from space for the first time – "Blue! Beauty!". 06.08.1961 SECOND cosmonaut G.Titov made the FIRST photographs and films of the Earth from space, which were used to verify models of the Earth's radiation field. The first and only academician among cosmonauts-researchers V.Savinykh celebrated his 80th anniversary. The first and only Doctor of physical and mathematical sciences among the cosmonauts-researchers G.Grechko would have celebrated his 90th birthday. Soviet achievements in space research were ahead of the rest thanks to manned space exploration. Theoretical and computational research was provided by three scientific schools on the radiation transfer theory and mathematical modeling – in Moscow, Leningrad and Novosibirsk. The huge theoretical and applied scientific potential created by Russian scientists at the dawn of the space age allows us to maintain a leading position in the world in the implementation of "Earth Future" Program. Studies of the Earth's radiation field are large-scale tasks that never have completion, since the atmosphere-land-ocean is constantly changing and never repeating – it is a dynamic system with an unpredictable state. The role of mathematicians, "computer sciences" and space for the implementation of the Program is increasing, since natural experiments are impossible to study the evolution of the natural environment and the planet's climate. At the initiative of T.A.Sushkevich, the radiation field was recognized as an "immaterial" component of the Earth's climate system. The priority is related direct and inverse tasks – computer modeling of radiation processes, predictive calculations of radiation characteristics and processing of huge data sets of global monitoring and remote sensing of the Earth from space.

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Recent developments of SL-AV numerical weather prediction model

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The global atmosphere model SL-AV [1] is applied for medium-range weather forecasts and subseasonal and seasonal probabilistic prediction. The same code is used for all the applications.

The medium-range ensemble prediction system based on this model is described. It consists of LETKF-based data assimilation system with ensemble centering into Hydrometcentre operational analysis [2], and the model incorporating stochastic parameter perturbations (SPP) [2] and stochastic perturbations of parametertization tendencies SPPT [3] (for temperature and vorticity only). The results of quasioperational runs are shown.

The development of the medium-range version of the model (10 km horizontal resolution) is presented. Parallel and I/O optimizations have allowed to accelerate the SL-AV code significantly.

The new long-range prediction system is depicted. Some results of seasonal forecasts starting from reanalysis data (hindcasts) are shown.

This work was partially (the part concerning long-range forecasts) supported by the Russian Science Foundation (grant 21-17-00254).

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Alternative designs of high load queuing systems with small queue

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In this paper, two alternative designs are constructing for queuing systems with a large load and a small queue. These modes are convenient from an economic point of view, since the service device is almost fully loaded. On the other hand, this mode is also convenient for users who will not be idle in the queue for a long time. The first design is an aggregation of a large number of single-channel systems into a multi-channel system. The second design is basing on the model of a single-channel system, in which random fluctuations are defining as the degree of tending to zero difference between the unit and the load factor. The exponent of this degree has a critical value, above which the stationary waiting time tends to zero, and below which it tends to infinity. A similar phase transition is founding in the multi-channel queuing system. The methods of the sources [1-4] are using.

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Taking into account a priori information is the most important stage in solving ill-posed problems

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What is a problem with a priori information? It is a problem, in which together with the basic statement there is an additional information on a solution (namely, constraints) that is absent in the original statement. But this information might contain important data on some properties of a solution. It should be noted that in the case of a non-uniqueness solution, (when a priori information is not used in the algorithm of the problem to be solved), the approximate solutions could not satisfy to physical reality. In the case of uniqueness of solution, attraction of the additional constraints permits to localize the desired solution and to raise its stability w.r.t. the errors in the input data. Majority of a priori constraints that arise in the applied problems can be presented in the form of the linear relations or systems of the linear and convex inequalities. We investigate various methods of taking into account a priori constraints, in particular, the most general and economical method on the basis of the Fejer mappings. Also, we consider the ill-posed problems, for which the solutions are found by the high-precision algorithms using a priori information [1–3].

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Study of algorithms for solving the motion equations in the particle-in-cells method

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The paper is dedecated to the study and creation of algorithms and programs for modeling the motion of plasma particles. The movement of charged particles in an electromagnetic field in a vacuum occurs under the action of the Lorentz force. Particle motion algorithms are part of the particle-in-cell method. Since the particle-in-cell method uses a very large number of model particles, it is important to economically calculate the velocities and coordinates of the particles at the time step. In 1970, Boris proposed a scheme that was economical in terms of the number of operations, which had a second order of approximation. In recent years, works have appeared in which modifications of the Boris method have been proposed. It was argued that new modifications would allow calculations for long physical times. A new economical and more accurate scheme is proposed for solving the equations of motion at a time step.

Since in practical calculations the values of the electric and magnetic fields at the location of the particle are obtained by interpolation from the nodes of the computational grid, the influence of interpolation on the running time of the algorithm was investigated. It turned out that the interpolation time in three-dimensional calculations takes an order of magnitude longer than it takes to calculate the motion of a particle. A method for reducing the cost of field interpolation is proposed.

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Section 1

METHODS OF COMPUTATIONAL ALGEBRA AND SOLVING MATHEMATICAL PHYSICS EQUATIONS

Solving the hourglass instability problem using rare mesh variation-difference schemes

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The hourglass instability effect is characteristic of the Wilkins explicit difference scheme [1] or similar schemes based on two-dimensional 4-node or three-dimensional 8-node finite elements with one integration point in the element.

The hourglass effect is absent in schemes with cells in the form of simplexes (triangles in two-dimensional case, tetrahedrons in three-dimensional case). But they have other disadvantages. In the paper [2], a rare mesh scheme was proposed, in which elements in the form of a tetrahedron are located one at a time in the centers of the cells of a hexahedral grid. This scheme showed the absence "hourglass" effect and other drawbacks with high efficiency.

This approach was further developed for solving 2D and 3D problems.

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About grid generation in constructions bounded by the surfaces of revolution

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For constructions bounded by the surfaces of revolution, structured grid generation technique is presented. Its technology has been elaborated within the variational approach [1] for constructing optimal grids. Grid generation has been designed for numerical solution of the differential equations modeling the vortex processes of multicomponent hydrodynamics [2]. The description of the technology for generation of grids has appeared in [4]. The technology [4] has started to be developed by the elaboration of the grid generation algorithms for the volume of revolution which has become the basic construction. The considered volume of revolution is obtained by the rotation through 180° about the axis of a generatrix consisting of straight line segments, arcs of circles and ellipses. Then the deformed volumes of revolutions are considered along with the generalizations of the volume of revolution which represent constructions obtained by the surfaces of revolution with parallel axes of rotation. The aim of the further development of the technology is to consider more and more complicated constructions and elaborate the technology for them. In the presentation, the current state of the development of the technology is given. Examples of generated grids are supplied.

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Smoothed particle hydrodynamics method for numerical solution of filtering problems of three-phases fluid

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This work is devoted to solving the problem of filtration of a mixture of water, gas and oil in a homogeneous porous medium. The basic equations of filtration theory [1] are converted into a special form for numerical approximation by the smoothed particle method. A numerical difference scheme is constructed on the basis of the smoothed particle hydrodynamics method [2]. An algorithm for setting the boundary conditions is proposed and a number of isothermal one-dimensional and two-dimensional test numerical calculations of the filtration process of a mixture of water, oil and gas are presented..

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The least-squares collocation method and its applications to problems of continuum mechanics

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The report is devoted to an application of the developed versions of the least-squares collocation (LSC) method to solving continuum mechanic problems. The efficiency of their combination with various methods of accelerating iterative processes is shown. Possibilities of the LSC method for solving boundary value problems for differential equations of various orders in canonical and irregular domains, including those with singularities, are investigated [1]. Mathematical modelling and numerical simulation of composite beam bending, calculation of thin plates bending, and numerical analysis of polymer fluid flows are carried out. Comparison with the results of other authors shows the advantages of the LSC method, as well as satisfactory agreement with experimental data in calculations.

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Numerical simulation of a stabilizing Poiseuille-type polymer fluid flow in the channel with elliptical cross-section

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Stabilization of the Poiseuille-type flows of an incompressible viscoelastic polymer fluid is studied using non-linear rheological relations from [1]. Channels of elliptical and circular cross-sections are considered. In [2] it was shown that the corresponding stationary formulation admits three different solutions. The process of stabilization of the flow after the jump of pressure gradient in the channel was simulated using the algorithm from [3]. The stabilized flow shows which of the three solutions of the stationary problem is implemented in practice. Simulations in a wide range of values of the physical parameters enable us to discover the effect of "switching" the limiting solution of the non-stationary problem from one solution of the stationary equations to another. The scenario of this switch is discussed in detail.

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The discontinuous shapeless particle method for quasi-linear transport

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Simulation of gas dynamic problems deals with the appearance of discontinuities, more precisely, strong gradients. The quality of computational methods is assessed primarily by their ability to convey this behavior of a solution as adequately as possible. In our opinion, the discontinuous particle method [1-3] allows one to cope with these difficulties better than alternative, traditionally more commonly used difference and finite element methods. This is achieved because the particle method is based on the Lagrange approach, and this, in turn, provides automatic mesh generation.

A new variant of the discontinuous particle method is presented. We use a new particle rearrangement criterion without analyzing particle overlaps. It is assumed that the nonlinear elastic transport preserves not only the mass of the particles, but also the mass located between the centers of these particles. This requirement leads to the fact that the change in the distance between the particles in the process of their movement and the conservation of mass in the space between them leads to a change in the density of one of the particles. The new version applies to solving the one-dimensional and two-dimensional quasi-linear transport equation problems. The main feature of the new variant is minimal smearing of discontinuities.

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On the optimal approximation of functions in the boundary layer

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In this study we consider the problem of approximation of functions belonging to the class of functions with high gradients in boundary layer. For such functions we build an algorithm of approximation both in one-dimensional and multidimensional cases. The idea of the algorithm is based on the results for optimal approximations of specific functional classes [1-3]. These classes include functions with modules of derivatives having power-type singularity that is a function of distance from the point to the boundary of the domain.

In order to develop the proposed algorithm we introduce the specific functional class and use the apparatus of continuous local splines providing approximation of functions from the mentioned class that is optimal with respect to accuracy. Solving model problems demonstrate the efficiency of the proposed method.

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On one iterative method for solving the amplitude-phase problem

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Methods for solving amplitude and phase problems for one and two-dimensional discrete signals are proposed. Methods are based on using nonlinear singular integral equations. In the one-dimensional case amplitude and phase problems are modeled by corresponding nonlinear singular integral equations. In the two-dimensional case amplitude and phase problems are modeled by corresponding nonlinear bisingular integral equations. Several approaches are presented for modeling two-dimensional problems:

1) reduction of amplitude and phase problems to systems of nonlinear singular integral equations;

2) using methods of the theory of functions of the complex variable, problems are reduced to nonlinear bisingular integral equations.

To solve the constructed nonlinear singular equations, methods of collocation and mechanical quadrature are used. These methods lead to systems of nonlinear algebraic equations, which are solved by the continuous method for solution of nonlinear operator equations. The choice of this method is due to the fact that it is stable against perturbations of coefficients in the right-hand side of the system of equations. In addition, the method is realizable even in cases where the Frechet and Gateaux derivatives degenerate at a finite number of steps in the iterative process.

Some model examples have shown effectiveness of proposed methods and numerical algorithms.

Numerical simulation of the dynamics of a heated turbulent mixing zone in a linear stratified medium

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Evolution of localized regions of turbulized fluid (turbulent spots) has a decisive effect on the formation of fine microstructure of hydrophysical fields in the ocean [1].

Based on an algebraic model of Reynolds stresses and fluxes, a numerical model of the dynamics of a flat localized region of turbulent perturbations of non-zero buoyancy in a linearly stratified medium was constructed. Presence of non-zero buoyancy leads to increase in the geometrical dimensions of the turbulent spot and generation of internal waves of greater amplitude in comparison with a spot of non-zero buoyancy. The work is a continuation and development of research [2].

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A-WENO schemes based on adaptive artificial viscosity

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We will introduce new finite-difference A-WENO schemes for hyperbolic systems of conservation laws. The proposed schemes are fifth-order accurate in space and stable. Unlike the original A-WENO schemes [1], the stabilization is achieved using the adaptive artificial viscosity (AAV) approach introduced in [3]: the AAV terms are made proportional to the weak local residuals originally introduced in [2]. The performance of the proposed schemes will be demonstrated on a number of challenging benchmarks.

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Dual approach as empirical reliability for fractional differential equations

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We consider fractional differential equations with derivatives in the Gerasimov-Caputo sense. Computational methods for these equations exhibit essential instability. Even a minor modification of the coefficients or other entry data may switch good results to divergent. The goal of this talk is to suggest a reliable dual approach which fixes this inconsistency. We suggest to use of two parallel computational methods based on the transformation of fractional derivatives through (1) integration by parts and (2) substitution method. The by-parts method is known whereas the substitution method is novel. We prove the stability theorem for the substitution method and introduce a proper discretization scheme that fits the grid points for both methods. The solution is treated as reliable (robust) only if both schemes produce the same results. In order to demonstrate the proposed dual approach, we apply it to linear, quasilinear and semilinear equations and obtain very good precision. The provided examples and counterexamples support the necessity to use the dual approach because either method, used separately, may produce incorrect results. The order of the exactness is close to the exactness of the approximations of fractional derivatives.

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The CFD-DEM numerical model for simulation of a fluid flow with large particles

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The mathematical model for considering flows consists of the Navier – Stokes equations for a viscous incompressible fluid flow and a set of motion and rotation equations for every particle. The no-slip boundary condition posed at the surface of the particles connects these two different sets of equations. In the numerical model, it is assumed that the fluid occupies the entire flow region, including the space occupied by particles. The influence of the particles on the fluid flow is realized by adding a special force acting from the immersed boundary. The direct forcing scheme is used [1] to satisfy the no-slip condition on the immersed boundary and evaluate the total force acting on every particle.

The CFD part of the numerical model consists of the SIMPLE-like algorithm on the staggered mesh to solve the Navier – Stokes equations. A moving Lagrangian mesh with an almost uniform distribution of nodes represents the boundaries of particles. In general, the nodes of these two meshes don’t coincide, and a discrete delta function is used to interpolate the variables. The discrete element method (DEM) is used to track, rotate and collide particles by integrating all motion and rotation equations. The main feature of the DEM is integration with a very small time step. Empirical formulae [2] form the basis for the interaction of particles through a thin layer of fluid.

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Levinson type algorithms for solving scattering problems for the Manakov model of nonlinear Schroedinger equations

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We have presented a numerical approach for solving the inverse and direct spectral scattering problems for the focusing Manakov system. We have found an algebraic group of 4-block matrices with ordinary matrices in diagonal blocks and with off-diagonal blocks consisting of special vector-like matrices that help generalize the scalar problem's efficient Levinson type numerical algorithms [1, 2] to the vector case of the Manakov system. The inverse scattering problem solution represents the inversion of block matrices of the discretized system of Gelfand-Levitan-Marchenko integral equations. Like the Zakharov – Shabad system's scalar case, the Toeplitz symmetry of the matrix of the discretized GLM equations system drastically speeds up numerical computations as in the Levinson algorithm. The reversal of steps of the inverse scattering problem algorithm solves the direct scattering problem. Numerical tests performed by comparing calculations with the known exact analytical solution, the Manakov vector soliton, have confirmed the proposed algorithms' efficiency and stability, sufficient for applications. The application of the algorithms illustrated by the numerical simulation of the polarized

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A combined analytical and numerical approach to solve spatial bending problems of composite beams

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The spatial problem of the theory of elasticity with small parameter is solved in application to the bending of composite beams. Using the asymptotic splitting method [1, 2] the problem is reduced to consecutive solving of two and one-dimensional problems, where two-dimensional problems are defined on the cross-section of the beam and one-dimensional problem is defined along beams length. In the general case of complex cross-section geometry, numerical solutions are obtained using the least-squares collocation method [3] and finite-element method.

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Modelling of burning coke sediment at catalyst grain

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Recovery of the catalyst activity is an essential part for industrial catalytic processes. One of the least costly regeneration methods is oxidative regeneration – burning out coke sediments from the catalyst grain by oxygen-containing gas [1-3]. The formation of surface complexes on the catalyst grain is observed during oxygen adsorption [4]. Heat exchange and the exothermic nature of the effect of coke burning inevitably leads to an increase in the temperature of the grain. One of the undesirable consequences of the oxidative regeneration process can be overheating of the catalyst layer, leading to its irreversible changes [1, 5]. Another issue requiring special attention is toxic carbon monoxide, which manifests itself during the decomposition of adsorption complexes. If the permissible limit is exceeded, the using of special procedures to reduce the concentration is required.

The article is devoted to numerical modelling of the nonlinear regeneration process, which is described by the partial differential equations system. Modelling results are visualized. Comparison with the experiment revealed the admissible deviation of the calculated data from the experimental data.

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Algorithm for the numerical solution of the pure Neumann problem in fractured porous media

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The paper considers some variants of boundary value problems for the pressures and filtration rates of a liquid in fractured porous media [1]. For non-flow conditions at the external reservoir boundaries, the pressures inside the media are determined ambiguously. A variant of the pure Neumann problem arises [2]. For such a problem, the condition of unique solvability is derived. Classical and mixed generalized problem statements that include the constraint on the pressures explicitly are investigated. An algorithm for numerical solution of the problem using the mixed finite element method is presented. The properties of the proposed algorithm are discussed on the examples of numerical solutions of model problems.

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On conjugate residual methods for solving non-symmetric SLAEs

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The aim of this work is to develop and study iterative methods in Krylov subspaces for solving systems of linear algebraic equations (SLAEs) with non-symmetric sparse matrices of high orders arising in the approximation of multidimensional boundary value problems on the unstructured grids and which are also relevant in many applications, including diffusion-convective equations. The considered algorithms are based on the construction A^TA – orthogonal direction vectors calculated using short recursions and providing global minimization of the residual at each iteration. Methods based on Lanczos orthogonalization, A^T – preconditioned conjugate residuals algorithm, as well as left Gaussian transformation for the original SLAE are implemented. In addition, the efficiency of these iterative processes was investigated when solving algebraic systems preconditioned using an approximate factorization of the original matrix in the Eisenstat modification. The results of a set of computational experiments for various grids and values of convective coefficients are presented, which demonstrate a sufficiently high efficiency of the approaches under consideration.

Schemes for solving filtration problem of a heat-conducting two-phase liquid in a porous medium

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This work is a continuation of the study of the problem of the motion of a two-phase liquid in a porous medium [1]. In addition, the dependence of the oil viscosity on the temperature is determined, and the energy equation is included in the system of equations. In the framework of the single-temperature model, the energy equation is reduced to the heat equation, which describes the conductive mechanism of heat propagation in a in a porous structure and in a heat-conducting liquid, as well as the convective heat transfer by the filtration flow. The heat equation is written in a mixed generalized formulation. By analogy with the IMPES scheme, the convective term is considered on the explicit time layer, and the integration of the conductive term is carried out using the implicit scheme. This approach to the numerical solution of the heat equation allows to save the value of the integration step and reuse previously developed codes for filtration problems. The representation of phase velocities in the form of components co-directed with the total flow, and oppositely directed components [2] provides a strict balance of heat in the grid elements. The properties of the proposed algorithm are discussed on the examples of numerical solutions of model problems.

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Simulation of heat transfer with considering permafrost thawing in 3D media

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An approach to mathematical modeling of heat transfer with permafrost algorithm [1, 2] in 3D based on the idea of localizing the phase transition area is considered. The paper presents a problem statement for a non-stationary heat transfer and a description of a numerical method based on a predictor-corrector scheme. For a better understanding of the proposed splitting method the approximation accuracy was studied taking into account inhomogeneous right-hand side. The phase changes in the numerical implementation of permafrost thawing is considered in the temperature range and requires recalculation of coefficients values of heat equation at each iteration step in time. A brief description of parallel algorithm based on a three-dimensional decomposition method and the parallel sweep method [3] is presented. A study of parallel algorithm implementations on the high-performance computing system of the Siberian Supercomputer Center of the SB RAS was performed. The results of the permafrost algorithm work on models with one and several wells are also presented.

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The numerical modelling of satellite motion by the symmetric multi-step methods in the predictor-corrector mode

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The orbital motion is described by the system of second-order ordinary differential equations which numerical integration by the Stormer-Cowell multistep methods leads to a longitude error which increases quadratically in time. This presents a problem when performing long-time integration. J. Lambert and I. Watson proposed the symmetric methods [1], that possess a periodicity property when the product of the step-size and the angular frequency lies within a certain interval called the interval of periodicity. The numerical integration of orbit by the symmetric methods with the step-size from the interval of periodicity gives the longitude error which increases linearly, whereas the energy error remains roughly constant.

The symmetric methods are not uniquely determined even if their order and explicitness are specified. We construct and investigate the high-order symmetric explicit and implicit methods in the "Predict-Evaluate-Correct-Evaluate" (PECE) mode. The methods were selected according to size of the stability interval $P(EC)^kE$ mode, the value of an error constant, behavior of the roots of the stability polynomial, and an accuracy of the numerical solution of test problems.

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Adaptive preconditioning for a stream of SLAEs

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The paper considers the way of reducing the time consumed to solve SLAEs with iterative methods by reusing the data structures obtained in the solution of a previous SLAE, or selecting a preconditioner from the available set of preconditioners to minimize the time of solving the next SLAEs.

Such adaptive preconditioning [1, 2] is used to solve time-dependent nonlinear problems. SLAEs generated at the Newton iteration *n-1* of every computation step are solved using the SLAE structure of the first Newton iteration and the selection of a preconditioner from the given set allows reducing the time of solving SLAEs of a varying complexity at different time steps.

The adaptive preconditioning idea and its application are demonstrated for a stream of SLAEs in some RFNC-VNIIEF's codes.

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On integral convergence method for analyzing the shock capturing schemes accuracy

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This work is a continuation of the research [1] on the justification of the method of integral convergence [2] for studying the accuracy of finite-difference shock-capturing schemes. We determine the integral convergence order using a series of numerical calculations on a family of embedded difference grids, which allows us to model a space-continuous difference solution of the corresponding Cauchy problem. We use this approach to study the accuracy of the Rusanov, TVD and WENO5 finite-difference schemes.

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On the solution of 3D boundary subproblems in subdomains in the domain decomposition method

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The domain decomposition method without intersection of subdomains with direct approximation of the Poincaré – Steklov equation at the interface [1] is considered. Decomposition is carried out by a uniform parallelepiped macrogrid. Each subdomain has its own uniform subgrid. When iterating over subdomains on each subgrid, the Dirichlet boundary subproblem is solved. An experimental study of methods for solving subproblems on subgrids is carried out. The following features are taken into account: 1) a relatively small number of nodes in subgrids, 2) multiple repetition of the solution in a subdomain with varying values at the boundary. Recommendations on the application of the methods are given.

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Application the quasi-invariants method to CABARET schemes for numerical calculation of gas dynamic problems

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The standard algorithm of the CABARET scheme [1], which approximates a hyperbolic system of conservation laws, assumes that this system can be written in the form of invariants. However, if the hyperbolic system of differential equations does not allow writing in the form of invariants, then to construct the CABARET scheme it is necessary to use quasi-invariants, which in the general case are determined ambiguously [1]. In this work, we present a general formulation of the quasi-invariants method when constructing a CABARET scheme approximating a hyperbolic system of conservation laws that cannot be written in the form of invariants. A comparative analysis of these modifications accuracy in the calculation of the Sod discontinuity decay for a polytropic gas is carried out. Based on this analysis, the optimal form of quasi-invariants has been identified, which allows the CABARET scheme to localize strong and weak discontinuities of the exact solution with high accuracy.

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Numerical solution of mean field problem with limited management resource

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Here we propose the computational algorithm for the formulation of MFG problem with the limited management resource during control realization. The Mean Field equilibrium leads to a coupled system of two parabolic partial differential equations: Fokker-Planck-Kolmogorov and Hamilton-Jacobi-Bellman ones with an additional constraint in the form of the inequality. Based on the Karush-Kuhn-Tucker theorem [1], this statement is reduced to finding the saddle point of the Lagrangian with an additional condition of complementary slackness. To approximate the problem, the (Euler-Lagrange) difference schemes are used, which is presented in [2]. An iterative algorithm is presented for solving the obtained discrete problem with justification of the convergence of its elements. The convergence of the algorithm as a whole is illustrated by a numerical example.

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On the accuracy of semi-discrete central-upwind schemes

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On the basis of the method proposed in [1], we studied the accuracy of the second-order semi-discrete finite-volume central-upwind scheme [2] in calculations of shocks propagating with variable velocity. It is shown that in the shock influence domain, the scheme orders of the integral and local convergence decrease to the first one, while on the smooth solutions this scheme has the second order of accuracy. Test calculations are presented.

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Methods for solving saddle-point SLAEs in filtration problems

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Iterative processes in Krylov subspaces for solving large ill-conditioned saddle-type SLAEs with sparse matrices arising as a result of finite element approximation using Raviart–Thomas basis functions on a regular rectangular grid of the Neumann problem for two-phase filtration in a mixed statement.

The regularized Uzawa method proposed by Greif is used. Combined two-level iterative algorithms using the effective Chebyshev acceleration and the variational method of conjugate directions. The resource intensity and computational performance of the proposed algorithms are investigated using examples of three-dimensional filtering problems. The effectiveness of the proposed numerical methods is demonstrated on a representative series of methodological problems.

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Combination of semi-Lagrangian approach finite difference scheme for three-dimensional parabolic equation

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We consider three-dimensional parabolic equation with initial and boundary conditions. Left-hands side of equation consists of transport and elliptic diffusion operators [1]. To approximate transport operator, we use conservative semi-Lagrangian approach [2]. For this purpose we consider two integrals at adjacent time levels. Integration domain of one of them is a cube. Another domain is a curvilinear cuboid. Boundary of cuboid is designated by characteristic trajectories [1-3]. To compute integral over curvilinear cuboid, we approximate it by 6 tetrahedrons [3]. For diffusion operator we apply finite difference scheme [4]. Finally, we get a system of linear algebraic equations. We investigate a restriction for ratio between time and space grid steps to reach non-positive off-diagonal elements of system and diagonal dominance. To compute solution of system, we use iterative methods. The proposed algorithm has the first-order convergence that is confirmed by computational experiments.

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A method to compute liquid-gas equilibrium based on the balance of evaporation and condensation rates

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A model is proposed that makes it possible to estimate the rates of evaporation and condensation processes in a two-phase medium (liquid-gas). The proposed model provides the preservation of the overall composition of the mixture. The method for calculating liquid-gas equilibrium is developed basing on this model and Peng-Robinson equation is used there as an equation of state for the mixture of the substances. A numerical method for time evolution calculations of the components concentration in the liquid and gas phases is proposed. The problem of calculating liquid-gas equilibrium for the mixture of hydrocarbons is considered as one of the application examples for the proposed model. The computational results for the equilibrium (stationary) state of hydrocarbons mixtures obtained using the proposed method and the results obtained using the method of successive substitutions, which is widely used for similar purposes, are compared.

High-order heterogeneous multiscale finite element method for elasticity problems

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Numerical modeling of physical processes in heterogeneous media is an important step of research and applied problems, for example, modeling of elasticity deformation for the subsequent study of the effective properties of rock samples or composite materials containing many scattered and randomly located inclusions. In this case, various modifications of the multiscale finite element method are used, which are adapted to a specific class of problems. Traditionally, for ease of implementation, algorithms are based on first-order shape functions on parallelepiped supports (in the three-dimensional case), in which case an increase in the accuracy of a multiscale solution is possible only by a grid refinement. However, the reduction of the macro-elements is not always possible, due to the method requirements for the ratio of the sizes of macro-elements and inclusions. In this paper, we investigate the efficiency of increasing the order of basis functions on tetrahedral supports and shape functions on polyhedral supports for the heterogeneous multiscale finite element method applied to the problem of elastic deformation of a solid with inclusions.

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Multidimensional computational models of gas combustion in heterogeneous porous medium

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A two-temperature multidimensional computational model of filtration combustion of gas is proposed [1, 2]. The model is based on the approximation of a system of conservation laws by the mixed finite element method in spatial variables and the splitting method in time. Particular attention is paid to improving the performance of the computational model by using parallel computing.

We investigated the process of filtration combustion of gas in inhomogeneous porous media in the case of a jump in the heat capacity of the frame and a jump in porosity. In the case of a jump in the heat capacity, we showed that the formula for the instantaneous velocity of the front works adequately away from the media boundary, i.e. it reflects the real process of what is happening before and after the jump of physical characteristics, namely, the combustion front slows down when approaching the boundary, and it reaches a new constant value of the velocity after the transition to a new medium. In this case, the process stabilization does not take place and the speed of the combustion front is not zero. In the case of a jump in porosity, its stabilization is observed, that is, the front stops abruptly at a certain critical value of the jump in porosity. In the latter case, the balance relation for the invariance of the process with respect to shear stops working for natural reasons - the invariance of the problem with respect to shear disappears in the presence of a jump in the parameters of the problem.

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Implementation of planar 3D model of hydraulic fracture in rock with layered compressive stress

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The paper proposes a description of the Planar 3D hydraulic fracture model implemented at the Institute of Thermophysics SB RAS. Two dimensional fluid flow in the fracture is described using Reynolds equation that is approximated by finite volume method as in fully 3D model [1]. Fracture opening is connected with fluid pressure by hypersingular integral equation [2]. Fracture front propagation is described by asymptotic solution lake in [3]. The system on nonlinear equation (SNE) at each step of fracture propagation is solved by Newton method. Results obtained by P3D model have been compared with classic 1D model solutions.

The model is planned to be used both for simulation of plane fracture propagation and for test of various convergence improving technics for SNE.

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(m, k)-methods for DAEs of index 2

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Authors derived non-iterative (m, k)-schemes for solving the Cauchy problem for differential-algebraic systems of index not exceeding 2. For these schemes, including freezing regularizing matrix, authors obtained and studied accuracy and stability conditions. Formulas for transformation of (m, k)-schemes parameters are given.

L-stable (3, 2)-method of order 2 is derived. It requires two calls of a function, single evaluation of the Jacobian matrix, and single LU-decomposition per integration step. The integration algorithm of alternating step size is based on the new method. The algorithm allows to solve differential-algebraic equation systems of index not exceeding 2. Numerical results confirming the efficiency and reliability of new algorithm are given.

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Non-conforming finite element modelling of coupled heat and mass transfer processes in phase-change media

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Today, mathematical modelling is one of the ways to study natural phenomena and physical processes taking place in the world around us. In heterogeneous media with phase-changing physical properties, mathematical modelling of coupled heat and mass transfer processes is complicated by the geometrical multiscale of systems under study, the nonlinear dependence of physical fields, and the high contrast of the physical medium properties. The formulated features determine the requirements for a computational scheme, which should naturally preserve the regularity properties of mathematical models of physical processes at a discrete level. For solving the problems in media with time-varying inter-fragments boundaries, non-conformal finite element methods are most suitable. In the paper, we propose modified computational schemes of the multiscale discontinuous Galerkin method for approximating the system of Navier-Stokes-Darcy equations and Stefan's problem. As a representative of the family of non-conforming methods, the discontinuous Galerkin method provides freedom in the choice of function spaces and trace operators. The form of operators is determined by the specifics of the problem being solved. To discretize physical fields, we use hierarchical bases of the $\mathbf{H}$(div) and H^1 functional spaces. To solve finite element discrete analogues, algebraic multilevel solvers are applied.

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A conservative sixth-order algorithm for the direct Zakharov – Shabat problem

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Improving the accuracy and efficiency of numerical algorithms for the direct Zakharov – Shabat (ZS) problem is an urgent problem in optics. We present a family of conservative sixth-order schemes for the ZS problem. The schemes are based on the generalized Cayley transform. In particular, we present an exponential scheme similar to [1] and schemes based on rational approximation, which allowed the use of fast algorithms. The schemes are compared with $CF_4^{[6]}$ scheme [2]. Numerical experiments have shown the efficiency of the new schemes.

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About one method for solving problems with quasispherical symmetry

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An approach based on the use of the apparatus of spherical vectors [1] is demonstrated for solving problems of mathematical physics with symmetry close to spherical. Several problems are shown, for which an analytical solution has been obtained. It helps to discover the qualitative features of the dynamics of the object under study. The problem of free rotation of an elastic quasi-ball is considered. The possibility of global movement of the axis of stable stationary rotation in the body is shown. The solution is obtained for the problem of the motion of a viscous fluid between non-concentric spherical and ellipsoidal surfaces. It was found that the solution contains a radial flow. The possibility of generating a magnetic field by the found flow is investigated.

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Preconditioning methods based on spanning tree algorithms and Schur complement techniques

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This work continues the evaluation of tree-based preconditioners started in [1, 2]. The new approach suggests using Schur complement [3] to invert the preconditioning matrix instead of using direct solvers for building the preconditioner. This allows to reduce both memory footprint and computation time. Also, this approach is a good candidate for parallelization. We compare its convergence rate and performance with some well-known preconditioners and solvers. The comparison is performed using SLAEs from the University of Florida's sparse matrix collection [4].

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Comparative analysis of methods for solving SLAE in three-dimensional initial-boundary value problem

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An experimental study of the performance of rendering methods for systems of linear algebraic equations (SLAE) in implicit approximation schemes for three-dimensional boundary value problems in modeling non-stationary heat conduction processes with phase transitions is carried out [1, 4]. Algorithms of finite volumes on an unstructured grid [2] and various approaches to temporal approximation [5] are considered. To improve the performance of the preconditioned iterative processes used in the Krylov subspaces [3], the technique of choosing the optimal initial residuals at each time step is used. The effectiveness of the proposed approaches is demonstrated in a representative series of methodological experiments.

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Crystal structures and continued fractions

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We consider a model of the crystal structure based on the representation of finite continued fractions by unimodular morphisms of a plane integer lattice. The specified representation and properties of these unimodular morphisms are obtained in [1]. The model constructed here allows us to explain the existing limitations of the sets of Weiss parameters (the rational ratio of the lengths of the edges of the forming cell) of the crystal lattice by the Gaussian distribution of natural numbers in the representation of continued fractions.

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On the application of a modified genetic algorithm to optimize the parameters of methods for solving systems of linear algebraic equations

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The solution of a system of linear algebraic equations (SLAE) is among the most frequently encountered stages of mathematical physics problems. In a number of computational fluid dynamics (CFD) applications, this stage takes more than 90% of the overall calculation time. Reducing the simulation time (and hence the time for solving SLAEs) can significantly speed up the calculations.

This work presents a modified genetic algorithm for automated parameters selection for the SLAE solution methods. The algorithm includes a neural network model that generalizes the SLAE solution statistics and limits the search area for the optimal parameters set. The performance of the algorithm is shown on SLAEs for the model Poisson equations and SLAEs from CFD calculations. An increase in search efficiency is shown when the neural network model is included in the basic genetic algorithm. The quantitative results of solution accelerating for SLAEs of various sizes are presented (30 % acceleration in comparison with manual parameters selection).

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Approximation of nonhomogeneous fractional differential equations

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This talk is devoted to the well-posedness and approximation for nonhomogeneous fractional differential equations in Banach spaces E. First of all we get the necessary and sufficient condition for the well-posedness of nonhomogeneous fractional Cauchy problems in the Holder spaces. Secondly, by using implicit difference scheme and explicit difference scheme, we deal with the full discretization of the solutions of nonhomogeneous fractional differential equations in time variables, get the stability of the schemes and the order of convergence. In [1–2] the stability and the order of convergence of homogeneous fractional differential equations for implicit difference scheme and explicit difference scheme were obtained. In this talk, we will consider the fulldiscrete approximation of the nonhomogeneous fractional differential equation in the space C([0, T];E).

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ODE solver based on methods with extended stability domains

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Many processes in chemical kinetics and electric circuit theory are modelled with stiff systems of ordinary differential equations (ODE), which in case of large dimension of system can be solved using explicit Runge-Kutta methods. Stability control of Runge-Kutta numerical schemes allows to increase efficiency of integrating algorithms significantly [1]. Methods described in [2] can be used in adaptive algorithms where number of stages may vary from one integration step to another providing large stability interval where needed and saving computational efforts where there is no requirement to stability characteristics of numerical scheme.

Here is presented ODE solver that includes a library of several algorithms, based on methods with extended stability domains. We use estimation of maximum eigenvalue of Jacobi matrix as stability control criteria allowing to switch between different numerical schemes. Algorithms of variable step, order and number of stages are build. Software package allows to create an algorithm by given number of stages, type of an algorithm and the shape of stability domain and then to solve a problem using it.

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Iterative method for solving difference problems of gas dynamics in mixed Euler – Lagrangian variables

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The method is intended to solve implicit conservative operator difference schemes for the grid initial-boundary value problems on a simplex mesh for the system of equations of gas dynamics in mixed Euler-Lagrangian variables. To find a solution to such a scheme at a time step, it is represented as a single equation for a nonlinear function of two arguments from space – the direct product of the grid spaces of gas-dynamic quantities. To solve such an equation, a combination of the generalized Gauss-Seidel iterative method (external iterations) and an implicit two-layer iteration scheme (internal iterations at each external iteration) is used. The feature of the method is that, the equation, which is solved by internal iterations, is obtained from the equation of the difference scheme using symmetrization – such a non-degenerate linear transformation that the function in this equation has a self-adjoint positive Frechet derivative. Using the operator properties of the difference scheme, it is possible to select a block-diagonal, symmetric, factorized operator of the upper layer of the iterative scheme with a template that does not exceed the size of the function template in the original equation.

Description of the dynamics of nonlinear localized waves of the sin-Gordon equation in the framework of the model with three attracting impurities

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One of the simple model equations used to study nonlinear wave processes in theoretical and mathematical physics is the sine-Gordon equation (USG) [1]. When using USG on real physical models, there is a need to modify it by adding additional terms and functions. They can describe the presence of an external force, the heterogeneity of the parameters of the medium, etc. The modified USG does not have exact analytical solutions, but there are a number of widely used analytical methods (the method of collective coordinates). In this paper, we study the dynamics of impurity modes in the sine-Gordon model with three identical point attracting impurities located at the same distance from each other.

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Numerical aspects of solving Fredholm integral equations of the 1st kind by projection methods

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For the approximate solution of integral equations, a large number of numerical methods have been developed, including projection methods, when an approximate solution is sought in the form of a linear combination of basis functions. However, the practical use of these methods for solving Fredholm integral equations of the 1st kind leads to a computational problems, the main of which is the choice of the number of basis functions. The report discusses as this problem as other problems in the numerical solutions of integral equations.

Application of the polynomial convergence in Bernstein ellipses for numerical analysis of initial boundary-value problems with fronts

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Numerical analysis of the non-stationary problems with fronts and blow-up-type solutions using rational approximations reveals a close connection between the evolution of solutions and the motion of their singular points in the complex plane (poles, branch points, etc.), see [1, 2]. Such singular points can behave quite complex and at certain moments of time come close to the real-valued domain of the problem, which leads to the appearance of fronts, peaks, blow-up effects.

To account for this type of singularities we use the forward and converse theorems of convergence of Chebyshev approximations in Bernstein ellipses and special mappings, which enable us to obtain the nonlinear differential equation describing the trajectory of singular point in complex plain. Then, the rational barycentric interpolations can be used to find the solution with the high rate of convergence, see [2]. The proposed method was tested on the example of initial boundary-value problem.

The research has been done under the financial support of the Russian Science Foundation (project No. 20-71-00071)

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Semi-Lagrangian approximation and the finite element method for solving the Navier – Stokes equations of a viscous heat-conducting gas

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An algorithm for the numerical solution of the Navier – Stokes equations of a viscous heat-conducting gas is proposed. The equations are written in the form necessary to fulfill the laws of conservation of mass and total energy. The semi-Lagrangian approach is used to approximate the convective part of the equations. The space-wise discretization of the remaining terms of the equations on each layer in time is carried out by the finite element method with piecewise bilinear basis functions and the use of simple quadrature formulas [1]. The constructed difference scheme has the first order of accuracy in time and space. The numerical experiment confirms the stability of the scheme and the first order of convergence of the numerical solution [2].

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Hyperbolic SVD for obtaining solutions of SU(2) Yang – Mills equations

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We use the hyperbolic singular value decomposition [1] and the method of two-sheeted covering of orthogonal group by spin group to present all constant solutions of the Yang – Mills equations with SU(2) gauge symmetry for an arbitrary constant non-Abelian current in arbitrary pseudo-Euclidean space [3]. Using the ordinary singular value decomposition, we solve the same problem in arbitrary Euclidean space [2]. Nonconstant solutions of the Yang-Mills equations are considered in the form of series of perturbation theory.

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On five-diagonals splitting for cubic spline wavelets with four vanishing moments on a segment

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In this study, we use a zeroing property of the first four moments for constructing a splitting algorithm for cubic spline wavelets. First, we construct a system of cubic basic splines satisfying the homogeneous Dirichlet boundary conditions [1]. Then, using four zero moments [2] the corresponding wavelet space, realizing orthogonal conditions to all polynomials up to third degrees on the closed interval, constructed. The originality of the study consists of obtaining implicit relations connecting the coefficients of the spline decomposition at the initial scale with the spline coefficients and wavelet coefficients at the nested scale by a tape system with almost five non-empty diagonals of linear algebraic equations. After excluding the even rows of the system, in contrast to the case with two zero moments [3], the resulting transformation matrix has five (instead of three) diagonals. The presence of a strict diagonal dominance over the columns [4] is proved which confirm the stability of computation process without any transformation of the boundary wavelets as in [1, 3]. For comparison, we use the results of calculations using wavelets orthogonal to polynomials of the first degree and interpolating cubic spline wavelets with the property of the best mean square approximation of the second derivative of the function being approximated [5].

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On seven-diagonals splitting for cubic spline wavelets with six vanishing moments on an interval

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In this study, we use a zeroing property of the first six moments for constructing a splitting algorithm for cubic spline wavelets. First, we construct a new system of cubic basic spline-wavelets, realizing orthogonal conditions to all polynomials up to fifth degrees [1]. Then, using the homogeneous Dirichlet boundary conditions [2], we adapt spaces to the closed interval. The originality of the study consists of obtaining implicit relations connecting the coefficients of the spline decomposition at the initial scale with the spline coefficients and wavelet coefficients at the nested scale by a tape system of linear algebraic equations with a non-degenerate matrix. After excluding the even rows of the system, in contrast to the case with two zero moments [3], the resulting transformation matrix has five or seven (instead of three) diagonals. For a seven-diagonal matrix, the presence of a strict diagonal dominance over the columns [4] is proved. The comparative results of numerical experiments on approximating and calculating the derivatives of a discrete function are presented.

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Hierarchical basis on tetrahedra for mixed finite element formulation of the Darcy problem

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The solution of a certain class of applied problems in the oil industry involves the use of mathematical models that describe complex processes associated with the intensification and development of hydrocarbon fields. Mixed variational formulation turn out to be effective for determining the explicit behavior of the normal velocity component at the boundary of the modeling domain, however, they involve finding a solution in two spaces [1]. In this paper the problem of constructing a specialized hierarchical basis systems on tetrahedral finite elements in the H^1-space for pressure and in the H^{div}-space for velocity is investigated and also the influence of this basis on the properties of a matrix of a discrete analogue of a non-conformal mixed formulation based on the discontinuous Galerkin method is studied [2].

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The wave process in the anisotropic medium for various types of electromagnetic field excitation

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Electromagnetic measurements are the main of non-destructive research in a wide range of engineering, medical and geophysical applications. Geological media often exhibit anisotropic properties and cannot be described by scalar electrophysical characteristics. The construction of an adequate measurement and interpretation system should consider the anisotropic properties of the medium. This paper presents the interaction of electromagnetic harmonic radiation in the kHz range with an anisotropic medium when the field is excited by distributed and lumped voltage sources. Various types of medium anisotropy are considered: transversely isotropic medium, orthotropic medium, and medium described by a dense second-order tensor. Modeling is conducted by the vector finite element method on simplicial finite elements [1] in a special variational formulation that considers the medium's tensor electrical conductivity [2].

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Particle motions for the gas dynamics equations with the special state equation

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The gas dynamics equations with the state equation of special form are considered. The state equation is a pressure equal to the sum of two functions. The first function depends on density, and the second function depends on entropy [1]. The system admits a 12-dimensional Lie algebra. An optimal system of dissimilar subalgebras of the Lie algebra was constructed in [2]. Invariant submodels are calculated for 2- and 3-dimensional subalgebras. Exact solutions were found for some submodels.

The motion of particles and volumes according to the exact solutions is considered due to using the computer mathematics system Maple.

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The coupling of the vectorial and scalar boundary element methods

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The vectorial boundary element method is a tool applied to solve electromagnetic problems in a media with consideration of eddy currents [1]. It’s also known as the boundary element method for eddy current problems [2, 3]. The use of this method brings certain difficulties, one of which is the problem of zero wave number in the subdomains adjacent to the domain where the eddy currents should be considered. As a means to mitigate the computational difficulty, we present in this paper the coupling with the scalar potential. The scalar boundary element method for the Laplace equation is in use for the corresponding adjacent subdomains with zero wave number and the associated scalar potential. In this study, we present a coupling similar to the one demonstrated in [4].

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On the numerical solution of some multidimensional differential-algebraic systems

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In the work a multidimensional differential-algebraic system with a special structure of a multiparameter matrix pencil is considered. Such systems combine hyperbolic and parabolic equations. Structural features of a multiparameter matrix beam constructed from the coefficients of the system do not allow the use of the fractional steps method and the alternating direction method for its numerical solution. For its numerical solution the spline-collocation method is applaed [1, 2].

The results were obtained within the framework of the state assignment of the Ministry of Education and Science of Russia under the project "Theory and Methods of Research of Evolutionary Equations and Controlled Systems with Their Applications" (state registration number: 121041300060-4).

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On the protective layer boundary determining error in the thermal conductivity inverse problem

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The article studies the problem of determining the error introduced by the inaccuracy of determining the thickness of a protective heat-resistant coating for composite materials. The mathematical problem is the equation of heat conduction on an inhomogeneous half-line [1, 2]. The temperature on the outer side of the half-line is unknown, it is measured at the media section.

An analytical study of the direct problem was carried out in the work [3]. The projection regularization method is used to estimate the modulus of conditional correctness [4].

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Role of conservativeness property for providing solvability condition at numerical solving the 3D Neumann problem of laser-induced plasma evolution in a semiconductor: direct and iterative methods

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In the report, we present a robust approach for numerical solution of 3D nonlinear set of PDEs describing problem of 3D semiconductor plasma generation. The process is governed by equation concerning laser pulse intensity and equations governing evolution of semiconductor characteristics. The Poisson equation describes the laser-induced electric field potential with inhomogeneous Neumann boundary conditions. Because of the nonlinear feedback presence, the Neumann problem solvability condition [1] violation could occur at using a direct method for numerical problem solving. We demonstrated coincidence of the solvability condition with the conservation law for the problem [2]. Violation of this law leads to problem solvability violation. Therefore, using an iterative method for solving the Neumann problem for the Poisson equation is caused by the fundamental property of the problem.

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Invertibility and estimates for norms of inverse bi-infinite matrices with diagonal dominance

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As is known, finite matrices having the property of diagonal dominance are invertible. The estimate for the norm inverse to the diagonally dominant matrix was obtained by Ahlberg J. and Nilson E.N. in 1963 [1]. Later, Shivakumar P.N., Williams J., and Rudraiah N. found that the diagonal dominance of infinite matrices does not guarantee their invertibility [2]. The report is devoted to an analogue of the concept of diagonal dominance for bi-infinite matrices. Such matrices are infinite in both directions and have an infinite number of diagonals. The main results are theorems that ensure the invertibility of bi-infinite matrices and give estimates for norms of inverse matrices. In the report, it will be shown also how these results are applied in the theory of splines. Such estimates are required in problems of extremal interpolation (see [3]).

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Determination of the external and internal attached pipe mass

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Resistance of continuous media with accelerated movement of a pipeline is considered. An undeformable pipe of infinite length, surrounded by an ideal incompressible fluid, moves with acceleration perpendicular to its axis. The pipeline has a circular cross section. It is assumed that the gas flow in the axial direction occurs inside a liquid circular cylindrical region. The perturbed movements of the internal gas, liquid, and external continuous media caused by the acceleration of the pipeline are described by the Laplace equations in polar coordinates relative to the velocity potentials. Solutions of equations are made in the form of one-term approximations. The time derivatives of the desired functions in the solutions are determined from the boundary conditions on the cylindrical contact surface of the phases of the gas-liquid medium as well as on the inner and outer surfaces of the pipe. It is shown that the ratio of the added masses of the liquid with and without taking into account the flow of particles of the gas-liquid mixture in cross sections is a function of the geometric dimensions of the pipe and the density of the media. Numerical calculations were performed for specific values of the input parameters.

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Semi-Lagrangian method for the numerical solution of the continuity equation on unstructured triangular meshes

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The paper presents a Semi-Lagrangian method [1] for the numerical solution of the continuity equation. The method is based on an integral conservation law connecting the two-dimensional integrals of the solution on adjacent time layers and the flux integrals at the input and output from the region [2, 3]. A discrete analog of the conservation law is substantiated for the numerical solution when passing from one layer in time to the next layer.

Involving the Lagrangian approach in the approximation of the transport operator (with the Eulerian approach for the remaining operators) allows significantly improving the properties of the obtained discrete problems. First, for the approximation of the continuity equation (the mass conservation law), the Courant-Friedrichs-Levy constraint for the time step is eliminated by adapting the stencil of a discrete equation. At high speeds, the stencil stretches along the transport direction in the combined time-space coordinates. Second, it is not necessary to match space difference grids on adjacent time layers. This opens up the possibility of flexible (often local) condensation of the difference grids at each time layer.

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Interier point method

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A family of algorithms for solving optimization problems is considered, which have become very popular since the 80-s all over the world, to which thousands of publications are devoted, which have now supplanted the simplex method in the curricula of many countries. Pioneering developments and theoretical studies of the algorithms under consideration have been carried out since the beginning of the 70s only in Russia at ISEM SB RAS, Computing Center of RAS (I. Dikin, Yu. Yevtushenko, V. Zorkaltsev, V. Zhadan). The initial impetus in the development of these algorithms was the 1965 idea of LV Kantorovich of approximation of "objectively determined estimates" of resources in a non-optimal design by the least squares method based on the complementary slackness condition. A great deal of experience has been accumulated in the application of these algorithms in models of energy, economics and ecology in linear and nonlinear optimization. Families of algorithms with various special useful properties will be presented.

Section 2

NUMERICAL STATISTICAL MODELING AND MONTE CARLO METHODS

Stochastic model of the joint spatio-temporal field of precipitation and wind speed in the southern part of the Lake Baikal region

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The report presents a numerical stochastic model of the joint spatio-temporal field of the wind speed with a three-hour resolution and semidiurnal precipitation. The model proposed is constructed on the basis of long-term observation data at an irregular network of meteorological stations positioned in the area of Lake Baikal. The model is developed under the assumption of the daily non-stationarity of the real joint meteorological field and its spatial heterogeneity, induced by the physical and geographical features of the considered terrain. The quality of interpolation of the simulated precipitation field on a regular spatial grid and the possibility of using the model proposed to study extreme precipitation regimes in the river basins located in the southern part of the Lake Baikal region are discussed.

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Setting unsteady inflow boundary conditions of a stochastic turbulence with the desired autocorrelation

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In computational fluid dynamics, synthetic turbulent velocity fields are commonly used for the imposition of inflow boundary conditions for the LES zone. The inflow artificial turbulent field should be unsteady and have the same properties, such as autocorrelation, as real turbulent fields. In the work presented, the artificial turbulent fields are generated with the help of Randomized Spectral Method [1, 2] as the sum of stochastic Fourier modes, with the time dependence at the boundary using random frequencies, following [3]. An appropriate model has been chosen on the base of time correlation analysis–both theoretical and numerical, given by test LES computations of turbulence in the cube. For comparison, the results for a time filtering method are also presented.

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Application of an economic algorithm for modeling of random variables for simulation of a Poisson point process

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Statistical solution of the problems of analysis, synthesis and filtration for systems of the diffusion-discontinuous type, requires simulation of inhomogeneous Poisson point process [1]. In order to simulate the latter, sometimes an algorithm based on the ordinariness property of the process is used. In this article, a modification of the algorithm is being constructed by using an economic method for modeling of random variables [2–4]. The developed method is verified by solving test problems

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Double randomization method for estimating the moments of solution to the coagulation equation

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The problem of estimating the probability moments of linear functionals from the solution to the Smoluchowski equation with random coagulation coefficients is considered. For this purpose, we modify the algorithms previously proposed by the authors for solving kinetic problems [1, 2] using the double randomization method. In addition, a splitting method is proposed to reduce the computational costs of the algorithms [3].

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Application of the Monte Carlo method to study the features of aerosol cluster motion

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In this work we applied the previously developed Monte-Carlo algorithm [1] designed to calculate photophoretic and viscous forces acting on the aerosol cluster in the rarified gas medium to study sedimentation of clusters.

According to calculations, the photophoretic force significantly changes the qualitative and quantitative characteristics of the cluster motion. It is shown that in the absence of light, the sedimentation velocity of cluster consisting of equal-sized spherical particles is close to the sedimentation velocity of a single spherical particle. The relationship between the cluster velocity and its fractal dimension and the number of spherical particles in the cluster is revealed. Light significantly changes the character of sedimentation. The vertical velocities of clusters are distributed within a broad range. Some of them move up against gravity. This is an effect of photophoretic (gravito-photophoretic) levitation. The computer model simulates the characteristic movement of the aerosol cluster at gravito-photophoresis, the upward spiral movement, which was previously observed in the experiments.

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Using the modified superposition method in the computational system NMPUD

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The computational system NMPUD (Numerical Modelling of Probabilistic Univariate Distributions) was developed in the Laboratory of Mathematical modelling of Lyceum No. 130 of the city Novosibirsk, Russia, in 2020 [1, 2]. The NMPUD system is used primarily as a helpful (or even necessary) tool for choosing the necessary economically simulated probability distributions for researchers involved in the elaboration and (or) use of computational stochastic models for solving urgent applied problems.

The main content of the bank of the NMPUD system is elementary densities (that is, those that are effectively simulated by the inverse distribution function method; see Chapter 2.6 of the book [3]). These densities can be obtained in sufficient quantities using the technology of sequential (inserted) integral substitutions; see Chapter 14.2 of the book [3].

In this paper, the expediency of creating blocks within the NMPUD system for simulating distributions with polynomial and piecewise polynomial densities using the modified superposition method (see Chapters 11.2, 11.3 of the book [3]) is substantiated.

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Numerical modeling of boundary value problems for differential equations with random coefficients

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The article is devoted to the numerical modeling of differential equations with coefficients in the form of random fields. Using the Karunen-Loeve expansion, the coefficients are approximated by the sum of independent random variables and real functions. This allows us to use computational probabilistic analysis and, in particular, we apply the technique of probabilistic extensions to construct the probability density functions of the processes under study. As a result, we present a comparison of our approach with the Monte Carlo method in terms of the number of operations and demonstrate the results of numerical experiments for boundary value problems for differential equations of elliptic type.

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Markov chain based stochastic modelling of HIV-1 and SARS-CoV-2 intracellular replication cycles

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Understanding the dynamics of the intracellular virus replication is crucial for antiviral drug development. We present the detailed deterministic models of the life cycles of HIV-1 [1] and SARS-CoV-2 [2] in target cells. The Markov chain based models are formulated to study stochastic aspects prominent at low variable numbers. The hybrid simulation algorithm based on direct Gillespie method [3] with automatic switching between stochastic and deterministic methods when variables exceed a specified threshold is implemented in C++. The stochastic models are used to predict (1) the probability of target cell infection as function of multiplicity of infection, (2) the heterogeneous structure in the evolution of the viral progeny number distribution, (3) the processes having the biggest impact on the total progeny number, (4) the integrated provirus number distribution in HIV-infected cells [4]. The model extensions to describe the innate IFN-I response and the evasion mechanisms by which HIV-1 and SARS-CoV-2 antagonize it are discussed.

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Solution of stochastic optimal control problems

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The report is devoted to solution of the problem of stochastic optimal control of dynamical systems, which are described by stochastic differential equations (SDE's) of the Ito type [1]. The coefficients of the SDE of the problem being solved depend on the random process, which is the control at each time item. In the problem, it is required to define a control such that optimizes the mathematical expectation of the functional of the controlled process. The determination of the optimal control is carried out on the basis of the principle of dynamic programming and solving the HJB equation. Numerical solution of problems of this type is considered.

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Numerical simulation of a two-dimensional electron gas transfer in a quantum well heterostructure

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In this work, a question of an influence of quantum well subbands number on a drift velocity of a two-dimensional electron gas in strong and weak electric fields is investigated by numerical modeling. A semiconductor heterostructure AlGaAs/InGaAs/GaAs used as a sample. Self-consistent numerical solution of Poisson's equation for electrostatic potential *V(z)* and Schrödinger's equation for energy levels E_i and their corresponding wave functions ψ_i lets us to define zone structure of the semiconductor [2, 3]. The obtained data on the wave functions and the distribution of the charge carriers across the layered structure are used to solve the Boltzmann kinetic equation and to determine the electron drift velocity. It describes the transfer of two-dimensional electron gas in the layered heterostructure [4, 5]. The model of electron gas transfer takes into account the electron scattering by optical and acoustic phonons, and scattering at the roughness of the heterointerface.

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Numerical stochastic models of non-stationary time series of bioclimatic indices in West and East Siberia

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The report presents the results of numerical modeling of time series of several bioclimatic indices used to study the unfavorable weather conditions during the cold season. The considered stochastic models of unconditional and conditional time series reproduce the diurnal cyclicity of the real bioclimatic processes. For a number of weather stations located in West and East Siberia the results of comparison of estimates of the occurrence probability, duration and other characteristics of adverse meteorological conditions characterized with extreme behavior of the bioclimatic indicators are presented.

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Application of kernel regression in nonlinear adaptation algorithms as applied to multidimensional objects

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The application of the time series smoothing algorithm based on the construction of nuclear regression [1] in the problems of nonlinear synthesis of control for continuous and discrete multidimensional objects is considered.

The illustrative examples of application of the proposed algorithm (biochemistry, immunology, economics, and other fields of knowledge) are provided along with their statistical results of numerical simulation.

The results obtained would be useful in designing a smart control system and for real-time decision making support as it concerns the problems of stochastic control over a wide range of poorly formalized objects from different applied areas.

There are grounds for believing that the synthetic use of two popular nonparametric forecasting algorithms will lead to a more efficient forecasting algorithm, at least for solving a certain class of control problems [2, 3].

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Comparative analysis of various projective algorithms of the Monte Carlo method in problems of the theory of particle transfer

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A comparative analysis of various variants of the projective algorithm of the Monte Carlo method [1] for estimating the particles flow through a layer of medium with scattering of the Henyi-Greenstein type is carried out.

For detailed optimization of the algorithms, a test problem is used that allows an analytical iterative approximation of the solution.

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The Monte Carlo method as a tool for the development of the apparatus of applied mathematical statistics and ensuring the correctness of statistical inferences in applications

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The apparatus of applied mathematical statistics formed to date includes a hard-to-see set of methods used to estimate the parameters of various probabilistic models, and criteria for testing various statistical hypotheses, which make it possible to build models and check their adequacy.

At the same time, the return on the use of the existing apparatus in applications turns out to be small. There are many reasons. Many promising methods and criteria are not being applied due to their lack of publicity. Due to the complexity, the use of many methods is impossible without the corresponding software, which may not be available.

But more often the problems turn out to be more serious. The correct application of any criterion is conditional on the fulfillment of certain assumptions that may not be fulfilled in a particular application. In this case, the statistical conclusion formed on the basis of this criterion may turn out to be incorrect.

Under non-standard conditions of applications, the properties of the methods for estimating parameters change, the distributions of statistics of the applied criteria change, corresponding to the validity of the hypothesis being tested.

The properties of the estimates and the distributions of the statistics of the tests are reflected in the presence of round-off errors, as a result of which, in this case, the possibility of using the existing asymptotic results is also excluded.

Solving the problems of applying statistical methods and criteria in non-standard conditions of applications by analytical methods requires large intellectual costs and, in general, turns out to be unproductive.

At the same time, good results are demonstrated by the use of computer technologies based on the computing apparatus of applied mathematical statistics and the Monte Carlo method. This approach makes it possible to successfully investigate probabilistic and statistical patterns in conditions of various violations of standard assumptions. Moreover, the study of the required patterns can be carried out interactively (in the course of the statistical analysis). And further, the found regularity or distribution of the criterion statistics can be used to form the correct statistical inference.

Using this approach, the problems of applying chi-square goodness-of-fit tests in non-standard conditions were investigated. When testing complex hypotheses, the problems of applying a set of nonparametric goodness-of-fit tests were investigated, and models of the statistical distributions of these tests were constructed. Models of distributions of statistics for multi-sample criteria of homogeneity of laws were used. The properties of a set of parametric and nonparametric criteria used to test the homogeneity of variances were investigated. The properties of sets of criteria for normality, uniformity, exponentiality, criteria for testing hypotheses about the absence of a trend, and others were investigated.

The software implements the possibility of correct application of the considered criteria, including in conditions of influence on the distribution of rounding statistics

Estimation of the probability of two consecutive passages through the resonant regions in the descent of an asymmetric rigid body in a rarefied atmosphere

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A two-frequency nonlinear system of ordinary differential equations is considered, which describes the perturbed motion of a rigid body with considerable asymmetry in the rarefied atmosphere. If the frequencies of the system coincide, the occurrences of capture or passage through the principal resonance are random [1]. In addition, the application of well-known expression [1] made it possible to estimate the probability of a single capture into the principal resonance during the descent of a spacecraft with small asymmetry in dense atmosphere [2]. The aim of this work is to obtain an estimate of the probability of two consecutive passages through the resonance regions during the descent in the rarefied atmosphere of Mars of a rigid body with considerable geometric and aerodynamic asymmetries. The veracity of the obtained estimate is confirmed by the Monte-Carlo method.

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Stochastic modelling of financial securities with a systemic risk component

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We propose and study a new jump-diffusion model for pricing multiple assets, where systemic-risk security is combined with several conditionally independent base assets. This approach allows for analyzing and modelling a portfolio that integrates high-activity security, such as an Exchange Trading Fund (ETF) tracking a major market index (e. g., S&P500 or TSX) with several low-activity assets. The latter may have missing and asynchronous pricing data when the assets are not traded frequently on financial markets. The proposed framework allows for constructing several models, including the following: (a) a diffusion-type model without jumps where all asset price processes are Geometric Brownian Motions; (b) a jump-diffusion model with only common jumps [1]; (c) a jump-diffusion model with both common and asset-specific jumps [2]. We discuss the properties of the proposed model, the estimation of its parameters using the Maximum Likelihood Estimation method, and the pricing of European-style basket options. The NSERC Discovery Grant program supported this work.

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Monte Carlo simulation of halos in crystal clouds

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In this paper, we try to answer the question: how multiple scattering, sun elevation, shape and orientation of ice crystals in the cirrus clouds affect a halo pattern. To study the radiation transfer in optically anisotropic clouds we have developed the software based on Monte Carlo method [1] and ray tracing. In addition to halos, this software enables one to simulate “anti-halos”, which above the cloud layer can be seen by observers [2]. We present the visualization of halos and anti-halos generated by the cirrus clouds for different shapes and orientation of ice crystals.

The study was carried out under the CSC (China Scholarship Council) and the State Contract with ICMMG SB RAS (0251-2021-0002).

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Study of asymptotics of particle transfer process with multiplication in a random medium

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Simulation is carried out using weight modeling and double randomization in order to estimate the average particle flow from a random medium in which particle multiplication occurs.

The main goal of this work is to study the possibility of superexponential asymptotics being realized for a standard model of an isotropic random field of density of the medium.

At the same time, for small correlation radii, a radical reduction in the complexity of calculations could be achieved by replacing double randomization with randomized modeling of trajectories taking into account the value of the correlation length.

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A vector Monte Carlo algorithm for large systems of linear equations

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A Monte Carlo randomization algorithm for solving large systems of linear algebraic equations is presented. This algorithm combines the randomized stochastic matrix based algorithms proposed in [1], and an iterative method of solving integral equations suggested in [2] which has no spectral restrictions on its convergens in contrast to the conventional Neumann series based method. We develop a special transform of the original non-negative matrix to a column stochastic matrix which is then conveniently used for calculation of matrix iterations. The algorithm of randomized calculation of matrix iterations proposed in [1] operates by sampling random rows and columns instead of matrix-matrix and matrix-vector multiplications. To solve a system of linear algebraic equations with a matrix whose eigenvalues are greater than 1, we apply the transformation and the relevant iterative procedure given in [2]. We analyze the correctness, laboriousness and efficiency of the method for various matrix sizes. As a byproduct, a vector random walk on grids and a modified random walk on boundary algorithms for three-dimensional potential problems are constructed.

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A randomized iterative method for solving integral equations of the second kind

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In this presentation we deal with an extension of the conventional Neumann series based Monte Carlo method for solving integral equations of the second kind. This approach is based on a randomized evaluation of the iterative procedure proposed by Polozhy in [1]. In contrast to the simple iteration method, this iterative procedure converges without any spectral restriction on the integral operator. The major challenge encountered in the present study is the analysis of the variance behavior as a function of the number of iterations. Preliminary simulations carried out for boundary integral equations of the potential theory indicates that this behavior is most likely not linear. A discrete version of this stochastic algorithm implementation of the Polozhy iterative method has been developed and presented in [3] where a vector randomization of the matrix iterations suggested in [2] has been applied.

This work is supported by the Russian Science Foundation under grant № 19-11-00019, and the Russian Fund of Fundamental Studies under Grant 20-51-18009 in the part of random walk process implementations.

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Using DSMC calculations to estimate heterogeneous reaction constants based on experimental data

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The direct simulation Monte Carlo method (DSMC) is widely used in solving problems of the rarefied gas dynamics. At the present stage, one of the promising areas of its use is the study of the interaction of gas with surfaces as applied to the problem of gas "activation" on catalytic surfaces. Various approaches to modeling heterogeneous reactions by the DSMC method are being developed. By virtue of the structure of the DSMC method, it is fundamental for all the approaches to use microscopic reaction probability when a particle collides with a surface. The amount of data on microscopic probabilities required for modeling heterogeneous reactions is limited, therefore, the urgent task is to develop approaches for estimating these probabilities based on experimental data. The work presents the results of using the DSMC method to estimate the microscopic probabilities of heterogeneous reactions based on data obtained by two experimental techniques: measurement of the gas composition at the outlet of the cylindrical channel and measurement of heat transfer between a heated wire and hydrogen atmosphere.

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Economic and mathematical model of the dynamics of the Baikal omul population

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In 2017, the Russia Government imposes a restrictions on the catches of Baikal omules, which are due to a significant reduction in its population [1]. By the way, such restrictions led to an increase in poaching and shadow trade. Unfortunately, the assumed measures have not solved the problem of the recovery of fish stocks. The development and study of economic measures to regulate the volume of catches of omules would be useful. The report is devoted to an economic and mathematical model of the development of the stock of Baikal omule, taking into account both natural fish mortality and the intensity of poaching. At the same time, the delivery of a commercial omule on the shore of Lake Baikal from other regions and from specially established fish-breeding plants is considered to be one of the regulators of catches, as a result of which excessive catches of omules in oz. Baikal is no longer profitable. The report addresses methodological problems in estimating individual model parameters. [2].

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Vector autoregressive process. Stationarity and modeling

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The conditions for stationarity of vector processes with a discrete parameter that satisfy the autoregressive equation or a mixed autoregressive and moving average model are investigated. In a mixed model, stationarity is determined by the autoregressive part of the model. Algorithms for modeling processes in the stationary case are presented.

For similar one-dimensional processes, the stationarity condition is equivalent to the fact that the characteristic polynomial determined by the autoregression coefficients has roots modulo less than one.

In the vector case, Hennan [1] showed how to find the characteristic polynomial, which in the stationary case has roots modulo less than one. In this paper, an example is given in which the roots of the characteristic polynomial are less than one in modulus, but the process is not stationary. Additional conditions, ensuring stationarity of the process [2], are found.

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Numerical study of randomized projective estimator and combined kernel-projective statistical estimator

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In this talk, we discuss two particular statistical estimators. One of them is the randomized projective estimator which is based on the projection expansion on the orthonormal polynomial basis. Though this estimator seems to be the promising one and has been applied to solve a number of problems [1, 2, 3], the conversion rates vary sufficiently depending on the basis that has been chosen. Another estimation in consideration is a combined kernel-projection statistical estimator that was suggested in work [4] for the two-dimensional distribution density. It was constructed in the following way: for one of the variables the classical one-dimensional kernel estimator is formed and for other – the projection estimator. The optimal parameters for such an estimator were obtained in [5] within the assumptions made about the convergence rate of the orthogonal decomposition in use. The numerical study was conducted on the number of problems of atmospheric optics.

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Monte Carlo method for solving the problem of predicting the steadiness of the functioning of an automated control system in the conditions of massive computer attacks

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The application of the Monte Carlo method for solving the problem of predicting the stability of the functioning of an automated process control system (APCS) in the conditions of massive computer attacks (MCA) is considered. The field of research is of practical and theoretical interest, since the methods developed by the theory of reliability are focused on simple, stationary, failure flows.

Under MCA conditions, the attack period is commensurate with the recovery time of the automated process control system, so the application of the simple flow model leads to a significant error. To ensure reliability, it is necessary to use the model of the alternating process, where the recovery time is commensurate with the study period and has a finite value. However, the analytical model is very cumbersome and has no practical application.

In [1], the Monte Carlo method is implemented for modeling processes in the automated process control system for MCA conditions with three different attack implementation scenarios. As a result, it became possible to model alternating processes for distribution laws other than exponential ones, including discrete ones. The method is applicable for modeling when organizing an information security audit [2, 3].

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Monte Carlo method for solving the problem of predicting the computer network resistance against DoS attacks

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DoS and DDoS attacks are the most effective types of attacks, as they allow to bring almost any poorly designed computing system to failure, without leaving legally significant evidence. To conduct a successful attack, the attacker selects potentially weak nodes of the computer network.

The article considers the application of the Monte Carlo method for solving the problem of identifying weak nodes and evaluating their security against DDoS attacks. The field of research is of practical and theoretical interest since the methods developed by the theory of reliability are focused on simple stationary failure flows. In the context of DDoS attacks, the flow of attacking requests is not Poisson flow, so the existing analytical models give an unacceptable error.

The opportunity to select the distribution function of arrival time of incoming attacking requests and their duration and response time of attacked nodes are required to make results reliable.

In conjunction with [1, 2], it is possible to adequately simulate DDoS attacks and identify unprotected nodes. The method is applicable for modelling a computer network in conducting an information security audit [3, 4].

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Error analysis of single scattering approximation for 2D and 3D impulse ocean sounding models

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In this report the problem of finding the volume scattering coefficient of sound in an ocean based on the angular flux distribution was examined. Acoustic sounding was done by a point impulse source and single scattering approximation was used to solve the problem [1, 2]. The analysis of single scattering approximation error, caused by multiple scattering in the medium with high-frequency probing (roughly 100 kHz) at a distance of up to 0.5 km, was conducted. It was established that the first order scattering approximation error in a 2D case significantly exceeds that of a 3D case. Images of restored volume scattering coefficient based on a considered scattering multiplicity in the medium are presented.

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High-speed null collision Monte Carlo method for plasma processing tasks

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The article discusses a high-performance null collision method for modeling collisions in plasma. A distinctive feature of the proposed approach from the classical [1] is that it does not use trigonometric functions at all, which can significantly reduce the program execution time on modern processors. The approach is based on the interaction of each particle with an "average" (having averaged properties of all particles in the cell) particle (instead of the classical approach based on pairwise interaction [2]). The most subtle point in this approach is the conservation of energy and momentum of the entire system when changing the trajectories and velocity of the particles. Approaches to solving this problem are given, experimental results are discussed. The effectiveness of the proposed approach is shown.

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Section 3

MATHEMATICAL GEOPHYSICS

Intellectual environment for studying parameters of seismic acoustic fields

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The work analyze and structure the data that have been obtained by recording the seismic effects of the SV-100 source and the group of seismic and hydroacoustic receivers at the Baikal Lake in March 2021. The results modeling have also been studied for these experiments.

The scientific intelligent system “Active seismology” has been arranged for storage, visualization, and numerical analysis of these data

An intellectual web environment has been developed for the online investigation of the acoustic fields.

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On a determination of speed and elastic parameters of a focal zone by the hodographs of earthquakes

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An algorithm for solving the inverse kinematic problem of seismic with internal sources, which is based on the method of multidimensional data approximation on chaotic grids [1], is considered. The arrival times of *P* and *S* waves fixed by seismic stations are considered to be the most reliable kinematic data on earthquakes occurring at great depths. The earthquake hodographs constructed by the method of multidimensional approximation make it possible to calculate the velocities V_p of longitudinal and V_s of shear waves under the assumption that they obey the eikonal equation [2, 3]. The V_p/V_s ratio, which can be calculated already at any point in the study area, determines the elastic parameters of the medium, such as Poisson's ratio, as well as Young modulus and Lamé parameters as functions considered in units of the density of the medium. The results of calculations based on real data are presented.

The work was partially supported by RFBR according to the research project RFBR-DFG No. 19-51-12008.

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Spectral portraits in tasks of recognition of moving objects

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The paper presents the consideration of tasks of passive geometric environmental monitoring associated with seismic and acoustic detection of man-made noise sources affecting the deterioration of the surrounding environmental background. Another task is related to the problem of automatic classification of noise sources by dividing them into disjoint sets in the space of their corresponding informative parameters. Obtaining information about the object of radiation of the wave field is effectively solved by methods of spectral analysis. Spectral analysis is the most informative method for analyzing various seismic and acoustic processes, including those caused by moving sources. However, in the case of a moving source, a complex spectral picture arises, connected with the peculiarity of the radiation of a particular object in various modes of its operation.

The classification problem based on spectral analysis requires a priori information about the object. With this approach, it is effective to analyze the features of the wave field of the radiation object and present the information obtained in the form of spectral portraits. In this case, spectral portraits mean the projection of a three-dimensional frequency-time function onto a two-dimensional plane “frequency-time”. This projection allows to select the time-frequency windows that characterize the analyzed seismic and acoustic vibrations. The latter are used to construct clusters displaying the position of individual objects in the space of informative parameters of moving objects. On the basis of experimental data, the paper presents the consideration and results of the listed stages of solving the problems of passive geophysical monitoring.

3D ray shooting algorithm in heterogeneous isotropic media

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The problem of numerical modeling of seismic waves propagation in three-dimensional heterogeneous isotropic media is of practical interest in seismic imaging and seismic exploration [1]. We solve this problem by the ray tracing method [2]. The purpose of the work is to develop effective algorithms and programs for calculating the times and directions of arrival of seismic waves in a given 3D grid of receivers.

An algorithm for 3D ray shooting has been developed. This algorithm can be applied for a point source and also for a more general case when the initial position of the wave front is given as a surface. The algorithm requires a velocity to be a smooth function. As far as this requirement is limitative we use smoothing algorithm based on a spatial low-pass filtering. We use an operator which describes the operation of a digital-to-analog converter (DAC), well known in digital signal processing theory [3].

The cases of different velocity structure of the medium are considered: homogeneous, gradient, etc., as well as various types of the initial wave front position surface. The results of numerical experiments are presented.

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Exact Navier – Stokes solutions for oil and gas problems

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The system of Navier-Stokes equations is considered, which describes the flow of a viscous incompressible fluid in a porous medium. The simplest model of a porous medium consists of a discrete set of points - grid nodes, which is the boundary of the flow region, in which the adhesion boundary condition is satisfied. Classes of exact solutions corresponding to vortex flow are presented [1]. The study of exact solutions is necessary for the development of a core simulator and simulation of fluid dynamics in a porous medium, its response to dynamic effects of various types and the creation of a domestic technology "digital field" [2].

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Investigation of the propagation of nonlinear waves in a two-fluid medium caused by an analogue of the Darcy coefficient

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The extreme difficulty of analyzing nonlinear waves, especially strong turbulence, led to another tendency in the development of their theory - the transition from complex equations of nonlinear random waves to simpler model equations [1, 2]. In this paper, a system of quasi-linear equations of hyperbolic type is obtained from a system of non-stationary equations of two-velocity hydrodynamics [3-5]. It is believed that the energy dissipation occurs due to the analogue of the Darcy. We study the Cauchy problem for a given system of equations in the class of bounded measurable functions based on the Kruzhkov method.

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Three-dimensional stationary flows of viscous fluids of a two-phase continuum with phase equilibrium with respect to pressure with a singular source in the disipative case

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In this paper, an overdetermined system of equations is obtained from the system of non-stationary equations of two-velocity hydrodynamics in the dissipative case [1-4]. It is believed that the energy dissipation occurs due to the analogue of the Darcy. Construction of a solution for describing three-dimensional stationary flows of viscous fluids of a two-phase continuum with phase equilibrium with respect to pressure with a singular source in the dissipative case.

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Numerical modeling and physical effects of interwave interactions

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The problems of studying the interaction of conjugate geophysical wave fields of different nature, arising from natural and man-made sources simultaneously in different environments: seismic in the lithosphere, acoustic in the atmosphere, hydroacoustic in the hydrosphere, optical, meteorological in the atmosphere are considered. The solution of the problems under consideration is due to the urgent problems of environmental monitoring in connection with noise pollution by various types of transport, industrial and natural sources. As a result, geoecological risks are generated that affect the social environment, first of all, on humans, as well as on buildings. Multivariate numerical models of interwave interactions and their mechanisms are presented and analyzed. As a result of interactions, various physical effects are generated that determine the degree of influence of conjugate wave fields on the medium. On the basis of numerical modeling and the results of field experiments, estimates of increased geoecological risks are given.

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Modeling of the Sun's magnetic field from the kinematics point of view-the gravitational ion dynamo model

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The first of a large number of works on the generation of the magnetic field of the Sun (MPS) and planets is considered to be the work (Lehrmor 1920), which discusses the need to introduce a self-excitation mechanism to amplify a weak electron current and obtain a strong MPC. In many subsequent works, models of self-excitation of an electronic current are investigated. In the previous [1] and this paper, the current generating the MPC is the motion of a positively charged liquid or gas. It is known that the current density is proportional to the charge density and the velocity of their movement. According to the known estimates of the parameters of the structure of the Sun the calculated charge densities and currents create magnetic fields (MP) for seven of the top layers of the Sun: chronosphere, chromosphere, photosphere and four layers of the convective zone. The maximum permissible estimates of currents and MPS are obtained. From these estimates of the kinematics-gravitational ion dynamo model, it follows that all layers of the model, taking into account certain restrictions, can participate in the generation of MPS.

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Numerical characteristics of technogenic noise in geoecological monitoring tasks

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One of the tasks of geoecological monitoring of the environment is related to the assessment of levels of technogenic noise representing a danger to people.

In this situation, there is a necessity of signals extraction from external noise and their parameters measurement. Other problem is related to the considered problem - noise source direction determination. In this work characteristics of seismic and acoustic wave fields, created by technogenic sources, are investigated. Railway, heavy tracked and wheeled transport as well as CV-40 seismic vibrator [1] are considered as sources.

In this work, the approach based on combining the algorithms of quadrature accumulation [2], polarization analysis [3], controlled directional reception [4] and directional coefficient determination [5] is considered for signals extraction and noise source direction determination.

The study of the characteristics of the noise sources under consideration is of interest for the problem of geoecological monitoring of the social and natural environment and in other problems.

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Mathematical modeling of wave fields to determine the sensitivity of the vibroseismic monitoring method

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The paper presents the application of mathematical modeling of wave fields in the problem of studying the sensitivity of the method of active vibroseismic monitoring to small changes in velocity parameters in the inner areas of the Earth's crust. The change in the parameters of the wave field recorded on the surface is determined depending on the size of the areas of changes, its location relative to the source and receivers, and the wavelength of the probing signal. Analytical estimates are obtained for variations in vibroseismic vibrations recorded on the surface for spherical inhomogeneity in a homogeneous model of the Earth's crust in contact with the upper mantle, as well as variations in the total wave field for a realistic model of the Earth's crust and inhomogeneous inclusion based on the application of the finite difference method to solve the problem of dynamic theory of elasticity. The results of mathematical modeling are compared with experimental data of active vibroseismic monitoring of the Baikal rift zone.

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Mathematical modeling of electromagnetic fields of main pipelines cathodic protection systems in electrically layered and anisotropic soils

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The geometric and physical properties of the containing pipeline soil play a significant role in the distribution of electric and magnetic fields generated in the cathodic anticorrosive electrochemical protection systems.

The paper considers mathematical models that are more adequate to practice (in comparison with those currently in force in accordance with GOST), taking into account the layering [1] and anisotropy [2, 3] of the specific electrical conductivity of the medium. The problems are solved by the method of fictitious sources. The results of confirming comparative computational experiments are presented.

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Signals of electromagnetic tool with toroidal coils in highly deviated wells

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This study propels the research direction related to the electromagnetic logging tool with toroidal coils [1]. Its main goal is to expand the tool's applicability from vertical well sections to those of highly deviated wells, based on 3D finite-difference simulation [2] and multi-aspect analysis of the signals. The latter were obtained in geoelectric models of oil-, gas- and water-saturated reservoirs with a different number of horizontal boundaries, varying reservoir thicknesses, including the case of fine layering.

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Earthquake record processing algorithms to form a strong motion database

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This study is devoted to the development of algorithms and software for earthquake record processing. The algorithms are based on the methodology used by the Pacific Earthquake Engineering Research Center for the implementation of the scientific project NGA-West2 [1]. The purpose of processing is to determine reliable values of ground acceleration and other parameters of earthquakes from the available records of velocity time series. To analyze the operation of the algorithms, earthquake records (simultaneously recorded time series of acceleration and velocity), taken from the European Rapid Raw Strong-Motion database [2], were used. The developed algorithms and the implemented software will allow in the future to form a database of strong motions for building regional attenuation models on the territory of the Russian Federation.

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Grid method for estimating the velocity characteristic of complex medium

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An important problem in solving inverse problems in seismology associated with determining the geographic and energy characteristics of a seismic source is obtaining a priori information about the propagation velocities of seismic waves. In heterogeneous media, in particular in the areas of volcanoes and faults, obtaining a velocity pattern is sharply complicated due to the nonlinearity of the travel time curve of seismic waves [1–3]. The paper proposes an approach to the calculation and assessment of local velocities of seismic P-waves in the area of the Mount Karabetova mud volcano (the Taman mud volcanic province) based on the use of the grid method. The numerical algorithm is tested on experimentally obtained arrival times of waves from a vibration source of the SV-10/100 type for the Mount Karabetova mud volcano. Using the approach proposed a zone of inhomogeneity introduced by the volcano and its approximate geometric dimensions have been identified. The obtained results of the distribution of local velocities are consistent with the geological structure of the study area [4] and indicate the prevalence of higher velocities in the area of the anticlinal fold passing through the volcano zone.

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Resolution of acoustic emission events recovery in core samples

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An approach to localizing the events of acoustic emission by the Time Reversal Mirror (TRM) approach [1, 2] with the analysis of the total energy of the wave process is proposed. Based on numerical modeling results, the resolution of the method was investigated depending on the dominant frequency of acoustic emission signals and the number of recording channels. It was shown that even for frequencies of the order of 250-500 kHz, it is possible to localize acoustic emission events on samples of standard size with a diameter of 30 mm.

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Seismic source recovery in cluttered media by the Time Reversal Mirror approach

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The problem of detecting and localizing objects embedded in some randomly inhomogeneous medium arises in many important applications, such as ultrasound medical imaging [1], non-destructive testing of materials [2], seismic inversion, etc.

The paper considers the problem of source recovery in geological cluttered media (randomly inhomogeneous media) based on a seismogram recorded on the free surface. To restore the source's location, the Time Reversal Mirror method [3] is applied to a set of statistically equivalent media modeled by a random function of space. The results of numerical experiments are presented.

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Numerical modeling of fault structures in the Kurai basin of Gorny Altai based on data from direct current methods

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We present the results of three-dimensional modeling of fault structures in the southern and central parts of the Kurai basin according to the data of direct current methods. The southern site is located in the junction zone of the Southwestern and Eshtykel deflection, where vertical electrical soundings were performed, and a preliminary fault-block depth model was built based on the results of interpretation of field data using a horizontally layered model [1-2]. Comparison of geoelectric and seismological data showed the coincidence of the identified assumed faults with the zones of distribution of earthquake epicenters. In the central site, three profiles of electrotomography were made through a step, which is well expressed in the relief. Three-dimensional modeling was used to verify and clarify the structural features of both sections. Моделирование выполнено с помощью программ The simulation was performed using the EMF_DC3Dmod (GPU) programs - an accelerated version of the EMF_DC3Dmod [3] program for vertical electrical sounding and SCALA-48 (GPU) [4] for the electrotomography method.

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The wave process in the anisotropic medium for various types of electromagnetic field excitation

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Electromagnetic measurements are the main of non-destructive research in a wide range of engineering, medical and geophysical applications. Geological media often exhibit anisotropic properties and cannot be described by scalar electrophysical characteristics. The construction of an adequate measurement and interpretation system should consider the anisotropic properties of the medium. This paper presents the interaction of electromagnetic harmonic radiation in the kHz range with an anisotropic medium when the field is excited by distributed and lumped voltage sources. Various types of medium anisotropy are considered: transversely isotropic medium, orthotropic medium, and medium described by a dense second-order tensor. Modeling is conducted by the vector finite element method on simplicial finite elements [1] in a special variational formulation that considers the medium's tensor electrical conductivity [2].

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A divide-and-conquer algorithm for seismic data approximation by the Laguerre series

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The Laguerre transform has been used in various fields of mathematical simulation to solve acoustics and elasticity equations, Maxwell and heat conduction equations, and spectroscopy problems. These problems are of considerable interest for mathematical modeling and spectral analysis methods. An algorithm of the Laguerre transform for approximating functions on large intervals is proposed. The idea of the considered approach is that the calculation of improper integrals of rapidly oscillating functions is replaced by a solution of an initial boundary value problem. A divide-and-conquer algorithm based on shift operations made it possible to significantly reduce the computational cost of the proposed method. Numerical experiments have shown that the methods are economical in the number of operations, stable, and have satisfactory accuracy for seismic data approximation.

The numerical implementation of proposed algorithms was carried out under state contract with ICMMG SB RAS (0251-2021-0004), the study of proposed algorithms was financially supported by RFBR and Novosibirsk region (Project No. 20-41-540003).

Self-similar solution of lava flows spreading problem in the condition of partial slip on the underlying surface for fissure eruptions

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The lava is a strongly viscous fluid, but no-slip condition on the underlying surface for lava flows not always realized. Often on the underlying surface there is a sublayer containing a considerable fraction of rock fragments which are not sticks to it. It is forms due to two facts: firstly, lava flows can spreaded over an earlier-erupted material and, secondly, they can be coated by a crust which cracks, owing to cooling, and falls down ahead of the flow. Previously, this phenomenon was considered for the axisymmetric case of lava flows spreading [1-3]. Problem similar to [2-3] for fissure eruptions, when lava erupts through linear volcanic vent, is being considered in present work: it is solved in the case of flat two-dimensional formulation.

Lava is modeled by the incompressible Newtonian or non-Newtonian fluid. The underlying surface is assumed to be flat and horizontal. The condition of partial lava slip in the form of generalized Navier slip condition is used. In the thin layer approximation the problem reduces to the solution of one nonlinear partial differential second-order equation with an additional integral condition. The self-similar solution is obtained in the case of the power-law time dependence of the lava flow rate from the vent under some restrictions. It is shown that the lava propagation velocity can be considerably higher, when the slip is taken into account.

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Applying the R-solution method for design a tsunami observing system

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One of the promising methods of the early warning of a tsunami near a source zone is obtaining data of the wave heights based on the numerical solution of the inverse tsunami problem by using the least-squares method and the truncated singular value decomposition method. The problem is considered within the framework of the linear theory of wave propagation. The technique proposed allows one to avoid the inevitable instability of the numerical solution. It is possible to choose the most informative directions for the placement of the observation stations, which is based on the analysis of the energy transfer by the spatial mods generated by each right singular vector. As it has turned out, the best location of the stations is closely related to the directions of the most intense distribution of the tsunami energy. One of the significant advantages of the approach presented is the possibility, without additional calculations of the tsunami wave propagation from a reconstructed source, to obtain the tsunami wave heights at the points at which there are no observations but which are associated when calculating the matrix of the direct problem operator. An example of the approach proposed to the real event of the Chilean Illapel Tsunami of September 16, 2015, is presented.

The research proposed was carried out under the State Budget Program with ICMMG SB RAS (0315-2021-0005).

Section 4

MATHEMATICAL MODELS OF ATMOSPHERIC PHYSICS, OCEAN AND ENVIRONMENT

Application of the methods of direct and inverse modeling for processing airborne measurements results of air composition

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The report presents an approach to processing the results of aircraft measurements using the results of direct and inverse modeling. For direct modeling, the WRF-Chem v.4.2 model was used. The resulting meteorological fields were used for inverse modeling. For inverse modeling, the IMDAF [1] model was used. As a result of the approach used, it became possible not only to estimate the total contribution of local sources to the measured values, but also to highlight the influence of a particular source.

This work was supported RFBR grant No. 19-05-50024, 18-45-700020 (modeling are carried out), and the studies of small gaseous constituents of the atmosphere and aerosols were carried out with the support of the Ministry of Education and Science of the Russian Federation.

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Modelling of multiphase multi-velocity unsteady flows in pipes with elevation difference

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This research aims at studying the behaviour of flows of multiphase mixtures in pipes, when there is a difference in elevations. The study method is based on computer modelling using a simulator of multiphase flows created by the authors [1]. The simulator is appropriate for describing the flow of multiphase mixtures in complex systems, with implementation of two-velocity motion model of various phases. In liquid-gas mixture, it results in different velocities of phases motion [3]. The analysis results demonstrate that velocities differ substantially. The presence of gravitational component greatly affects the nature of flow, and, in some cases, leads to a change in flow regimes [2]. The work shows that regimes can also be implemented without reaching steady-state conditions.

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The problem of retrieval the methane profiles in the Earth's atmosphere from high-resolution IR spectra

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Here we present some results of modified Levenberg-Marquardt method [1] applicability for solving inverse problems of greenhouse gases remote sensing in Earth's atmosphere. The computational experiments were performed to retrieve the vertical profile of the main methane isotopologue from the thermal IR synthetic spectra of IASI/MetOp spectrometer. The noise parameters were set equivalent to sensor characteristics. The optimal estimation method implemented in FIRE-ARMS software [2] was used for solving the inverse problem. The data of the retrospective climate analysis CAMS GHG Flux Inversions [3] were used as an initial guess and a statistical set of profiles. The computational experiment showed convergence and accuracy of the proposed method, which, however, turned out to be more computationally expensive than Gauss-Newton method.

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Modelling of internal solitary waves in a multilayer stratified fluid

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We present a hyperbolic model describing the propagation of internal waves in a stratified shallow water with a non-hydrostatic pressure distribution in two external layers and an arbitrary number of internal hydrostatic layers, which is an extension of the models from [1, 2]. The construction of the hyperbolic model is based on the use of additional instantaneous variables. This allows the reduction of the dispersive multi-layer Green–Naghdi model to a first-order system of evolution equations.

Stationary solutions of the motion equations are investigated and conditions for the formation of the solitary waves are formulated. The model was verified by comparison with the results of field observations and calculations using two-dimensional equations. Numerical simulation of the propagation of non-stationary nonlinear wave packets in a multilayer fluid has been performed.

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Particle filters in data assimilation problems for chemical kinetics models

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Methods of data assimilation based on the particle filter [1, 2] are quite a new and promising direction. The advantage of the algorithms is that they allow us to estimate not only the value of the model state function based on measurement data, but also the density of the probability distribution of its values. Particle filters are well parallelized and require only an algorithm for solving a direct problem for their calculation. We are actively working on the development of particle filters for multidimensional nonlinear problems of geophysics with an emphasis on atmospheric and oceanic applications. The paper considers the application of methods based on a particle filter in nonlinear problems of assimilation of chemical kinetics data [3]. The efficiency of the algorithm is numerically investigated.

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Hyperbolized "soft cover" model for calculating stratified flows with a free boundary in a non-hydrostatic approximation

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The original system of equations describing the dynamics of a stratified fluid with a free surface in the Boussinesq approximation, presented in terms of density and pressure variations is elliptic and it is necessary to solve the Poisson difference equation in its numerical implementation. With a large number of computational nodes, this procedure requires significant computational resources and complicates the algorithm parallelization on multiprocessor computers.

The hyperbolization of the problem based on the weak compressibility approximation is an alternative option. In this approach, an equation of state establishes a linear dependence of pressure on the parameter θ. This parameter characterizes the degree of volume deviation of the Lagrangian particle from the initial state: $\Delta P = c^2(\theta - \theta_0)$, $\theta_0 = 1$. Even though its change is described by the continuity equation this parameter does not coincide with the density. Parameter *c* is an artificial sound speed. It is determined by the condition that the parameter θ does not deviate from the initial value by more than one percent. The density equation is a transport type.

The pressure force acting on the free surface returning it to the state of static equilibrium. It can be called "soft cover" mechanism. This pressure depends on the magnitude of deviation of the free surface from the equilibrium position. A standard kinematic condition is also set at the liquid boundary.

The explicit-implicit CABARET scheme is used to solve the hyperbolized system, explicit in horizontal directions and implicit in depth. It makes it possible to use large time steps on grids with thinning of layers to a free surface. The proposed non-hydrostatic model is verified by laboratory experiments, in which the formation and propagation of internal bottom waves formed during the rapid extraction of a lock gate separating a denser part of the liquid with a controlled vertical salinity distribution from a homogeneous liquid in a long channel are investigated. The results are compared with laboratory measurements and calculations using a hydrostatic model.

Validation of the CABARET-MFSH hydrostatic model for modeling the flows of stratified fluids with a free surface in laboratory experiments

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This paper is devoted to the results of validation on two series of laboratory experiments of the new low-dissipative multilayer hydrostatic model CABARET-MFSH, which describes the dynamics of a fluid with variable density and a free surface. The computational algorithm of the new model is based on representing a multi-layer environment as separate layers interacting across interfaces. We call this method hyperbolic decomposition. An explicit CABARET scheme is used to solve the system of hyperbolic equations in each layer. The scheme has a second order of approximation and is time reversible. To regularize the multilayer hydrostatic model, mass and momentum exchange between the layers and the filtration of flux variables are used. The filtration parameters are determined empirically from the condition of the stability of the algorithm and the minimality of the scheme viscosity.

In laboratory experiments, the emergence and propagation of bottom internal waves is investigated. They are formed when the gate is quickly pulled out between a liquid with a controlled vertical salinity distribution and a homogeneous liquid.

The calculation results are in good agreement with the experimental data.

Changes in the state of the Siberian Arctic seas in the last two decades

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This report discusses issues related to climatic changes in the ice and water state of the shelf seas of the Siberian sector of the Arctic. The research is based on analyzing observational data and modeling results using a numerical three-dimensional model of the Arctic Ocean. Changes in the timing of the formation and melting of ice, an increase in heat input into surface sea waters, an increase in the heat content of the seas are analyzed. The extreme rise in surface water temperature in shelf seas can be classified as the existence of marine heatwaves. To identify marine heatwaves, the method described in (1) was applied.

This work was supported by the Russian Science Foundation (19-17-00-154).

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Simulation of the interaction of long surface waves with semi-submerged structures with an uneven bilge

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The study is devoted to the problem of the interaction of long surface waves with semi-submerged fixed structures with an uneven bilge. Numerical algorithms [1] are constructed for one-dimensional nonlinear shallow water models with and without frequency dispersion [2]. The influence of bilge irregularities on the characteristics of the reflected and transmitted waves is investigated. The obtained numerical solutions are compared with the results of other authors [3].

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Some nonlinear models of transport theory

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A wide class of problems in physics and engineering leads to the study of integro-differential equations of transport theory. The foundations of mathematical and numerical modeling of particle transport processes were laid in the works [1-4]. We consider stationary and non-stationary problems for nonlinear systems of integro-differential equations of transport theory [5]. The issues of correctness of statements of the corresponding mathematical problems, properties of their solutions and algorithms for numerical solution are discussed. The theoretical study of the problems uses the methods of ordered function spaces.

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Local ensemble optimal nonlinear filtering algorithm

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A shortcoming of the classical particle filter method is that observation data are used only to calculate the weight coefficients with which the elements (particles) of an ensemble are summed. An approach to solving the nonlinear filtering problem based on a representation of the distribution density as a sum of Gaussian functions has been used. If the distribution density is represented as a sum of Gaussian functions, a sum with weights of estimates obtained in Kalman filters corresponding to Gaussian distribution densities is the optimal estimate. In the report, an approach to solving the nonlinear filtering problem with the distribution density represented as a sum of Gaussian functions is considered. The ensemble π-algorithm, which was proposed earlier by the author, is used to implement the algorithm [1, 2]. The algorithm is local and can be implemented in separate subdomains. This allows its implementation in high-dimensional geophysical models. The results of numerical experiments with a 1-dimensional nonlinear model are presented.

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Data assimilation problems for production-destruction models with parameter identification

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To predict and assess the state of rapidly changing processes, stable data assimilation algorithms are widely used. An example is the process of changing the chemical composition of atmospheric air. To study the dynamics of pollutants in urban conditions, methods of mathematical modeling are used with the assimilation of measurement data of the pollution level obtained at monitoring posts. Data assimilation algorithms restore the missing information about the parameters of the mathematical model in the process of modeling with the input measurement data for the past and current values of the model state functions. We will understand the data assimilation problem as a sequence of related inverse problems [1, 2]. As a basic inverse problem, let us consider the problem of evaluating the initial data and parameters of the product-destruction model from the data of point measurements of the state function. Optimization algorithms are used to solve it.

The results of the operation of data assimilation algorithms, when the measurement data become available in some portions in time, and algorithms for solving the inverse problem, when all data are available at the time of the start of calculations, are numerically compared. The computation time and accuracy are analyzed.

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Analysis of the annual water balance of the Lena river basin and variability of river flow

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It is known that the hydrological system of the Arctic is especially sensitive to an increase in temperature, and it is also influenced by precipitation, evapotranspiration, processes on the land surface: the development and distribution of taliks, the dynamics of the depth of the seasonally thawed layer [1]. Analysis of fluctuations in water balance components in a changing climate based on MERRA reanalysis data for the period 1980–2020. [2] makes it possible to identify the most important factor controlling the increase in river flow.

The purpose of this work is to analyze changes in meteorological processes and their influence on the variability of river flow.

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Modelling of Earth thermosphere-ionosphere coupled dynamics

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One of the central directions in Earth system models development is inclusion of upper atmosphere and ionospheric models. Such models create possibilities not only to study the atmospheric upper and lower layers interaction but also to apply them to solving the practical problems, such as radio waves propagation through ionosphere. The difficulty in constructing such models lies in variations of atmospheric characteristics and specificity of the low-temperature plasma dynamics in the Earth's magnetic field, in addition it is necessary to account a large amount of small gas impurities responsible for both radiation heat fluxes and ionization processes, etc.

In our talk we discuss the problem of thermosphere-ionosphere coupled dynamics and present a new coupled model of Earth's thermosphere and ionosphere global dynamics (altitudes 90-500 km). The model is based on a three-dimensional thermospheric general circulation model and a dynamical model of the ionospheric F region, which takes into account plasma-chemical processes, ambipolar diffusion, and advective ion transport due to neutral wind and electromagnetic drift. Realistic upper atmospheric processes main characteristics in model is shown and quantitative estimates of thermosphere – ionosphere interaction are obtained based on presented coupled model.

Eddy transport in a stably stratified atmospheric boundary layer over rough surface: a study with of nonlocal model turbulence

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The features of the atmospheric boundary layer (ABL) depend it is on atmospheric stratification (effects of buoyancy) and the dominating mechanism of turbulence generation. The boundary layer becomes stably stratified when the underlying surface is colder than the air. In these conditions turbulence can be generated by shear and destroyed under the influence of negative buoyancy and viscosity. Because of the different shear and buoyancy effects, turbulence in the stable boundary layer (SBL) is inhibited in comparison to the neutral and convective boundary layers (CBL). In this study, the turbulent momentum and heat fluxes are calculated with explicit algebraic models obtained with use of symbolic algebra from the transport equations for the momentum and heat fluxes in the approximation of weakly equilibrium turbulence [1, 2]. The nonlocality of the mechanism of turbulent momentum and heat transfer in the atmospheric boundary layer over a rough surface manifests itself in the form of limited regions of countergradient of momentum and heat transfer, which are diagnosed from analysis of balance terms in the transport equation for the variance of temperature fluctuations and from calculation of the coefficients of turbulent momentum and heat transfer invoking model of "gradient diffusion". It is show is that the countergradient heat transfer in the local regions is caused by turbulence diffusion or by the term of divergence of triple correlation in the balance equation for the temperature variance.

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The use of satellite data in the problems of evaluating the characteristics of emission sources and atmospheric parameters

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Images from space make it possible to visually record the trajectories of smoke plumes from industrial chimneys. Based on this information, it is possible to quickly track the spread of impurities in the atmosphere.

The paper analyzes the trajectories of smoke plumes using the equations of hydrothermodynamics and transport of impurities in the lower atmosphere. With the use of satellite observation data in relation to emissions from high-rise chimneys of thermal power plants located in the Baikal natural territory, estimates of additional heights of rise of smoke plumes were obtained according to the previously developed method [1]. Comparison with calculations based on known relationships, including the heat flux of buoyancy and the dynamic impulse of emissions, is carried out [2].

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One approach to restoring conditions on inner boundary in the hydrothermodynamics problem

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In this work a domain decomposition method based on theory of optimal control and adjoint equations [1] is considered. The initial domain is divided into subdomains by introducing an inner boundary. To formulate interface conditions 'additional unknows' are introduced to the system. The domain decomposition approach allows to solve the problem, restore boundary conditions on inner boundary and obtain solution of the system. The domain decomposition method is numerically studied in the problem of hydrothermodynamics modelling. The numerical experiments with using the domain decomposition algorithm are presented and discussed. It could be noted that described domain decomposition method could be applied together with variational data assimilation [2].

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Enviro-HIRLAM seamless modelling approach for environmental studies: recent research and development

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The Enviro-HIRLAM (Environment - HIgh Resolution Limited Area Model) is seamless/ online integrated numerical weather prediction (NWP) and atmospheric chemical transport (ACT) modelling system capable to simulate simultaneously meteorology – atmospheric composition on multi-scales ranging from regional to sub-regional – urban scales.

The main areas of the modelling system research and development include: (i) downscaling/ nesting for high resolutions, (ii) improved resolving planetary boundary layer and surface layer structures, (iii) urbanization and sub-layer processes, (iv) improvement of advection schemes, (v) integration of natural and anthropogenic emission inventories, (vi) implementation of gas-phase chemistry mechanisms, (vii) implementation of aerosol dynamics and microphysics, (viii) implementation of aerosol feedback and interactions mechanisms.

The Enviro-components includes the following: (i) gas-phase chemistry; (ii) aerosol microphysics with nucleation, coagulation, condensation of sulfate, mineral dust, sea-salt, black and organic carbon together with aerosols' dry and wet deposition, sedimentation processes; (ii) parameterisations of urban sublayer with modifications of the interaction soil–biosphere–atmosphere scheme; (iv) sulfur cycle mechanism with dimethyl sulfide, sulfur dioxide and sulfate; (v) radiation scheme improved to account explicitly for aerosol radiation interactions for 10 aerosol subtypes; (vi) aerosol activation implemented in condensation-convection scheme with nucleation dependent on aerosol properties and ice-phase processes; (vii) locally mass-conserving semi-Lagrangian numerical advection scheme; (viii) natural and anthropogenic emission inventories.

The Enviro-HIRLAM utilises extraction and pre-processing of initial/ boundary meteorology-chemistry-aerosol conditions and observations for data assimilation (from ECMWF's ERA-5 & CAMS), pre-processing of selected emission inventories for anthropogenic and natural emissions. The latest version has been run on CRAY-XC30/40 and Atos BullSequana HPCs machines, and it has been developed through the research and HPC projects such as Enviro-HIRLAM at CSC and Enviro-PEEX & Enviro-PEEX(Plus) at ECMWF, as well as other research projects.

The further (since 2017; Baklanov et al., 2017) research, development and science education of the modelling system and its applications will be demonstrated on examples, where the Enviro-HIRLAM is used as a research tool for studies in domain of the Pan-Eurasian Experiment (PEEX; https://www.atm.helsinki.fi/peex) programme. These studies include: aspects of regional-subregional-urban downscaling with focus on metropolitan areas of St.Petersburg and Moscow; influence of dust transport from artificial tailing dumps and Cu-Ni smelters of the Kola Peninsula on pollution of environment and health of population; aerosol feedbacks and interactions at regional scale in the Arctic-boreal domain; estimation of spatio-temporal variability of elevated black carbon episodes; influence of land cover changes on regional weather conditions/ patterns and its consequences on meteorology for cases of extreme (with heatwave, heavy rains and snowfall) meteorological; evaluation of atmosphere-land-sea surfaces interactions, and in particular, heat-moisture exchange/ regime between these surfaces and for better understanding and forecasting of local meteorology in the Arctic; assessment of potential pollution regional atmospheric transport resulted from wildfires in the Chernobyl zone; analysis of urban meteorology and atmospheric pollution with integrated approach to high-resolution numerical modelling; and others.

The science education component (as part of the PEEX Educational Platform) for the Enviro-HIRLAM model is also realised, and though the organization and carrying out of the research training weeks. The latest face-to-face trainings took place in April 2019 (Helsinki; Enviro-PEEX project) and June 2019 (Tyumen, Russia; AoF ClimEco project), and next ones arranged and temporarily postponed into autumn 2021 (Moscow, ClimEco & MegaCity projects) and spring 2022 in St.Petersburg; EDUFI PEEX-FRESReN project) in Russia. Short term visits and trainings of young researchers are also expected as a part of the activities in the Enviro-PEEX(Plus) project, MEGAPOLIS Russian Megagrant, and PEEX-CarbonPolygon collaboration, and others.

The model application areas are the following: aerosols-chemistry feedbacks studies on various meteorological variables; effects of various interactions of aerosols and cloud formation processes and radiative forcing on urban-regional scales; boundary layer and sublayer parameterizations; urbanization processes impact on changes in urban weather and climate on urban-subregional-regional scales; studies on atmospheric pollution and its local impacts; improving prediction of extreme weather events; providing meteorology-chemistry input to assessment studies for population and environment; integration modelling results into GIS environment for further risk/vulnerability/consequences/etc. estimation, and others.

Influence of tsunami wave parameters on its passage through straits

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The experience of historical tsunamis shows that when the tsunami wave passes the straits it loses a significant part of its energy and becomes certainly lower in amplitude. Using numerical modeling, the influence of wave length (period) on the ratio of tsunami height before and after it passes a narrow strait is considered.

The study was carried out both in the model configuration of the straits, and in the case of real geography and the bottom relief.

Modeling of atmospheric diffusion taking into account wind impacts and building

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The paper proposes a modification of the Margolus Neighborhood Cellular Automata (CA) [1], its spatial implementation with the addition of such factors that affect the propagation of pollutant as wind and gravity, which brings the model closer to the simulated process. We implement CA-diffusion in *three-dimensional space* with various kinds of obstacles. When modeling the interaction of a substance with an obstacle, each block in the basic substitution is associated with a binary type parameter, as a result of which all blocks are subdivided into two types: internal and boundary. The entered parameter in the result determines the need to rotate the block when performing basic substitution. Wherein, the boundary of the modeling area can be specified in the form of planes (plates) and parallelepipeds. It is also possible to simulate the effect of wind on the admixture at a given angle. The transfer of substances in the absence of obstacles is modeled by a synchronous shift of the cells of the state array with probabilities proportional to the corresponding components of the wind speed vector [2].

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Study of the interaction of a reservoir with an ideal compressible fluid with an elastic half-space

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We solved in a flat formulation the problem of harmonic oscillations for a basin with an ideal compressible fluid on an elastic half-space exposed to a localized surface vibration load. The problem was reduced to an integral equation (IE) of the first kind for the amplitude of the contact hydrodynamic pressure with a kernel that depends on the difference and the sum of arguments [1]. IE was solved by the factorization method [2].

A semi-analytical method is presented for determining the main parameters of the contact interaction in hydroelastic systems "liquid-soil" taking into account the effect of natural and man-made vibration loads on them, which makes it possible to identify the conditions for the occurrence of dynamic modes that are dangerous for construction integrity and to estimate their frequencies range depending on the defining characteristics of the system.

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Sensitivity-operator-based inverse modeling framework with heterogeneous measurements

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Air quality monitoring systems vary in temporal and spatial coverage, the composition of the observed chemicals, and the data's accuracy. The developed inverse modeling approach [1] is based on sensitivity operators and ensembles of adjoint equations solutions. An inverse problem is transformed to a quasi-linear operator equation with the sensitivity operator. The sensitivity operator is composed of the sensitivity functions, which are evaluated on the adjoint ensemble members. The members correspond to measurement data elements. This ensemble construction allows working in a unified way with heterogeneous measurement data in a single operator equation. The quasi-linear structure of the resulting operator equation allows both solving and analyzing the inverse problem. More specifically, by analyzing the sensitivity operator's singular structure, we can estimate the informational content in the measurement data with respect to the considered process model. This type of analysis can estimate the inverse problem solution before its actual solution and evaluate the monitoring system efficiency with respect to the considered inverse modeling task [1, 2].

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Numerical comparison of a sensitivity operator based and metaheuristic algorithms on parameter identification problems for production-destruction models

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Various meta-heuristic algorithms are widely to identify parameters of the mathematical models. Usually, these algorithms take only direct problem solution and can be easily applied to various problems without serious modifications. The trade-off for this universal character is the use of a limited number of inverse problem properties. The objective of this paper is to compare the performance of the sensitivity operator-based algorithm [1] and standard implementations of metaheuristic algorithms [2] on a realistic scenario of parameter identification problems for atmospheric chemistry and bio-chemical models.

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Variational principles for Earth system models and data assimilation

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The problem of matching mathematical models of the Earth system using the variational principle was considered in [1]. These studies were developed in the creation of methods for solving environmental problems. Indeed, processes in the environment affected by anthropogenic factors occur in various components of the Earth's system: in the atmosphere, hydrosphere, on the Earth's surface, in the upper layers of the soil, etc. The models, which describe these processes, must be consistent with each other. We combine all these models into a united system based on variational principles in formulations with weak constraints, allowing for the presence of uncertainties in all objects of the modeling system and in the observational data. The latter are included in the modeling system using data assimilation methods. Currently, most of the data from existing monitoring systems comes from the atmosphere and the Earth's surface. In problems of the Earth system, the process models and observational models act as tools of spatio-temporal extrapolation-interpolation for estimating state functions and parameters in solving direct and inverse problems for the system as a whole in continuation mode.

The work was done according to the state task of the ICMMG SB RAS (0251-2021-0003) in the development of variational approach and partially supported by RFBR (grant 20-01-00560) in solving the continuation problems.

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The problem of determining the sources of greenhouse gases in a given region based on a time series of observations

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The problem of determining the sources of greenhouse gases in a given region is one of the most important at present. An algorithm based on the statistical optimization method to estimate a parameter that is constant in time is considered. To implement the algorithm, a variant of ensemble smoothing is used, which is an optimal estimate of the desired parameter based on observational data and forecast for a given time interval. This report presents the implementation of the algorithm for real observational and forecast data. The results of a three-dimensional transport and diffusion model (MOZART) are taken as a mathematical model, and satellite measurement data (AIRS) are used as observational data. Greenhouse gases fluxes are estimated in subregions of the Earth's surface for specified time intervals. The report contains a mathematical formulation of the problem, a scheme for its numerical implementation. The results of numerical experiments with model and real data are presented.

Climate system modeling and some methods diagnostic of midlatitude extreme weather in Northern Hemisphere

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Recent decades have seen accentuated warming and precipitous decline of sea ice in the Arctic, in keeping with the so-called Arctic amplification anticipated from the increasing greenhouse gas forcing.

Accompanying the Arctic change are the more frequently observed weather extremes in the Northern Hemisphere midlatitudes. Locations for the occurrence of weather extremes and their trends and a better understanding of their regional impact on weather is importance. Circulation pattern that can lead to such extremes, the blocking event, is a synoptic-scale phenomenon that blocks the jet stream, resulting in persistent weather. Atmospheric blocking has received attention for many decades and is still very much a topic of actuality because of its relationship to extreme weather. Recently, [2] have proposed local wave activity (LWA) as a diagnostic of local wave anomalies and blocking events. LWA is a generalization of the finite-amplitude wave activity theory [3] into its local counterpart, quantifying waviness as a function of latitude and longitude, and is capable of measuring regional disturbances in the atmospheric circulation. In this work we quantifies LWA using Z500, which has been used to diagnose weather extremes in the troposphere such as blocking events [4–6].

The study used the INM-CM48 climate system model [1], developed at the INM RAS and taking into account many factors of climate change.

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Modeling of admixture transport from Baikal region sources under winter atmospheric conditions

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The report presents some scenarios for modeling the transport of impurities from high pipes of industrial enterprises and thermal power plants in the Baikal region in winter atmospheric conditions. Scenario calculations were performed on the basis of the mesoscale model of atmospheric dynamics developed in the ICMMG SB RAS. The initial distributions of the fields of meteorological elements and the conditions at the upper boundary of the modeling domain were set from the calculations of the COSMO-SIB6 prognostic mesoscale model.

The work on the development of basic mathematical models is carried out within the framework of the state task of the ICMMG SB RAS No. 0251-2021-0003. The implementation of special scenarios for solving the problems of continuation is supported by the RFBR under grant No. 20-01-00560.

Numerical analysis of the processes of aerosol pollution of the Baikal natural territory

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Using model descriptions of the processes of atmospheric transport of impurities and data from monitoring studies of pollution of vegetation and snow cover of the Baikal natural territory (BNT), the formulation of problems of low-parameter estimation of concentration fields and characteristics of sources is discussed. To increase the stability of the solutions of the considered inverse problems, algorithms for optimizing the placement and assessing the information content of monitoring systems are used.

Examples of approbation of the proposed methods for assessing pollution fields in the vicinity of large industrial facilities of BNT are given. The quality of the obtained results is checked by comparing the measured and calculated concentrations of impurities at the control points of observation, comparing the experimental and numerical results with the data of satellite observations.

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Joint realisation of algorithms for variational assimilation of salinity, temperature and sea level at the open boundary

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An approach to taking into account open boundaries in hydrothermodynamics modeling, based on the theory of inverse problems, the use of adjoint equations and methods of variational data assimilation, is considered. The formulation of boundary conditions at open boundaries is an actual problem in the modeling of circulation of seas, bays and other open water objects. The algorithms for variational assimilation of salinity, temperature and sea level [1] at the open boundary are presented, the results of the numerical experiment on their joint realisation in the hydrodynamics model are discussed. The simulation results are compared with the observational data from various sources.

This work was supported by the Russian Foundation for Basic Research (grant 19-01-00595).

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Construction of a model of the Earth's ion-magnetosphere, which determines the dynamics of the propagation of a radar pulse

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The expansion of the scale of the tasks solved by the supporting space systems requires the improvement of methods and algorithms used for processing trajectory measurements in order to increase their reliability and accuracy of determining the motion of the aircraft.

Various factors influence the accuracy of the estimation of motion parameters.

To solve the set tasks, it is necessary to build a mathematical model of the Earth's ion-magnetosphere, close to the real one. In this case, it is necessary to take into account the various properties and characteristics of the Earth's ion-magnetosphere.

Effect of the shape of moving external load on ice deflections and strains distribution in a frozen channel

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Deflections of an ice cover in a frozen channel caused by a moving load are considered. The channel has a rectangular cross-section. The fluid in the channel is inviscid, incompressible and covered with ice. The ice cover is modeled as a thin elastic plate with constant thickness. The flow caused by the ice deflections is potential. The problem is solved within the linear theory of hydroelasticity [1]. The load is modeled by a pressure distribution and moves along the channel at a constant speed. The load is of arbitrary shape and vary in calculations. The problem using the Fourier transform along the channel is reduced to the problem with respect to the deflections profile across the channel, which is solved by the method of normal modes [2]. The solution is obtained as the sum of the integrals of the inverse Fourier transform. It is shown that parallel or sequential motion of loads can increase stresses in the ice cover both on the channel walls and between loads. The numerical and analytical study of the considered problem is presented. The problem of the motion of an external load along unbounded ice was studied in [1], along the central line of the channel in [3].

The work is supported by the State Assignment of the Russian Ministry of Science and Higher Education entitled `Modern methods of hydrodynamics for environmental management, industrial systems and polar mechanics' (Govt. contract code: FZMW-2020-0008, 24 January 2020).

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Solution of advection-diffusion-reaction problems on a sphere

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The new algorithm proposed in [1] is applied for solving linear advection-diffusion-reaction problems and nonlinear diffusion problems on a sphere. Discretization of differential problems in space is performed by the finite volume method using the Gauss theorem for each grid cell. For time discretization, the method of symmetrized two-cycle componentwise splitting and the Crank-Nicholson scheme are used. The obtained numerical method has the second order of approximation in space and time. It is implicit and unconditionally stable; in addition, operator splitting provides a direct (non-iterative) and fast implementation of all implicit schemes. The theoretical results are confirmed numerically by simulating various linear processes on the sphere (diffusion in a spherical sector, diffusion flux through the pole, advection flux through the pole, dispersion of a pollutant emitted from multiple point sources) and nonlinear diffusion processes (spiral waves, nonlinear temperature waves, HS, LS and S blow-up combustion modes and solutions of the Gray-Scott model). Numerical experiments [2] show a high accuracy and efficiency of the method that correctly describes the processes of advection-diffusion on a sphere (including processes near the poles and through the poles) and the mass balance of matter in forced and dissipative discrete systems. Moreover, in the absence of external forcing and dissipation, the method conserves both the total mass and the L2-norm of the solution.

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Mathematical modeling of the flow in a wake behind an impact of an elastic body on a thin liquid layer

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The study is motivated by the results of experiments on droplet deposition in an annular gas-liquid flow and mass transfer between gas and liquid film [1]. A two-dimensional problem of the impact of an elastic body on a thin layer of liquid is considered. The body is modeled by a thin plate. At the beginning of impact the liquid layer is at rest. At the initial moment of time, the elastic plate touches the liquid at a single point. After the impact, the plate moves in the positive x-direction and penetrates into the liquid layer (Oxy is the Cartesian coordinate system). The coupled problem of deflections of an elastic plate and the fluid motion under the plate is studied in [2] in the leading approximation. After determining the deflections of the plate and the behavior of the fluid under the plate, the problem of fluid dynamics in the wake is solved by the method of characteristics and asymptotic methods. Similar problems are studied in [3]. The results of the numerical and analytical solution of the formulated problem are presented. The main focus of the report is given to the first terms of the asymptotic decomposition and the jet formations on the free surface in the wake.

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A numerical modelling of urban air quality with mesoscale atmospheric models

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The results of the numerical prediction of meteorological parameters and some indicators of atmospheric air quality in the city of Tomsk using the mesoscale numerical weather forecast model TSUNM3 [1] and the model of pollutant transport taking into account chemical reactions [2] are presented. For individual historical dates, the study of the relationship between meteorological conditions and air quality in the city was carried out using mathematical modeling methods. Particular attention is paid to the formation of aerosol particles in the atmosphere of the city. The calculation results are compared with the observational data obtained at the TOR-station of the IAO SB RAS, and with the calculations of the CAMx air quality model.

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New method for analytical continuation of the planetary potential fields and terrain topography

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A new effective technique based on the modified S-approximation is proposed for constructing analytical description and continuation of terrain topography and potential fields. The modern digital elevation models are, most frequently, regular grids of cells of a given size or irregular triangular grids. Analytical topography models are another type of representation of the terrestrial or planetary surface data [1]. In contrast to digital models with a piecewise continuous dependence of elevation of the observation point on its projection coordinates, analytical models imply a more complex relationship between the elevation of the observation point above the surface and the geographical coordinates of the point. This lends the possibility to study structural features of the Earth's surface, smooth the relief data for different-scale mapping and also analytically continue the fields under investigation [2]. The approximation accuracy and degree of detail in the description of the terrain features are very important in this research. This paper addresses the results of the mathematical experiment using optical satellite data for a test region with urban elements and combining various continental landforms (hill and mountain terrain, a plain, ravines, and river mouth).

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Non-isothermal problem of fluid filtration in a poroelastic medium

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The process of nonisothermal filtration of a viscous fluid in a deformable porous medium is considered. The mathematical model is based on the equations of conservation of mass for liquid and solid phases, Darcy's law, rheological relation, the law of conservation of balance of forces and the equation for temperature [1, 2]. The viscosity of the porous skeleton is a function of temperature. In the isothermal case, the problem was investigated in [2–4]. This paper investigates the issues of justifying the model.

This work was completed within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation on the topic "Modern methods of hydrodynamics for problems of nature management, industrial systems and polar mechanics" (project FZMW-2020-0008).

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Soil moisture analysis for the multilayer soil scheme of the global atmospheric model SLAV

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The study presents a new soil analysis system for the SLAV global atmospheric model, based on a simplified point-wise Extended Kalman filter (SEKF). This analysis system was developed within the framework of the offline version of the surface model ISBA and the multilayer soil scheme of the INM RAS for the initialization of the soil fields in the numerical weather forecast model. This system is compared with the land assimilation system that uses a full atmospheric model to compute Jacobians of the observation operators in finite differences. By comparing the Jacobians of both analysis schemes, it was shown that the assumption of the linearity of these operators is better fulfilled in the offline version. Another advantage of the offline approach is the reduction in computation time, which makes the SEKF method compatible with the operational requirements.

The elements of the Jacobi matrix of the observation operator for two soil layers and the spatial structure of the analysis increments are presented. The interval from June to August 2014 was taken as the estimation period. Comprehensive data assessments are presented regarding the screen-level temperature and relative humidity observations, irregular observations of soil temperature and atmosphere. It was shown that using the SEKF improves forecast quality of the SLAV model.

This work was partially (the part concerning long-range forecasts) supported by the Russian Science Foundation (grant 21-17-00254).

New versions of models of hydrodynamics and distribution of impurities in Lake Baikal

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New versions of the implementation of large-scale models of hydrothermodynamics and the distribution of impurities in Lake Baikal are presented. One of the main goals was to improve the spatial resolution and, consequently, effective implementation on parallel computers. In the framework of the variational approach, the initial object of the numerical implementation of the models is the integral identity, in which all equations with boundary and initial conditions participate. Further, based on this identity, using the ideas of the splitting method for physical processes and for spatial variables, finite-difference approximations are constructed. The most time-consuming are the splitting stages, when it is necessary to solve two-dimensional problems for the level surface and three-dimensional problems for pressure fields. Finally, iterative methods with incomplete factorization are applied to solve systems of linear algebraic equations. The OpenMP standard is used to build parallel versions. The results of comparative experiments on the efficiency of implementation and examples of solving continuation problems related to the modeling of large-scale hydrodynamic processes and the propagation of impurities in the lake are given.

The work was carried out within the framework of the State Task of the ICMMG SB RAS code 0251-2021-0003 in terms of the development of basic models of the lake and with the financial support of the Russian Foundation for Basic Research (project code 20-01-00560) in solving the problems of continuation.

Meteorological effects of forest canopy under the conditions of steep orography

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It is often difficult to perform observations within areas covered by various kinds of vegetation, especially under conditions of steep underlying surface. The lack of data can often be compensated by using an appropriate mathematical model to describe the effects of canopy on the structure of the atmospheric boundary layer. Specifically, in this study a simulation is carried out with a numerical mathematical model of a compressible atmosphere based on finite elements [1, 2] to estimate the effects of some parameterization schemes of forest canopy on distributions of meteorological variables in a domain covered by tall forests over a steep terrain.

The simulation results appropriately reproduce well-known meteorological phenomena in forest areas, for example, stable thermal stratification near the surface during the day, neutral or slightly unstable state at night and, in general, a reduced wind speed in the forest cover.

This work was supported by ICMMG SB RAS under state contract 0251-2021-0003 (the numerical simulation) and the Russian Foundation for Basic Research under grant 17-01-00137 (the formulation and development of the numerical algorithms).

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Mathematical modeling of space-time distributions of emissions from local anthropogenic sources and emission estimates

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The paper presents new effective mathematical methods for estimating emissions of local anthropogenic sources, using high-resolution images obtained from a satellite of the Resurs-P series [1] and methods of asymptotic analysis used to solve inverse problems of reconstructing model parameters. The work is aimed to improve the input data for regional chemical transport models such as SILAM [2], METI-LIS [3], and increasing the efficiency of their use, namely, obtaining an adequate forecast of the state of atmosphere in order to prevent extreme situations associated with deteriorating air quality in regions with a high degree of the anthropogenic pollution.

This work was financially supported by the Russian Foundation for Basic Research (project code 18-29-10080).

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Emergence of optimal disturbances in stratified turbulent shear flow under the stochastic forcing

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Large-scale inclined organized structures in stably stratified turbulent shear flows were revealed in numerical simulations and indirectly confirmed by field measurements in the stable atmospheric boundary layer [1-2]. Spatial scales and forms of these structures coincide with those of optimal disturbances of the simplified linear model [3]. In this talk we clarify the relation between the organized structures and the optimal disturbances, providing the analysis of time series of turbulent fields obtained by the RANS model with eddy viscosity/diffusivity and stochastic forcing generating the small-scale turbulence.

The work was supported by the RSF (grant No. 17-71-20149, numerical experiments with optimal disturbances) and the RFBR (grant No. 20-05-00776, development of DNS and RANS models).

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Hydroelastic waves in a frozen channel with nonuniform thickness of ice

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Hydroelastic waves propagating along a channel covered with ice are considered. The channel has a rectangular cross section. The fluid in the channel is inviscid, incompressible and is covered with ice. The ice is modeled as a thin elastic plate with nonuniform thickness. The ice thickness changes linearly, symmetrically relative to the center of the channel, with a minimum value in the center and a maximum value on the walls of the channel. A similar problem in the case of constant thickness of the ice is studied in [1] and in the case of free edges of the ice cover in [2]. The solution is sought in the form of periodic waves propagating along the channel. The problem is reduced to the problem of the wave profiles across the channel. The solution of the last problem is obtained in the form of a series of the vibration modes of an elastic beam with nonuniform thickness [3]. These modes are a combination of Bessel's functions. It is shown that with the decrease in the change in the ice thickness, the vibration modes approach the normal modes of an elastic beam with a constant thickness. The behavior of the hydroelastic waves depending on the parameter describing the change in the ice thickness is studied.

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Section 5

SUPERCOMPUTER COMPUTATIONS AND PROGRAMMING

Numerical simulation of aerodynamic properties of split elements of space-rocket systems in LOGOS software package

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The work describes simulation results of the aerodynamic properties of split elements of the space-rocket systems in LOGOS software package [1]: the review of the advanced methods for aerodynamic properties has been carried out, the advantages of the computer simulation when solving such problems were demonstrated, verification and validation computations of the simulation problems for the split elements were performed, the produced results were compared with the reference data from available publications [2-4]. The analysis of the results confirmed the applicability of the LOGOS software package for computing aerodynamic properties of the split elements.

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BEREN3D: parallel code for particle in cell simulation colliding laser wakefield

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This paper presents a 3D3V PIC code for simulating collisions of laser pulses. The "BEREN3D" code is based on a kinetic model using Monte Carlo methods to simulate field ionization processes. The possibility of both representing laser pulses in the form of a virtual ponderomotive force and a direct solution of Maxwell's equations is supported. Using the problem of generating THz electromagnetic radiation by colliding laser wakefield as an example, the main capabilities of the code and its scalability are shown.

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Numerical modelling of open magnetic trap using parallel computers

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We consider two-dimensional problem of beam-plasma evolution in open magnetic trap. The result of the high current ion beam injection into the central region of the trap and its interaction with the magnetic field and the background plasma of the trap may lead to the plasma confinement [1]. The lack of the physical experiments compels using of numerical modelling, based on the problem-oriented parallel algorithms. We present the complex work on the model, the parallel algorithms and the simulation results for the 2D3V case in cylindrical coordinates.

The work was performed within the framework of the state task of ICM&MG SB RAS supported by the Foundation 0251-2021-0005.

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Developing a direct sparse solver for the Elbrus processors

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In software development, solutions working well for x86 processors are not necessarily good for another architecture. In out talk, we tell about issues that arose during developing a parallel direct solver for servers equipped with the Elbrus processors and what we did to resolve the issues. Although the obtained results are not final, the story about achieving the performance goals is instructive.

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In-memory data grid-based analysis of multi-energy system vulnerability

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The vulnerability assessment of multi-energy systems (MES) [1] is based on modeling their functioning under disturbances of various classes [2]. A MES multi-period model can be constructed by combining the models of particular energy systems using the system interdependencies. Disturbances are described as scenarios of changes of the structural and functional parts of the system models. It should be noted that scenarios of natural disasters tend to be formulated after careful meteorological data series analysis [3].

The MES vulnerability analysis at different levels of the territorial hierarchy is implemented in the form of separate scientific application packages that reflect the peculiarities of energy modeling at these levels. A common feature of these packages is the use of the in-memory data grid technology to process the disturbance consequences data [4]. The article compares the performance of the Apache Ignite in-memory data grid for various configurations of a distributed computing environment in computational experiments related to the identification of critical elements. The determination of critical elements is a type of the MES vulnerability analysis [2].

Implementation of an approach to modeling MES under disturbances taking into account the analysis of meteorological data series is supported by the Russian Foundation of Basic Research and Government of Irkutsk Region, project No 20-47-380002.

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Application of various ice accretion simulation approaches in the LOGOS software package

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The software package LOGOS [1–3] implements various techniques, including algorithms to model ice accretion on aircraft. This paper presents ice accretion simulation approaches and methods implemented in the LOGOS-Aero module of the LOGOS software package. Performance of LOGOS software components employing Lagrangian and Eulerian multi-phase flow models is demonstrated by test simulations of some NACA problems [4] intended for verification of the Lewice software package.

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Comparison of MKL matrix multiplication routines for one practical example

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Nowadays, math libraries (MKL [3] and Netlib BLAS [1]) are used to get the best performance of application. Extensive libraries' functionality often allows applied program to be implemented via various library procedures that have different levels of optimization. As a result decision about which routine should be used is a non-trivial task. A roof-line model [2] can help to identify some weak points of the software and prepare required experiments that identify the optimal library procedure. Given one specific practical example, it was shown that MKL BLAS gemm routine preferable over the similar MKL BLAS gemv procedure for the target set of the input data.

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LOGOS software package. Heat-transfer problem solving method with the account for ablation process

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An approach to simulate 3D heat-transfer problem with the account for the surface ablation process is realized in the *LOGOS Thermal Analysis* product [1]. The urgency of the work comes from the need for the adequate thickness definition of the low-conductivity coating of the flying vehicle during its operation.

Stefan exterior problem is solved for the computation of the boundary nodes displacement in the grid model. Grid internal nodes motion is computed using an elastic smoothing method. Quality preservation of the grid model during the computation is the application condition for the approach. Three cell quality criteria are considered, as well as additional possibilities to preserve grid topology.

A step-by-step computational algorithm is proposed using the example of the heat-transfer problem solution with the account for the design shape changing; it includes the computation until the stopping criterion is met, remeshing and proceeding with the computation.

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Some approaches to the creation of supercomputer technologies for solving compute-intensive problem

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The issues of using supercomputer technologies developed by the authors of the article to solve compute-intensive problems are discussed. The developed technology of creating algorithmic and software for supercomputers contains three related stages: co-design, by which we understand the adaptation of the problem statement, the mathematical method, the computational algorithm to the parallel architecture of the supercomputer at all stages of the problem solution; study of the scalability of computational algorithms for the most promising supercomputers based on simulation modeling; evaluation of the energy efficiency of algorithms for various implementations on a given supercomputer architecture [1]. It is proposed to further develop the proposed approach with the use of intellectual support for solving computationally complex problems using the ontology of computational methods and algorithms for solving the problem, the ontology of computational heterogeneous architectures and decision rules [2]. For clarity, illustrations are presented that schematically display the various components of the process of solving a geophysical problem, from stating to implementation on a supercomputer, and also how those are interconnected [3]. An example of field observation processing for one of the areas of Western Siberia using the developed system is presented [4].

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Thermal efficiency and computing productivity metrics for data center operations

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Data Centers (DCs) provide scalable on-demand computing and networking services to a growing number of businesses, government, health organizations, and end-users. Naturally, DCs' power demand for cooling and IT equipment has increased over the last few years [1]. However, some energy utilized in DCs is wasted for both inefficient cooling and applications that do not run properly on computing clusters [2]. We present a framework for the investigation of (a) hidden thermal pitfalls using thermal metrics [3] and guidelines [4] as well as machine learning for assessment of thermal factors affecting individual servers [5] and (b) energy waste that is caused by ineffective computations and can be translated into carbon waste evaluation with the help of a proposed metric [6]. The framework has been tested on job scheduling reports and (a) thermal meters of CRESCO4 and CRESCO6 clusters in ENEA Portici DC. The work results in a set of recommendations on how the productivity assessment could drive a new power and thermal efficiency management strategy.

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Simulations of viscous incompressible fluid flows on grids with unmatched interfaces in the LOGOS software package

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At present, numerical simulations of industry-specific hydrodynamic and aerodynamic problems are based on solving three-dimensional Navier-Stokes equations on arbitrary unstructured grids [1, 2]. Dividing complex initial geometries into simpler fragments makes it easier to construct grid models and yields higher-quality grids. Such grid models are usually composed of unmatched grid fragments. CFD simulations on this kind of grids require special unmatched grid interfaces to be developed.

This paper describes a numerical method, which considers specific aspects of solving the Navier-Stokes equations in viscous incompressible flow simulations in the vicinity of interfaces between unmatched arbitrary unstructured grid fragments. The numerical method presented in this paper is implemented based on the Russian LOGOC software package [3]. Performance of this method is demonstrated by three-dimensional simulations of a turbulent flow in a circular diffuser.

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Iterative refinement approach for improving convergence of the mixed precision linear solvers

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The use of the lower precision floating point calculations is an evident way to speed up the solution of systems of linear algebraic equations. The widely used approach for iterative methods assumes the use of the mixed precision calculations when the preconditioner is performed with the lower precision. In practice it can provide 10-15 % calculations speedup. The more attractive way is the use of the lower precision for the whole solver, which can reduce the calculation time by a factor of 1.6-1.8, but may affect the convergence rate.

The current talk discusses an alternative variant of introducing the mixed precision calculations, which provides the double precision solution accuracy, but allows to perform most of the calculations in the single precision [1]. The algorithm is based on the iterative refinement procedure and combines two nested iterative methods: the simple outer method (e.g., Jacobi) performed in double precision and the more robust method (e.g., BiCGStab + AMG preconditioner) performed in single precision. It is shown that the proper choice of the inner solver stopping criteria is the key aspect of achieving the appropriate convergence rate, and the overall convergence can be equal to the basic double precision method configuration, providing the decrease in the calculation time by a factor of 1.6-1.7.

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Numerical simulation of propellers rotation under cavitation conditions

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Cavitation influences the design of propellers considerably, so the research on their operation under cavitation conditions is critical [1]. The work describes numerical simulation of cavitation processes when a model VP1304 propeller is rotating. Volume of Fluid (VOF) method is used for numerical simulation, which is realized in LOGOS software package. It allows numerical simulation of two-phase problems with free surface [2]. Cavitation is accounted for when the method is supplemented with the account for the phase-to-phase mass exchange; cavitation models are used to compute its rates [3, 4]. The work shows a physical-mathematical model, briefly describes a numerical method used, as well as cavitation models; the models are compared afterwards. Numerical simulation of the rotating propellers is demonstrated using the problems of flow-past of the model VP1304 propeller under the conditions of developed cavitation.

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Research on the accuracy of numerical simulation of acoustic perturbations in a fluid basing on Navier – Stokes equations

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The work is devoted to the necessary space and time resolution when simulating the propagation of acoustic perturbations in a fluid, analysis of the accuracy of the solution as a function of the parameters of the iteration procedure and numerical discretization of the equations. A popular SIMPLE method [1] together with finite-volume discretization of the equations on the basis of the home software package LOGOS [2] is used as a numerical method. A problem of perturbations propagation from a harmonic-oscillations source in a fluid is described for the assessment [3]. Space and time resolution necessary to provide acceptable accuracy of the solution is estimated. The produced estimations are validated using the problem of propagation of harmonic waves from a point source in a fluid.

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Algorithms and implementation of active knowledge in LuNA system

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Active knowledge development problems in the domain of numerical simulations on supercomputers is discussed. Basic components of the LuNA system, which supports active knowledge, are concerned. Peculiarities and limitations of the system, as well as its current condition and abilities are discussed. Applications of LuNA for a series of tests are analyzed.

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Execution trace based optimization of fragmented programs performance

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Profiling and tracing of parallel programs execution is a source of information on quantitative characteristics of efficiency, such as computing nodes load over time, communication subsystem load, memory consumption, etc. It is essential, that the characteristics can be measured with connection to source code locations of the program executed. This information can often be used to significantly improve performance of parallel programs. In particular it is important for systems and tools for automatic parallel programs construction, since a program can be reconstructed according to profiling and trace information automatically. In the work we propose facilities for LuNA system, capable of optimizing fragmented programs efficiency based on trace information. Experimental results are presented.

Research on the numerical method and grid parameters as they influence the simulation accuracy for the floating bodies

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The work studies the grid parameters, the time step size, the order of approximation by space and time as they influence the accuracy of the problem solution with damped free vibrations of the cylinder on the water surface [1, 2]. The numerical simulation method of the floating bodies is based on the solution of a system of Navier-Stokes equations together with VOF method [3, 4]. The motion of the body is accounted for by the deformation of the computational grid [5]. CFS model is used to account for the surface tension forces [6]. The method is realized on the basis of the home LOGOS software package [7].

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Optimizations of computations on manycore processors and accelerators for elastic waves simulation

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The solution of compute-intensive problems of mathematical modeling requires the development of parallel programs. The choice of various mathematical methods, algorithms and computational architectures for solving such problems, as well as the development of high-performance codes is a complex task. In solving it, the researcher can be helped by the developed system of intellectual support based on the ontological approach [1]. In this system, it is necessary to lay the knowledge about the impact of different approaches to organizing computations and working with memory on the final performance for different types of codes.

In this work, finite-difference 3D modeling of the propagation of elastic waves is considered [2]. Using the example of solving this problem founded wide application, the influence of various optimization strategies for parallel programs for various manycore architectures is investigated. Specific optimizations for different types of architectures are considered, including improving the cache memory usage, balancing the computational load, vectorization and accelerator memory usage.

Based on the research carried out, the software has been developed for various computing systems with high rates of strong and weak scalability.

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Solution approaches to numerical gas-dynamic problems with changing boundaries in LOGOS software package

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Approaches in simulation of the gas dynamic processes are of both scientific and practical interest. Transient modes in operation of engineering equipment that come from the motion of the element constituents of the unit cause growing attention in the engineering practice. Numerical simulation of this class of problems in LOGOS engineering software package [1] is available using two approaches different in the ideology: computing method on the deforming grids preserving links topology [2] and computing technology on overlapping grids [3].

The choice of a particular approach comes from the immediate task setting. Nevertheless, there are some problems where it is not possible to prefer either of the alternatives because it is impossible to describe completely the physical processes using one approach only.

The work reviews the realized physical-mathematical models for the problems of numerical gas dynamics with moving structural components. It provides the examples of characteristic problems in aviation industry that show operability of the realized models of the LOGOS software package.

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Using Didal distributed data library for implementation of parallel fragmented programs for distributed memory supercomputers

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Distributed data library Didal [1] is designed to facilitate development of efficient parallel programs for distributed memory supercomputers. The aim of the library is to provide high-level distributed data structures coupled with different strategies for data partitioning, distribution and load balancing, to develop parallel programs with. The library approach allows to use all existing tools for parallel program development, debugging and profiling, as well as optimized C/C++ codes. One of defining features of Didal is its support of fragmented programming [2]. In fragmented programming a parallel program is represented as sets of data and computational pieces (fragments), number and sizes of fragments being static or dynamic parameters. Results of implementation of several parallel programs with Didal library and fragmented programming approach are presented. Details of parallel fragmented programs implementations, as well as key aspects of Didal's design, are provided. The programs' performance is measured and compared with other parallel programming models.

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Multi-grid starting initialization as a way to achieve higher convergence rates in industry-specific hypersonic aerodynamic simulations

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The paper presents a multilevel geometric initialization-based algorithm [1–2] to speed up external aerodynamics simulations. This method provides higher convergence rates and stability of numerical results in the flow structure formation and settling phase. The concept of the method is to generate a series of coarse grids [3] based on a parent grid to find solutions on each of the grids and to subsequently interpolate them to a finer grid. The solution calculated on the finest of the grids constructed in series is then interpolated to the parent grid, thus representing the starting initialization on it. The algorithm can be used on unstructured grids with an arbitrary cell shape. As a cell combination criterion to form new control volumes in the successive grid coarsening, the algorithm uses a relationship calculated from face areas and cell volumes. The cell combination process is based on the analysis of the weighted graph. Solution stability and convergence analysis was performed by test simulations of a supersonic flow in a channel with a wedge [4] and a hypersonic flow over a cone [5]. As a result, the geometric multi-level initialization algorithm shortened the runtime by 23 percent.

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Implementation of the imitation method of the propeller rotation to simulate marine propellers

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Model implementation of a virtual propeller for the numerical simulation of the ship-related dynamic problems on the water surface is described in LOGOS software package [1]. The model is based on the imitation of the marine propellers operation of a ship with the help of a given source of bulk forces, which is set in the area of the 3D location of the propeller [2, 3]. As rotating solid blades are actually absent in the rated operating conditions, the screw stop, the moment and the efficiency of the propeller as a preliminary specified function of the pitch ratio are introduced to account for the geometric rotating properties of the immediate propeller. The realized approach has been tested and implemented to solve industrial problems of ship cruising using moving grids.

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Verification of the LOGOS software package for multi-material flow simulations

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In this paper, we consider convective flow approximations, which are used to simulate incompressible low-velocity multi-material flows on unstructured grids. The simulation technique is based on the SIMPLE algorithm [1], which serves for numerical simulations of incompressible and low-compressible flows. Using the problem of a propane jet injected into an air flow as an example, we explore effects of convective flow discretization schemes, including the first-order UD, higher-order LUD (Linear Upwind Differences), and second-order hybrid CD+0.1UD schemes [2, 3]. The calculations were performed on different types of grids, including block-structured and arbitrary unstructured tetrahedral and polyhedral grids. Data reported in this paper demonstrate that LOGOS delivers acceptable results for multi-material flow simulations on unstructured grids with a characteristic grid size of 4 and 6 times smaller [2, 4] than the grid size of block-structured grids. Based on the results of the calculations, recommendations are given for the optimal characteristic grid size in the region of mixing streams to ensure acceptable results on the chosen grids of different types.

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Section 6

INVERSE PROBLEMS

On the stability of determining the position and shape of local acoustic inhomogeneities when solving an inverse problem using the BaL algorithm

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In [1], the so-called BAL algorithm is proposed for stable solvng of the 3D scalar inverse problem of acoustic sounding of an inhomogeneous medium. The data for the solution is the complex amplitude of the wave field measured in a layer outside the region of inhomogeneities. The inverse problem is reduced to solving 1D Fredholm integral equations of the first kind, to the subsequent calculation of the complex amplitude in the region of inhomogeneity, and then to finding the required sound velocity field in this region. The algorithm allows solving the 3D inverse problem on a PC of average performance for sufficiently fine 3D grids in tens of seconds. Now we present the numerical study of the stability of determining the position and shape of local inhomogeneities using the BAL algorithm in the case of many such inclusions with different geometries.

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Algorithm for inversion of resistivity logging-while-drilling data in 2D pixel-based model

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Multi-frequency and multi-component extra-deep azimuthal resistivity measurements with depth of investigation a few tens of meters provide advanced possibilities for mapping of complex reservoir structures. Inversion of the induction measurements set becomes an important technical problem. We present a regularized Levenberg – Marquardt algorithm for inversion of resistivity measurements in a 2D environment model with pixel-based resistivity distribution. The cornerstone of the approach is an efficient parallel algorithm for computation of resistivity tool signals and its derivatives with respect to the pixel conductivities using volume integral equation method. Numerical tests of the suggested approach demonstrate its feasibility for near real time inversion.

Properties of solenoidal vector and 2-tensor fields given in domains with conformal Riemannian metric

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Helmholtz decomposition of a vector field on potential and solenoidal parts is well known [1]. The decomposition is much more natural from physical and geometric point of view then representations through the components over coordinate systems in Euclidean space. A profound generalization of Helmholtz decomposition to a case of the symmetric tensor fields, given in a compact Riemannian manifold, was suggested in [2]. The structure, representation through potentials and detailed decomposition for 2D and 3D symmetric m-tensor fields in the case of the Euclidean metric was established in [3, 4]. In the case of the Riemannian metric similar results are known partially only for vector fields. We investigate here the properties of the solenoidal vector and 2-tensor fields given in the Riemannian domain with conformal metric and established the connections between the fields and the metric. The solenoidal fields of the general type and their partial case of toroidal fields is considered.

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Recovery of a vector field in the cylinder by 2D ray transforms and NMR-data

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We consider the problem of recovery of a three-dimensional vector field in the cylinder [1]. The data for the problem are two-dimensional integral ray transforms and NMR-data [2]. We explain the features of this problem in the cases of different vector fields and present algorithms for solving. Simulation showed good results.

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On one linear inverse problem for a mixed type equation of the first kind in a undo bounded prismatic domain

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In the process of studying non-local problems, a close relationship of problems with non-local boundary conditions and inverse problems was revealed. To date, the inverse problems for classical equations such as parabolic, elliptic and hyperbolic types have been studied quite well. [1, 2]. For equations of mixed type, both the first and the second kind in bounded domains, it was studied in papers. [3, 4].

Inverse problems for equations of mixed type in unbounded domains are much less studied. We will try to partially fill this gap within the framework of this work.

In this paper, to study the unique solvability of inverse problems for equations of mixed type in an unbounded prismatic domain, we propose a method based on reducing the inverse problem to direct problems for infinite loaded systems of integro-differential equations of mixed type in an unbounded prismatic domain.

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Inverse problem determinating location domain-source of diffusion proccess

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Consider diffusion process from source to environmental for system four nested domains (3D cubes). 3D numerical realization balayage process H. Poincare depicts iterative process density diffusion from source Ω to source environmental (for grid: from 1 point source to 6 surrounding nodes). If we have 2D domains of sweeping densities with constant mean ("Plateu") on the boundaries of the 3D domain V (may be space-time domain) then we interpret the source Ω, as the domain in the center.

Some computing experiments for the interior of domain, the overgrown interior of domain, the annular domain are considered.

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Method of differential constraints and its application to the solution of inverse problems in the mechanics of composites

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Mathematical problems of solving inverse problems of mechanics of composite structures are formulated. The problems of strength calculation and optimal design of anisogrid structures and composite overwrapped pressure vessels are investigated.

The solutions of the optimization problem have been recieved and verified by solving the direct problems with obtained design parameters using the classical and improved shell theories [1–3].

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Highly accurate algorithms for solving scattering problems for the Zakharov – Shabat equations

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We proposed a new numerical method for solving the inverse scattering problem based on solving the Gel'fand – Levitan – Marchenko system of equations. The existence and uniqueness of the solution of the GLM equations is proved. To approximate the integrals, quadrature formulas are used up to the fourth order of accuracy. The resulting system of equations is reduced to a system of equations only with unknowns necessary to determine the required potential. The algorithm allows to determine the potential independently for any point x from a given interval $0 \le x \le L$, which allows parallelization.

Estimation of ocean depth from sensing by impulse source and affected multiple reflection of radiation from a surface

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The report deals with the issues relating to mathematical modeling of the processes of pulse sounding in the ocean for the problem of the seabed relief restoration. In previous articles [1, 2] solutions of the direct and inverse problems for the nonstationary radiation transfer equation were obtained in the single-scattering approximation for bathymetry problems. In this paper, the main attention was given to the calculation of the pulsed radiation in the case of multiple reflection from the Lambertian surface and to the analysis of the influence of multiple bottom scattering on the solution of the inverse problem. The complexity of calculations was caused by the type of source and receiver, as well as the specifics of their location in space due to the physical formulation of the bathymetry problem.

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Inverse kinetic problem in complex non-isothermal processes

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Development of a kinetic model in a chemical reaction requires solving the inverse problem of restoring the values of kinetic parameters: the rate constants of the stages and the activation energy. The inverse problem is defined as the calculation of the kinetic parameters, the calculated concentrations from which allow describing the experimental data.

In this paper, a non-isothermal chemical process is considered. Therefore, the residual functional in inverse kinetic problem includes experimental data component concentrations and changes in temperature [1]. The inverse kinetic problem is a one-criterion optimization problem: variable parameters – vector of stage rate constants k, physicochemical restrictions on variable parameters - area D_k; optimality criteria or residual functional $Z(k)$: Z_Y, Z_T. Then it is necessary to determine $\min_{\mathbf{k}\in D_{\mathbf{k}}} Z(\mathbf{k}) = Z(\mathbf{k}^*) = Z^*$.

The residual functional Z:

$$Z = Z_Y + Z_T \rightarrow \min;\ Z_Y = \sum_{i=1}^{I}\sum_{l=1}^{L}\frac{\left|y_{il}^e - y_{il}^c\right|}{y_{il}^e};\ \ Z_T = \sum_{i=1}^{I}\sum_{l=1}^{L}\frac{\left|T_{il}^e - T_{il}^c\right|}{T_{il}^e}.$$

Here Z_Y and Z_T – concentration and temperature components of the residual functional; y_{il}^e and y_{il}^c, T_{il}^e and T_{il}^c – experimental and calculated values of component concentrations and temperatures, L – number of time points in observed substances during the reaction, I – number of observed substances.

In the mathematical model, the temperature change is taken into account according to the values of the thermodynamic characteristics of the reaction components [2].

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Application of kernel regression in nonlinear adaptation algorithms as applied to multidimensional objects

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The application of the time series smoothing algorithm based on the construction of nuclear regression [1] in the problems of nonlinear synthesis of control for continuous and discrete multidimensional objects is considered.

The illustrative examples of application of the proposed algorithm (biochemistry, immunology, economics, and other fields of knowledge) are provided along with their statistical results of numerical simulation.

The results obtained would be useful in designing a smart control system and for real-time decision making support as it concerns the problems of stochastic control over a wide range of poorly formalized objects from different applied areas.

There are grounds for believing that the synthetic use of two popular nonparametric forecasting algorithms will lead to a more efficient forecasting algorithm, at least for solving a certain class of control problems [2, 3].

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3D inverse problems of magnetic susceptibility restoration from experimental data

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Retrieval of magnetic parameters using magnetic tensor gradient measurements receives attention in recent years. Traditional magnetic inversion is based on the total magnetic intensity data and solving the corresponding mathematical physical model. In recent years, with the development of the advanced technology, acquisition of the full tensor gradient data becomes available. In work [1], the problem of restoring magnetization parameters has been solved. In this problem three scalar functions(components of the magnetization vector) were recovered using data by five scalar functions(independent components of the magnetic tensor). In our work [2] we consider the problem of magnetic susceptibility restoration using magnetic tensor gradient measurements. In this work we have recovered one scalar function(magnetic susceptibility) using data by five scalar functions(components of the magnetic tensor). As we are dealing with the physically overdetermined problem we expect to receive better results than if the problem was just physically determined. At the current moment, we have provided testing calculations using simulated data. Now we are testing our approach on real data.

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Determination of the bottom scattering coefficient discontinuity lines in multibeam ocean sounding

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In this report, the problems of acoustic sounding of the sea bottom with using side-scan multibeam sonar are studied. Within the model based on radiative transfer equation and diffuse reflection conditions at the boundary, the problem of determining the coefficient of bottom scattering from the data of a multi-beam receiving antenna [1, 2]. Unlike previous works of the authors, the problem of determining only the singular support of the reflection coefficient is formulated, and not the reflection coefficient itself. Numerical method for solving the inverse problem is developed. Results shows that it is be able to use in highly scattering environments. Analysis of the quality of the bottom scattering coefficient discontinuity lines depending on scattering level in the ocean, range and number of sounding angles is done.

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Identification of agent-based mathematical model of COVID-19 propagation in Russian Federation regions, UK and USA

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The agent-based mathematical model of COVID-19 propagation in fixed region is characterized by stochastic nature of epidemiological process, demographic features of the region and epidemiological parameters (reproduction number, initial asymptomatic infectious individuals, test rate, etc.). The sensitivity-based identifiability analysis based on the Bayesian approach is carried out to three types of data: daily confirmed, critical and death cases of COVID-19 [1-2]. As a result, the set of more sensitivity parameters is investigated. The scenarios of COVID-19 propagation on Siberia [3], UK and USA are modelled and discussed.

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Non-destructive testing of the state of the insulating coating of the main pipeline according to the UAV-magnetometry data

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Monitoring the state of trunk pipelines is an urgent practically important task for trouble-free operation. Determination of the transient resistance at the "pipe/soil" boundary according to magnetometry data using unmanned aerial vehicles is the inverse problem of mathematical geophysics to determine the coefficient function of the boundary condition of the third kind.

The paper considers mathematical models of direct [1, 2] and inverse problems, algorithms for their solution based on the search for the extremal of the regularizing A.N. Tikhonov’s functional. The results of computational experiments are discussed.

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The Gerchberg-Papoulis method in non-scalar tomography problems with limited data

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The problem of recovery a scalar field by limited data [1] has some difficulties. One of the methods for solving this problem is the Gerchberg-Papoulis iterative method [2]. Problem with limited data may also be considered for non-scalar fields. This report contains a generalizations of this method for the case of vector and 2-tensor fields. The results of numerical simulations are presented.

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Comparative analysis of the Gerchberg-Papoulis method in the problems of scalar and vector tomography

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The paper discusses the methods of solving the inverse problems of a few-views and limited angle data of two-dimensional tomography using iterative procedures in Fourier space. Partial absence of angular data can be approximately compensated by extrapolation in the Gerchberg-Papoulis iterative method [1]. In particular, these algorithms should be complemented by a priori information and regularization procedures [2–3]. The computational experiment compare reconstruction errors of mathematical models of scalar and vector problems.

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The problem of identification an unknown substance by the radiographic method

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The paper considers the problem of partial identification of the chemical composition of unknown medium by the method of multiple transillumination of this medium with X-ray radiation. Sample of unknown substance is assumed to be homogeneous in chemical composition, and the photon flux, collimated both in direction and in energy. A mathematical model is formulated for the identification problem. The proposed approach to solving the problem is based on the method of singular value decomposition of a matrix [1, 2]. At the first stage of solving the problem is reduced to finding singular numbers and singular vectors for the series systems of algebraic equations linear with respect to products of unknown quantities. Then, based on the received data, a special function is built, called an indicator of the distinguishability of substances, which enables the sufficient conditions for the distinguishability of various substances [3]. Based on tabular data [4], calculations were made for a number of specific groups of chemical elements.

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Optimization of solution of inverse problem for stochastic differential equation

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The problem of drift and volatility parameters identification in stochastic differential equations (SDEs) using additional measurement of single trajectory of stochastic process is investigated. The classical way for solving such a problem is to reduce it to a Fokker-Planck equation [1] and minimize a data fidelity functional, that is unstable. For higher-dimensional systems of SDEs, the numerical solution of the Fokker-Planck equations becomes infeasible.

We propose regularized Landweber iteration algorithm [2] with fidelity functional based on mathematical expectations, for easier parallelization of solution. Parameters are implemented in solution-dependent form, for implicit time-dependency, with Fourier series for reducing number of variables. In addition to that adjoint problem is deterministic. We conduct this process on synthetic data for validation of an algorithm and regularization for variety of input data with Tikhonov regularization.

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Numerical solution of inverse problem for acoustic equation, based on a modified version of GLK-approach

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In this talk we consider the coefficient inverse problems for the acoustic equation in 1D and 2D cases [1–3]. We propose the new version of the Gelfand – Levitan – Krein approach to reduce the non-linear inverse problem to a set of linear integral equations. We study the possibility to use the method in case of general time form of the sounding wave. In 2D case we also consider the modification of the method that uses the data, obtained by the areal data collection system. The results of numerical experiments are presented.

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Mean field games for modeling of disease propagation

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The mean field game (MFG) that describes the control of a population with a large number of interacting agents [1] is numerically investigated. MFG is based on Kolmogorov (Fokker – Planck) equations that characterize the distributions of agents in four groups (susceptible, infected; recovered and cross-immune people) and system of Hamilton-Jacobi-Bellman equations that describes the optimal strategy of isolation: if a person is not infected and the number of non-isolating people in population is arising, person's profit decreases to comply with the restrictions. Otherwise, if a person is infected, then he is inclined to comply with restrictions. The optimality conditions are derived. The scenarios of COVID-19 propagation in Siberia depend on restrictions [2] are modelled and discussed.

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On the singular value decomposition of the ray transforms operators acting on 2D tensor fields

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We consider the problem of the 2D m-tensor tomography. Namely, it is necessary to reconstruct a 2D symmetric m-tensor field by values of its ray transforms. We propose to solve the problem with usage of the singular value decomposition method. The singular value decompositions of the ray transforms operators acting on vector and 2-tensor fields were constructed earlier [1, 2].

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On the singular value decomposition of the dynamic ray transforms operators acting on 2D tensor fields

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We consider the problems of the dynamic 2D vector and 2-tensor tomography. The initial data are values of the longitudinal and/or transverse and/or mixed dynamic ray transforms. An object motion is known and consist of rotation and shifting [1]. Properties of the dynamic ray transforms operators are investigated. The singular value decompositions of the operators with usage of the classic orthogonal polynomials are constructed [2, 3].

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Regularization methods for solving the continuation problem

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When conducting experiments for heat and mass transfer, the main studied values are the heat flux density and temperature. The most commonly used field and local methods that have high accuracy, in particular infrared thermography.

There are no direct methods for measuring the heat flux density at a distance. There is a need to estimate the flow density from temperature measurements.

A method for inverting a finite-difference scheme is developed and implemented, a gradient method for solving the inverse problem is implemented, and a gradient formula is obtained. A comparative analysis of the developed methods is carried out. The methods are tested on experimental data.

The work was carried out with the financial support of the Russian Foundation for Basic Research (project code 20-51-54004).

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Regularization of inclusions of differential equations solutions based on the kinematics of a vector field in problems of stability of a set of trajectories

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In the papers of specialists on stability problems, it is proposed to investigate stability problems for a set of trajectories of nonlinear dynamics under the influence of arbitrary perturbing influences [1]. In this report, to estimate the stability of the sets of solutions, the boundaries of the sets of solutions will be efficiently and accurately computed applying symbolic formulas for solutions of ordinary differential equations [2] and evaluating the parameters of the kinematics of the vector field. The parameters of the vector field kinematics perform regularization, which eliminates the excessive growth of the boundaries of the inclusions. The examples show the advantages of this approach to solving stability problems for a set of trajectories.

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Regularization of the global error estimation for numerical solutions of differential equations based on tracking approximate trajectories

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The main idea of the regularization of the global error estimate is that new variables or new relations are introduced that make it possible to reduce (or even eliminate) the influence of the Lyapunov instability on the bounds of the numerical solutions and to refine these estimates. Such a regularization was performed in several works of the author, for example, in [1]. In this report, it is proposed to consider the perturbed system as a modified model based on pseudo-trajectories (approximate) trajectories, the effect of numerical errors on the pseudo-trajectories, including round-off errors, leads to the actual study of the trajectory with some approximation. The report proposes to use pseudo-trajectories to consider the data space as a space of problems and to estimate the relationship between a defect, local and global errors of numerical solutions. Examples of numerical estimates of the global error are given.

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Kinetic modeling of propane pyrolysis: parameters identifiability and estimation

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One of heavy olefins upgrading processes is pyrolysis. As it is a complex process involving many chemical reactions, the mathematical model of pyrolysis process often has more kinetic parameters than can be estimated from the data. In this article, a kinetic model for propane pyrolysis processing is proposed. It is proved that the model is practically identifiable. Practical identifiability analysis is based on simulated model outputs and their sensitivities with respect to parameters [1, 2]. As a result of the analysis of identifiability, the least and most sensitive parameters to measurements were identified. The minimization problem was solved through the genetic algorithm method that is widely applied for stochastic global optimization. It has been demonstrated that kinetic model describes the experimental data of the observed substances of the reaction.

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Multiplicative control problems for semilinear reaction-diffusion-convection equation

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The interest in the study of boundary value and control problems for linear as well as for nonlinear models for mass and heat transfer does not fade over sufficiently long time (see [1, 2] and References in there). In this paper, we consider multiplicative control problems for the semilinear reaction-diffusion-convection equation. The coefficients in both the equation and the boundary condition of the model under consideration depend on the solution of the boundary value problem (see [2]). The diffusion coefficient plays a role of a multiplicative control. The solvability of a multiplicative control problem under consideration was proved in [2]. For concrete reaction and mass transfer coefficients we obtain optimality systems and based on their analysis we establish local stability estimates for optimal solutions.

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On the inverse boundary value problem solution for parabolic equation in a cylindrical coordinate system

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This work solves the problem the inner wall temperature determination of a hollow cylinder consisting of composite materials. The problem is reduced to an ordinary differential equation using the Fourier transform in time and the Fourier transform is found for the exact solution of the desired inverse boundary value problem.

The projection regularization method [1] is used to solve it. This method makes it possible to obtain a stable solution to the problem and to estimate the error of the approximate solution. Working with Bessel functions [2] complicates the technique of obtaining the error estimate. This problem is of known interest in connection with the theory of thermocouples and devices for measuring current.

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Direct method for solving the problem of identifying the coefficients of an elliptic equation

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A direct method for solving the inverse coefficient problem for an elliptic equation with piecewise constant coefficients is presented. The method allows much faster, in comparison with the implementation of iterative procedures for this problem, to restore the unknown coefficients of thermal conductivity. The values (measurements) of the solution at the break points of the coefficients are used as additional information.

A numerical study of the algorithm has shown its efficiency. For unperturbed additional information, piecewise constant coefficients are reconstructed exactly regardless of the number of parts that make up the object under study. An analysis of the sensitivity of the algorithm to the disturbance of additional information showed that for bodies consisting of a small number of parts, with a disturbance of up to 5 %, the result of restoring the coefficients can be considered satisfactory. With an increase in the number of breakpoints of the coefficients, the sensitivity to data perturbation increases.

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Numerical solution of the inverse problems of magnetic cloaking shell design

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In recent years, the inverse problems of designing devices serving to cloak material bodies from static magnetic fields have been actively studied. The first solutions obtained in this field have a number of disadvantages. The main one is the difficulty of technical implementation. To simplify this difficulty, firstly, the work assumes that the designed device consists of a finite number of concentric layers, each of which is filled with a homogeneous isotropic medium. Second, the inverse problems under consideration are reduced by the optimization method [1] to finite-dimensional extremum problems in which the role of controls is played by magnetic permeabilities of each layer. To find the required controls, a numerical algorithm developed on the particle swarm optimization method is used [2]. The obtained optimal solutions correspond to highly efficient and technically easily realizable devices in the considered class of inverse problems [3].

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On solution of the slice-by-slice three-dimensional vector and 2-tensor tomography problems by the approximate inverse method

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A numerical solution of the problems of recovering the solenoidal part of a three-dimensional vector and symmetric 2-tensor fields using the incomplete tomographic data are proposed. The initial data of the problems are values of the ray transforms for all straight lines, which are parallel to at least one of the planes from a finite set of planes [1]. We consider two sets of planes, the number of planes in which are: two and three for vector case; three and six for 2-tensor case. The recovery algorithms are based on the approximate inverse method [2, 3].

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An inverse problem for a system of nonlinear parabolic equations

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An inverse problem for a system of nonlinear parabolic equations is considered in the present paper. Namely, it is required to restore the initial condition by a given time-average value of the solution to the system of the nonlinear parabolic equations. An exact in the order error estimate of the optimal method for solving the inverse problem through the error estimate for the corresponding linear problem is obtained. A stable approximate solution to the unstable nonlinear problem under study is constructed by means of the projection regularization method which consists of using the representation of the approximate solution as a partial sum of the Fourier series and the auxiliary boundary conditions method. An exact in the order estimate for the error of the projection regularization method is obtained on one of the standard correctness classes. As a consequence, it is proved the optimality of the projection regularization method. As an example of a nonlinear system of parabolic equations, which has important practical applications, a spatially distributed model of blood coagulation is considered. Numerical examples are given to confirm the theoretical results.

This work was supported by Act 211 Government of the Russian Federation, contract № 02.A03.21.0011.

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Determination of the variable density of the rod from the natural frequencies of longitudinal vibrations

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Rods of various configurations are elements of many structures and machines. Therefore, the acoustic and vibration diagnostics of such parts has been widely developed [1-3]. The paper considers the problem of determining the variable density of the rod from the natural frequencies of longitudinal vibrations. It is assumed that the density changes along the axis and is described by a power function. This approach allows one to determine the law of density variation from a finite set of eigenvalues. The results of the study can find applications for finding hidden defects in steel and composite rods, which arise during the production process or due to corrosion.

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Method for improving the reconstruction quality in pulsed x-ray tomography

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Recently, successful development of short-pulse X-ray sources along with appearance of high timing resolution detectors give wider opportunities to construct new schemes of tomographic imaging [1]. The paper is devoted to a method of improving quality of imaging based on serial irradiation of medium with x-ray pulses of different durations. We investigate an inverse problem for non-stationary radiation transfer equation that consists of determining an attenuation coefficient. The time-integral intensity at the domain boundary is considered to be known. The vanishing rate of the scattered component was estimated with the probe pulse duration. The estimation is used to extrapolate the transfer equation solution and to construct an approximate method for medium imaging. Extrapolation methods are not unfrequently used to improve reconstruction quality of various imaging modalities. However, algorithms applied to resulting image or its spectrum are prevailing. Our approach differs from the previous methods in that we apply an extrapolation method to projection data with approximation function taking into account the nature and structural features of the measured signal. We carried out numerical experiments using a well-known digital phantom [2]. The results obtained show the effectiveness of the algorithm proposed to suppress a scattering effect in X-ray tomography.

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Tensor train optimization for the source problem of the partial differential equation using high performance computing

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The source problem for the diffusion-logistic model based on a nonlinear partial differential equation, which describes the process of information dissemination in social networks [1], is considered. The problem of recovering a source from additional data about process in fixed time points is reduced to the problem of minimizing the misfit function. The function is reduced to tensor form and minimization problem is formulate as a problem of searching the minimal element in considering tensor. The optimization problem is solved by a global method based on the expansion of the large dimension tensor in the tensor train format [2]. The program code is spread across 48 CPUs.

This work is supported by the Council for Grants of the President of the Russian Federation (project no. MK-4994.2021.1.1).

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Section 7

INFORMATIONAL AND COMPUTATIONAL SYSTEMS

Optimal lossless encoding of string and numeric data in arrays

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The problem of optimal coding of various types of data in information arrays is considered. Effective compression of such data leads not only to a decrease in their physical size, but also to increase the speed of query execution, as well as to a decrease of memory size used. The most common data types used in arrays are strings and numeric data. An encoding algorithm is proposed that allows efficiently compressing both types of data. The "bitmap" method [1, 2] is used to encode numeric data. We use the Ziv-Lempel compression method [3] to encode string data.

It is shown that the method allows one to increase the compression ratio and encoding and decoding rate compared to previously known methods.

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Integration of geophysical information resources

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The paper proposes an ontological approach to integration of information resources in geophysics. Ontology can form a framework of knowledge base, create a basis for describing the basic concepts of the subject area and serve as a basis for integrating databases containing factual knowledge necessary for effective work of researchers. This approach allows you to provide the user with a data source at a conceptual level and address the user query to several heterogeneous data sources.

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Automation of the process of updating personal accounts in the GIS Housing and Communal Services system

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The article describes the implementation of the process of automating the process of updating personal accounts in the GIS Housing and Utilities GIS system, the automation functions are formed and interaction with the SOAP API services of the GIS Housing and Utility Services is implemented.

Currently in Russia there is a comprehensive automation of the information resource in the housing sector. The following automation functions have been implemented: loading data from GIS Housing and Communal Services and linking these data to enterprise data; viewing and checking related data with the ability to manually edit the links; viewing and checking personal accounts and their data for the selected house or management campaign; sending selected personal accounts to the GIS Housing and Communal Services using the organization's data.

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Computing fringes of equal thickness via ray tracing

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Trends of modern photorealistic computer graphics (PhCG) are to visualize (to render) more and more detailed images of objects that are computer models of real objects. Fringes of equal thickness (FET) are classical optical phenomena that are investigated and explained in books on physical optics, e.g., [1]. A well-known FET are Newton’s rings. Existing renderers do not allow computing of interference patterns, and, consequently, FET. This problem requires: 1) more detailed physically based mathematical models of real objects then renderers use; b) the corresponding complication of the information associated with the ray. However, such improvements still do not allow the calculation of FET, since, as a rule, interfering mathematical rays have zero thickness and do not intersect on the picture plane, but in front of it or behind it, see [2]. In [3], it is proposed to use rays in the form of Gaussian beams and apply complex ray tracing. The authors calculated several interference patterns for too simple scenes, including Newton's rings. This solution is unacceptable for a PhCG that renders scenes from a huge number of elements.

This report is devoted to our solution based on the physically based assumption that the ray is the direction of energy transfer by a light wave. In contrast to [3], we use zero-thickness ray tracing. The rays potentially interfering on the picture plane are represented as spherical waves, and the calculation is performed for them. We describe our approach and demonstrate FET images calculated for scenes of the glass wedge type. We would like to note that for the first time, images of Newton's rings were calculated based on zero-thickness ray tracing.

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Library to process linear polarized light rays by spherical lenses

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In [1], an approach to calculating the interaction of transparent optically isotropic objects with polarized light rays is proposed. While mathematical modeling spherical lenses are the most commonly used elements of 3D scenes, which are computer counterparts of an optical experiment setups.

To facilitate the use of such lenses in experimental programs, a library of spherical lenses was developed. Each lens is constructed using set-theoretic intersections of the inner or outer space of geometric primitives: a sphere, a cylinder, a cone, and a half-space (plane). For a linearly polarized light ray incident on the lens, the library calculates the output linearly polarized light rays: the reflected and the required number of transmitted rays.

Obviously, there are several huge software products like TracePro®, ASAP®, which allow to solve analogous tasks. However, systems are huge, expensive, autonomous and do not allow to use some parts in a user program. On the contrary, the proposed lens library can be used in C++ applications dedicated to carrying out and demonstrating optical experiments.

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Support tools for functional programming distance learning and teaching

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The Cloud Sisal language carries on the traditions of previous versions of the Sisal language while remaining a functional data-flow language focused on writing large scientific programs and expanding their capabilities by supporting cloud computing [1]. The cloud parallel programming system CPPS is based on the Cloud Sisal language [2]. This paper considers the online environment [3] of the CPPS system which allows a user on any device with Internet access to develop and execute Cloud Sisal programs.

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A circular layout algorithm for attributed hierarchical graphs with ports

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Information visualization based on graph models is a key component of support tools for many applications in science and engineering [1]. The Visual Graph system [2] is intended for visualization of big amounts of complex information on the basis of attributed hierarchical graph models [3]. In this paper, a circular layout algorithm for attributed hierarchical graphs with ports and its effective implementation in the Visual Graph system are presented.

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NUMA-aware MPI broadcast algorithms for shared memory systems

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Broadcast is an important communication operation in high-performance computing. For a significant number of parallel algorithms and packages of supercomputer simulation, the performance of broadcast operation is critical. The MPI standard defines an MPI_Bcast routine for single source non-personalized broadcast operation, in which data available at a root process is sent to all other processes. On HPC systems, MPI applications usually run several processes per compute node and therefore the latency of intra-node communications can significantly impact the performance of the overall application. Thus, optimization methods that leverage intra-node shared memory become increasingly crucial. We consider a data broadcasting only between processes reside on a same compute node. It is a typical situation for hierarchical (topology-aware) collective operations to form a separate MPI communicators for each node and execute an algorithm of collective operation level-by-level.

The most used double copy algorithms (copy-in/copy-out) involve a shared buffer space used by local processes to exchange messages. The root process copies the content of the message into the shared buffer before the receiver reads from it. In this paper we propose kernel-assisted (CMA, KNEM and XPMEM) and CICO-based NUMA-aware algorithms for MPI_Bcast operation. In contrast to other works our algorithms explicitly allocate memory for queues from local NUMA nodes even with active linux page cache readahead subsystem. We show how to find optimal size f of buffer and length s of the queue what takes no more than b bytes and provides minimum algorithm time. On NUMA machines with Xeon Nehalem and Xeon Broadwell processors, our implementation based on Open MPI achieves on average 20–60% speedup over algorithms of Open MPI coll/sm and MVAPICH (mv2_shm_bcast).

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Aggregation errors in project schedulling

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The problem of resources evaluation in network projects models with constant and variable intensity of operations is discussed. The exactness of plans depends on a degree of resources aggregation and a time scale, which consists of some intervals (quanta). A quantum is the least time period (called so by analogy with physics) for measuring resources and other purposes in scheduling. A sum of quanta is equal to planning period. Resources demands for schedules are calculated separately per each quantum taken as a whole. A decrease of a number of quanta (one way of aggregation) reduces models dimensions, but at the same time it leads to growth of systematic mistakes of resources calculation, which doesn’t allow seeing schedules in proper perspective. The results of numerical experiments using the package for solving network optimization problems [1] are presented.

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The diameter vulnerability of two-dimensional optimal circulant networks

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This paper studies the effect of changing the diameter of circulant networks of dimension two with unreliable elements. The well-known (Deg, D, D1, S)-problem is to find (Deg, D)-graphs with maximum degree Deg and diameter D such that the subgraphs obtained from the original graph by deleting any set of up to S vertices (edges) have diameter at most D1. For a family of optimal circulants of degree four we found the ranges of orders of the graphs that preserve the diameter of the graph for one (two) vertex or edge failures. It is proved that in the investigated circulant networks in case of failure of one or two edges (vertices), the diameter can increase by no more than one, and in case of failure of three elements by no more than two (edge failures) or three (vertex failures). It is shown that the graphs investigated, in comparison with two-dimensional tori, have a better diameter in case of element failures.

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Application of Big Data technologies to assess the natural moisture of the territory

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Due to the sharp changes in climatic conditions in Western Siberia, the most pressing problem is food security associated with forecasting crop yields [1–2]. There is a need to estimate the natural wetness of the area on the basis of agroclimatic indicators, among which the sum of active air temperatures and precipitation is currently the most widely used. However, for a comprehensive assessment of the wetness of the territory, it is necessary to take into account the climate energy resources associated with evaporation of different time resolutions (day, decades, months, vegetation period, year). The initial meteorological parameters are described in the form of poorly structured information of a large volume [3]. Therefore, various technologies and algorithms of machine processing are used in the work. With the help of the high-level Python programming language and engineering libraries, a comprehensive assessment of the territory was carried out using the example of Mirny of the Kochenevsky District of the Novosibirsk Region in the context of long-term average data and two years 2019 and 2020. that the use of machine processing technologies related to NoSQL data requests, creation of data set and big data slices allows to store and process meteorological parameters using cloud services of different time resolution. This makes it possible to significantly reduce the time for a comprehensive assessment of the territory according to agroclimatic parameters. As a result of the work, precipitation distribution, temperature, relative air humidity, evaporability, humidification coefficients (Ivanov-Vysotsky [4] and Selyaninov hydrothermal coefficient [5]) were obtained.

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Paley graphs and Cartesian product for designing promising topologies for networks-on-chip

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The purpose of this work is to study promising network-on-chip (NoC) topologies. Classical NoC topologies (mesh, ring, torus) are well studied, but their configuration parameters are not the best among all existing ones. In this work, we study circulant topologies and their modifications, as well as evaluate their parameters in the context of NoC design. Recently, in a number of works [1, 2], a proposal to use circulant topologies for designing NoC has appeared. The use of a new topology with better parameters of the diameter and average distance in comparison with the classical regular topologies made it possible to significantly advance in solving the problem of finding optimal topological structures. At the same time, the use of circulant topologies has a number of disadvantages associated with the need to find optimal routing algorithms and avoid deadlocks and livelocks in the network. There are also other approaches to generating new structures of circulant graphs, namely, the use of Paley graphs [3] and the direct product of circulant graphs. The result of a study of these approaches proved their relevance and the need for further research in this direction.

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Co-authorship network structure analysis

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Co-authorship networks of scientists belong to the class of complex networks [1]. Analysis of these networks reveals features of academic communities which help in understanding collaborative scientific works and identifying the notable researchers. A network is defined as follows. The set of co-authorship network's nodes consists of authors. There exists an undirected edge between authors u and v iff they produced a joint paper.

Empirical measurements allow us to uncover the topological measures that characterize the network at a given moment. The bibliometric data used for this study has been retrieved from the distributed RePEc [2] database. We use the simple network model represented by an undirected, unweighted graph. The data was analyzed using statistical techniques in order to get such parameters as the number of papers per author, the number of authors per paper, the average number of coauthors per author and collaboration indices. We show that the largest component occupies near 90 % of the network and the degree distribution follows the scale-free power-law with a small fraction of scientists having a large number of coauthors. An important phenomena of many real networks is the small-worldness. Therefore we investigate two quantities of interest: the degree of clustering and the average path length and show that the network on study deviates from a random

Erdős – Rényi model [3] of similar size and average connectivity and can be classified as a small world network [4].

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Decision-making system based on data analysis

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The article is devoted to the analysis of the functional capabilities and future trends of the developed system of managing the scientific and educational process based on the analysis of scientometric and academic data. It also describes the reasons for its creation, the main architectural and technological features, the services provided and the prospects for development. The issues of using ontologies for integrating data from heterogeneous sources and knowledge base organizing are considered. The system is used to test various evaluation-based decision-making procedures. The main attention is paid to the example of decision-making in the procedure for appointing teaching staff to positions. The approximate application of the system shows its analytical advantages as an adaptable tool for the study of a wider range of tasks in scientific and academic activities. The application of the system shows its analytical advantages as an adaptable tool for the study of a wider range of tasks in scientific and academic activities. The practical significance and effectiveness of the system is confirmed by the expanding list of functions that are assigned to it in the field of preparing management decisions.

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Section 8

COMPUTER BIOLOGY, MEDICINE AND BIOTECHNOLOGY

Molecular evolution of proteins, containing phospholipase A2 domain in flatworms

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Phospholipases are a group of enzymes (a class of hydrolases) that catalyze the hydrolysis of phospholipids. Depending on the position of the hydrolyzed bond in the phospholipid, there are 4 main classes of phospholipases: A, B, C, and D. In this work we will consider phospholipases A2, which cleave SN-2 acyl chain [1]. Phospholipases A2 are known for being snake venom toxins. These proteins are also widely represented in mammals and perform a number of important basic functions at the cellur level and the whole organism [2]. Disruption of human phospholipase A2 functions is often associated with cancer [2].

The parasitic worms pose a threat to the health of Siberian population (high incidence of opisthorchiasis in Western Siberia). The disease may cause complications (cholelithiasis or cancer) [3]. In this regard, phospholipases are of interest for study because they can participate in the process of "parasite-host" interactions. The aim of this work is to study the peculiarities of the structure, functions and evolution of proteins containing phospholipase A2 domain in flatworms. A bioinformatic approach for detecting phospholipase A2 family proteins in flatworms has been proposed. In flatworms, classes of phospholipases A2 of 11 families were identified for the first time.

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In silico design of new ethylene sensors in plants based on genome-wide analysis of EIN3 transcription factor binding sites

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ETHYLENE INSENSITIVE 3 (EIN3) transcription factor is the master regulator of gene expression in response to plant hormone ethylene. It binds a short nucleotide sequence referred to as EBS to induce transcription. Arabidopsis thaliana reporter EBS:GUS driven by the classical variant of the EIN3 binding site is widely used as a sensor for detection of ethylene signaling. However, very little is known about the role of structural variants of EBS in EIN3 functioning. Here we accomplish a systematic bioinformatics analysis of EIN3 bound sequences in Arabidopsis genome.

We used publicly available ChIP-seq data on EIN3 binding, RNA-seq data on ethylene-induced transcriptomes in Arabidopsis seedlings [1] and DAP-seq data [2]. We used Homer [3] for de novo motif search in the peaks, and MCOT [4] for enrichment analysis of EBS repeats. Associations of EBS configurations with peaks and genes features were estimated with Fisher's exact test. We discovered a previously unknown EBS architecture that is enriched in EIN3 bound sequences to a much greater extent than a single EBS motif. This new configuration is a tail-to-tail inverted repeat of EBS-like sequences with 1 bp overlap referred to as 2EBS(-1). We also demonstrated that the inverted repeat of the coreEBS with the overlap of the motifs but not with a spacer is enriched in the Arabidopsis genome. We further showed that of all EBS configurations under study only 2EBS(-1) was significantly associated with transcriptional response of EIN3 targets to ethylene treatment. Moreover, it tended to cause a more pronounced transcriptional response than other EBS configurations. Based on these findings we consider that 2EBS(-1) is a preferred EIN3 binding site in A. thailana genome. We applied these findings to design a new genetic sensor for highly sensitive detection of ethylene signaling. Taken together, this work provides new insight on the molecular mechanisms utilized for regulation of transcriptional response to ethylene in plants and offers a workflow for the inference of the cis-regulatory code.

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Changes in transcriptome profiles during enzymatic degradation of cell walls in fig (*Ficus carica* L.) leaves

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Isolated protoplasts provide an opportunity to study a wide variety of cellular processes. As usual, the isolation of protoplasts from plant tissues occurs due to the cell wall enzymatic degradation. While this process, the pattern of gene expression changes from that characteristic to a mature cell towards undifferentiated cells. In this work, we analyzed the leaves of a typical variety, "Sabrucia Rosea", obtained from microshoots grown *in vitro* were incubated in an enzymatic mixture. Several successive steps in the protoplast isolation protocol served as sampling points. For control, RNA was obtained from the original tissue. For all mRNA isoforms, expression levels were normalized relative to expression levels at the point corresponding to the transcriptome of untouched leaves. Based on the principal component analysis and k-means clustering, we identified groups with similar behavior. Among them, several mRNA isoforms showed significant changes in the expression level throughout the experiment. These data could be used to search for genes that act as "time markers" while enzymatic degradation of leaf tissue in order to optimize and test the protoplast isolation protocols.

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New possibilities of the PCA-Seq method in the analysis of time series

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When decomposing a one-dimensional time series using SSA, two PCs correspond to one frequency. But they can be modulated by a third PC without breaking orthogonality [1, 2].

In the PCA-Seq method [3], PCs are calculated through a matrix of distances between fragments of a time series. The original and modulating signals can be separated by fragments pre-normalizing. A reliable zero correlation with the time axis may testify in favor of the hypothesis that the found regularity really exists and can be continued in both directions from the interval under study. We use traditional solar activity data as an example.

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Automatic abdominal aneurysm segmentation using deep learning

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Abdominal aortic aneurysm is a serious disease, delayed diagnosis and surgical treatment of which is often fatal. Early detection and subsequent observation of the dynamics of the development of aneurysmal transformations of the aorta allows for advance planning of surgical intervention, which significantly reduces the risk of postoperative complications and mortality in patients. The main method for diagnosing this disease at the moment is laborious visual analysis of three-dimensional computed tomography images of the patient. Creation of a tool for automatic segmentation of an abdominal aortic aneurysm will simplify the diagnosis of this disease. The paper considers the creation of an abdominal aortic aneurysm segmentation tool based on deep learning methods. The algorithm is built by adapting the U-net architecture, which has proven itself for solving biomedical problems [1], to the analysis of three-dimensional images of computed tomography of patients.

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Three-dimensional shape reconstruction of abdominal aortic aneurysm for hemodynamic modeling

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Abdominal aortic aneurysm (AAA) is a degenerative disease that significantly increases the rupture risk of arterial wall. It’s a localized enlargement of the abdominal aorta such that the diameter is greater than 3 cm or more than 50 % larger than normal. So an accurate prediction of AAA rupture is critical.

In this study, algorithm for automatic 3D reconstruction of AAA, obtained from tomographic images, was developed and implemented. Accurate reconstruction of the geometry is necessary for automatic mesh processing with a high quality in hemodynamic simulations. Moreover, the developed program can be applied to measure important volume geometric characteristics of AAA [1]. The results of the work will be included in the software package for predicting the rupture risk.

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Formalization of target invariants of the system of anaerobic biological wastewater treatment

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A model of a two-stage process of anaerobic fermentation in a bioreactor-mixer is considered, the mathematical description of which is a system of nonlinear differential equations [1].

The aim of the study is to apply a new approach to organizing energy-saving control based on the principles of nonlinear adaptation on target manifolds with an attractive property [2], called invariants or laws of behavior of the target system of the object under study.

In this regard, a necessary preliminary study is the formalization of these target invariants as given (desired) laws of the control object's behavior.

Further, on their basis, an algorithm is proposed for the analytical synthesis of a vector controller with compensation for systematic and random disturbances along the control channel ofthe system of anaerobic biological wastewater treatment [3].

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Mathematical models for dynamics of HIV infection acute phase

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There are considered mathematical models for dynamics of HIV infection acute phase. The first mathematical models describing the dynamics of HIV infection appeared as early as 1986 [1], three years after the discovery of HIV. The basic mathematical model of the dynamics of HIV infection includes three key cell populations: uninfected target cells, infected target cells, and free virus particles. This basic model allowed to obtain such important quantitative characteristics of the infectious disease as the virus replication rate and an average half-life of a virus particle, the rate of decrease of the viral load, a life span of infected T-lymphocytes and the rate of virus production by a single infected cell (basic reproduction number, R_0). The next generation of dynamic models is an extension of the basic model by considering various types of cells in the immune system, types of infection (acute, latent), localization in the compartments (blood, lymphatic system), mutated strains of the virus, etc. [2, 3].

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Random graphs as structural models of biological networks

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Modern methods of experimental research allow reconstruction of biological networks of various types, including gene, metabolic, interatomic networks, gene co-expression networks, disease networks, etc.

Structural models as a random graphs can be used for testing various statistical hypotheses on networks, searching for network biomarkers, studying the influence of structural patterns in biological networks on their function.

In this paper, we use the method for generating a random graph with restrictions in the form of frequencies of structural motives of various sizes. The process corresponds to a Markov chain, at each step of which two non-adjacent edges of a graph are swapped in a random way. A computational experiment was carried out to analyze the process of the Markov chain convergence to a stationary distribution when generating a random graph from a set of starting positions. In addition, in order to estimate the optimal number of steps of the Markov chain, methods of "multiple short runs" and "one long run" were applied. A computational experiment was carried out to verify these estimates on mouse liver PPI network.

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Computer analysis of the gene network that controls appetite in human

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The drive to consume food is one of the most primitive of instincts promoting survival. Appetite disorders can lead to human diseases (anorexia nervosa, hyperphagia, obesity). Gene network involving 120 human genes and proteins that control appetite was built. This network also included miRNAs that regulated the expression of proteins, as well as diseases associated with network objects. It was found that the subsystem of anorexigenic genes included more elements, had an additional mechanism of expression regulation involving miRNA, and, on average, was associated with a greater number of diseases compared to the subsystem of orexigenic genes. The study of the evolution of the genes based on PAI [1] showed that "middle-aged" genes predominated in the network. An evolutionary stage was identified, corresponding to the moment of the emergence of placental organisms, at which more genes "arose" than could be expected for random reasons. The number of cases when the gene encoding the cell surface receptor was older than the gene encoding the corresponding ligand (signaling molecule - hormone, neuropeptide, etc.) significantly exceeded the number of cases when the opposite situation was observed. It turned out that most of the genes of the network undergo stabilizing selection, but the genes encoding signaling molecules are less susceptible to it.

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ANDDigest: A web tool for finding information in scientific publications and patents in the biological field

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We propose the ANDDigest tool [1], which is a new module of ANDSystem [2], dedicated to the search of relevant scientific literature in the field of biology, considering many types of objects from the ANDSystem's ontology as well as sets of keywords, provided by the user. In contrast to the previous version of ANDDigest, a proposed tool allows performing search not only in the sets of PubMed abstract, but also in patents, full-text publications, and texts of pre-prints. The user has possibility to select one or several sources of the information. Another approvement of the system is addition of the possibility to perform more complex searches. The system has a user-friendly interface, providing sorting, visualization, and filtering of the found information, including mapping of mentioned objects in text, linking to external databases, sorting of data by publication date, citations number, J. H- indices, etc. The system provides data on trends for identified entities based on dynamics of interest according to the frequency of their mentions in PubMed by years. The tool can be applied to the interpretation of experimental genetics data, the search for associations between molecular genetics objects, and the preparation of scientific and analytical reviews. It is presently available at https://anddigest.sysbio.ru/.

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Reconstruction of associative gene networks using text mining methods

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The ANDSystem software [1] was developed for the purpose of scanning literature for extracting relationships between diseases, pathways, proteins, genes, microRNAs and metabolites and reconstruction of associative gene networks on the base of this information. The ANDSystem incorporates utilities for automated extraction of knowledge from Pubmed published scientific texts and analysis of factographic databases. The ANDVisio [2] is provided with various tools supporting filtering by object types, relationships between objects and information sources; graph layout; search of the shortest pathway; cycles in graphs. An associative gene network is a heterogeneous network, the vertices of which, along with molecular genetic objects (genes, proteins, metabolites, etc.), can represent entities of a higher level (biological processes, diseases, environmental factors, etc.) connected with each other by regulatory, physicochemical or associative interactions. A new direction for the study of molecular genetic mechanisms is the prioritization of biological processes based on the analysis of associative gene networks. Methods for prioritizing or ranking candidate genes according to their importance in accordance with specified criteria based on the analysis of gene networks are widely used in biomedicine to search for associations of genes with diseases, predict biomarkers, pharmacological targets, etc. At the same time, there is a tendency to use them in other areas of knowledge, in particular in crop production. This is largely due to the development of technologies for solving the problems of marker-oriented and genomic selection, which require knowledge of the molecular genetic mechanisms underlying the formation of economically valuable traits. Using ANDVisio, biological processes were prioritized according to the degree of their connection with gene networks, presented in the ANDSystem knowledge base. With this approach it was analyzed a set of human diseases and the response of plants to cadmium, salt stress and drought conditions.

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Algorithm for the study of the biomechanics of the shoulder joint in rehabilitation

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The variability of anatomical and physiological features is often an additional risk factor for structural pathologies and injuries of the shoulder joint. Studies of the kinematic patterns of the shoulder joint and the upper limb as a whole, as well as, their variability in norm and pathology are actively carried out in biomechanics, rehabilitation, and sports medicine. Injuries to the structures of the shoulder joint are account for 16 to 55% of all injuries of large joints [1, 2]. Clinical studies conducted in FSRCC FMBA in Krasnoyarsk. The objects of observation were men and women 18–55 years old in the early and late recovery periods after surgical treatment of injuries of the shoulder joint [3]. The series of MRI images were studied using Shearlet transform and color-coding algorithms [3, 4]. Demonstrated MRI images of patients with additional imaging. Improved the study of joint morphology and geometry. The obtained data reflect the state of all components of the unified kinematic model of the shoulder joint at a particular moment in the rehabilitation process. The proposed complex approach significantly improves the quality of the step-by-step diagnostics for injuries of the shoulder joint which opens up prospects for its application in biomechanics and practical medicine. The dependencies in indicators allow more accurately to plan the exercise cycle for a patient.

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Experimental research: search and definition of texture markers

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Research suggest the formation of a methodology for the effective detection, texture analysis and visualization of pathological changes in the lungs, in particular, the determination of pulmonary fibrosis in the early stages of the development of pneumonia from COVID-19 [1–4]. The purpose of the study is to improve the visualization of areas with pathology in order to improve the accuracy of diagnosis and expand the radiological conclusion. As part of the used technique, segmentation and contouring of objects of interest with contrasting color coding are performed to identify features and obtain quantitative estimates of changes associated with Covid-19 [5, 6]. An assessment of the area of the involved lung parenchyma is also performed to supplement and expand the clinical and radiological picture and conclusion. During study was used the data set of CT images of the FSNCTs of the FMBA of Russia. It includes data of patients with confirmed Covid-19 taking into account distribution depending on the severity of pathology. The paper presents the results of experimental studies aimed at improving the accuracy of analysis and interpretation of images of lung pathology with Covid-19, which include assessments of the corresponding indicators (markers) in the format of modern radiomy technology, as well as assessments of dynamic changes in the patient's lungs to adequately predict the results.

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Chronic hepatitis B modelling within the Marchuk – Petrov model

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The dynamics of infection diseases and immune responses are modeling with systems of delay differential equations. Stable non-trivial steady states and stable periodic solutions to such models can be interpreted as chronic diseases. In this talk we present a technology, which we developed in [1, 2] for computing steady and periodic solutions of time-delay systems, and discuss the results of computing such solutions of the Marchuk-Petrov model [3] with parameter values corresponding to hepatitis B with low viral load. These solutions are of particular interest since the corresponding forms of chronic disease cannot be diagnosed by conventional methods. However, they become dangerous in the case of organ transplantations, since the low level infection can turn into an acute form of disease with a high viral load following immunosuppressive drugs treatments, which is necessary after such operations.

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Mutation hotspots of SARS-CoV-2 RNA motifs conserved in betacoronaviruses

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The pandemic of the coronavirus infection COVID-19, which began at the end of 2019 and caused by the SARS-CoV-2 virus, has led to unprecedented consequences in the world. By the end of May 2021, in the world there were 167 million infected and 3.5 million died directly from infection [1].

SARS-CoV-2 is a beta coronavirus, so it shares many conserved fragments with other known viruses of this type [2]. Since the beginning of the spread of the COVID-19, one of the important issues of research of the

SARS-CoV-2 virus has been the search for its conserved RNA motifs and their functional annotation. These motifs are potential targets for the treatment and diagnosis of a disease caused by the virus.

This report examines the structural RNA fragments of SARS-CoV-2, similar to the corresponding fragments in other beta coronaviruses [2]. For these RNA motifs the nucleotide variability during the spread of the virus, depending on their secondary structure, was investigated. All the motifs display the similar background variability although contain hypervariable positions.

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Meta-analysis of auxin-induced transcriptomes unveiled signal transduction pathway from auxin to its PIN transporters

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Auxin is a plant hormone that plays a key role in ontogenesis. Protein families of ARF and Aux/IAA provide the auxin signal transduction. However, the specific participants of auxin signaling pathway to its PIN transporters are certainly unknown. We have developed bioinformatics algorithm for the meta-analysis of auxin-induced transcriptomes of *Arabidopsis thaliana*. We selected genes differentially expressed in response to auxin in coordination with PIN1, PIN3, PIN4, PIN7, and identified possible participants in the ARF-Aux/IAA signaling pathway that regulate the expression of each PIN gene. We suggested that the regulation of PIN expression by auxin occurs through several ARF-Aux/IAA regulatory circuits, in which ARF4, ARF10 and IAA4, IAA12, IAA17, IAA18, IAA32 are combined. Some combinations are specific for the auxin-mediated regulation of transcription of certain PIN genes, while others, on the contrary, are common to several PIN genes.

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Algorithm for analyzing computed tomography images to assess initial ischemic changes

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The report presents an algorithm that solves the problem of evaluation the state of the patient's brain in the first hours of the growth of an ischemic stroke. Using the data of computed axial tomography (CAT) of the brain, it is necessary to evaluate the initial ischemic changes using the Alberta Stroke Program Early CT Score (ASPECTS) scale. The purpose of the work is to build a tool that will analyze CAT images within the ASPECTS scale and indicate the areas in which early signs of ischemic changes are determined.

The brain regions supplied with blood by the middle cerebral artery were divided into ten separate sections in accordance with the ASPECTS scale, which leads to the problem of image segmentation. Finding areas of interest according to some common patterns and determining the degree of damage to a part of the brain is traditionally carried out using convolution neural networks.

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Comparison of genomes of different species of coronaviruses using spectra of periodicities

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The periodicities presented in the genomes of related organisms play an important role in classification. The complete spectra of periodicities identified by the authors in genomes are quite compact and visible even for relatively long genomes, which makes them a convenient tool for differentiating closely related objects. Genomes of SARS, MERS and SARS-COV-2 coronaviruses are being considered

The first confirmed case of Middle East respiratory syndrome-related coronavirus (MERS-CoV) was reported in Jeddah, Saudi Arabia in April 2012. By July 2015, MERS-CoV cases had been reported in over 21 countries, in Europe, North America and Asia as well as the Middle East. Severe acute respiratory syndrome coronavirus (SARS-CoV or SARS-CoV-1) caused the 2002–2004 SARS outbreak. Coronavirus disease 2019 (COVID-19) is a contagious disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). The first known case was identified in Wuhan, China, in December 2019. The disease has since spread worldwide, leading to an ongoing pandemic.

This work was carried out within the framework of the state contract of the Sobolev Institute of Mathematics (project no. 0314-2019-0015)

A computational model of the cereal leaves hydraulics

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Environmental factors and plant architectonics significantly determine its water regime, namely, the water content and its movement through the tissues forced by the difference in water potentials, turgor pressure in cells, etc. In turn, the cumulative water regime affects the functioning and growth of cells, photosynthesis, and, as a result, the plant's growth. The leaf contributes to the formation of the water regime and characterizes the contour of the plant's adaptive system. Nevertheless, the data on the contribution of leaves to the total resistance to water transport in the plant and the structure of the hydraulic resistance of the leaf itself is still contradictory.

This paper presents the formulation and justification of the monocots leaf hydraulics model based on Darcy's law. The model was tested in computational experiments in the Comsol 4.3b package on idealized geometric models of leaf blades. Simulations showed the dependence of water potential distribution in xylem vessels and leaf mesophyll on the permeability of these tissues and on microclimatic parameters around the leaf. The adequacy of the model parameters selected as a result of testing is discussed.

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Modeling the influence of the availability of NAD+ for the SIRT1 enzyme on the interaction of the circadian oscillator with the inflammatory response system to bacterial infection

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A mathematical model of the influence of the availability of NAD + for the SIRT1 enzyme on the interaction of the circadian oscillator with the inflammatory response system to bacterial infection has been developed and verified on experimental data. To verify the model, we used data on the daily dynamics of gene expression in the liver of wild-type mice and with knockouts of circadian genes, information on biologically justified intervals of parameter values, etc. Sensitivity analysis for the parameters of the oscillation period and the amplitude of the change in the main variables of the model made it possible to identify the important parameters.

Modeling showed a pronounced circadian character of changes in Sirt1 and NFkB activity, and made it possible to assess age-related changes in the functioning of the circadian oscillator, the NAD + consuming enzymes, and the level of NF-kB activation induced by LPS.

Thus, the developed model makes it possible to predict diurnal and age-related changes in the activity of the inflammatory response to bacterial infection through NF-kB, and the results of modeling serve as a justification for a chronotherapeutic approach in the treatment of inflammatory diseases.

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Destabilizing selection against under-expression of human immunostimulatory and immunosuppressive genes both provokes and prevents rheumatoid arthritis, correspondingly, as a self-domestication syndrome

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Using SNP_TATA_Comparator [1], we studied of single-nucleotide polymorphisms in promoters of human rheumatoid arthritis (RA)-related genes and found destabilizing selection of immunostimulatory and immunosuppressive genes provoking and preventing RA, respectively, , as a self-domestication syndrome. Among known differentially expressed genes (DEGs) of pet vs wild animals, amount of DEGs in pets corresponding to worsened RA in humans exceeds those in their wild congeners (10 vs 3), while less DEGs in pets relate relieved RA in humans than those in Wild (1 vs 8). This is reliable according to binomial distribution, χ^2 and Fisher's exact tests.

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Identification and classification of long noncoding RNAs

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Motivation and Aim: Long non-coding RNAs (lncRNAs) are typically defined as transcripts of more than 200 nucleotides length and without any protein coding potential. The functions are poorly understood, however, a number of well-known plant lncRNAs play diverse roles in X inactivation, imprinting and gene expression. Thus lncRNAs are involved in important plant development processes such as phosphate homeostasis, flowering, photomorphogenesis and stress response in this connection, their study is relevant. Information is obtained from transcriptomes, but bioinformatic annotation methods are not sufficiently presented, especially for plants. This raises the challenge of developing approaches to automatic annotation and prediction of lncRNA functions in plants.

Methods and Algorithms: In this paper a computational pipeline for the identification and annotation of lncRNA in the plant transcriptome has been developed, steps: 1. Identification of lncRNAs – lncFinder [1]. 2. Alignment lncRNA on referense genome – GMAP [2]. 3. lncRNAs classification – gffcompare [3]. lncRNAs structural features analysis. The pipeline is implemented using the Snakemake workflow management system language.

Results: The pipeline was used to analyze ~ 800 *Zea mays* transcriptomes comprising 3148430 transcripts in total. We identified 2741504 (87%) lncRNAs; of them 98% were aligned to the reference genome. We identified 334069 exon antisense, 4390 intron antisense, 231970 multi-exon, 81163 retained introns, 512753 intergenic. Antisense lncRNAs alignment (exon, intron, 338459 tr.) on structure of the target gene, showed that the predominant amount of lncRNA is aligned on exon 1 of the target gene.

Conclusion: The proposed pipeline made it possible to identify 1164345 new lncRNAs in the maize genome, annotate them and evaluate their structural features.

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New motif discovery approach

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The development of new high-throughput experimental methods has led to the accumulation of a huge amount of new data on regulatory DNA sequences. This has put forward new requirements for de novo motif discovery approaches. Empirical approaches that are widely used today effectively reveal well-represented motifs. However, they do not guarantee finding a global optimum and identifying poorly represented motifs. We have significantly accelerated our previously proposed new brute-force method based on CUDA technology and using video accelerators [1]. It allows the detection of very poorly represented context signals in regulatory DNA sequences. Its higher efficiency is shown in comparison with existing widely used methods.

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Section 9

METHODS OF ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

Russian-English dataset and comparative analysis of algorithms for cross-language embedding-based entity alignment

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The problem of data fusion from data bases and knowledge graphs in different languages is becoming increasingly important. The main step of such a fusion is the identification of equivalent entities in different knowledge graphs and merging of their descriptions [1]. This problem is known as identity resolution, or entity alignment problem. Recently, a large group of new methods has emerged to look for so called "embeddings" of entities and establish the equivalence of entities by comparing their embeddings [2]. This paper presents experiments with embedding-based entity alignment algorithms on a Russian-English dataset for. Also, the future directions of research are outlined.

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RWeakly-supervised semantic segmentation of tomographic images in the diagnosis of stroke

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The early diagnosis of acute stroke is of primary importance for deciding on a method for further treatment. In order to distinguish the brain areas affected by stroke, it is required to engage a highly qualified radiologist. It is known that even a highly qualified specialist can make erroneous predictions with sufficiently large probability (up to 10%). Also, the process of manual annotation of a large number of computed tomography digital images is difficult and time-consuming, thus a specialist may label areas affected by stroke inaccurately.

In this report, a method for automatic semantic segmentation of acute stroke using non-contrast computed tomography brain images is presented. Under the weakly-supervised task we understand the scenario, when some images are labeled accurately and some images are labeled inaccurately. To solve this problem, we use the traditional computer vision methods [1] and a convolutional neural network based on U-net architecture [2]. We propose a modified loss function with weights obtained from the information of the images.

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A lobster-inspired multi-robot control strategy for monitoring non-stationary concentration fields

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We propose a new lobster-inspired chemotaxis decentralized control strategy for monitoring a non-stationary concentration field using a team of nonholonomic mobile robots. The task of the team is to locate and trace the movement of the point (or points) with the highest field value (i.e. source), provided that the robots are not aware of the dynamics of the field and can only periodically sample the field at their locations. The proposed strategy combines the lobsters' plume localization behavior and flocking mechanisms to efficiently solve the problem even with a small group of robots. Simulations and experimental works on physical unicycle robots are performed to validate the effectiveness of the approach for the cases of stationary and non-stationary fields.

Data-driven turbulence modelling using symbolic regression

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The study is focused on the performance of machine learning (ML) methods applied to improve prediction of main features in canonical turbulent flows by the Reynolds-averaged Navier–Stokes (RANS) equation models. A key issue here is to approximate the unknown term of the Reynolds stress (RS) tensor arising after Reynolds averaging, which is needed to close the RANS equations.

Turbulent flows in channels with bumps on the bottom having the extensive LES and DNS data sets for various Reynolds number cases are chosen to examine possibilities of GEP (gene expression programming) [1] to formulate accurate RANS models. Such a symbolic regression technique allows us to get a new explicit model for the RS anisotropy tensor. Results obtained by the new model produced using GEP are compared with those from high-fidelity LES and DNS data (serving as the target benchmark solution during the ML algorithm training) and from the conventional RANS model with the linear Boussinesq hypothesis for the RS tensor.

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Weakly supervised semantic segmentation of tomographic images in the diagnosis of stroke

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The early diagnosis of acute stroke is of primary importance for deciding on a method for further treatment. In order to distinguish the brain areas affected by stroke, it is required to engage a highly qualified radiologist. It is known that even a highly qualified specialist can make erroneous predictions with sufficiently large probability (up to 10 %). Also, the process of manual annotation of a large number of computed tomography digital images is difficult and time-consuming, thus a specialist may label areas affected by stroke inaccurately.

In this report, a method for automatic semantic segmentation of acute stroke using non-contrast computed tomography brain images is presented. Under the weakly supervised task we understand the scenario when some images are labeled accurately and some images are labeled inaccurately. To solve this problem, we use a convolutional neural network based on U-net architecture [1], since it is known that in the problems of semantic segmentation of medical images fully convolutional neural networks show a better performance in comparison with classical machine learning methods [2]. We introduce the model of inaccuracy that shows the likelihood that the label is correct. The resulting values obtained from the inaccuracy model are used as weights in the loss function. The proposed method improves the quality of segmentation; its effectiveness has been tested on real computed tomography images.

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Automated construction of a scheme for solving compute-intensive problems based on the ontological approach and Semantic Web technologies

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The paper describes the means for supporting researchers in the development of parallel code. They are based on the ontology of the knowledge area "Support for solving compute-intensive problems of mathematical physics on supercomputers". The main result of these tools work is a scheme for solving the problem, built according to its specification provided by the user. The scheme includes the most suitable mathematical models for solving the problem, numerical methods, algorithms and parallel architectures, links to available fragments of parallel code that the user can use when developing their own code. The construction of the scheme is carried out on the basis of ontology and expert rules built using the Semantic Web technology.

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Machine learning methods to develop Reynolds-stress models in turbulent flows

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Possibilities to build explicit algebraic models of Reynolds stresses needed for closing the averaged Navier–Stokes equations in the RANS method for calculating turbulent flows are considered. To calibrate the new models, following [1], machine-learning methods are used that allow expressing the Reynolds stress anisotropy tensor via the basic tensors including the linear and quadratic dependence on deformation and strain tensors.

To train the models, we use the high-fidelity data of LES in a turbulent channel flow with the curved backward-facing step [2] and those of DNS in an annular channel flow performed by the authors. To validate the obtained Reynolds-stress tensor expressions, DNS and measurement results for flows of similar geometry or for the same flows at varied Reynolds numbers are taken from the available databases.

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Towards real time fluid motion estimation by particle images based on convolutional neural networks

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A task of motion estimation can be found in various fields from surveillance security systems, industrial inspection and non-destructive testing to computer graphics increasing rendering speed and visual motion capture. Additionally whole-field quantitative assessment of mechanical stresses and velocity in the strain gauges and fluid velocity sensors can be mentioned. Optical flow processing algorithms are frequently applied when using dense motion estimation [1]. This technique is based on conservation of local intensity to track displacements of moving objects within the image [1]. Two-dimensional motion estimation for fluids is usually performed with high power pulsed laser illumination, and it is difficult to guarantee similar intensity profiles between pulses. Developing alternative fast motion estimation algorithms that can be adjusted for specific intensity variation conditions is relevant. This work presents test results of application of a convolutional neural network model PWC-Net [2] for on-line estimation of dense velocity field using pairs of particle images of VGA size. The original model was fine-tuned by 15 k synthetic moving particle image pairs [3] modeling different turbulent flow configurations as well as additional 1 k real experimental images. Currently achieved inference time as low as 70 ms (14FPS) can be improved further modifying the model configuration sacrificing spatial resolution and accuracy of the results.

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The use of neural networks for predicting concentration limits of flammability

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Neural networks were used to predict the flammability’s concentration limits of chemicals of various classes, based on a combination of descriptor and neural network approaches. Fragmentary descriptors are used in forecasting. They are calculated automatically using the structural formula of substance. It was detected that the results obtained in the article for predicting the concentration limits of flammability make an insignificant error in comparison to the experiment.

For a comparative analysis of the developed methods capabilities, the equations of domestic and foreign researchers are taken.

The research suggests and studies the methods combining the neural network and descriptor approaches for predicting the concentration limits of chemicals flammability. The best data are found using the “atom-bond-atom” descriptors.

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Selective regularization of linear regression model

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The paper considers the construction of a linear regression model with regularization of the matrix of the system of normal equations. Unlike traditional ridge regression, which consists in adding some positive parameter to all diagonal elements of the matrix [1], the proposed method increases only those diagonal elements that help to reduce the condition number of the matrix and, consequently, reduce the variance of the coefficients of the regression equation. These are the smallest diagonal elements of the triangular matrix obtained by the Cholesky decomposition of the correlation matrix of the original data set [2]. The effectiveness of the method is tested on a known dataset, and the comparison is made not only with the ridge regression, but also with the results of the widely used algorithms Lasso and LARS [3].

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Researching zero-shot learning methods for automatic speech recognition

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Speech recognition systems require datasets that will contribute to high quality recognition. However, such systems often do not meet this characteristic due to the lack of labeled data. The lack of labeled data, in turn, entails an imbalance: the high accuracy of the model will turn out to be "false" – the input data will be biased towards a particular class, which will affect the trained model. We propose a new in speech recognition termins method of dealing with this problem: training generative models [1, 2] on objects of one set of classes (seen) and classifying objects of another set of classes (unseen) using additional information. Using generative models helps us generate signal features for invisible classes using semantic information. A generative networks generates signal characteristics based on the semantic attributes of a particular class.

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Convolutional neural networks and readability evaluation for Russian texts

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Automatic evaluation of the age of the reader is a task of current interest in applied linguistics [1]. An algorithm that makes it possible to evaluate the age at which a text, on the one hand, will be understandable, and on the other, interesting, has a broad spectrum of potential applications in education and recommendation systems.

The classical methods for evaluating the readability of a text are linear regressions on a small number of simple features leading to their low reliability. The development of natural language processing methods and the use of neural network algorithms can significantly improve the estimation accuracy. In this paper, a new algorithm based on convolutional neural networks is presented. The main advantage of this approach is the set of chosen features. We use combination of classical features such as average sentence length, semantic vectors and some manually constructed abstract features. Training sample is collected from experimental data on the real pReferences of Russian school students increasing the practical value of our work.

The reported study was funded by RFBR, project number 19-29-14224.

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Computer system for searching for chemicals with predefined properties

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An important area of scientific research is the search for patterns between the structures of substances and their various properties, including biological ones. The problem of predicting new promising compounds is solved using data mining and machine learning methods. They allow you to filter and filter out unnecessary compounds and leave a small percentage of compounds that can be experimentally investigated. Methods and models for predicting the physico-chemical, medicinal, and biological properties of organic substances using factographic databases have been developed. A virtual screening procedure has been created, which includes an automated review of the database of chemicals and the selection of those for which the desired properties are predicted [1]. The developed mathematical modeling methods and computer technologies allow us to significantly limit the search area for chemicals with the required properties.

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Application of convolutional neural networks for agricultural land classification

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The main application of space images in agriculture is classification of land cover, agricultural crops, soil cover mapping, and yield forecasting [1–3]. Multispectral data from MODIS [4–6], Landsat-8 [1–2] and Sentinel-2 [7–9] are most widely used. Space images of Sentinel-2, covering parts of the land and water surface up to 290 km, are characterized by higher spatial and spectral resolution as compared to Landsat-8. Sentinel-2 imagery was used in this work in order to classify agricultural lands using Omsk Region as an example. In the course of classification it is necessary to distinguish the groups of lands that determine the direction of development of adaptive-landscape farming systems taking into account natural and economic factors (relief, climate, soils and soil-forming rocks, limiting factors). For this purpose, quantitative methods of Random Forest and Convolutional Neural Networks (CNN) recognition are used in this work. The theoretical foundations of CNNs have been developed for several decades according to the concept of computer vision. Modern architectures of convolutional networks allow the processing of large raster data by automatic extraction of feature space through the use of autoencoders. This significantly reduces the processing time of big data. Different vegetation indices are used to improve the recognition accuracy: normalized difference vegetation index (NDVI), normalized difference water index (NDWI), enhanced vegetation indexes (EVI) and textural features.

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Predicting a steady fluid flow over bluff bodies for shape optimization using machine learning

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In this study we apply a Machine Learning methods to the problem of the flow over a bluff body which shape is to be optimized using Convolutional Neural Network (CNN) and Reinforcement Learning (RL). In work of Viquerat et al. [1] it was shown that neural networks trained with RL algorithm are able to find optimal shapes for aerodynamics. Due to the high computational costs required by CFD solvers, it was proposed to use CNN to approximate stationary solutions of the Navier – Stokes equations [2]. The advantage of this solution is a significant reduction in time required to obtain a solution (about 2-3 orders) in comparison with the direct calculation by CFD solver at the cost of a small error rates. This acceleration makes it possible to reduce the computational costs in the problem of finding the optimal hydrodynamic shape using the Reinforcement Learning algorithm, where it is necessary to obtain a large number of solutions when searching for optimal parameters of bluff body geometry.

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Identification of argumentative sentences in scientific and popular science texts

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In this study we analyze the applicability of specific machine learning algorithms to the task of detecting argumentative sentences in Russian text. We employ a collection of scientific and popular science texts with manually annotated argumentation to evaluate the quality of identifying argumentative sentences in terms of precision, recall, and F-measure. The experiment involves three algorithms: MNB, SVM, and MLP in Scikit-learn implementation. The bag of words model is used for representing texts. Lemmas of words in analyzed sentences serve as features for the classification. We perform the automatic selection of informative features in accordance with Variance and χ^2 criteria combined with weight-based filtration of lemmas (via TF*IDF and EMI). The training set includes around 800 sentences, while the test set contains 180. The MNB algorithm demonstrates highest F-measure and recall scores on almost all feature, while the MLP algorithm shows the best precision for about a half of feature selection variations.

The study was carried out within the framework of the state contract of the Sobolev Institute of Mathematics (project no. 0314-2019-0015).

Extended methodology for deriving formal concepts

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In the study we analyze two methodologies for deriving formal concepts: the classical one, which focuses on the posterior analysis of the object's properties of the studied knowledge domain [1], and non-classical, the cornerstone of which is the priori formation of the set of measured object's properties and the determination of existential relations on this set [2]. Firstly, in the technological chain of the target transformation of the source data we fix a position where the difference between considered methodologies really shows itself. Secondly, we establish the commonality of these two approaches in the aspect of the unity of their hypothetical-deductive basis. We demonstrate the need for the joint use of the considered methodologies at processing incomplete and inconsistent empirical data about studied knowledge domain [3].

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Pattern recognition for bubbly flows with vapor or gas-liquid interfaces using U-Net architecture

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We apply deep learning algorithms to images of the water pool boiling in order to detect the evolution of the vapor bubbles. It can allow us to simultaneously analyze each separated bubble and obtain all key parameters including the bubble growth rate, departure diameter and time and nucleation site's activation. For analysis the data obtained in experiments at pool boiling conditions in pressure range 9-101 kPa were taken for the basis [1]. The camera is directed upwards and focuses on the heat substrate itself, which makes it easier for the network to distinguish surface bubbles from one that floats up. Using our technique the evolution of each bubble was automatically measured based on video recording of the experiment. As a basic network U-Net with ResNet 50 encoder was used [2]. The network was trained on manually labeled dataset augmented with random rotations, flips, extra surface bubbles, background bubbles and background noise. We demonstrated the capabilities by tracking the appearance, growth and separation of the bubbles from the heating surface, which can be used for the mechanistic analysis of the heat transfer rate during liquid boiling at various pressures.

This work was supported by RFBR and TUBITAK according to the research project № 20-58-46008.

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Approach to automatic population of ontologies of scientific subject domain using lexico-syntactic patterns

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The paper presents an approach to automatic population of ontologies of scientific subject domain (SSD) using lexico-syntactic patterns and corpus of texts related to modeled domain. These patterns are built on the basis of ontology design patterns (documented descriptions of practical solutions to typical problems of ontological modeling) [1] provided by the system for the automated development of SSD ontologies [2].

This research was supported by the Russian Foundation for Basic Research (grants No. No. 19-07-00762).

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Mini-symposium

MULTISCALE AND HIGH-PERFORMANCE COMPUTING FOR MULTIPHYSICAL PROBLEMS

DG-GMsFEM for problems in perforated domains with non-homogeneous boundary condition on perforations

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In this work, we present the Discontinuous Galerkin Generalized Multiscale Finite Element Method (DG-GMsFEM) for problems in perforated domains with non-homogeneous boundary conditions on perforations.

In this method, we divide the perforated domain into local domains and construct local multiscale basis functions.

We present the construction of the two types of multiscale basis functions related to the outer and perforation boundary of the local domain. Construction of the basis functions contains two steps: snapshot space construction and solution of the local spectral problem in order to reduce the size of the snapshot space. The snapshot space for outer boundary contains a local solution of the problem with various boundary conditions on the interfaces between local domains and homogeneous boundary conditions on perforations. For generation of the snapshot space for perforation boundary, we set various boundary conditions on perforation boundary of the local domain and homogeneous boundary conditions for outer local domain boundary. We present construction of the method for different model problems: elastic and thermoelastic equations with non - homogeneous boundary conditions on perforations. The different concepts for coarse grid construction and definition of the local domains are presented and investigated numerically.

Numerical investigation of the presented method is performed for two test cases with homogeneous and non-homogeneous boundary conditions. For the case with homogeneous boundary conditions on perforations, we present results using only outer boundary basis functions. For non-homogeneous boundary conditions, we show that both outer and perforation boundary basis functions are needed in order to obtain good results with small errors.

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Multiscale model reduction for a piezoelectric problem in heterogeneous media using generalized multiscale finite element method

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We consider a static piezoelectric problem in heterogeneous media. The mathematical model consists of a system of equations for the mechanical displacements and the electric potential. We use a finite element method for fine grid approximation. For coarse grid approximation, we use the Generalized Multiscale Finite Element Method. We implement the multiscale method and compute errors between the multiscale and fine-scale solutions. The results show that the proposed method can provide good accuracy with a few degrees of freedom.

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Implementation of the SPH-IDIC method for modeling multiscale problems of dynamics of polydisperse gas-dust media on GPU

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The report presents the results of three-dimensional modeling of the regular expansion of a gas-dust ball with two dust fractions. A characteristic feature of this process is the constancy of the density over the volume of the sphere and the linear dependence of the velocity on the radial coordinate. Despite the fact that the expansion is spherically symmetric, the simulation was performed in a three-dimensional setting on a GPU using nVidia CUDA technology. In problems of the dynamics of polydisperse media, characteristic times of equalization of the phase velocities appear, which can differ by orders of magnitude, which leads to the need to greatly reduce the time step. In this work, the interphase interaction was calculated using the implicit method IDIC (Implicit Drag in Cell) [1, 2] of friction in cells in combination with the method of smoothed hydrodynamic particles SPH (Smooth Particle Hydrodynamics). This method makes it possible to carry out calculations with a time step limited only by the CFL (Courant-Friedrichs-Lewy) condition. The results obtained are in good agreement with both the analytical solution of the problem of regular expansion of a purely gas sphere and with the corresponding physical features of the process.

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Supercomputer model of dynamical dusty gas with intense momentum transfer between phases based on OpenFPM library

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The paper considers the solution of model gas-dynamic problems (propagation of a one-dimensional sound wave, one-dimensional problem of discontinuity decay, three-dimensional problem of a point explosion in a continuous medium) in the case of a gas-dust medium. The interaction of dust and gas was taken into account using the IDIC method [1, 2] within the SPH method used to solve gas-dynamic equations.

An important feature of the work is the use of the open computational package OpenFPM, which makes it easy to carry out parallel computations. The main advantage of this package is the ready-made (implemented by the authors of the package) and intuitive, automatically parallelizable vector data structures, the use of which is identical both in the case of calculations on a personal computer and in the case of using supercomputer resources. The paper analyzes the efficiency of parallelization of numerical solutions of the considered problems.

The research was supported by the Russian Science Foundation grant number 19-71-10026.

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Numerical solution of a 2d inverse gravimetric problem

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A 2d inverse gravimetric problem is considered. The aim is to recover the shape of an homogeneous ore body from the observation of the vertical gravity at the ground surface. To overcome the ill-posedness of such problem we restrict the unknown body to a star shaped domain. The numerical solution of the direct problem is based on solving an auxiliary boundary value problem in a bounded computational domain coupled with the surface integral. According to that, for solution of the inverse problem we present an iterative algorithm based on conjugate gradient method and specific regularization term. To demonstrate efficiencies of the proposed method we investigate a model problem of a simplified body with the analytical solution and noised input data.

Edge generalized multiscale finite element method for scattering problem in perforated domain

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In this work we consider scattering problem in perforated domain. The mathematical model is described by Helmholtz problem related to wave propagation with absorbing boundary condition. For the solution of the problem using classic finite element method, we construct unstructured fine grid that resolve perforation on the grid level. Such classic approximations lead to the large system of equations. To reduce size of the discrete system, we construct a novel multiscale approximation on coarse grid. We use the Edge Generalized Multiscale Finite Element Method, where we construct a multiscale space using solution of the local spectral problems on the snapshot space related to the coarse grid edges. We present numerical results for the Helmholtz problem in perforated domain with Dirichlet boundary condition on perforations. Proposed method are studied for a different wave numbers and numbers of the edge multiscale basis functions.

Embedded discrete fracture model on structured grids

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An approximation of the embedded discrete fracture model EDFM by the finite element method is considered. The paper proposes to use exponential functions instead of the Dirac delta function [1]. With this approach, instead of a separate computational mesh for fractures, a mesh for a porous medium can be used. The results of numerical experiments demonstrate the efficiency of the proposed approach.

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Multiscale finite element technique for mathematical modelling of multi-physics processes in the near-wellbore region

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In borehole physic, the results of the direct mathematical modelling of multi-physical phenomena are used to control drilling and well operation. Electromagnetic and acoustic measurements are the most accessible indirect methods for determining the thermal, transport and mechanical properties of rock samples in the near-wellbore zone. Mathematical modelling is one of the technologies used for solving multi-physical problems. A multi-physical problem is formulated as a system of partial differential equations with special interface conditions coupling mathematical models of physical processes. The near-wellbore region is characterized by a multi-scale geometric structure, high contrast and anisotropy of physical parameters. The discretization method should take into account the specifics of the problem and preserve the global regularity of mathematical models at a discrete level. The paper presents modified variational formulations of multiscale non-conforming finite element methods for mathematical modelling of electromagnetic and acoustic fields in fluid-saturated media at various temperatures and mechanical loads. To solve the discretized mathematical models, special multilevel solvers are developed. The results of three-dimensional mathematical modelling using model rock samples from the near-wellbore zone are presented.

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Analysis of ionospheric irregularities based on multi-instrumental data

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The most complex ionospheric phenomena occur in the areas of auroral ovals. These areas are characterised by intense small-scale ionospheric inhomogeneities that exist in both calm and disturbed geomagnetic conditions. Such irregularities could result in radio wave scattering, GNSS (global navigation satellite system) positioning quality deterioration, failures in radio communication, etc. GNSS ROTI (rate of total electron content index) datasets along with other datasets are available to study complex dynamics of ionospheric irregularities. This report analyses the auroral oval dynamics datasets, based on GNSS global network, coherent radars data, and satellite data. The SIMuRG system (https://simurg.iszf.irk.ru/) is employed. The auroral oval regions corresponds to high values of ROTI, therefore it is possible to separate their location from mid-latitude data. Coherent scatter radars record signal scattering from the oval boundary. The SuperDARN-like radars located in Russia were employed. Satellite data shows sharp variations in field-aligned currents. During magnetic storms the oval expands equatorward, and small-scale irregularities shifts to mid-latitudes. All the data show close positions of the oval boundary. The latter makes it possible to use the datasets of different modalities to estimate the oval boundary. Some advance was achieved by computer vision techniques to find the auroral oval boundary in the Northern hemisphere. The techniques implemented mathematical morphology to expand data and decrease data gaps, Otsu techniques and K-means to cluster image data.

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Mixed generalized multiscale finite element method for flow problem in thin domains

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In this work, we consider the construction of the Mixed Generalized Multiscale Finite Element Method approximation on a coarse grid for an elliptic problem in thin two-dimensional domains. We consider the elliptic equation with homogeneous boundary conditions on the domain walls. For reference solution of the problem, we use a Mixed Finite Element Method on a fine grid that resolves complex geometry on the grid level. To construct a lower dimensional model, we use the Mixed Generalized Multiscale Finite Element Method, where we present the construction of the multiscale basis functions for velocity fields. The construction is based on the definition of the local snapshot space that takes all possible flows on the interface between coarse cells into account. In order to reduce the size of the snapshot space, we solve a local spectral problem. We present a convergence analysis of the presented multiscale method. Numerical results are presented for two-dimensional problems in three testing geometries along with the errors associated to different number of the multiscale basis functions used for velocity field. Numerical investigations are conducted for problems with homogeneous and heterogeneous properties respectively.

Multiscale mathematical modeling of the seepage into the soil under cryolithozone conditions

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In this work, the numerical modelling of fluid seepage in the presence of permafrost in heterogeneous soils is considered. The multiphysics model consists of the coupled Richards' equation and the Stefan problem. These problems often contain heterogeneities due to variations of soil properties. In the paper, we design a multiscale simulation method based on Generalized Multiscale Finite Element Method (GMsFEM). For this reason, we design coarse-grid spaces for this multiphysics problem and design algorithms for solving the overall problem. Numerical simulations are carried out on two-dimensional and three-dimensional model problems. For the case of a three-dimensional, somewhat realistic geometry with a complex surface structure is considered. We demonstrate the efficiency and accuracy of the proposed method using several representative numerical results.

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Generalized Multiscale Finite Element Method for the poroelasticity problem in multicontinuum media

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In this paper, we consider a poroelasticity problem in heterogeneous multicontinuum media that is widely used in simulations of the unconventional hydrocarbon reservoirs and geothermal fields. Mathematical model contains a coupled system of equations for pressures in each continuum and effective equation for displacement with volume force sources that are proportional to the sum of the pressure gradients for each continuum. To illustrate the idea of our approach, we consider a dual continuum background model with discrete fracture networks that can be generalized to a multicontinuum model for poroelasticity problem in complex heterogeneous media. We present a fine grid approximation based on the finite element method and Discrete Fracture Model (DFM) approach for two and three-dimensional formulations. The coarse grid approximation is constructed using the Generalized Multiscale Finite Element Method (GMsFEM), where we solve local spectral problems for construction of the multiscale basis functions for displacement and pressures in multicontinuum media. We present numerical results for the two and three dimensional model problems in heterogeneous fractured porous media. We investigate relative errors between reference fine grid solution and presented coarse grid approximation using GMsFEM with different numbers of multiscale basis functions. Our results indicate that the proposed method is able to give accurate solutions with few degrees of freedoms.

A generalized multiscale finite element method for neutron transport problems in SP3 approximation

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The SP3 approximation of the neutron transport equation allows improving the accuracy for both static and transient simulations for reactor core analysis compared with the neutron diffusion theory. Besides, the SP3 calculation costs are much less than higher order transport methods (SN or PN). Another advantage of the SP3 approximation is a similar structure of equations that is used in the diffusion method. Therefore, there is no difficulty to implement the SP3 solution option to the multi-group neutron diffusion codes.

In this paper, we attempt to employ a model reduction technique based on the multiscale method for neutron transport equation in SP3 approximation. The proposed method is based on the use of a generalized multiscale finite element method (GmsFEM). The main idea is to create multiscale basis functions that can be used to effectively solve on a coarse grid. From calculation results, we obtain that multiscale basis functions can properly take into account the small-scale characteristics of the medium and provide accurate solutions. The application of the SP3 methodology based on solution of the lambda-spectral problems has been tested

for the some reactor benchmarks. The results calculated with the GMsFEM are compared with the reference transport calculation results.