

INSTITUTE OF COMPUTATIONAL MATHEMATICS
AND MATHEMATICAL GEOPHYSICS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

International conference
ADVANCED MATHEMATICS, COMPUTATIONS
AND APPLICATIONS – 2014

ABSTRACTS



June 8-11, 2014
Akademgorodok, Novosibirsk, Russia

УДК 519.6
ББК 22.19

Abstracts. The International conference "Advanced mathematics, computations and applications – 2014". Institute of Computational Mathematics and Mathematical Geophysics of Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia. June 8–11, 2014. Novosibirsk: Academizdat, 2014. 122 p.

ISBN 978-5-9904865-8-4

The International conference on advanced mathematics, computations and applications (AMCA'14) is dedicated to the 50th anniversary of the Institute of computational mathematics and mathematical geophysics (the former Computing Center) of Siberian branch of the Russian Academy of sciences (ICM&MG SB RAS), founded by academician G. I. Marchuk. The goal of this conference is to bring together well-known experts involved in numerical analysis, applied mathematics, computational technologies, challenging applications and to discuss the topical issues facing the mathematical community.

The topics of AMCA'14 are the four major areas of interest of the ICM&MG SB RAS:

- numerical analysis,
- applied mathematics and mathematical modeling,
- parallel and distributed computations,
- information systems.

The topics of "AMCA'14" include, but are not limited to the following: computational algebra, numerical solution of differential and (or) integral equations, computational geophysics, inverse problems, statistical modeling and Monte Carlo methods, high performance computing, advanced problems in scientific programming, data-intensive processing and communications.

The conference is supported by the Russian Foundation for Basic Research,
grant 14-01-06038

Platinum sponsor	Gold sponsor	Silver sponsors	Partners of the conference
IBM Corporation	Hewlett-Packard Corporation	NVIDIA Corporation Schlumberger Corporation RSC Group	LEDAS Company Nonolet Company Novosibirsk Institute of Program Systems Center RITM Company

Informational support:

“Poisk” newspaper
“Science in Siberia” newspaper

The web-site of the conference: <http://conf.nsc.ru/amca14>

ISBN 978-5-9904865-8-4

PROGRAM COMMITTEE

Chairman

B. G. Mikhailenko (ICM&MG SB RAS, Novosibirsk, Russia)

Vice-chairmen

S. I. Kabanikhin (ICM&MG SB RAS, Novosibirsk, Russia)

Y. A. Kuznetsov (University of Houston, Houston, USA)

V. V. Shaidurov (The Institute of Computational Modeling SB RAS, Krasnoyarsk, Russia)

Secretary M. A. Boronina (ICM&MG SB RAS, Novosibirsk, Russia)

Members

S.M. Abramov	Moscow, Russia	T. Liu	Beijing, China
P. Bjørstad	Bergen, Norway	V.E. Malyshkin	Novosibirsk, Russia
S. Brenner	Baton Rouge, USA	A.G. Marchuk	Novosibirsk, Russia
B.N. Chetverushkin	Moscow, Russia	S.B. Medvedev	Novosibirsk, Russia
N. T. Danaev	Almaty, Kazakhstan	G.A. Mikhailov	Novosibirsk, Russia
J. Dongarra	Oak Ridge, USA	M. Pagano	Pisa, Italy
V.P. Dymnikov	Moscow, Russia	V.V. Penenko	Novosibirsk, Russia
M.I. Epov	Novosibirsk, Russia	O. Pironneau	Paris, France
Y.L. Ershov	Novosibirsk, Russia	V.K. Popkov	Novosibirsk, Russia
M.P. Fedoruk	Novosibirsk, Russia	V.G. Romanov	Novosibirsk, Russia
A.M. Fedotov	Novosibirsk, Russia	K.K. Sabelfeld	Novosibirsk, Russia
V.M. Fomin	Novosibirsk, Russia	R.M. Shagaliev	Sarov, Russia
B.M. Glinsky	Novosibirsk, Russia	M. Shashkov	Los Alamos, USA
R. Glowinski	Houston, USA	G.I. Shishkin	Ekaterinburg, Russia
S.K. Godunov	Novosibirsk, Russia	Y.I. Shokin	Novosibirsk, Russia
S.S. Goncharov	Novosibirsk, Russia	V.M. Sveshnikov	Novosibirsk, Russia
V.P. Ilin	Novosibirsk, Russia	T. Tang	Hong Kong, China
M.N. Kalimoldaev	Almaty, Kazakhstan	E.E. Tyrtshnikov	Moscow, Russia
N.A. Kolchanov	Novosibirsk, Russia	P. N. Vabishchevich	Moscow, Russia
A.N. Konovalov	Novosibirsk, Russia	V.V. Voevodin	Moscow, Russia
V.I. Kostin	Novosibirsk, Russia	Y.S. Volkov	Novosibirsk, Russia
L.A. Krukier	Rostov-on-Don, Russia	V.A. Vshivkov	Novosibirsk, Russia
V.I. Kuzin	Novosibirsk, Russia	M. Wheeler	Austin, USA
M.M. Lavrentiev	Novosibirsk, Russia	O. Widlund	New York, USA
Y.M. Laevsky	Novosibirsk, Russia	J. Xu	University Park, USA
R. Lazarov	College Station, USA		

ORGANIZING COMMITTEE

Chairman B.G. Mikhailenko (ICM&MG SB RAS, Novosibirsk)

Vice-chairmen (ICM&MG SB RAS, Novosibirsk, Russia) V. P. Ilin, S. I. Kabanikhin, V. V. Kovalevsky

Secretary L. V. Vshivkova (ICM&MG SB RAS, Novosibirsk)

Members (ICM&MG SB RAS, Novosibirsk, Russia)

A. V. Burmistrov, I. G. Chernykh, B. M. Glinsky, Y. L. Gurieva, K. K. Imomnazarov, I. N. Ivanova, S. E. Kireev, S. N. Kosova, I. M. Kulikov, M. A. Marchenko, A. V. Penenko, A. V. Petukhov, O. D. Sokolova, A. G. Usov, O. G. Zavarzina, Y. M. Zybarev.

INVITED PLENARY TALKS

Multiscale coarse spaces and domain decomposition methods for problems with discontinuous coefficients

P.E. Bjørstad

In this talk, we first provide some motivating examples of a frequently discussed model problem characterized by having a highly discontinuous coefficient.

Next, we discuss how iterative methods based on domain decomposition, may be seen as an extension of some multi-scale algorithms that have gained acceptance in industrial applications.

We proceed with a discussion of multi-scale coarse spaces and how they help achieve robustness and better convergence properties of the overall domain decomposition methods. We outline the key steps in a convergence analysis based on the standard additive Schwarz framework. The analysis offers some new, improved results, but also reveals limitations of this class of methods.

We briefly discuss an alternative, incorporating eigenmodes in an adaptive way in order to better tailor the method to the actual problem at hand. We end by discussing several numerical examples that highlight some of the methods that have been considered.

Joint work with Atle Loneland and Du Rui, all in Bergen Norway.

Rate optimality of adaptive algorithms

C. Carstensen

The Four axioms (A1) – (A4) link estimators and distance functions on a set of admissible refinements together and imply optimality of a standard finite element routine on an abstract level with a loop: solve, estimate, mark, and refine. The presentation provides proofs and examples of the recent review due to C. Carstensen, M. Feischl, M. Page, and D. Praetorius: The axioms of adaptivity, *Comput. Math. Appl.* 67 (2014)1195–1253 and so discusses the current literature on the mathematics of adaptive finite element methods. The presentation concludes with an overview over several applications of the set of axioms.

Implicit iterative algorithms for solving Navier – Stokes difference equations

N.T. Danaev

This report describes new approaches to finding a solution of auxiliary difference equations, arising from the use of splitting schemes for Navier – Stokes equations in "velocity, pressure" variables and theorems on the convergence rate of considered iterative algorithms are proven. For stationary Navier – Stokes equations in "velocity, pressure" variables new iterative schemes are proposed, for which it is shown that in the case of a linear Stokes problem convergence rate does not depend on the number of nodes of a finite-difference grid. For incompressible fluid equations in "stream function, vorticity" variables mathematical issues of stability, convergence and numerical implementation of two-dimensional differential problem, defined on a symmetric pattern of the finite-difference grid are studied with method of a priori estimates. Approximate boundary conditions for the vorticity are chosen as Tom's and Woods formulas. In case of a linear Stokes problem, considered various numerical implementation algorithms for which convergence rates are obtained. In case of non-linear Navier – Stokes equations estimations of the convergence of the problem solution to the differential problem solution and the estimation of the convergence of considered iterative algorithm are obtained under condition equivalent to condition of the uniqueness of nonlinear difference problem.

Results of the numerical experiment are provided.

Modeling of the Earth System

V.P. Dymnikov, V.N. Lykosov, V.B. Zalesny, V.Ya. Galin, E.M. Volodin, A.V. Glazunov, A.S. Gritsun, N.A. Dianski, M.A. Tolstykh, N.G. Iakovlev, A.V. Gusev, S.V. Kostrykin, D.V. Kulyamin, R. Yu. Fadeev, V.V. Shashkin

The report is devoted to a problem of mathematical modeling of the Earth System, which includes such components, as the atmosphere, ocean, land, cryosphere (continental and sea ices, permafrost) and the biosphere. Dynamics of the Earth System is regulated by physical, chemical, biological and other processes that demands interdisciplinary approaches at its research. In the report the main attention is paid to three global aspects of this problem: the supercomputer numerical technologies based on modern methods of applied mathematics; the description of processes taking place in the system, explicitly at the scales resolved by model, and in the parametrized way – at subgrid scales; mathematical questions (methods of the theory of dynamic systems and the sensitivity problem). The results received with climatic model of the Institute for Numerical Mathematics of the Russian Academy of Sciences (INM RAS) within the international project of comparison of such models (reproduction of modern climate and an assessment of its possible changes in the future) and with an operational weather forecasting model of INM RAS/Russian Hydrometeorological Center (including, at a seasonal scale) are presented. Finally, perspectives of further development of models of the Earth System for investigation of fundamental problems of its dynamics and for practical applications are considered.

Современный подход к математическому моделированию процесса сварки металлов взрывом

С.К. Годунов

В докладе будет представлен обзор результатов, полученных к настоящему времени в задаче о моделировании процесса волнообразования при сварке взрывом, задаче, активно изучавшейся в СО РАН начиная с начала 60-х годов прошлого века.

Задача по существу распадается на выбор уравнений, моделирующих процесс, и проведение расчетов, основанных на этом выборе с дальнейшим сравнением результатов расчетов и натуральных экспериментов. На самом деле надо иметь ввиду, что пока это только прикидочные расчеты, которые должны быть в дальнейшем дополнены аккуратным подбором коэффициентов в использованных уравнениях состояния на основе прецизионных экспериментов. Важно также аккуратно сформулировать область применимости разрабатываемых моделей.

В поле зрения автора доклада и его соавторов были две возможные модели явления. Одна основывалась на применении расширенной теории упругости, в которую включались пластические деформации, возникающие при больших касательных напряжениях и переход пластического состояния среды в жидкое в определенной области температур и нормальных напряжений. Эта модель разрабатывалась в Институте математики СО РАН и ИВМиМГ СО РАН. Вторая модель, основанная на методе молекулярной динамики, разрабатывалась в ИТПМ СО РАН. Все работы по моделированию велись при активном участии экспериментаторов из Института гидродинамики СО РАН.

В докладе будет достаточно подробно описана использованная упруго-пластическая модель и результаты расчетов, выполненных на ее основе, а также приведено сравнение этих результатов с расчетами, проведенными по методу молекулярной динамики и с реальными экспериментами.

Литература

1. Годунов С.К., Киселев С.П., Куликов И.М., Мали В.И. Численное и экспериментальное моделирование образования волн при сварке взрывом // Труды Матем. Ин-та им. В.А. Стеклова. 2013. Т. 281. С. 16–31.
2. Годунов С.К., Пешков И.М. Термодинамически согласованная нелинейная модель упругопластической среды Максвелла // ЖВММФ. 2010. Т. 50, № 8. С. 1481–1498.
3. Годунов С.К., Пешков И.М. Симметрические гиперболические уравнения нелинейной теории упругости // ЖВММФ. 2008. Т. 48, № 6. С. 1034–1055.
4. Киселев С.П., Мали В.И. Численное и экспериментальное моделирование образования струи при высокоскоростном косом соударении металлических пластин // ФГВ. 2012. Т. 48, № 2. С. 100–112.
5. Киселев С.П. Численное моделирование методом молекулярной динамики деформации пластин при их косом соударении // Физическая мезомеханика. 2013. Т. 16, № 3. С. 45 – 53.

6. Grignon F., Benson D., Vecchio K.S., Meyers M.A. Explosive welding of aluminum to aluminum: analysis, computations and experiments // Intern. J. of Impact Engineering. 2004. Vol. 30, I. 10. P. 1333–1351.

7. Wang X. et al. Numerical study of the mechanism of explosive/impact welding using Smoothed Particle Hydrodynamics method // Materials & Design. 2012. Vol. 35. P. 210– 219.

GPU computing for systems biology

G. Mauri

The analysis of dynamical properties of biological systems in physiological and perturbed conditions usually requires the execution of a large number of simulations, which generally results in prohibitive running times. The use of GPGPU as massively parallel processors can offer a substantial help in this direction, providing power-efficient high-performance computing at a relatively low cost.

With the goal of offering to researchers in life sciences efficient and easy to use simulation tools, we developed GPU-powered implementations [1-5] for parameter estimation, parameter sweep analysis, sensitivity analysis, reverse engineering of biochemical networks, which can rely either on numerical integration methods or stochastic simulation algorithms.

References

1. M.S. Nobile, D. Besozzi, P. Cazzaniga, G. Mauri, D. Pescini. cupSODA: a CUDA-powered simulator of mass-action kinetics. Proc. of 12th Int. Conf. on Parallel Computing Technologies (PaCT 2013) (V. Malyskin, ed.), LNCS 7979, 344-357, 2013.

2. M.S. Nobile, P. Cazzaniga, D. Besozzi, G. Mauri. GPU-accelerated simulations of mass-action kinetics models with cupSODA. Journal of Supercomputing, submitted.

3. M. Bellini, D. Besozzi, P. Cazzaniga, G. Mauri, M.S. Nobile. Simulation and analysis of the blood coagulation cascade accelerated on GPU. PDP2014 - Special Session "Advances in High-Performance Bioinformatics, Systems and Synthetic Biology", 12-14 February 2014, Torino, Italy.

4. P. Cazzaniga, M.S. Nobile, D. Besozzi, M. Bellini, G. Mauri. Massive exploration of perturbed conditions of the blood coagulation cascade through GPU parallelization. BioMed Research International, submitted.

5. M.S. Nobile, P. Cazzaniga, D. Besozzi, D. Pescini, G. Mauri. cuTauLeaping: a GPU-powered tau-leaping stochastic simulator for massive parallel analyses of biological systems. PLOS ONE, in press.

Direct and inverse problems of geophysics

B.G. Mikhailenko, S.I. Kabanikhin

The main goal of Geophysics is to solve inverse problem, i.e. to find the structure and properties of the Earth (atmosphere, hydrosphere and lithosphere) using some information about geophysical processes (seismic, electromagnetic, acoustic and others). But the main tool of Geophysics is the direct (forward) problems, i.e., numerical modelling of geophysical processes while the structure and properties are supposed to be known. We will discuss both direct and inverse problems (theory and numeric) and describe several new algorithms of numerical solution.

The errors of standard biased estimates in Monte Carlo method

G.A. Mikhailov, G.Z. Lotova

The collisional model of transfer process with acceleration in external force field is considered. The time steps are used in numerical-statistical modeling of a particle free path. In this work the new estimate of the corresponding deterministic relative error is constructed. It allows to choose the suitable step value.

The standard statistical "local estimates" of particle flux density are biased when the contribution of collisions in "local sphere" with small radius is excluded to perform the variance finiteness. In the report the practical efficient estimates of corresponding relative error are presented.

We suppose that the sample statistical ensemble has "poisson" behavior. In this assumption the uniformly optimal partition for functional estimates of the histogram type is constructed. It appeared that the deterministic error is close to the statistical one.

The work was supported by grants of RFBR №№ 13-01-00746, 12-01-00727, 12-01-00034, 13-01-00441, 12-05-00169 and grant HIII-5111.2014.1.

A space-time finite element method for PDEs posed on evolving surfaces

M.A. Olshanskii

Partial differential equations posed on surfaces arise in mathematical models for many natural phenomena: diffusion along grain boundaries, lipid interactions in biomembranes, pattern formation, and transport of surfactants on multiphase flow interfaces to mention a few. Numerical methods for solving PDEs posed on manifolds recently received considerable attention. In this talk we briefly review some existing approaches and focus on an Eulerian finite element method for the discretization of elliptic and parabolic partial differential equations on surfaces. The method uses traces of volume finite element space functions on a surface to discretize equations posed on the surface. The approach is particularly suitable for problems in which the surface is given implicitly by a level set function and in which there is a coupling with a problem in a fixed outer domain. If the surface evolves, then the method employs DG space-time finite elements for a space-time weak formulation of a surface PDE problem. In this case, trial and test surface finite element spaces consist of traces of standard volumetric elements on a space-time manifold resulting from the evolution of a surface. We present an error analysis, a posteriori estimates, adaptivity, and discuss algebraic properties of the method.

A problem of a determination of coefficients in viscoelasticity equations

V.G. Romanov

An inverse problem of recovering coefficients and kernels of integral operators is studied for integro-differential equations of viscoelasticity. It is supposed that supports of unknown functions are contained inside a compact domain. A series of direct problems for which a pulse source is located at a point y , that belongs to the boundary of the domain, is considered. The point y is a parameter of the problem. A given information on a solution of the direct problem is the trace of the solution to Cauchy problem with zero initial data on the boundary of the domain for all possible y and a finite time interval. Main results of this paper are uniqueness theorems for the problem under consideration.

The work is partially supported by RFBR under grant 14-01-00208.

Semi-lagrangian approach in finite element method for Navier – Stokes equations of viscous heat-conducting gas

V.V. Shaydurov, G.I. Shchepanovskaya, M.V. Yakubovich

The algorithm is proposed for numerical solving the Navier – Stokes equations for two-dimensional motion of viscous heat-conducting gas. The discretization of equations is performed by a combination of a special semi-lagrangian method for transport derivatives and the finite element method with piecewise linear basis functions for other terms. The results of numerical studies of the structure of a supersonic flow around an obstacle for a wide range of Mach numbers and Reynolds numbers will be presented. Velocity and pressure fields and the vortex structure of flow are studied in the circulation area of the obstacle.

Current situation and present-day tasks in the development of national supercomputing technologies

R.M. Shagaliev, A.S. Kozelkov

As evidenced by the worldwide practice, today supercomputing technologies belong to the most critical factors governing the rate of development and competitiveness of strategic industries.

FSUE RFNC-VNIIEF occupies leading positions in Russia in the design and development of national supercomputing technologies and their practical application in high-tech industries.

The paper presents the key results in the design and development of the basic product line of supercomputers, the provision of computing resources to Russian companies, and the development of national software for supercomputer-based simulations, pilot versions of virtual models of complex engineering systems in the aircraft industry, nuclear power, car manufacturing, and aerospace engineering. Examples of above industry-specific practical simulations using the software developed are provided.

In conclusion, the paper summarizes current tasks in the development of national supercomputing technologies for high-tech industries that need to be addressed nowadays by the scientific and engineering community of Russia.

Development of the method of minimal residuals

E.E. Tyrtysnikov

We consider prerequisites of the GMRES as a method of minimization of the residual on the Krylov subspaces generated by a given nonsingular matrix and by initial residual, the optimality results and convergence estimates starting from the pioneering paper [1], and some recent developments including the convergence theory for special classes of matrices [2, 3].

The work is supported by the RFBR grant 14-01-00804.

References

1. G. I. Marchuk, Yu. A. Kuznetsov, Iterative methods and quadratic functionals (in Russian). Translated as *Methodes iteratives et fonctionnelles quadratiques*, in *Sur les methodes numeriques en sciences physique et economique*, J. Kraus and U. Langer, eds., Nauka, Novosibirsk, Dunod, Paris, 1972, 1974, pp. 3-132.
2. B. Beckermann, S. A. Goreinov, E. E. Tyrtysnikov, Some remarks on the Elman estimate for GMRES, *SIMAX*, Vol. 27, Issue 3 (2006), 772-778.
3. E. E. Tyrtysnikov, N. L. Zamarashkin, A. Yu. Yeremin, Clusters, preconditioners, convergence, *Linear Algebra Appl.*, 263 (1997), pp. 25-48.

Monotone finite volume discretizations of the diffusion and convection-diffusion equations on polyhedral meshes

Yu.V. Vassilevski

We consider two approaches to the design of a monotone cell-centered finite volume discretization of the steady diffusion and convection-diffusion equations. The diffusion tensor may be heterogeneous, full and essentially anisotropic. The convection-diffusion operator may have the dominated convection part. The conformal computational mesh is assumed to consist of convex polygonal or polyhedral cells. The schemes possess the minimal stencil containing the closest neighboring cells only. The cornerstone of the approaches is the nonlinear discretization of diffusion and advection fluxes derived on faces of mesh cells. The first approach [1,2,3,4] is based on the two-point diffusion fluxes and preserves non-negativity of the differential solution. The second approach [5] uses the multi-point diffusion fluxes and provides the discrete maximum principle.

References

1. Lipnikov K., Svyatskiy D., Vassilevski Yu. Interpolation-free monotone finite volume method for diffusion equations on polygonal meshes. *J.Comp.Phys.*, 2009, 228: 703-716.
2. Lipnikov K., Svyatskiy D., Vassilevski Yu. A monotone finite volume method for advection-diffusion equations on unstructured polygonal meshes. *J.Comp.Phys.*, 2010, 229: 4017-4032.
3. Danilov A., Vassilevski Yu. A monotone nonlinear finite volume method for diffusion equations on conformal polyhedral meshes. *Russian J. Numer. Anal. Math. Modelling*, 2009, 24: 207-227.
4. Nikitin K., Vassilevski Yu. A monotone nonlinear finite volume method for advection-diffusion equations on unstructured polyhedral meshes in 3D. *Russian J. Numer. Anal. Math. Modelling*, 2010, 25: 335-358.
5. Lipnikov K., Svyatskiy D., Vassilevski Yu. Minimal stencil finite volume scheme with the discrete maximum principle. *Russian J. Numer. Anal. Math. Modelling*, 2012, 27: 369-385.

Supercomputers, steam locomotives and atomic stations

V. V. Voevodin

It is widely recognized that capabilities of modern supercomputers are great but their efficiency on a huge range of applications is very low. What are the reasons? Unfortunately, there can be dozens of reasons of performance degradation and we need to analyze a supercomputer environment very thoroughly to detect root causes. The main trend of the last years is unprecedented growth in the number of components in supercomputers. Number of cores, processors, compute nodes, memory modules, ports, cables, fans,

sensors, and etc. is enormous and each component can be potentially a reason of low efficiency. How to detect failures, bottlenecks and efficiency losses on time? How to increase ROI in supercomputing centers? How to control myriads of hardware and software components? All these questions are important today in the post-petascale era.

Ensuring the effectiveness of the largest supercomputing center in Russia we have developed a concept of holistic monitoring and total control over supercomputer infrastructures, and this is the only way of living in the extremely parallel computing world in future.

Section 1. NUMERICAL METHODS OF SOLVING DIFFERENTIAL AND INTEGRAL EQUATIONS

Thermodynamically compatible hyperbolic conservative model of compressible multiphase flow

A.A. Belozerov, E.I. Romenski, I.M. Peshkov

Computational modeling of compressible multiphase flows is of a great interest in environmental sciences and industry. Nevertheless most publications on this topic deal with mathematical and numerical aspects for two-phase flow whilst multiphase case consideration is quite rare. We present a new model of multiphase compressible flow generalizing the two-phase model proposed in (Romenski et al., J. Sci. Comput. 2010) to arbitrary number of phases. The design of the model is based on the thermodynamically compatible systems theory which allows us to derive compressible multiphase flow governing equations as a hyperbolic system of conservation laws. A model is formulated and numerical method is developed for the case of arbitrary number of phases taking into account dissipative processes of interfacial friction and phase pressures relaxation. The MUSCL-Hancock method in conjunction with the GFORCE flux is used for solving of governing equations of the model and numerical results for some test problems are presented.

The uniform boundedness families Galerkin projectors and the convergence of algorithms posteriori adaptation for the elliptic singular perturbed boundary value problems

I.A. Blatov, U.I. Shustikova

The study of uniform boundedness families Galerkin projection underlies evidence asymptotically best possible error estimates in different projection methods, including non-Hilbert norms. The report presents the results of the uniform boundedness in C-norm Galerkin projections for singularly perturbed elliptic boundary value problem with an exponential boundary layer domain with smooth curvilinear boundary using meshes and Shishkin piecewise smooth finite elements of the first order. The results are applied to prove the convergence of algorithms posteriori adaptation of the computational grid. The results of numerical experiments are presented.

Numerical solution of unsteady advection-diffusion equation on unstructured grids

V.V. Churuksaeva, A.V. Starchenko

Obtaining the solution of convection-diffusion equation is an important part of calculating the contaminant dispersion in the environment (atmosphere or water stream). To describe processes occurring in nature, as a rule, it is necessary to obtain a solution in the field of complex geometry so as unstructured grids become preferable.

This paper presents the results of numerical solution of contaminant dispersion in the atmosphere which can be mathematically described by the Neumann problem for the two-dimensional unsteady convection-diffusion equation on unstructured triangular meshes. Numerical methods for solving stated problem have been obtained using the finite volume method on several types of unstructured grids.

Computational example of momentary point source has been carried out for investigation and applying established models. Results of computational experiments showed consistency with the exact numerical.

On some algorithm for the numeric solution of linear partial differential-algebraic equations of high index

S.V. Gaidomak

The linear differential-algebraic system of partial differential equations of the first order of mixed type (hyperbolic and parabolic) is considered. It is assumed that the pencil matrix-functions of the system under consideration is a regular in the domain of definition and has a special form. Maximal multiplicity of the zero and infinite eigenvalues of matrix pencil define the index of differential-algebraic systems. The

problem is that the high index of the system do not allow to apply classic methods for numerical solving it. The new algorithm for the numerical solving of the considered systems with a high index is proposed.

The asymptotic expansion of the transversal correlation function for isotropic turbulence

V.N. Grebenev, A.N. Grishkov, M. Oberlack

The behavior of the correlation functions presents significant interests for the theory of turbulence since this leads to various types of the so-called integral invariants. Loitsyansky and Birkhoff integrals are most famous integral invariants. We present the asymptotic behavior of the transversal correlation function for large values of the correlation distances for the geometry of the correlation space determined by the two-point velocity correlation tensor in the case of homogeneous isotropic turbulence. The question about the asymptotic expansion of the correlation functions in the physical space with the standard Euclidian metric is still open. The asymptotic expansion obtained is based on the algebraic constructions as in Conformal Field Theory. This construction is associated with a nontrivial central extension of the infinite-dimensional Lie algebra of conformal transformations in the corresponding Riemannian space. Here a central charge measures the so-called internal degrees of freedom of the system and is defined by the same bilinear skew-symmetric form as for the Witt algebra.

Boundary layer phenomena in the theory of singularly perturbed ordinary differential equations

G.M. Kenenbaeva

Various "phenomena" and "effects" can arise when known conditions of "existence, uniqueness and stability of the solution" of the corresponding degenerate equation (system) of singularly perturbed equation (system) do not hold, including phenomena of computational splitting, stretching singular cycle, [1]. The last one is a base for more delicate ones such as "deeping splash". In general, we call phenomena arising in neighborhood of a fixed point in the domain of unknown functions "boundary layer ones". We proposed framework definitions of these notions [2] and found necessary conditions of their occurrence. We are going to propose definitions and find sufficient conditions of arising new types of boundary layers.

References

1. Imanaliev M.I., Pankov P.S., Kenenbaeva G.M. (in Russian) (2004) Phenomenon of deeping boundary layer in the theory of singularly perturbed ordinary differential equations. Studies in integro-differential equations, issue 33, pp. 15-18.
2. Kenenbaeva G.M. (2012). Theory and methodic of searching new effects and phenomena in the theory of perturbed differential and difference equations (in Russian). "Ilim", Bishkek, 203 p.

Optimum splitting algorithms for numerical solution of Euler and Navier – Stokes equations

V. M. Kovenya

Efficient finite difference and finite volume algorithms based on predictor–corrector and factorization methods for numerical solution of equation Euler and Navier – Stokes viscose compressible heat-conducted gas are described. Special splitting procedure over physical processes and the spatial directions is introduced at the predictor stage. It allows using scalar tridiagonal matrix algorithm to solve equations at fractional steps. Algorithms conservatism is restored at the corrector stage that guarantee fulfillment of integral laws. The results of flow of viscous gas in the flat channel with gas injection from a part of its surface and the results of flow around a body with complicated configuration modeling flow in the inlet are also given. Calculations of a supersonic flow of the cylinder with a needle are carried out. The mode of the pulsation flow observed in experiments is received.

Работа выполнена при частичной финансовой поддержке Российского фонда фундаментальных исследований (код проекта 14-01-00191) и интеграционных проектов СО РАН № 76 и 130

On real accuracy of WENO schemes at shock capturing calculations

O.A. Kovyrkina, A.N. Kudryavtsev, V.V. Ostapenko

The paper proposes a method which allows to estimate the accuracy of approximation of the Rankine-Hugoniot conditions through the shock wave front by shock capturing schemes. The method concerns the calculation of the order of integral convergence of a finite-difference solution itself (as opposed to using its absolute value as in the norm L_1) on the intervals crossing the shock. In such integration the error arising in front of the shock due to its smearing, can be compensated by the similar error of the opposite sign after the front. Provided examples demonstrate that this approach allows to obtain a high order of integral convergence on the intervals crossing the shock for some of the classical non-monotone difference schemes (e. g., the Rusanov scheme). In the present work it is also shown that the order of integral convergence of WENO schemes is reduced to the first one on intervals crossing the shock regardless of their accuracy for smooth solutions.

The study was carried out with the support of the Council on Grants of the Presidium of the Russian Academy of Sciences for the Support of Young Scientists (grant MK-3477.2013.1).

A new class of solutions of Yang – Mills equations

N.G. Marchuk

Yang–Mills equations are used in Standard Model of elementary particles for description of electroweak and strong interactions. Consider an eigenvalue problem for the Yang – Mills operator. We've found one nonzero eigenvalue and corresponding eigenvector for the Yang – Mills operator. On this basis we present a new class of gauge invariant solutions of the Yang – Mills equations.

On invariant manifolds for some equations of hydrodynamic type (AMCA'14), June 8-11, 2014, Akademgorodok, Novosibirsk, Russia

S.B. Medvedev

Few examples of exact invariant manifolds for some equations of hydrodynamic type are present. Also there are discussed non-existence of invariant manifolds and invariant formulation for some types of motions.

Multigrid techniques in computational fluid dynamics

G. V. Muratova, L. A. Krukier, E.M. Andreeva

We present some aspects of applying Multigrid techniques in computational fluid dynamics (CFD). The fundamental basis of almost all CFD problems are the Navier – Stokes equations, which define any single-phase (gas or liquid, but not both) fluid flow. The other most common equation in the computational fluid dynamics field is the convection-diffusion equation. Mathematical models that involve a combination of convective and diffusive processes are among the most widespread in all the sciences. Research of these processes is especially important and difficult when convection is dominant. Some approaches for solving Navier – Stokes equations and convection-diffusion problems by MGM are considered. For the Navier – Stokes equations it has been shown that by mixing the method of characteristics and the finite element method we are able to obtain first and second order accurate conservative schemes of the upwinding type. We suggest modification of MGM with special iterative methods as smoothers for convection-diffusion problems with dominant convection.

An integration algorithm for moderately stiff problems with using stages of the Dormand – Prince method

E. A. Novikov, A. E. Novikov

Solving of stiff high-dimensional problems demands using algorithms, based on explicit numerical schemes. Integration algorithms, based on implicit or semi-explicit methods usually use decomposition of

the Jacobi matrix. In this case, a decomposition is a separate time-consuming problem. In such a situation it is preferable to use algorithms, based on explicit formulas, if stiffness of a problem allows to obtain an approximation to a solution for a reasonable time. Usually an algorithm for control of step of integration is based on accuracy control of a numerical scheme. It is natural, because the main criterion in calculations is accuracy of a solution. However, applying of integration algorithms, based on explicit formulas leads to loss of efficiency and reliability. This is due to the fact that in a settling area of a solution a contradiction between accuracy and stability leads to large amount of additional calculations of a solution and a step is chosen significantly less than the maximum allowable. It can be avoided by using control of stability of the numerical scheme. Here an inequality for stability control for the Dormand – Prince method of eighth order of accuracy is constructed. A first-order method with an enhanced stability region, based on first seven stages is constructed. Numerical results confirming increase of efficiency due to using alternating order are given.

This work was supported RFBR (project 14-01-00047).

Numerical method for the elasticity problems in the domain with reentrant corner

V.A. Rukavishnikov, S.G. Nikolaev

It is known that the speed of convergence of the classical finite element solution to the Lamé system in the domain with the reentrant corner on the boundary depends on the corner's size and is always less than one. Mesh refinement near the singular point, decomposition of the solution into regular and singular components, and other special techniques of increasing convergence rate lead to the "deterioration" of the stiffness matrix of the linear equations system.

We develop the weighted finite element method for the boundary value elasticity problem with changing of the boundary conditions kind posed in the two-dimensional domain with reentrant corner greater than $3\pi/2$. The rate of convergence of this method in the norm of the weighted Sobolev space $W_{2,\nu}^1(\Omega)$ does not depend on the corner's size and equals $O(h)$.

For this, the notation of the R_ν -generalized solution is introduced for the posed problem. It is proved that this solution exists and is unique in the special weighted Sobolev set. Results of the numerical experiments confirm high efficiency of the constructed method.

Solution stability of a standard difference scheme in the presence of computer perturbations for a singularly perturbed convection-diffusion problem

G.I. Shishkin (Invited talk)

A Dirichlet problem approximated by the standard monotone finite difference scheme on the uniform grid is considered for a singularly perturbed ordinary differential convection-diffusion equation with the perturbation parameter ε ($\varepsilon \in (0, 1]$), multiplying the highest-order derivative. We study stability of the grid solutions in the presence and absence of computer perturbations. Results of numerical experiments are considered that illustrate the theoretical results.

This research was supported by the Russian Foundation for Basic Research under grant No.13-01-00618.

Теория переноса излучения и освоение космического пространства (история и перспективы)

The theory of radiation transfer and exploration of space (history and prospects)

T.A. Сушкевич (Invited talk)

Посвящается 50-летию Института вычислительной математики и математической геофизики СО РАН – преемника Вычислительного центра СО РАН, основанного в 1964 г. академиком Гурием Ивановичем Марчуком (08.06.1925-24.03.2013), и 80-летию член-корреспондента РАН Геннадия Алексеевичу Михайлову (06.03.1934). Оба своими корнями связаны с Институтом Келдыша, основанного в 1953 г. как Отделение прикладной математики Математического института им. В. А. Стеклова АН СССР (ОПМ МИАН СССР) на правах института, а в 1966 году получившего название Институт

прикладной математики АН СССР. Заместителем Келдыша был Андрей Николаевич Тихонов, который и предложил кандидатуру Н. Н. Яненко на пост первого ученого секретаря ОПМ.

Двадцатый век в истории земной цивилизации – это век научно-технической революции (НТР), связанной с тремя великими открытиями:

- проникновение в тайны строения вещества и овладение ядерной энергией,
- покорение космического пространства и выход человека в космос,
- изобретение электронно-вычислительных машин и информационных технологий.

Компьютер явился главным действующим лицом, основным двигателем НТР: использование ядерной энергии, полет в космос, информационные технологии, естественно, были бы невозможны без ЭВМ. Два эпохальных научных проекта – атомный и космический – способствовали колоссальному развитию советской науки, которая могла конкурировать с мировой наукой XX века. Впервые для реализации инженерно-конструкторских проектов создания "ракетно-ядерного щита" потребовалось решение больших задач на ЭВМ и были заложены основы новой технологии, которую позже назвали "математическое моделирование" или "computer science". Разработка информационно-математических аспектов этих двух проектов привела к расцвету кинетической теории переноса нейтронов, заряженных частиц, излучения разной природы в широком диапазоне спектра длин волн, лежащей в основе ДЗЗ.

В докладе пойдет речь о научной деятельности и участии в обоих проектах блестящих математиков Г.И.Марчука и Г.А.Михайлова и создании основ "computer science". Это неоспоримое свидетельство важнейшей роли математики и фундаментальной науки в научно-техническом прогрессе 20-го века, развитии естествознания и гуманитарных наук, технологий и техники в 21-м веке.

P.S. Историческая справка. Подготовка этого доклада проходила в условиях, когда в соответствии с Федеральным законом от 27 сентября 2013 года № 253 "О Российской Академии наук, реорганизации государственных академий наук и внесении изменений в отдельные законодательные акты Российской Федерации" Распоряжением правительства от 30 декабря 2013 г. № 591-р все академические институты были переданы в ведение вновь созданного Федерального агентства научных институтов и тем самым закончилась 290-летняя история Академии Наук, а управление наукой передали чиновникам. Но это будет другая история науки. Потому так важно писать и говорить об объективной фактической истории науки и наших достижениях, пока еще живы свидетели и участники великих научных свершений цивилизации в открытии космической эры и освоении космического пространства, которыми руководила Академия Наук, чтобы предостеречь потомков и историков от искажений и домыслов.

Работа поддержана Российским фондом фундаментальных исследований (проекты № 12-01-00009, № 14-01-00197) и Российской академией наук (проект 3.5. ПФИ ОМН РАН)

Difference scheme of high order accuracy to solution decomposition method for singularly perturbed problems

L.P. Shishkina, G.I. Shishkin

A technique is considered for constructing ε -uniformly convergent (in the uniform norm) grid approximations of high accuracy order on uniform grids for singularly perturbed problems with the perturbation parameter $\varepsilon (\varepsilon \in (0, 1])$, multiplying the highest-order derivative. Application of the Richardson extrapolation technique in combination with the solution decomposition method allows us to construct finite difference schemes of high order accuracy, using uniform grids.

This research was supported by the Russian Foundation for Basic Research under grant No.13-01-00618.

Two-grid method using Richardson extrapolation for nonlinear convection-diffusion problem

S.V. Tikhovskaya, A.I. Zadorin

A boundary value problem for a second-order nonlinear singularly perturbed ordinary differential equation is considered. We use Newton and Picard iterations for a linearization of the nonlinear problem.

We apply a modified Samarskii and central difference schemes on a Shishkin mesh for solving problem at each iteration. To decrease the required number of arithmetical operations for implementation of the difference scheme, a two-grid method is proposed. To improve the accuracy of difference schemes, we investigate Richardson extrapolation method.

The results of some numerical experiments are discussed.

Fractional differential equation for earthquake aftershocks dynamics

V.V. Uchaikin (Invited talk)

As known, the first shock of an earthquake is normally accompanied with a sequence of aftershocks. The aftershocks follow one after another in random time intervals at random points. On assumption that the time intervals and distances between points be independent between one another and among themselves (what doesn't contradict observation data, at least obviously), the random sequence of aftershocks is suggested to be considered as a trajectory of some Markov chain in the coordinate-time phase space (Helmstetter and D.Sornette, 2002).

In the framework of this model, the average density of shocks in a homogeneous boundless seismic medium obeys the linear integral equation

$$n(\mathbf{x}, t) = \int_0^t \int_{\mathbb{R}^3} K(\mathbf{x} - \mathbf{x}', t - t') n(\mathbf{x}', t') d\mathbf{x}' dt' + \delta(\mathbf{x})\delta(t)$$

where $K(\mathbf{x} - \mathbf{x}', t - t')d\mathbf{x}'dt'$ is the probability that the next shock will occur in $d\mathbf{x}'dt'$ if the preceding one happened at \mathbf{x}', t' , and the last term in the equation relates to an initial shock. Our development of the model is based on the factorization hypothesis assuming separation of spatial and temporal variables in the transition probability, which leads to correspondent splitting of the equation. The second hypothesis laid into the base of the model is formulated by involving the fractal assumption for spatial and temporal interval between consecutive aftershocks. The resulting equations contain partial time- and space-derivatives of fractional orders. They are numerically solved by using Monte Carlo technique and results are discussed.

Three-level explicit schemes for parabolic and hyperbolic equations

P.N. Vabishchevich (Invited talk)

Standard explicit schemes for parabolic equations are not very convenient for computing practice due to the fact that they have strong restrictions on a time step. More promising explicit schemes are associated with explicit-implicit splitting of the problem operator (Saul'yev asymmetric schemes, explicit alternating direction (ADE) schemes, group explicit method). These schemes belong to the class of unconditionally stable schemes, but they demonstrate bad approximation properties. These explicit schemes are treated as schemes of the alternating triangle method and can be considered as factorized schemes where the problem operator is splitted into the sum of two operators that are adjoint to each other. Here we propose a multilevel modification of the alternating triangle method, which demonstrates better properties in terms of accuracy. We also consider explicit schemes of the alternating triangle method for the numerical solution of boundary value problems for hyperbolic equations of second order. The study is based on the general theory of stability (well-posedness) for operator-difference schemes.

Theoretical justification of integral semi-lagrangian scheme

A.V. Vyatkin, V.V. Shaydurov

We consider two-dimensional continuity equation equipped with suitable known coefficients, initial and boundary conditions. To solve this problem we describe integral semi-lagrangian scheme based on exact equality of two spatial integrals over different domains located at the neighboring temporal levels. The order of convergence depends on accuracy of integral approximation. To compute integrals we use bilinear interpolation of integrand and domain approximation with fourth order of accuracy. It allows us to make the theoretical justification of numerical scheme convergence with first order of accuracy. Furthermore theorem which permits to take into account a volume of substance passed through a boundary is presented. Additional advantage of presented algorithm consists in the exact validity of integral conservation law for

bilinear interpolation of discrete numerical solution. Theoretical investigations are confirmed by numerical experiments. Introduced algorithm allows to avoid algebraic relation between temporal and spatial steps which traditionally implied by Courant-Friedrichs-Lewy condition for numerical methods.

This work was supported by the Russian Foundation of Basic Research, grants № 14-01-31203 and № 14-01-00296.

Investigation of error accumulation in the problem of heat conductivity equation solved by finite difference methods

V.P. Zhitnikov, N.M. Sherykhalina, R.R. Muksimova

A mixed problem for one-dimensional heat conductivity equation with a few variants of initial and boundary conditions is under consideration. The explicit and implicit schemes are applied for the solution. The sweep and the iteration methods are used for the equations system solving for the implicit scheme. Analysis of a calculating method error and a roundoff error is bases on the numerical filtration of a finite set of results, each corresponding to a different mesh, and a number of mesh knots n increases. Moreover, the results obtained for several mantissa lengths are compared for investigation of the roundoff error.

The results of computational experiment show, that the numerical method error is represented as a sum of a few power components $c n^{-k}$ with integer degrees ($k=k_j > 0$). The roundoff error is accumulated along with the increase of mesh knots number as $c n^2$. This dependence on n has determinate character in contrast to the methods of numerical differentiation and integration. The coefficient c value either is bounded by the magnitude 10^{-M} (M is mantissa lengths) or a threshold error of the iteration method. The value of coefficient c changes chaotically with variation of the Courant number.

Section 2. ALGEBRA AND APPROXIMATION

On some algebraic and performance aspects of Krylov, a parallel sparse SLAE solver library

D.S. Butyugin, Y.L. Gurieva, V.P. Il'in, A.V. Petukhov, D.V. Perevozkin (Invited talk)

The issues of high performance implementation of the advanced algorithms for solving very large systems of linear algebraic systems (SLAEs) with sparse matrices are considered. Formally, the SLAEs, to be solved, are the general type systems (symmetric or non-symmetric, positive definite or indefinite) presented in some compressed format, CSR for example. But in fact, SLAEs are supposed to be constructed by grid approximation, FEM or FOM for example, of the original multi-dimensional, multi-physics boundary value problems, on the non-structured meshes.

Algorithms present two level preconditioned iterative process in Krylov subspaces, based on domain decomposition with parametrized overlapping subdomains and using different interface conditions on the internal boundaries. Restarted FGMRES is used as external solver. The parallel solving of SLAEs in subdomains are made by direct or iterative algorithms. Acceleration of external iterations is implemented by deflation or smoothed aggregation approaches. The library includes the algorithms of automatic construction of balancing algebraic decomposition, on the base of CSR format. Scalable parallelism is provided by hybrid programming, with using tools of MPI and OpenMP on the upper and down levels of iterations respectively.

The comparative analysis of the efficiency and performance of implemented method is made on the set of representative test problems. The structure and functionality of the library Krylov are presented.

Rational approximation of a nonstandard branch of $z^{-1/2}$ on the union of a positive and a negative real line segment

V. Druskin, S. Güttel, L. Knizhnerman (Invited talk)

Markov functions are commonly defined in the complex plane minus the negative real semiaxis. However, we have met a geophysical application (namely, constructing absorbing boundary conditions for discretized hyperbolic PDEs), where one needs good $[(m-1)/m]$ rational approximants on the union of a positive and a negative real line segment; it is assumed that the slit is shifted, so the function is analytic in a simply connected domain containing both segments (but not zero). These approximants are recalculated into complex end FD subgrids carrying out numerical absorption. We present a theoretically well-grounded algorithm for obtaining "almost best" approximants, our construction exploiting classical Zolotarev's and Gonchar's assertions. Our theorems are illustrated with the results of numerical experiments. We also present analogous statements and illustrations for another Markov function arising in the FD framework.

Дифференциальный метод вычисления коэффициентов Фурье

В.Г. Гасенко

Для вычисления коэффициентов дискретного преобразования Фурье (ДПФ) предложен новый дифференциальный метод Фурье (ДМФ), основанный на разностном решении дифференциальных уравнений первого или второго порядка с комплексными или действительными коэффициентами соответственно. При свертке комплексного либо вещественного вектора ДМФ метод требует вдвое-вчетверо меньшее количество операций умножения по сравнению с классическим ДПФ. Дифференциальный метод совместим с алгоритмом быстрого преобразования Фурье по основанию квазипростых чисел, и в этом сочетании превосходит все известные методы ускорения БПФ за счет регуляризации матриц преобразования. В частности, при вычислении ДПФ вектора размерностью 12 и 24 ДМВ методом вообще не требуются операции умножения, что существенно ускоряет, например, JPEG сжатие изображений.

On one problem of molecular trigger modeling

V.P. Golubyatnikov

We study molecular triggers models represented in the form of piecewise linear dynamical systems

$$dx_i/dt = L_i(x_{i-1}) - x_i, \quad i = 1, \dots, n. \quad (1)$$

Here $i-1=n$ for $i=1$, non-negative variables x_i are concentrations of species in reactions, threshold functions L_i are defined as: $L_i(x) = A_i = \text{const} > 2$ for $x \leq 1$, $L_i(x) = 0$ for $x > 1$. The domain $Q = [0, A_1] \times [0, A_2] \times \dots \times [0, A_n]$ is invariant for the system (1). Our task is to detect its cycles and to describe their positions.

Theorem 1. *If $n=3$, and $A_i > 2$ for $i = 1, 2, 3$, then the system (1) has exactly one cycle in Q .*

Theorem 2. *If $n=4$, and $A_1 = A_2 = A_3 = A_4 = A > 2$, then the phase portrait of symmetric system (1) contains only one cycle C_4 in Q .*

Direct measurements of the parameters A_i in cells can be done by invasive methods only, and the precision of these chemical measurements is low. So we consider periods of the cycles of the systems (1) as the non-invasive physical measurements data.

Theorem 3. *If $n=4$, and the conditions of the Theorem 2 are satisfied, then the parameter A is uniquely determined from the period of the cycle C_4 .*

Similar result holds for $n = 3$, $A_1 = A_2 = A_3$.

The work was supported by RFBR, grant 12-01-00074.

Numerical investigation of parallel DDM implementation with acceleration

Y.L. Gurieva

Parallel realization of DDM is investigated numerically for one particular 2D problem. Data structures for effective inter-domain communications are presented. Two-level iterative process has been proposed: the outer iterations are carried out according to BiCGStab method, while inner solver in a particular subdomain is PARDISO from Intel MKL. Different ways to reduce the total time of the solving process are under consideration: domain decomposition with intersections of the subdomains, Dirichlet – Neumann condition on subdomain boundaries, aggregation approach. Results of numerical experiments are presented and discussed.

Intel® Math Kernel library parallel direct sparse solver for clusters

A. Kalinkin, A. Anders, R. Anders

This paper describes a direct method for solving the equation $Ax=b$ with a sparse matrix A . The main idea of this method is decomposition matrix A on multiplication of lower-triangular, diagonal and upper triangular matrices and further solving of obtained subsystem. To achieve an efficient work balance on a large number of processes is proposed for the original matrix hereinafter referred to as "multifrontal" approach.

The multifrontal approach was proposed in Duff et al. (1983) and further expanded by Liu et al. (1992). The decomposition algorithm implementation includes several stages. The initial matrix is subject to a reordering procedure Karypis et al. (1996, 1998) first in order to represent it in the form of a dependency tree. Then the symbolic factorization takes place where the total number of nonzero elements is computed in LDU. Then a factorization of the permuted matrix in the LDU form is performed in Amestoy et al. (2003).

This paper continues previous works of authors in this direction. In Kalinkin et al (2013) the base of algorithm has been implemented for symmetric, positive definite matrix. In Kalinkin presentations (2013) the presented algorithm has been significantly improved by balancing dependence tree. In current paper existing algorithm expanded on non-positive definite matrices and non-symmetric case. Proposed algorithm of balancing tree and SMP parallelization on each MPI process allow us to achieve overall performance better than world-known package. The performance charts with comparison presented in example section

A fast method of sparse matrix-vector multiplication for FEM matrices from HPCG benchmark

A. Kalinkin, N. Shustrov, A. Anders, R. Anders

In addition to the traditional way of measuring the performance via the HPL benchmark used for Top500 ranking, a new HPCG benchmark enables comparing the performance of HPC systems solving problems with sparse data.

The HPCG benchmark performs four main steps:

- Sparse matrix-vector multiplication of a 27-diagonal matrix;
- Solving a sparse triangular system with 14-diagonal matrix;
- Projection for multigrid algorithm which corresponds multiplication on rectangular sparse matrix;
- Halo exchange.

One of the key functionalities in HPCG benchmark is sparse matrix-vector multiplication. The sparse matrix proposed for the HPCG benchmark comes from Finite Element Method (FEM) discretization of some differential equation. This fact allows us to represent the sparse matrix as a sum of a few dense matrices (with proper local variables numbering). Therefore we can replace the sparse matrix-vector multiplication of the whole sparse matrix ($Ax = y$) with the sum of independently executed dense matrix-vector multiplications followed by gather/scatter of input/output arrays. In what follows an algorithm is presented that allows to implement high-performance matrix-vector functionality for an HPCG matrix by using a special bypass over data and calling optimized Intel®Math Kernel Library (Intel®MKL) BLAS routines.

The proposed approach allows uploading different components of the vector y sequentially. So it is possible to effectively exploit both software and hardware prefetching, which is especially important for getting maximum performance on Intel®Xeon Phi™coprocessors. Based on these facts the performance of our algorithm is limited by achievable memory bandwidth.

Polygons imbedding algorithms

A.I. Kulikov

Currently, among a various number of application tasks, allocation problems are important. Their essence is in placing geometrical objects without intersections in a given domain. This paper considers the problem of imbedding for two polygons: one being fixed, the other moving due to the parallel translation and rotation. It is necessary to find all possible locations of a moving polygon, in which it is inside the fixed one contacting with it, at least, at two points.

The explicit analytical solution to this problem has been obtained.

The problem of convex polygons is separately investigated, whose solution is less labor-consuming.

The program implementation of the obtained algorithms is carried out in the MAPLE development environment and in the C language.

Local algorithms of smooth approximation preserving geometric shapes

A.I. Kulikov, A.A. Kopylov

For a local smooth approximation in 2- and 3-dimensional spaces, an efficient method based on the usage of biquadratic polynomials with isogeometric properties is proposed.

In the 2D case, the approximating functions of the class C^2 , having the first order accuracy, have been obtained. They are based on the linear transformations of the basic spline, which is a biquadratic polynomial. Therefore, such functions have an explicit analytical form. Constructing such an approximation is locally carried out thus allowing the parallelization of the algorithm. This kind of construction does not lead to oscillations. A preliminary calculation of values of the basic spline with a certain mesh size makes possible to calculate values of the approximating function. In the plane case, with non-degeneracy and uniqueness, the approximating transformations preserve convexity and monotonicity.

Surface approximation is based on the method proposed for the 2D case. First, splines along one coordinate are constructed, then along the other. Convexity criteria of the approximating surface in the vicinity of a grid point are proposed.

This method can be used in problems of visualization of information when building a smooth approximation of grid data preserving the geometrical form, drawing maps, fonts, in computer graphics and in the CAD.

On parallelization of MKL LAPACK SVD

S.V. Kuznetsov, N. Mozartova

The talk is devoted to modifications of a two-step algorithm for reducing a matrix to bidiagonal form. At the first stage the matrix is reduced to band matrix. A successive band reduction is then used to reduce a band matrix to bidiagonal form. Both stages apply two-sided orthogonal transformations to the matrix based on Householder reflectors. The underlying idea for our modifications is to use speculative computations of components of the Householder transformations. Performance comparisons between the Intel® Math Kernel Library (Intel® MKL), PLASMA bidiagonal reduction and our implementation are provided.

Constrained approximation by discrete weighted cubic splines

B. I. Kvasov

Keywords: monotone and convex approximation, discrete weighted cubic splines, automatic selection of shape control parameters, discrete weighted B-splines, control point approximation

This paper presents methods for constrained spline approximation when discrete weighted cubic splines are used. We consider algorithms that select shape control parameters (weights) automatically. We give two such algorithms: one to preserve the data monotonicity and other to retain the data convexity. These algorithms are based on the sufficient conditions of monotonicity and convexity for discrete weighted cubic splines and adapt the spline curve to the data geometric behaviour. The main point, however, is to determine whether the error of approximation remains small under the proposed algorithms. To this end we prove a theorem to estimate error bounds. We show that using special choice of shape parameters one can rise the order of approximation. Using general approach [4,5], we construct also discrete weighted cubic B-splines and consider control point approximation. Recurrence relations for discrete weighted B-splines offer valuable insight into their geometric behaviour.

References

1. Kim T., Kvasov B.I., A shape-preserving approximation by weighted cubic splines, J. Comput. Appl. Math. 236 (2012) 4383-4397.
2. Kvasov B.I., Methods of Shape-Preserving Spline Approximation, World Scientific, Singapore, 2000.

Optimal methods of local approximation by cubic splines

V.L. Miroshnichenko (Invited talk)

The report examines the algorithms of local approximation of functions of one and several variables by cubic splines. Best methods of local approximation for sufficiently smooth functions are obtained. Exact error bounds of function and its derivatives are given. The report is illustrated by numerical examples.

On finding the optimal smoothing parameter for the abstract smoothing spline

P.V. Mokshin, A.I. Rozhenko

In this talk, we present an improvement for the method of finding the optimal smoothing parameter α for an abstract smoothing spline σ_α to satisfy the residual equation $\|A\sigma_\alpha - z\| = \varepsilon$, where ε is the given estimate for the noise in the vector z of interpolated values. The method is based on the approximation of the residual operator $R_\alpha z = z - A\sigma_\alpha$ for any $\alpha > 0$ with series of powers of the operator R_{α_0} or $I - R_{\alpha_0}$ for the given α_0 (A.I. Rozhenko. "A new method for finding the optimal smoothing parameter for the abstract smoothing spline" // J. Approx. Theory. 2010. 162. P. 1117–1127). In this method, the accuracy

of approximation of the residual depends on the maximum power of operators used in the series. The new improved calculation schema essentially increases the accuracy of the approximation the residual for the given maximum power of operators by applying a refinement based on two approximations with different maximum powers (something like Richardson's extrapolation). The iterative algorithm based on residual approximation with proposed refinement has been implemented in the "Splines for Data Maning" (Sdm) library developed in Institute of Computational Mathematics and Mathematical Geophysics, SB RAS.

Efficient dynamic parallelization for the reduction of a banded matrix to tridiagonal form

N.S. Mozartova, A.A. Zotkevich

In the talk a new dynamic parallelization for the reduction of a banded matrix to tridiagonal form is considered. The reduction is one of the most time consuming step of Successive Bandwidth Reduction approach for general to tridiagonal matrix reduction. A sequence of optimization steps and their impact on performance is shown. Specifics of WY representation of bundle of the Householder transformations is described. Performance results between the Intel® Math Kernel Library (Intel MKL) and PLASMA tridiagonalization for cases with and without eigenvectors are provided on the Intel® Xeon® platforms.

The analysis of semi-conjugate direction (SCD) methods

E.I. Pak, V.P. Ilin

SCD methods are similar to GMRes approach in Krylov subspaces but the first one doesn't require additional Hessenberg matrices to be constructed. The investigation compares SCD methods for different set of SLAE which have been built for 3D problems of diffusion-convection and respective equations. Preconditioning types such as statical and dynamical have been explored, OpenMP parallelization effectiveness has been analyzed and evaluated.

Performance-oriented data structures and techniques for sparse matrix-vector multiplication

D.V. Perevozkin

Sparse matrix-vector multiplication is one of the key computational kernels in many areas of scientific computing. Because it is a significant resource consumer, its optimization is beneficial for application performance. Several attempts have been made to provide alternative data layouts and algorithms, though without much effect on the scientific community.

The emergence of graphical processing units has brought a new wave of research on the subject, since older implementations turned out to be unsuitable for the intricate new architecture. Multiple methods and data storage schemes have been proposed. However, it is noteworthy that the figures indicating these methods' advantage are mostly time-based, while other factors, e.g. power consumption, are generally overlooked.

This report attempts to partially systematize and compare these techniques, also providing the estimates and measurements of their performance and energy efficiency.

Performance optimization solutions tridiagonal systems

A.V. Petukhov

The report describes the "bottlenecks" sweep algorithm for tridiagonal systems of the order of 100 or more, at the current latency and throughput of arithmetic operations on the data type double precision, one thread. Proposed modifications of the algorithm (based on reordering data counter sweep algorithm, using SSE instructions and reducing the number of divisions) to allow two or more times to accelerate the solution of tridiagonal systems. Are times of the algorithms on processors firm Intel: Nehalem, Westmere.

Cubature formulas on a sphere invariant under the octahedral group of rotations with inversion

A.S. Popov

The definition of the best cubature formula invariant under the octahedral group of rotations with inversion on a sphere is given (the cubature formulas of this symmetry type are called also the fully symmetric cubature formulas). The unified algorithm of searching for the best cubature formulas of this symmetry type is described. The table which contains the main characteristics of all the best today cubature formulas invariant under this symmetry group up to the 59th algebraic order of accuracy is given.

Comparative analysis of quintic spline construction's algorithms

S.S. Primakov

Yu. S. Volkov proposed algorithm of construction an interpolation quintic spline, based on decomposition of second or third derivative of spline by cubic or parabolic B-splines. The report deals with problem of choice boundary conditions for these algorithms and answered, which of them are useful in computations.

MKL Sparse BLAS: performance optimizations on modern architectures

S. G. Pudov

Sparse BLAS was integrated into MKL 8.0 and it was continuously optimized for upcoming architectures. MKL Sparse BLAS supports many sparse formats and is comprised of Fortran-style interfaces. The interfaces are very universal; they support a lot of interesting features like usage sparse submatrices, etc. Also computational kernels make almost no assumptions about sparse data storage except for several cases (e.g. solving routines). Current MKL key functionality demonstrates substantial performance results. But this all-mode approach resulted in limited numbers of supported optimization algorithms. It is well known that effective optimization of sparse computations requires preliminary information about input matrices: the more information is available the better algorithm can be chosen. This information is usually time-consuming and cannot be found for every function call. Traditionally computations are divided into two steps – analysis and execution – so matrix is analyzed only once and this information is used in further function calls. For iterative methods and for algorithms with the same matrix sparsity structure this approach can provide a lot of benefits.

Hereby current MKL Sparse BLAS universal interfaces come into conflict with optimizations on modern parallel many-core architectures because they are unable to take into account sparse matrix specifics. To resolve this issue a research project has been initiated in MKL for developing new Sparse BLAS interfaces that should support two-steps execution mode for providing auto-tuning functionality. We mainly investigate SpMV routines as they are most actively used. Several experiments on modern many-core architectures have been performed. Performance results are very promising but there are several options for final interface implementation to be chosen based on customer usage analysis.

Maximum consistency method for data fitting under interval uncertainty

S.P. Shary

For the linear regression model $b = a_1x_1 + a_2x_2 + \dots + a_nx_n$, we consider the problem of data fitting under interval uncertainty. The intervals \mathbf{a}_j and \mathbf{b}_i are supposed to represent the input data and output responses of the model, such that $a_1 \in \mathbf{a}_{i1}, a_2 \in \mathbf{a}_{i2}, \dots, a_n \in \mathbf{a}_{in}, b \in \mathbf{b}_i$ in the i -th experiment, $i = 1, 2, \dots, m$. It is necessary to find the coefficients x_1, x_2, \dots, x_n , that best fit the above linear relation for the data given.

Values of the parameters x_1, x_2, \dots, x_n , are called *consistent* with the interval data $(\mathbf{a}_{i1}, \mathbf{a}_{i2}, \dots, \mathbf{a}_{in}), \mathbf{b}_i, i = 1, 2, \dots, m$, if, for every index i , there exist such representatives $a_{i1} \in \mathbf{a}_{i1}, a_{i2} \in \mathbf{a}_{i2}, \dots, a_{in} \in \mathbf{a}_{in}, b_i \in \mathbf{b}_i$ that $a_{i1}x_1 + a_{i2}x_2 + \dots + a_{in}x_n = b_i$. As an estimate of the parameters in the data fitting problem, we take the values x_1, x_2, \dots, x_n that provides maximum of the so-called recognizing functional which gives a consistency measure between data and parameters. We discuss properties of the recognizing functional, interpretation and features of the estimates obtained by the method.

Computing aspects of the spline-wavelet transformation theory

B.M. Shumilov (Invited talk)

Wavelet refers to as small or quickly fading wave, which hierarchically organized compressions and displacements form a set spanning some space of the bounded functions on the whole numerical axis. As to orthonormal and bi-orthogonal wavelets they have not analytical representation and graphically are similar to fractal curves. Semi-orthogonal spline wavelets are deprived these defects, that makes them convenient for use in interpolating graphical objects. However these wavelets are supported on the rather wide interval. The reduction of supports was achieved by construction of Hermite spline multi-wavelets, at which more than one basic function are associated to each node. Here we shall construct basic multi-wavelets, orthogonal to polynomials, on space of Hermite splines of odd degree. New approach to calculation on the basis of block three-diagonal method of Gauss is suggested. Along with this, we shall consider some examples of multi-wavelets with dismissed supports and we shall prove the new approach to calculation on the base of the finite implicit relations of decomposition with splitting at even and odd nodes. Moreover, in case of first degree spline-wavelets we shall consider the situation where data are given on nonuniform grid.

Multifrontal hierarchically semiseparable direct solver for 3D discretized PDEs

S.A. Solovyev

This paper presents a fast direct solver for 3D discretized linear systems using the supernodal multifrontal method together with low-rank approximations. For linear systems arising from certain partial differential equations (PDEs) such as elliptic equations, during the Gaussian elimination of the matrices with Nested Dissection ordering, the fill-in of L and U factors loses its sparsity and contains dense blocks with low-rank property. Off-diagonal blocks can be efficiently approximated with low-rank matrices; diagonal blocks approximated with semiseparable structures called hierarchically semiseparable (HSS) representations. Matrix operations in the multifrontal method are performed in low-rank arithmetic. To compress dense blocks into low-rank or HSS structures, we use effective adaptive cross approximation (ACA) approach. We also use idea of adaptive balancing between robust arithmetic and low-rank matrix operations while performing the elimination. In memory and performance tests we compare our solver with Intel MKL PARDISO – the high performance direct solver. Numerical results show up to 3 times performance and memory gain for the 3D problems with more than 10^6 unknowns.

Low-rank matrix approximations for large SVD computations

S.A. Solovyev, S.Tordeux

The SVD analysis is nowadays at the heart of solving and analyzing inverse problems in geophysics. However, the computation of the SVD of large sized problem is very expensive. In this paper, we present an algorithm to compute the Truncated SVD (T-SVD) of a matrix A, whose singular values are decreasing very fast (such as Born approximation matrices). This method is based on a Low-rank approximations which extracts the most important information contained in the matrix. The largest singular values and their left and right singular vectors can then be approximated numerically without performing any operation using the full matrix. This property decreases significantly the memory usage and increases the performance while getting the T-SVD. The low-rank approximation is computed thanks to the Cross Approximation (CA) technique. Validations tests demonstrate the accuracy of the method, both in terms of singular values and singular vectors. High performance of proposed algorithm is archived by using BLAS and LAPACK components from Intel Math Kernel Library (Intel MKL) that is optimized for Intel architecture. Performance tests showed up to ten times performance on one-thread system.

Approximation of variational eigenvalue problems in a Hilbert space

S.I. Solov'ev

We consider the eigenvalue problem for a positive definite bounded symmetric bilinear form with respect to a compact positive symmetric bilinear form in an infinite-dimensional Hilbert space. This

problem has a nondecreasing sequence of positive eigenvalues of finite multiplicity with a limit point at infinity, which correspond to complete orthonormal system of eigenelements. The Hilbert space and the two bilinear forms are the data of the problem. The original problem is approximated by a problem in finite-dimensional subspace. We establish new error estimates for the approximate eigenvalues, eigenelements and eigensubspaces via the errors contributed in the data of the problem. The theoretical results are used to derive optimal order estimates for the accuracy of finite element method with numerical integration for differential eigenvalue problems.

This work was supported by Russian Foundation for Basic Research (Project nos. 12-01-97026, 13-01-00908, 14-01-00755).

Optimal cubature formulas generated by projection-net approximation

N.A. Strelkov

Two approaches to the construction of optimal cubature formulae are considered. The approximation subspace is the span of lattice translations of the fixed function. This problem is closely associated with the finding of characteristics of the best projection-net approximations. For example in some cases the optimal lattice satisfies the following condition: the dual lattice generates the densest packing of Lebesgue sets of some function depending on the norm of Hormander spaces (for Sobolev spaces the problem comes to the densest lattice packing of spheres).

Extremal problems of interpolation, error estimates for approximation in connection with FEM, approximation of nonlinear operators on classes of smooth periodic functions

Yu.N. Subbotin

Some problems of interpolation and interpolation in average associated with splines, Kolmogorov widths and other extremal problems, in particular, related to the approximation of nonlinear operators, including operators of curvature of plane curves would be discussed in the report. In addition, in connection with the finite element method, it is expected to discuss the approximation properties of piecewise polynomial functions depending on the geometric properties of the triangulation (see [1], [2], [3] and references therein).

The research was supported by the Program NSH-4538.2014.1 and the joint integration projects of SB RAS and UrB RAS (project 12-C-1-1018).

References

1. Subbotin Yu. N. Extremal L_p interpolation in the mean with intersecting averaging intervals // *Izvestiya Mathematics*. 1997. V. 61, n. 1. P. 183–205.
2. Subbotin Yu. N. Approximation of smooth curvature classes of plane curves by elements of finite-dimensional subspaces // *Izvestiya Tulskogo gosudarstvennogo universiteta. Estestvennyye nauki*. 2012. Iss. 3. P. 41–47 (in Russian).
3. Baidakova N. V. Upper estimates for the error of approximation of derivatives in a finite element of Hsieh–Clough–Tocher type // *Proc. IMM RAS*. 2012. V. 18, n. 4. P. 80–89 (in Russian).

50 years convergence studying of spline interpolation: a review

Yu.S. Volkov (Invited talk)

In the Proceedings of first International Conference on Approximation Theory (1964) I.Schoenberg stated the problem: The convergence of spline interpolation. I.Schoenber is acknowledged to be the "father of splines". With the advent of computers, the spline functions have become a major tool for data fitting and computer-aided design. In our talk we present the overview of the study and results on the convergence problem of spline interpolation. Numerical analysis in spline theory is the one of areas covered by the Institute of Computational Mathematics and Mathematical Geophysics.

Interpolation formulas for functions with a boundary layer component and its applications

A.I. Zadorin, N.A. Zadorin (Invited talk)

An application of Lagrange interpolation formulas on an uniform mesh to functions with a boundary layer component can lead to significant errors. We offer two approaches to increase the interpolation accuracy: the construction of non polynomial interpolation formulas exact on a boundary layer component and the application of Lagrange polynomials on a Shishkin mesh, dense in a boundary layer. We obtained the estimates of the interpolation errors uniform in large gradients of the interpolated function in a boundary layer. We investigated the application of constructed interpolation formulas under the construction of quadrature rules and numerical differentiation formulas for functions with a boundary layer component.

This work is supported by RFBR, grant N 13-01-00618.

A new approach to the interpolation problem

V. G. Cherednichenko

Let a function $f(x)$ satisfy the Lipschitz condition on $[a, b]$, and let T_n be the classical interpolation polynomial for $f(x)$ with arbitrary distributed nodes x_1, x_2, \dots, x_{n+1} .

Introduce the distributed nodes, i.e., the correcting interpolant

$$T_{n+1} = T_n + \gamma(x - x_1) \dots (x - x_{n+1})$$

which, obviously, solves the same interpolation problem as T_n for every constant γ . The optimal $\gamma = \gamma_{n+1}$ is defined from the condition $\|f - T_{n+1}\| \rightarrow \min$, $T_{n+1} = 1/2(m_0 + M_0)$ where m_0 and M_0 are the least and greatest values of $f(x)$. At each step we choose an interpolation node and estimate the error.

Section 3. MONTE CARLO METHODS

Numerical models of homogeneous and isotropic random fields and corresponding radiative transfer problems

A.Yu. Ambos

Two types of piece-wise constant homogeneous and isotropic random fields are considered: a model based on the Poisson field of hyperplanes and a model based on the Voronoi diagram. Numerical estimates of various functionals like the transmission factor and their variances are studied relatively to different approximations for radiative transfer models using dependent sampling. These functionals are also compared with the same functionals for the corresponding deterministic model.

Number of alternatives in the competition algorithm

V.S. Antyufeev

A competition algorithm was proposed in [1]. The algorithm to solve pattern recognition problems and the method much differs from the common Artificial Neural Network. The convergence theorem (theorem of learning) for the new algorithm was proved [2]. The proposed algorithm in its initial form allows to distinguish just two alternatives: $\{z \in X\}$ and $\{z \in Y\}$ (here X is an unknown set and Y is the complement of the set X). To solve some applied problems we need often to distinguish a greater number of alternatives. A simple generalization of the algorithm is proposed to distinguish an arbitrary number of alternatives. The learning theorem is proved for the modified algorithm.

References

1. Antyufeev V.S. Solution of recognition problems by the Monte Carlo method // Russian Journal of Numerical Analysis and Mathematical Modelling. 2012, Vol.27, No.2, pp.113-130.
2. Antyufeev V.S. Theorem of learning for the competition algorithm // Numerical Analysis and Applications. Vol. 6, No 1, 2013, pp. 1-8.

Analysis of stochastic Navier - Stokes equations by Monte Carlo methods

S.S.Artemiev, V.D.Korneev (Invited talk)

In the Navier – Stokes equations sampling in spatial variables is carried out, which leads to a large system of ODEs. If further a random noise is added in the model, we will arrive at the SDEs system. Simulating a large ensemble of trajectories of such a system of SDEs on a multiprocessor supercomputer, we can estimate any probabilistic characteristics of SDEs solutions, as well as to obtain frequency characteristics of a laminar or a turbulent fluid flow, generalizing the integral curve and the phase portrait. The Navier – Stokes equations added to a random noise can be represented both as a process with independent increments (Wiener and Poisson processes) and processes correlated with increments with given distribution laws. Numerical experiments to simulate a random motion of the fluid in the "cavity" were conducted on the cluster NKS-30T of Siberian Supercomputer Center at the Institute of Computational Mathematics and Mathematical Geophysics, SB RAS.

Numerical analysis of systems with random structure

T.A. Averina

There are different probabilistic analysis problems of random-structure systems. For example, the estimation of the probability that the system is in some of its possible structures (so-called the structure probability), the estimation of expectation of a transition time from one structure to another and variance of this time, the estimation of the probabilistic characteristics of the solution. In this work the random-structure systems are considered and statistical algorithms for probabilistic analysis of these systems are developed. The statistical algorithms are based on the numerical solution of stochastic differential equations and Monte Carlo methods. The main features of the developed algorithms are the universality and the possibility to calculate the estimations of different probabilistic characteristics of a solution with high accuracy.

Simulation of the vehicular traffic flow within the kinetic model by Monte Carlo method

A.V. Burmistrov, M.A. Korotchenko

We consider an acceleration oriented vehicular traffic flow (VTF) model. A special feature of this model is introduction of the acceleration variable into the set of phase coordinates, which describe the state of a vehicle. In contrast to the gas dynamics, the interaction in the system results not in a velocity jump, but in an acceleration one. For the initial probabilistic VTF model, we construct an integral equation of the second kind, which is related to a linear many-particle model describing the vehicle system evolution. We also propose Monte Carlo algorithms for estimating the functionals of the solution to the obtained equation. We demonstrate the practical suitability of this approach to the solution of the VTF problems by numerical experiments in which we estimate velocity and acceleration distribution for various car densities and interaction profiles.

The work is a continuation of the research and a development of simulation methods started by the authors earlier. In particular, the approach suggested by the authors is applied for more realistic interaction profiles.

Application of numerical solution of stochastic differential equations to estimating solutions of parabolic equations with discontinuous coefficients

S.A. Gusev

A method for estimating solutions of a boundary value problem for linear parabolic equations with discontinuous coefficients is offered in the paper. For this kind of problems, it is proved in the paper [1], under fairly general assumptions, the existence and uniqueness of the generalized solutions, and existence of classical solutions under some additional smoothness conditions. The existence of the solution of such problem is proved by considering it as the limit of solutions of boundary value problems with smoothed coefficients. Based on the above, we propose to find an approximate solution of the problem with discontinuous coefficients as the solution of the corresponding problem with coefficients, smoothed by using the integral averaging. We apply to estimating solution of the parabolic problem the method of numerical solution of the stochastic differential equations. The paper presents some applications of the proposed technique to solving practical problems.

References

1. O.A. Ladyzhenskaya, V. Ya. Rivkind and N.N. Ural'tseva, On classical solvability of diffraction problems, Boundary-value problems of mathematical physics. 4, Tr. MIAN SSSR, 92 (1966), 116-146.

Large and supersize droplets influence on propagation of Lidar radiation in cloud's aerosole. Numerical statistical simulation

E. G. Kablukova, B. A. Kargin, A. A. Lisenko

Numerical simulation for propagation of ground-based lidar radiation in cloud layer is carried out by Monte Carlo methods utilizing averaged optical data for wavelengths from visible to submillimeter range, describing the clouds in temperate latitudes of Russian Federation, consisting of small, large and supersize droplets. Accounting large droplets in the optical model of the scattering layer increases the intensity of the echo signal from the cloud base to submillimeter wavelengths.

Stochastic models of non-Gaussian piecewise constant periodically correlated continuous-time processes

N.A. Kargapolova

A special type of non-Gaussian piecewise constant periodically correlated continuous-time processes is considered. Processes under consideration are based on stationary non-Gaussian discrete time processes and on point flow processes with constant time-interval between jumps (this time-interval is equal to time-step of stationary process). Formulas for correlation functions of processes are obtained. Processes obtained as a sum of described piecewise constant processes are also considered.

Statistical simulation as the solution of problems in testing composite hypotheses with nonparametric goodness-of-fit tests

B.Yu. Lemeshko (Invited talk)

In the case of testing composite hypotheses, the limiting statistic distributions of nonparametric goodness-of-fit tests depend on a number of factors: the kind of distribution corresponding to the tested hypothesis; the number and the type of estimated parameters; the estimation method used; sometimes, a specified value of parameter. Ignoring this problem of testing composite hypotheses leads to incorrect statistical inference.

It is impossible to solve such a great number of arising problems in the framework of the analytical approach. At the same time the Monte Carlo methods with the usage of parallelization of computational processes enable to simulate the empirical distribution of the test statistic with the required accuracy, and then to build approximate models of limiting distributions. Such study of statistic distributions can be carried out interactively (during performed statistical analysis).

On the basis of the results, obtained with the use of statistical simulation, the textbook on the application of nonparametric goodness-of-fit tests (Kolmogorov, Kuiper, Watson, Cramer-von Mises-Smirnov, Anderson-Darling and Zhang tests) has been developed. It includes a number of tables of percentage points and models of statistic distributions. This textbook will be useful to engineers, scientists, experts in various fields, who face the need of statistical analysis of the results of experiments, as well as to university teachers and students.

Application of random field models for wildland fire behavior analysis

N.E. Lepp, S.V. Ushanov

Dynamic processes on Earth's surface propagate in environment conditions which are spatially heterogeneous. Uncertainty in input data caused this variability is an important problem for users of computerized systems, for instance, systems prediction of wildland fire behavior. The rate of surface fire spread is a function of the physical characteristics of the fuel, moisture content of the surface fuel, meteorological conditions and topography. We propose method of preliminary estimation of influence spatial fuel heterogeneity on fire behavior based on the random field theory. The landscape is represented by a square lattice. The absolute value of the rate of fire spread in each cell is modeled as a realization of two-dimensional discrete Gaussian field. Probabilistic characteristics of the random field are determined according to Rothermel's surface fire spread semi-empirical model. Here the random field models assume a form of a priori knowledge about environment. Fire propagation across the landscape is simulated by wave-algorithm. The estimation of the mean perimeter and fire area is based on Monte Carlo methods. The results of simulation confirmed the effect of increasing the overall rate of fire spread, perimeter and area for spatially heterogeneous fuel. The proposed stochastic approach could be used for predicting forest fire spread and a decision-making process support.

The error analysis for spectral models of the sea surface undulation and the rogue waves

K.V. Litvenko, S.M. Prigarin

It is assumed that the sea surface roughness is sufficiently well described by a spatial-temporal random Gaussian field, which is stationary with respect to time and homogeneous with respect to space. Numerical models of the sea surface based on this assumption were used, in particular, for the simulation of rogue waves [1]. In this paper, numerical errors for models of the sea surface undulation based on spectral decomposition of the stochastic field of the water level are studied. The errors depend on the number of random harmonics in the spectral model and on the size of the domain, for which the spectral model is constructed. Numerical errors are studied for temporal and spatial spectral models.

The research was partially supported by the RFBR (12-05-00169), and by the Program for Leading Scientific Schools of Russia (NSh-5111.2014.1)

References

I. Prigarin S.M., Litvenko K.V. Conditional spectral models of extreme ocean waves, Russian Journal of Numerical Analysis and Mathematical Modeling (2012), V.27, No.3, P.289-302

Estimations of particles density, diffusion coefficient and diffusion radius in modeling of electron avalanches in gases

G.Z. Lotova

In the problem of modeling of electron avalanches in gases calculation of diffusion coefficient D is needed. When the values of relation E/p is greater than 300 V/(cm Torr) then the diffusion approximation is not applicable. Here E is the electric field strength, p is gas pressure. In this case we propose to calculate D by use of the particles density figure (polygon of frequencies). In the report the method of optimal step determination for the histogram and polygon of frequencies with respect to full mean square error is described. Moreover, additional methods of diffusion coefficient calculation are proposed. These methods are based on choosing of a suitable approximation of probability density using a combination of well-known densities.

The work was supported by grants of RFBR №№ 13-01-00746, 12-01-00727, 12-01-00034, 13-01-00441, 12-05-00169 and grant HIII-5111.2014.1.

Simulation of random variates with the Morgenstern distribution

O. A. Makhotkin

Five algorithms for the simulation of random vectors with the bivariate Morgenstern distribution density

$$p(x, y) = 1 + \alpha(2x - 1)(2y - 1), \quad (x, y) \in [0, 1]^2, \quad |\alpha| < 1$$

are described and realized. The run-time efficiencies of these algorithms are estimated so that the fastest one is determined. It uses the presentation of the Morgenstern distribution density as the sum of the bilinear finite elements.

Optimization of parallel Monte Carlo algorithm for simulation of trajectories of branching processes

M.A. Marchenko (Invited talk)

We consider a problem of optimization of parallel Monte Carlo simulation of trajectories of branching processes. To investigate efficiency of parallel computations, we implement Monte Carlo simulations on different architectures of supercomputers: massive parallel and hybrid ones. For the supercomputer with massive parallel architecture, we use software library PARMONC developed by the author earlier. To enhance efficiency of parallelization we use coprocessors, namely, NVIDIA GPUs and Intel Phi accelerators. To this goal, we modify our parallel Monte Carlo algorithm defining new levels of parallelization. This technique with several levels of parallelization enables one to load both the CPUs cores and accelerators cores in balanced way. Using this modification leads to sufficient acceleration of parallel Monte Carlo simulation.

The work was supported by grants of RFBR No. 13-07-00589, 13-01-00746, 12-01-00034, 12-01-00727 and President grant for Leading Scientific Schools Support No. 5111.2014.1.

Weight "collision" estimators with a priori finite variance

I.N. Medvedev

In this talk, the problem of constructing the weight Monte Carlo estimators with finite variance for estimating the solution of the integral equation of the second kind is studied. We construct biased weight "collision" estimator with a priori finite variance on the base the "l-fold" iteration of the recurrence for the basic weight "collision" estimator and the use of some similar integral equation to the given one.

The estimation of the bias of constructed weight "collision" estimator and mean squared error is presented. In addition, we consider the efficiency of the use of branching in Monte Carlo method. In particular, we construct and study efficiency of the weight "collision" estimators with the use of branching that depends on the weight value after next or some transition in simulated Monte Carlo chain.

Weight modification of direct statistical modeling with branching and randomization for the solution of the nonlinear kinetic equation

G.A. Mikhailov, S.V. Rogasinsky

For the approximate solution of the nonlinear kinetic Boltzmann equation the weight modification with branching and randomization is offered. Efficiency of this modification is confirmed on the example of the numerically statistical solution of a problem of two gases relaxation in the case of essentially differing concentration. When using the constructed modification the estimates of frequencies of the gas with small concentration significantly improve.

Numerical models of inhomogeneous meteorological fields

V.A. Ogorodnikov, O.V. Sereseva

Numerical stochastic parametric models of inhomogeneous spatio-temporal fields of meteorological elements on the grids are considered. All models are based on real data obtained on weather stations. The method of estimation the degree of inhomogeneity of the real fields is created. Studies of inhomogeneity of different real meteorological fields on the basis of this method are presented.

The approach to the modeling of inhomogeneous two-dimensional spatial fields is described. This approach is based on stochastic interpolation of the field values from the stations to the mesh points. With the help of this approach numerical stochastic model inhomogeneous in space and stationary in time spatio-temporal fields of meteorological elements are given. The results of the verification models are given. Several applications of proposed models for practical use are illustrated. In particular some spatio-temporal characteristics of an extreme weather conditions are described.

Approach to evaluation of time-dependence of sampled realizations in the DSMC method

M. Yu. Plotnikov, E.V. Shkarupa

The direct simulation Monte Carlo (DSMC) method is widely used nowadays for solving the steady problems of the rarefied gas dynamics. The statistical error is the most important property of the calculation results obtained in the frames of the Monte Carlo method. Nevertheless the statistical error is not commonly evaluated in the DSMC calculation because of its complexity. The statistical error in the Monte Carlo method is usually estimated by the standard deviation determined by the variance of the estimate and the number of its realizations. It is assumed that sampled realizations are independent. In distinction from the classical Monte Carlo method, in the DSMC method the time-averaged estimate is used and sampled realizations are dependent. The degree of dependence of sampled realizations has a substantial influence on the value of the statistical error. In the present work the new simple way to evaluate correlations without additional computations is proposed. This way is tested on the examples of the Fourier problem on heat transfer between two infinite parallel plates and Couette problem.

The work was supported by the Integration Grant of SB RAS N47, State Maintenance Program for the Leading Scientific Schools of the Russian Federation (NSH-5111.2014.1) and the RFBR (14-08-00534).

Stochastic models of fluctuation controlled bimolecular reactions: analytic analysis, simulation and some applications

K. K. Sabelfeld (Invited talk)

We suggest a stochastic model for fluctuation controlled bimolecular reactions based on a system of stochastic nonlinear integral equations we proposed to describe this kind of interactions with taking into account diffusion, tunneling, and capturing in recombination centers. The most difficult issue concerns the involving of different scales of diffusion and reaction rates: direct simulation is in this case practically impossible, so we introduce a "large random jump technique" which is a generalization of the "random walk on spheroids" we used in our Monte Carlo algorithms for linear diffusion equations [1]. Simulation of the processes studied is also much complicated by the random point source distributions which in the case of small concentrations requires additional averaging over these initial configurations. Application to

electron holes annihilation by tunneling and diffusion in the presence of nonradiative recombination centers is discussed.

References

1. K.K. Sabelfeld. Monte Carlo Methods in Boundary Value Problems, Springer, Heidelberg – New York – Berlin, 1991.

Stochastic collocation method for solving PDEs with random coefficients

I.A. Shalimova, K.K. Sabelfeld

We develop a technique for solving the Darcy equation governing flows in stochastically porous media, on the basis of combination of Karhunen – Loeve and polynomial chaos expansions. We use probabilistic collocation method (PCM) to determine the coefficients of the polynomial chaos expansion. For this purpose we solve the Darcy equation for different sets of collocation points, while the number of simulations in PCM is significantly reduced in comparison to the standard Monte Carlo method. Numerical results for both Monte Carlo and PCM simulations are given.

The work has been supported by HIII -5111.2014.1, RFBR under Grants N 12-01-00635-a, 14-02-00294-a and N 12-01-00727-a.

Monte Carlo algorithms for reconstructing the aerosol scattering matrix from polarized radiation observations

S. A. Ukhinov

The problem of determination of the atmospheric matrix scattering phase function from groundbased solar almucantar observations of radiation Stokes vector is considered. New iterative algorithms for solving this problem was developed as a combination of existing additive and multiplicative methods of refining the single-scattering contribution to the observed vector brightness of scattered radiation in the atmosphere. The objective of this study was to numerically substantiate the convergence of these methods. For this purpose, an algorithm of Jacobi matrices calculation for the iteration operators of the methods was developed, and calculations were carried out for various parameters of the atmosphere. Also a study of the influence of measurement errors on the reconstruction of the scattering matrix was carried out.

This work was supported by the Russian Foundation for Basic Research (project no. 13-01-00441-a).

Analytical description and optimization of adaptive discrete-stochastic algorithms for approximation of the complicatedly computable functions

A.V. Voytishchik

The special modifications of randomized algorithms for approximation of functions, for which the computation of individual values is complicated, are considered. The functional estimators of the Monte Carlo method are given as the main example of such algorithms. We propose to use the special self-organized and geostatistical techniques as the effective modifications of the corresponding discrete-stochastic numerical schemes. The special approaches for analytical description of these modifications are elaborated. The recommendations for the choice of the conditionally optimal parameters of the modified algorithms are formulated.

Section 4. MATHEMATICAL GEOPHYSICS

Fast parallel method for computing of 3D creeping flows on GPU with CUDA, modeling the salt diapirism

T.V. Abramov., B.V. Lunev (Invited talk)

We propose an algorithm and program implementation rate of 3-D creeping flows uniformly viscous Newtonian fluid with variable density under the action of gravity. The high efficiency of the algorithm is due to the using of the Green's function for the problem of the halfspace with a free surface. This makes it possible to significantly reduce the number of operations and effectively organize parallel computations. Computing acceleration in this case is proportionally to peak performance of parallel computing hardware, not to the throughput of memory, as for difference methods. It makes the algorithm especially suitable for GPU with CUDA. The paper presents calculations of the 3-D fluid flows with piecewise-homogeneous density distribution, modeling the processes of salt diapirism, the study of which is of considerable practical interest in connection with the search for hydrocarbon deposits.

Solving oil extraction problems using MapReduce Hadoop and MPI

D. Akhmed-Zaki, M. Mansurova, A. Shomanov, B. Kumalakov

We have designed an experiment to gain data on working implementations of three iterative Hadoop solutions for an oil extraction problem: single stand Hadoop, Hadoop-MPI combination, and Hadoop-MPI that uses memory-mapped files for data management. ×

Oil extraction problem is defined as follows. Consider hypercube of porous elastic anisotropic medium $\Omega = [0, T] \times K\{0 \leq x \leq 1, 0 \leq y \leq 1, 0 \leq z \leq 1\}$. Let (1) describe the fluid flow in W with initial condition (2) and boundary condition (3).

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left(\phi(x, y, z) \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left(\phi(x, y, z) \frac{\partial P}{\partial y} \right) + \frac{\partial}{\partial z} \left(\phi(x, y, z) \frac{\partial P}{\partial z} \right) + f(x, y, z) \quad (1)$$

$$P(0, x, y, z) = \varphi(0, x, y, z) \quad (2)$$

$$\left. \frac{\partial P}{\partial n} \right|_{\Gamma} = 0 \quad (3)$$

Here, G is the surface area of Ω . In (1) solution function $P(t, x, y, z)$ is the reservoir pressure at point (x, y, z) at time t ; $\varphi(t, x, y, z)$ is the diffusivity coefficient of reservoir; $f(t, x, y, z)$ is density of the sources, deposit of wells. We used implicit numerical Jacobi method to solve the problem de-fined in (1)–(3).

Hadoop implementation of hybrid iteration technology results in design and implementation of novel control mechanism for iterations of MapReduce Jobs; initialization module for the first iteration step; and, specialized class for updating data on each step of iteration.

Rock formation objects recognition and visualization software tools development using micro-seismic monitoring data

K.S. Alsynbaev, D.N. Gapeev, G.N. Erokhin, A.V. Kozlov

To analyze the results of micro-seismic monitoring, it is necessary to structure and visualize data obtained as a result of micro-seismic records processing. These data contain micro-seismic activity hypocenters that form clusters, which are indicators of heterogeneities and areas of fractures in rocks. The obtained processing results are represented by multidimensional pixel arrays of a volume up to several million elements. Interpretation of the data requires involvement of algorithmic and ergonomic issues. Rock formation objects recognition and visualization software tools using micro-seismic monitoring data have been developed. The software tools allow for interactive visualization of micro-seismic activity hypocenters and context information, event filtering, fracture zones and faults recognition representing them as flat polygons in 3D environment. The algorithms of faults and other rock formation objects recognition are based on cluster analysis, methods of computational geometry, classical and modified approximation methods.

This work was supported by RFBR grant 14-07-00699.

Numerical simulation of nonlinear stationary filtration problems with a multivalued law

I.B. Badriev, M.T. Singatullin

We study the established processes of the underground filtration of incompressible viscous fluids following a multi-valued filtration laws with a limiting gradient [1]. Generalized statement of the problem is formulated as a mixed variational inequality with inversely strongly monotone operator and convex, Lipschitz-continuous, generally non-differentiable, functional. To these problems the problems of determining the boundaries of maximum equilibrium pillars of viscoplastic residual oil [2] are reduced.

To solving the variational inequalities with monotone type operators it was suggested the iterative splitting method that do not require inverting of the original operator. The main difficulty is the solving of arising at each iteration the minimization problems. In the case of filtration problem the minimization problem was solved explicitly due to the fact that we can efficiently compute the subdifferential of the conjugated to a minimized one. The each step of the iterative process actually reduces to the solving of the boundary value problem for the Laplace operator.

It was developed the software, using MatLab environment. Numerical experiments for model problems are performed. It was investigated the dependence of the boundaries of dead zones (sets in the field of filtration, where the modulus of the pressure gradient is less than the limiting one, i.e, the motion of the filtered fluid is absent) on the magnitude of the jump in the multi-valued filtration law.

The work was financially supported by the Russian Foundation for Basic Research (projects nos. 12-01-00955, 12-01-97022, 14-01-00755).

References

1. Badriev IB Mathematical simulation of stationary problems of underground filtration with the multivalued law // Vestnik of Tambov University. Series: The natural-governmental and technical science. 2013. V 18, № 5-2. P. 2444-2446.
2. Entov V.M., Pankov V.N., Panko S.V. Mathematical Theory of Pillars of Residual Viscoplastic Oil. Tomsk: Tomsk State University, 1989. 196 p.

3D model of early stage of hydraulic fracture evolution

S.G. Cherny, V.N. Lapin, D.V. Esipov, D.S. Kuranakov, G.R. Aidagulov, O.P. Alekseenko

A fully-coupled 3D model of hydraulic fracture propagation has been developed. In the model rock is considered as linear elastic isotropic homogenous material; fracture growth is assumed to be quasistatic.

The proposed model couples effectively three sub-models with each one to describe one of the following processes. Rock deformation is described by 3D elastic equilibrium equations that are solved by Boundary Element Method. Fluid flow inside the fracture is governed by 2D lubrication equations that are solved using the Finite Element Method. Fracture growth condition for brittle elastic materials is used to describe rock failure. Interpolation formula is applied to calculate Stress Intensity Factors that are necessary to obtain fracture propagation direction and velocity.

The proposed model and its blocks have been verified for simplified statements where solutions are available. Simulations demonstrated physically consistent sensitivity to the main physical parameters. This includes simulation case when hydraulic fracture emanated from the openhole wellbore has to reorient towards the principal far-field stress direction which results in essentially non-planar fracture shape.

Numerical simulation of wave propagation in media with curved free surface

G.V. Demidov, V.N. Martynov, P.A. Titov

An algorithm for the simulation of wave fields in 2D-media with curved free surface is proposed. It is based on the construction of curvilinear grid agreed with the geometry of the free surface in the domain of interest, which is then to be mapped into "calculation" rectangular domain covered by a uniform grid. To solve the transformed problem in the "calculation" domain, previously proposed stepwise Laguerre time method and spatial differential method are used. Results of numerical simulation on a multiprocessor system for various forms of the free surface are presented.

Analytical modeling of wave fields for complex subsurface geometries and structures

A.G. Fatyanov (Invited talk)

In this work we propose an analytical method of modeling seismic wave fields for a wide range of geophysical media: elastic, non-elastic, anisotropic, anisotropic-non-elastic, porous, random-inhomogeneous,

etc. for super-remote (far) distances. As finite difference approximations are not used, there is no grid dispersion when computing wave fields for arbitrary media models and observation points.

The analytical solution representation in the spectral domain makes possible to carry out analysis of a wave field in parts, specifically, to obtain the primary waves. Based on the developed program of computing wave fields, we have carried out the simulation of water waves and seismic "ringing" on the Moon. The monotone displacement resonant to the lower frequency area with increasing the recording distance has been explained. Such a displacement was detected in experiments with a seismic vibrator.

Numerical interaction characteristics of geophysical fields on border "lithosphere – atmosphere – hydrosphere"

M.S. Khairtdinov

The problem of forecasting of geocological risks for the environment, generated by technogenic and natural explosions, in many respects depends on interaction of geophysical fields on border lithosphere – atmosphere – hydrosphere. The integrated characteristic of risks is specific acoustic energy of waves.

Its value is function of many parameters defined by conditions of radiation and distant propagation of acoustic fluctuations. This dependence can be presented in the form of some function: $E = F [Q, f_1(c, \varphi, w, \alpha), f_2(T), \delta(H), \psi(t)]$. Here Q - power of a source, $f_1(c, w)$ – functional dependence on a parity of speed c and directions φ propagation of an acoustic wave from a source; w and α are speed and azimuthal direction a wind accordingly; $f_2(T)$ - high-rise distribution of temperature of air; $\delta(H)$ the-function reflecting heterogeneity of a day surface of the earth; $\psi(t)$ the-factor of heterogeneity of the atmosphere, depending, in particular, from humidity of air. Thus, the problem of estimation of ecological risks is a multiple parametric problem.

Reception of analytical dependence of specific acoustic energy in full statement encounters complexities of its description from entering parameters. Reception of analytical dependence is possible for some special cases. Other way of overcoming of arising complexities is connected with reception of estimations of energy on the basis of experiments with application of vibrators as radiators acoustic fluctuations with high metrological characteristics. Both variants of the decision are considered in the present work.

Changes in Z-component of the geomagnetic field in the IGRF geocentric coordinate system in the period 1980-2005

V.A. Kochnev

Secular variations are calculated according to the global magnetic surveys every 5 years. Extensive literature devoted to the prediction of the secular variations of the geomagnetic field. Extrapolation of the observed changes implemented, for example, in the field model IGRF [1] and WMM [2], allows predicting changes for the next few years, but the task of forecasting long-term changes have not yet been solved.

Special feature of this work is that the change in the field is viewed along the Z-component and the results of solving the inverse problem demonstrate the change in the core sources.

The most likely option is the varying intensity of the core sources. Solving the inverse problem for the difference of magnetic fields using packet ADM-3D-earth [3], we obtain an increase in the intensity of the main sources of 230 A/m (12% or about 0.5 % per year) in the equatorial eastern and southern part of the northern hemisphere and in the eastern part of the southern hemisphere of the core. The largest decrease of intensity is about 200 A/m and situated in the southern part of the southern hemisphere of the core, which creates on surface South Atlantic magnetic anomaly. Uneven change of intensity of core sources can be explained by a non-uniform change in temperature in different parts of the core, resulting in a change in viscosity and ionization of the liquid substance of the core.

References

1. International Association of Geomagnetism and Aeronomy, Working Group V-MOD. et al. International Geomagnetic Reference Field: the eleventh generation // *Geophysical Journal International*. 2010. Vol. 183, № 3. P. 1216–1230.
2. Maus S. et al. The US/UK World Magnetic Model for 2010-2015, NOAA Technical Report NESDIS/NGDC. 2011.
3. Кочнев В.А., Гоз И.В. Нераскрытые возможности магнитометрии // *Геофизика*. 2006. № 6. P. 51–55.

Three-dimensional model of hydraulic fracture initiation

D.S. Kuranakov, D.V. Esipov, V.N. Lapin, S.G. Cherny, O.P. Alekseenko (Invited talk)

Three-dimensional model of hydraulic fracture initiation from a perforated wellbore has been developed. The model allows calculating the wellbore pressure required for rock failure as well as the location, shape

and orientation of the initial fracture. The boundary element method is used to obtain the rock stress state. The model utilizes the following fracture initiation criterion: tensile stress at some point of the cavity surface should overcome its critical value to cause the rock failure. The construction of the initial fracture is based on the assumptions that it is orthogonal to the cavity surface and to the maximal tensile stress direction, its penetration at each point is proportional to the maximal tensile stress. The influence of casing and cement sheath can be taken into account through setting special boundary conditions at the borehole surface.

Simulation results allow obtaining the optimal orientation of wellbore and perforation relative to given in-situ stress directions that provides the minimal initiation pressure. It is shown that wellbore and perforation orientation affects not only initiation pressure but also initial fracture location and orientation.

The monitoring system of cosmic rays nucleon component

V.S. Kuzmenko, V.L. Yanchukovsky

A global network of stations cosmic rays (CR) stations, located in different points of the globe, is a single instrument for the study of near-Earth and interplanetary space. The network includes about 50 standard neutron monitor 24NM-64 allows to perform long-term continuous observations of cosmic rays nucleon component. The obtained data is transmitted in Neutron Monitor Database (NMDB). CR observation conducted using four-section of the neutron monitor 24NM- 64 in Novosibirsk. For reporting data base NMDB mode on-line, as well as for the rapid assessment of the received information and diagnostic information and measuring system in real time needed modernization of the existing data gathering system (DGS). Now DGS has interactive graphical representation and collects, diagnostics and sends data in on-line mode. Statistical modeling (by means of LabVIEW) allowed us to exclude the construction of a non-trivial theoretical model of the neutron monitor functioning, it is a practical novelty of this work.

Combination of discontinuous Galerkin method with finite differences for simulation of seismic waves in presence of free-surface topography

V.V. Lisitsa, V.A. Tcheverda

This paper presents an original approach to simulation of seismic wave propagation in models with complex free-surface topography. In order to approximate the free-surface a discontinuous Galerkin method (DG) on tetrahedral (triangular) mesh is suggested to use. The choice of the method allows also increase the accuracy locally, using hp-adaptivity of the DG. However, computational intensity of the DG is much higher than that of the finite differences. Moreover, in seismic modeling extreme accuracy of the interfaces description is needed only for the sharpest ones such as free-surface and sea-bed, while the internal interfaces of the mode can be approximated by a regular rectangular grid. So in this paper we present a hybrid algorithm so that DG is used only in the near-surface part of the model while the finite differences are applied in the major part.

Applying modified multi-start optimization algorithm to solve inverse logging problem

O.V. Nechaev

The solution of inverse logging problem can be formulated as problem of minimization the function. The main feature of this problem is the set of possible solutions. By a solution we mean a local minimum in which the function value is less than a predetermined value. As well by solution can be understood some neighborhood of such local minimum. So the algorithm used to solve such a problem must find as much as possible solutions. A modified multi-start optimization method is considered to search the set of possible solutions. At each iteration, the algorithm sample the point from which starts a local optimization. In the standard algorithm start point is sampled from uniform distribution over an all search area. While the present algorithm sample the start point from uniform distribution over an unexplored domain of the search area. The effectiveness of the proposed algorithm is investigated numerically on a number of model problems.

Simulation of the nonlinear motion of saturated granular media

Yu.V. Perepechko, K.E. Sorokin, Kh.Kh. Imomnazarov

A nonlinear model of the saturated granular media based on a two-phase mixture model of viscous liquids is proposed. A mathematical model of the two-velocity dynamics of a granular medium involves the temperature phase equilibrium and the absence of the pressure phase equilibrium and is consistent from the thermodynamic standpoint. The obtained two-velocity model was verified by comparison with the results of numerical calculations for one-velocity model. Simulation of the convective and the pressure flows of the mixture of compressible viscous liquids for various conditions are presented.

Peculiarities and numerical modeling of seismic wave fields in Arctic Shelf regions

G.V. Reshetova, V.A. Tcheverda, V.G. Khaidukov (Invited talk)

Seismic study in Russian Far North and Arctic Shelf for the summer period is hampered essentially by the vast area of shallow waters. At the same time for a winter period thank to thick ice cover, there are no problems with installation of any seismic acquisitions and implementation of all necessary logistic operations. But unfortunately seismic data acquired for source – receivers onto ground-fast and floating ice are extremely noisy. The natures of this noise are various and sometimes not physically clear. In order to bring to the light the roots of this processes the large-scale 3D finite-difference simulation for realistic models is implemented and results analyzed in details. These results prove that the main impact to the noise observed in the real life data is connected with flexural waves. These intensive waves are very slow and excited by seismic source if installed onto ice cover. They propagate along the ice "plate" and converse to fast P- and S-waves, which are also very intensive and overlap seismic reflections from target geological objects.

Another series of numerical experiments was done to understand which modification of acquisition should be done to reduce the noise level.

The solving of some nonlinear non-stationary underground filtration problems

L.Sh. Ryazapova

We study the of nonlinear filtration process in a bounded domain with Lipschitz continuous boundary in elastic regime filtration [1]. Generalized statement of the considering problem is formulated as an integral identity. Investigation of the solvability is based on the general theory of monotone operators. A mesh approximations of the problem are constructed. For the model problems of the filtration theory, numerical experiments are performed. A numerical study of the behavior of sets boundaries, where the filtration velocity is zero (the so-called dead zones) is performed.

The work was financially supported by the Russian Foundation for Basic Research (projects nos. 12-01-00955, 12-01-97022, 14-01-00755).

References.

1. Bernandiner MG, Entov V.M. Hydrodynamic filtration theory of abnormal fluids. Moscow: Nauka, 1975. 199 p. (in Russian)

Development of algorithms and software for modeling volcanic structures on the hybrid cluster

A.F. Sapetina

Numerical simulation of seismic wave propagation in 3D inhomogeneous elastic medium is carried out on the basis of the complete system of elasticity equations solving with the corresponding initial and boundary conditions. Method to solve this problem is based on the explicit finite-difference scheme of second order approximation and auxiliary algorithm CFS-PML for the absorption of elastic wave reflections from the boundary of the computational domain.

As the field of modeling is considered a parallelepiped to simulate mud volcanoes with low height and three-dimensional domain with a curved boundary to simulate high magmatic volcanoes such as the Elbrus. Handling of curved boundaries carried out by the method of adaptive grids.

Since the beginning of active using graphic cards for general-purpose computations the problem of algorithms modification for the new architecture occurs. In this work the program, which solves the problem of numerical modeling of elastic wave propagation in 3D medium, is developed using CUDA and MPI on the hybrid cluster SSCC SB RAS with GPGPU technology. The scalability of the developed software is investigated and shown that the problem fits the hybrid architecture.

The using of double-layer potential for numerical solutions of the elastic mixed type boundary value problems

E.B. Sibiriakov

In this paper a new method of numerical solution of 3D elastic stationary oscillations boundary-value problem is presented. Its thrust is modification of the kernels for the boundary integral equations. It is

proposed to use as kernels the response on the finite analog of delta-loading derivative. It means that the frequency domain of loading is limited and therefore kernels are finite and smooth even at zero distance between points. It gives a possibility to find solutions on the surfaces with angles. This method can be used both for static and stationary oscillations problem. It is especially handy for the mixed type boundary problems.

The disjoining pressure for the grain medium was calculated. A representative volume of medium consisted on a solid sphere with six plane and symmetrical contacts areas. In several cases the disjoining pressures were calculated. It was shown that disjoining pressure significantly depends on the area of contact end weak enough depends on the kind of contact boundary condition type.

Spectral-difference parallel algorithm for the seismic forward modeling in the presence of complex topography

A. V. Terekhov

A spectral-difference parallel algorithm for modeling acoustic and elastic wave fields for the 2.5D geometry in the presence of irregular surface topography is considered. The initial boundary-value problem is transformed to a series of boundary-value problems for elliptic equations via the integral Laguerre transform with respect to time. The computational core of the proposed algorithm is a parallel SLAE solving procedure developed on the base of the fast preconditioning algorithms and the domain decomposition method. Efficiency of the preconditioning procedure, in terms of arithmetic operations, is attained due to using the fast Fourier transform and the dichotomy algorithm in the context of the method of separation of variables. The domain decomposition method allows efficient computation of wave fields for models of media for which it is possible to select macro-subdomains with small velocity variations, and also to efficiently solve difference equations for the surface topography and the PML boundary conditions. Thus, in addition to already available methods of modeling acoustic and seismic wave fields for models of media including the irregular topography, we have proposed a novel numerical modeling tool.

Fractional differential equations in geophysics: a review

V.V. Uchaikin

The report contains a survey of various differential equations of fractional orders which have found applications in mathematical description of different geophysical phenomena/problems such as atmospheric and oceanic turbulence, anomalous diffusion of water and oil through sand, soil and rocks, temperature fields in oil strata, seismic waves and earthquake aftershocks, hydraulic conductivity and underground flows. Climatology, meteorology, solar radiation transport and auroral ionospheric kinetics are also discussed from this point of view. But the central point and main aim of the review is to clarify the origin of the fractional operators in the description of this phenomena, its limitations and some unsolved methodological problems.

Highly-optimized TWSM algorithm for seismic diffraction modeling adapted for GPU cluster

N. Zyatkov, A. Ayzenberg, A.M. Aizenberg

We represent a highly-optimized TWSM (*tip-wave superposition method*) algorithm for diffraction modelling adapted for GPU cluster. We show the scheme of parallelization of the TWSM for several GPUs with analysis the resulting acceleration. Accuracy, stability and efficiency of the algorithm are illustrated by numerical examples for transmission through the W-shaped salt overhang and reflection from smooth interface with strong contrast.

Section 5. PHYSICS OF ATMOSPHERE, OCEAN AND ENVIRONMENT PROTECTION

Эффект "косых волн" в тангенциальном завихрителе водосброса

Б.А. Бельгибаев, А.М-М. Даурбаев

Сложность постановки граничных условий для давления на бетонной поверхности тангенциального завихрителя водосброса связана с возникновением эффекта "кавитации". Это усложняет математическое моделирование расчетных параметров потока на начальном участке шахты водосброса. Известные полуэмпирические модели основаны на поиске автомодельности течения в завихрителе и водосбросе с учетом шероховатости поверхности шахты, турбулентности потока и гидродинамических эффектов, которые зависят от конструкции завихрителя.

Экспериментально доказано, что эффект "косых волн" на начальном участке шахты водосброса возникает из-за "перехлестывания" струек тока воды в тангенциальном завихрителе. Этот эффект можно устранить за счет совершенствования конструкции завихрителя. Методами трехмерного компьютерного моделирования и анимации проведен расчет и анализ влияния конструктивных элементов завихрителя на возникновение эффекта "косых волн" в зависимости от угла наклона нижней полки тангенциального завихрителя.

Предложено простое и эффективное конструктивное решение на примере плотины Медео, обеспечивающее быстрый переход потока из пространственной структуры течения в осесимметричное течение воды, что позволяет эффективней гасить потенциальную энергию падающего потока за счет трения о стенки водосброса в поле центробежных сил.

Integrated information system for ecological monitoring of atmospheric air of an industrial city

A.A. Bublikov, A.V. Penenko, S.J. Rakhmetullina

In this work, we have presented tasks and the software architecture of the integrated solution system for ecological monitoring of industrial city atmospheric air. The system solves such important problems like modeling the diffusion process of contaminants in atmospheric air and the allocation of pollution sources. As input data, the system uses data of the automatic measurement system consisting of several devices providing concentration measurement data. Another necessary input data is weather conditions and in order to get the detailed weather forecast we use the Weather Research and Forecasting model (WRF). The results of modeling the diffusion are verified by comparison with the data of the automatic measurement system.

This work is supported by the Committee on Science and by the Ministry of Education and Science of the Republic of Kazakhstan under project "Development of information technology of the modeling of atmosphere pollution and allocation of pollution sources by using variational algorithm".

Mega-tsunami of the World Ocean and the problem of their hazard assessment

V.K. Gusiakov

Mega-tsunami is an event capable to produce severe damage and human fatalities at the opposite coast of an oceanic basin. Mega-tsunamis constitute less than 1% of the total number of historical tsunamis in the World Ocean, however, they are responsible for more than 50% of total tsunami fatalities and considerable part of the economic damage. The paper considers the problems of mathematical modeling of these extreme events and their input in overall tsunami hazard. The strongest possible tsunamigenic events that are characterized by run-up heights up to 40-50 m measured along the considerable part of the coastline (up to 1000 km) can make the major input in the overall tsunami hazard. The source of majority of transoceanic tsunamis is subduction submarine mega-earthquakes with magnitude 9.0 or higher having return period from 200-300 years to 1000-1200 years. Any long-term tsunami hazard assessment should take into account a possibility of occurrence of such mega-events at the nearest segments of a subduction zone.

Numerical Simulation of removing impurities from the atmosphere metropolis, located in mountain terrain

K.B. Jakupov

On the basis of new mathematical models of high viscous compressible gas flows series of numerical experiments carried out on the possible aspects of removing impurities from the air basin metropolis, located at the foot of the mountains in the windless areas. For the numerical solution of boundary value problems of a complex nonlinear dynamics equations, continuity and heat conduction developed and applied effective difference schemes using specific approximation equation of conservation of mass. The results of calculations of removing impurities by passing clean air through a tunnel in the mountain, education artificial pressure gradient at the top of the mountains, located in a special way in the city blown towers etc.

Development and integration of information systems and technologies in the field of hydrometeorology, oceanography and environmental monitoring

V.N. Kopylov

The All-Russian Research Institute of Hydrometeorological Information –World Data Center (RIHMI-WDC) is the leading research institution within the Federal Service for Hydrometeorology and Environmental Monitoring (Roshydromet) on the development and deployment of information systems and technologies for environmental information collection, exchange, processing and distribution. RIHMI-WDC has developed the technologies for preprocessing of data from meteorological, hydrological, agrometeorological and ship meteorological observation networks. These technologies are used in all divisions of Roshydromet. RIHMI-WDC has also developed the following: the Russian segment of the World Meteorological Organization (WMO) Information System (WIS); the Ocean Data Portal (ODP) of the International Oceanographic Data and Information Exchange Programme (IODE) of the Intergovernmental Oceanographic Commission (IOC) of UNESCO; the nation-wide Unified System of Information on the State of the World Ocean (ESIMO); the Integrated Information and Telecommunication System of Roshydromet; technologies for maintaining the Unified State Environmental Data Fund, hydrometeorological data service systems.

The general circulation of the atmosphere and climate changes

V. Krupchatnikov V., Yu. Martynova, I. Borovko

We examine the general circulation of the atmosphere and climate changes. An evidence of our understanding of the general circulation is whether we can predict changes in the general circulation that might be associated with future climate changes. It would be especially useful to predict changes associated with global climate change

We provide our study using the idealized climatic system model. This model consists of several modules: atmosphere, ocean, land surface module, module of soil, sea ice and biosphere.

In this report demonstrates that there exists considerable evidence that key-elements of the atmospheric circulation (Hadley Cell, storm tracks) have been moving poleward during the last few decades. Current theories as well as model experiments indicate that greenhouse gas increases and stratospheric ozone depletion is the most likely cause for the trends. However, there are many other aspects of these shifts that are not well understood.

This work is supported by RFBR grants 13-05-00480

Modeling and simulation of the urban-heat-island circulation in stably stratified environment

L.I. Kurbatskaya, A.F. Kurbatskiy

The urban-heat-island phenomenon and its associated circulation, driven by the energy generated by anthropogenic sources are found to be most intense at nighttime under clear skies and weak ambient wind. A thermal plume is generated by an underlying heat island in the form of an area source. In this case, a vertical plume and associated circulation will develop due to the temperature difference between the heat source and

its environs. The plume stops rising as temperature difference between the plume and its ambient vanishes due to the entrainment or mixing of fluid from a stable environment. The fundamental characteristics of most concern for a nocturnal heat island are its mixing height, intensity, temperature and turbulent kinetic energy distributions, and heat-island-induced circulation. At simulation of an urban-heat-island, structure it is necessary to describe correctly the turbulent penetrative convection in case of near-calm conditions when the ambient wind speed approaches zero and the turbulent motion at the urban center is dominated by the thermal buoyancy force. The mechanical forcing due to the urban roughness and wind shear is less important, except the immediate vicinity of an urban surface or within the urban canopy. The turbulence in most existent the mathematical models of an urban-heat-island is parameterized. The principal aim of this investigation is the development of turbulent transport model for the simulation of turbulent urban-heat-island structure in the stably stratified environment. The computationally efficient three-parametric turbulent-model describing an evolution of fully turbulent, low-aspect-ratio buoyant plume with no initial momentum under calm and stable stratified conditions is formulated and evaluated.

World Ocean as the part of the climatic system of the Earth

V.I. Kuzin (Invited talk)

Climate change due to natural and human factors are the result of complex nonlinear interaction of physical, chemical and biological processes in the atmosphere, ocean and earth. Since the study of the climate system is a search for an explanation of the climate behavior over a period of years to centuries, focuses on the study of mechanisms of interaction between Ocean subsystem and the climate system. The processes in the World Ocean are interconnected what is realized for example in the thermohaline circulation which is joined all the oceans. However each ocean has his own specific features. For example, the Atlantic ocean is the source of the so called Meridional Overturning Circulation (MOC) which is the part of the mechanism of global "Conveyor Belt" in the World Ocean. In this connection the Arctic Ocean plays the important role in these processes, because it gives 10% of total fresh water to the Atlantic and World Ocean. The Pacific Ocean plays the specific role in the climatic system because there exist such interannual and interdecadal climatic variations as El-Nino (ENSO) and the Pacific Decadal Oscillations (PDO). The investigations of these problems has the essential interest from the point of view of the understanding of the climatic system and the role of the Ocean in it.

The work was supported by the grants: RFBR № 14-05-00730, IP SB RAS № 69, 109.

Solution of direct and inverse problems of hydrophysical tsunami monitoring on parallel and hybrid computational architectures

M.M. Lavrentiev, An.G. Marchuk, K.V. Simonov, A.A. Romanenko, M.A. Kurako

Computational methods for restoration of a shape and parameters of tsunami source and for tsunami wave's propagation modeling are developed for the solution of direct and inverse problems of hydrophysical monitoring in a problem of tsunami in the Pacific Ocean.

Software toolkit consists of the following subsystems: monitoring of seismically active regions of the studied water area; calculation of positions of the nearest DART stations and preprocessing of input data; solutions of the direct problem of tsunami wave's propagation and the inverse problem of restoring a shape and parameters of tsunami source. Solution of the inverse problem is based on the results obtained by S. Yu. Dobrokhotov. The result is a map of distribution of maximal tsunami wave heights for assessment of hazard of protected coast.

The proposed computational technology is implemented in the form of parallel computational modules for SMP and GPU systems.

Numerical simulation of air flow over the city of Novosibirsk for ecological purposes

A.A. Lezhenin, V.A. Shlychkov, V.M. Malbakhov

A steady temperature vertical layer almost always observed over the city of Novosibirsk. The layer contains an inversion sublayer that prevents vertical air mass transfer. Air pollution from industrial

enterprise and traffic get trapped under these adverse meteorological conditions. A small-component model of atmospheric air circulation developed for a stably stratified boundary layer is proposed. The model is based shallow water equations with surface friction and turbulent transfer. The results of numerical simulations of airflow and pollution transport over the city of Novosibirsk are presented.

Gas hydrates as a possible source of the methane in the Arctic Ocean

V.V. Malakhova

Massive quantities of the greenhouse gas methane are stored beneath the Arctic Ocean as hydrates, and can be involved in the modern biogeochemical cycles under the global warming. In this study we simulate the dynamic behavior of the two types of hydrates: the deep-water marine gas hydrates and the shallow hydrates associated with subsea permafrost. Our goal is to study what is causing of increased concentrations CH₄ and emissions on the Arctic Ocean region, the dissociation of gas hydrates, or methane generation and migration.

The global thickness of gas hydrate stability zone was calculated applying the pressure-temperature equilibrium of the methane hydrate system, the model of heat transport in soil, bottom-water temperature, and geothermal gradient. The temperature of the Arctic Ocean water masses state was simulated for the period from 1948 to 2012 based on the regional model the Arctic Ocean-North Atlantic, developed in ICMMG SB RAS. The subsurface North Atlantic Layer is of particular interest here because it tends to hug the shelf break between 200 and 500 m depth, near the top of the hydrate stability zone. The analysis of the thermohaline characteristics of the Arctic continental shelf water in the model run showed the positive trend in the bottom temperature, which is in agreement with the observational data. The increase in its temperature will be release of additional amount of methane from gas hydrates. Most of the gas hydrates occur in sediments below the seafloor at such large water depths or under the subsea permafrost that they are not affected by warming. A three-dimensional mathematical model of the dissolved gas transport by the ocean currents with the parameterization of the oxidation process was used for the quantitative evaluation of the scale of a possible methane flux from the submarine sources. According to our numerical results obtained the methane emissions to atmosphere can be estimated to 1 Tg(CH₄) per year.

This work was supported by the IP SB RAS №109, RFBR № 14-05-00730-a projects.

The multi-scale algorithm for tsunami propagation modeling

An.G. Marchuk, A.P. Vazhenin

Tsunami sources are usually located in deep-water areas. Thus, if we want to estimate tsunami parameters near the coastline the computational domain must include both deep and shallow-water areas. A standard stability condition required that the wave advancement during one time step be lesser than a spatial grid-step. In this case we shall use a sufficient small enough time step (for computational stability in deep-water areas of the domain) which makes computations on a shallow shelf with unreasonably small time step be too time consuming. A scale-switching algorithm for computing the tsunami propagation from the initial source to the coastline has been developed. Computations that use Method of Splitting Tsunami (MOST) [1] are carried out on a sequence of grids with various resolutions where one is embedded into another. Tsunami wave parameters are transferred from the larger domain to the embedded smaller one by means of boundary conditions. With the method proposed the numerical modeling of tsunami near the Fukushima coast was carried out. The initial 3200x3200 knots computational domain A1 covers approximately 700x1000 km Pacific area near the north-east coast of Honshu island (Japan) with a grid step of 0.0024844 arc degrees (that is about 277 meters in the North-South direction). The size of the first embedded computational domain A2 is approximately 180x220 km with 0,0006211 arc degrees grid step (70 meters in the North-South direction). The final stage of this algorithm is numerical simulation of tsunami wave resulted from the previous computations in the domains A1 and A2. The third-level embedded domain A3 covers a harbor in the South of Sanriku coast. The 17 m grid step in this domain provides a very detailed tsunami inundation mapping. Comparison of the tsunami wave parameters obtained by computations with switching scale and without it reveals a certain difference of wave length and height inside a harbor.

References

1. Titov V.V. and Gonzalez F. Implementation and Testing of the Method of Splitting Tsunami (MOST) // Techn. Memorandum ERL PMEL-112, National Oceanic and Atmospheric Administration, Washington DC, 1997.

Direct variational data assimilation algorithm for multidimensional convection-diffusion-reaction models

A.V. Penenko

An algorithm for data assimilation to multidimensional convection-diffusion-reaction model is considered. Splitting technique is used to decompose the model to stages corresponding to one-dimensional convection-diffusion and reaction processes. Data assimilation is carried out on the separate splitting stages. Special control functions are introduced into the structure of the model equations to take into account various uncertainties. In the presence of measurement data this augmented model is treated with variation technique for the functional describing the misfit between measured and calculated values with the introduced control functions as the quantities to be minimized. In the case of convection-diffusion stage and one time step analysis window each resulting one-dimensional data assimilation problem has the form of tridiagonal block-matrix linear problem that can be solved with the matrix sweep method. Reaction stage processes are modeled with discrete-analytic schemes with respect to time. In the case of assimilation windows longer than one time step the result of the fine-grained algorithm analysis can be used as an initial guess.

Integrated models of dynamics and chemistry of the atmosphere for interrelated problems of ecology and climate

V.V. Penenko (Invited talk)

In recent years the attention of researchers is directed to creation of a new generation of models accounting the direct and feedback connections among hydrodynamics-chemistry-aerosols-radiation, etc, in an online mode. In ICMMG we develop a new variational technique for this class of models. Its theoretical basis is the variational principles in the formulation of strong and weak constraints. The last are convenient when dealing with uncertainties in the models and input data. To implement the models, the methods of decomposition and splitting as well as the technique of sensitivity theory to variations in model parameters and external sources are used. For creation of numerical schemes the method of discrete-analytical approximations based on the integrating factor's theory combined with the technique of adjoint equations is offered. Such approach is convenient for work with multi-scale processes described by convection-diffusion equations and stiff systems of chemical kinetics and dynamics of aerosols. The direct algorithms of variational data assimilation have special value for practical applications in online regime.

The work is partially supported by the Presidium of RAS (Program No 4), the Mathematical division of RAS (program N3), RFBR (project N 14-01-00125-a), as well as by the SB RAS through Integrating projects N 8 and 35.

Mathematical modeling of mesoscale atmosphere dynamics and pollution transport for solving environmental problems

E.A. Pyanova, L.M. Faleychik

A mesoscale mathematical model of atmospheric hydrodynamics and transport of pollutants over areas of significant thermal and orographic inhomogeneity is presented. A program package is developed for numerical realization of the model. The major components of the model are: motion equations, equations of heat and moisture, a parameterization of the surface layer and the direct solar radiation flux at inhomogeneous terrain. The input information about the underlying surface of the calculation domain is obtained by means of a GIS technology. Visualization and analysis of the results of some model experiments are carried out in a GIS environment.

Estimates of the state of the atmosphere based on a series of scenario calculations under typical meteorological situations for the lower Angara region, Baikal region, and Ust-Kamenogorsk area are made.

The information and computer technology presented above can be used to estimate air quality and to forecast possible microclimate changes in the areas under study for environmental assessments of technical objects (hydroelectric reservoirs, heat and power plants, etc.).

This work was supported by the Presidium of RAS under Program № 4, the RFBR under grant № 14-01-00125-a, the SB RAS through Integration project № 8, and project IX.88.1.6 of the SB RAS Basic Researches.

Models and methods for reconstruction of radioactive contamination from nuclear explosions and accidents

V.F. Raputa, T.V. Yaroslavtseva

The problem of quantification of radioactive environmental pollution as a result of nuclear explosions and accidents is very important. Application of direct modeling methods of transport of contaminants in principle makes it possible to completely correct description of the concentration fields, but in some cases this approach faces significant difficulties associated with providing the necessary input to the models used. Involvement of the same experimental information about the fields of contamination leads to the possibility of creating reconstruction models, allowing to establish a compromise between the model descriptions of the processes of pollution and observations.

Models for reconstructing of coarsely heterogeneous impurities fallout fields from an instantaneous source are discussed in the report. The process of aerosol impurities distribution in the atmosphere is described by the semiempirical equation of turbulent diffusion. To describe the particulate impurities distribution in the source over sedimentation velocities a two-parameter gamma distribution is used. Under this approach the numerical analysis of observations of local and regional areas pollution as a result of major radiation accidents was conducted ("Fukushima-1", SPA "Mayak", the Siberian Chemical Plant), ground nuclear explosions at the Semipalatinsk range.

Dependence of the equilibrium state from initial data in numerical global ocean climate model

A.V. Scherbakov

The three-dimensional seasonally forced large scale geostrophic model of climate of the World Ocean with realistic topography is presented. The model is based on solution of the three-dimensional equations of heat and salt transport on the regular five-degree latitude-longitude grid and on the irregular, condensed to the surface grid in vertical. The numerical method is based on using the implicit schemes. On the horizontal coordinates, the conservative nine-point difference scheme of the second order of approximation based on Richardson's extrapolation is applied, on the vertical coordinate - the second upwind scheme of the first order approximation is exploited. The main purposes of the model are reconstructions of the ocean large-scale thermohaline paleocirculation. The climatic model of the World Ocean is integrated for the periods the glacial cycle 120 000 years and simulates the penetrations of cooling and warming from the surface into the deep ocean. Sensitivity of large-scale numerical model of climate of the World Ocean from initial data on temperature and salinity is investigated in numerical global ocean climate model.

Study of the sensitivity of the numerical model of hard-branched river delta to boundary conditions on sea borders

V.A. Shlychkov, A.I. Krylova

To develop a hydrodynamic model of multi-channel sleeve in the river mouth area it is necessary to formulate the boundary value problem for the Sen-Venan equations describing the dynamics of water in the ducts. In this case full water flow is set in channel on the input boundary at the top of the delta. On the output boundaries multiple lines of partition of sea and river waters are where put cojugation conditions. The coincidence between the calculated levels of free surface in the sleeves and sea level is taken as these conditions. Significance level of the sea surface is usually defined by a constant equal to zero. Actually the sea level may vary considerably in space and time due to tides and surges. Simplification associated with unchanged level on the outlet boundaries of watercourses contributes a certain error in the model dynamics

of delta waters. The problem is to make an estimate of the error generated by boundary modes on the terminal targets of the delta. The objective is to form a mathematical model of the river delta on the example of mouth area Lena river and study the model sensitivity to variations in the level limits.

Modeling of air pollution transport on urban scales

A.V. Starchenko (Invited talk)

Developed at the Tomsk State University and at the Institute of Atmospheric Optics RAS modeling system and results of its application to numerical simulation of pollution transport in an urban airshed are presented. A core of the modeling system is a prognostic nonhydrostatic mesoscale model of atmospheric boundary layer, which allows to make numerical predictions in the nested domains of investigation. A transport of the atmospheric air pollutants is modeled on the basis of spatial prognostic equations of turbulent diffusion with taking in account dry deposition, chemical and photochemical reactions of pollution compounds. To make predictions of ozone and aerosol particles formation and transport, a modified kinetic mechanism based on the semi-empiric CSIRO Generic Reaction Set model is applied. Ten reactions between ten chemical compounds of antropogenic admixture are considered in the GRS-model.

Numerical results obtained with usage of multiprocessor computers are in good convergence with measurements of near surface meteorological parameters, nitric oxides, carbon monoxide and ozone concentrations, obtained at TOR-station of IAO.

On numerical implementation of Lake Baikal mathematical models

E.A. Tsvetova

To sum up the results of the Lake Baikal studies in ICMMG, a brief description of the set of numerical models of diverse dimensionality and complexity for studying hydrodynamics, transport and transformation of admixtures is presented. The 4D (space-time) models of hydrodynamics have been developed in two basic formulations: hydrostatic and nonhydrostatic ones. Some versions of them exist for the whole lake and for its local zones. There are a few models of admixtures' transport. As dictated by the statement of the problem, the processes of hydrodynamics and transport of admixtures are considered separately or jointly. In former case the admixture is a tracer which has no influence on hydrodynamics. In the latter case the presence of admixture changes the hydrodynamic characteristics of the surroundings. To construct numerical algorithms and approximations, a general concept of variational approach combined with splitting technique is applied in each of above mentioned models. Some numerical scenarios are discussed.

The work is partially supported by the Presidium of RAS (Programs No 4 and 23), the Mathematical Division of RAS (Program No3), RFBR (project 14-01-00125-a).

Mathematical modelling of the around-the-year temperature cycles for water bodies's

A.F. Voevodin, V.S. Nikiforovskaya, T.B. Grankina (Invited talk)

Complex mathematical models for research hydro-thermal processes in water bodies inside around the year cycle at natural and regular conditions with the account of ice creations are suggested. Here supposed that water body is the water economic system which can include at itself on the whole condition settings with the differing morphologic and hydrodynamic characters (individual water courses, water bodies, lakes, it's interconnection systems (for example, lake-river system with the tributaries/ outflows and so on)). Possible variety of such components in the research water economic systems or in their fragment is main difficult of mathematic modeling using within one's mathematic model. Suggested complex is the setting of mathematic models varied for investigate (one-dimensional, two-dimensional longitudinal-vertical models) and varied also for their possibilities to study those or other different physical factors and external influence over studied water body. Flexibility of employment of program complex is provided with foresee setting of correspond conjugating between research water body individual parts'. Hydrodynamic processes studying by numerical modeling at so varied water bodies structure's using necessary mathematic models combinations (1D or 2D) allow to provide the decrease of calculate expenditures and more effectively and economically to carry out computing experiments.

The research is fulfilled with support within the Program of RAS Presidium 4.8.

Tsunami waveform inversion by a truncated SVD approach

T.A. Voronina

An original approach to reconstructing the initial tsunami waveform in a tsunami source area is proposed. This approach is based on the inversion of remote measurements of water-level data without any a priori information on a source except for common information about its spatial localization. The direct problem of the tsunami wave propagation is considered within the scope of the linear shallow-water theory. The numerical simulation is based on the finite difference technique and the method of staggered grids. The ill-posed inverse problem of reconstructing initial tsunami waveforms is regularized by means of the least-square inversion using the truncated SVD approach. As a result of the numerical process, an r -solution is obtained. The obtained inverted field is a projection of the exact solution onto a linear span of the r first right singular vectors corresponding to the top singular values of a compact operator of the direct problem. In the present paper, the properties of the inversion operator are studied by means of numerical modeling. It is shown that the accuracy of the tsunami source reconstruction strongly depends on the signal-to-noise ratio, the azimuthal and temporal coverage of accumulated tide gauge stations relative to the target area, and bathymetric features along the wave path. The method presented allows one to control the instability of the numerical solution and to obtain an acceptable result in spite of the ill-posedness of the problem. The algorithm was verified by the numerical simulation with a real bathymetry of the Peru subduction zone and synthetic data.

Simulation of gravity currents in the atmosphere with FDM and FEM models

M.S. Yudin

Atmospheric gravity currents over obstacles of various shapes are simulated by hydrodynamic models of increasing complexity for the Navier – Stokes equations of compressible flow. The propagation of a gravity wave over a mountain is simulated by a 3D non-hydrostatic finite-difference model. Conservative difference operators are proposed for the advection terms inside the computational domain. Higher order radiation outflow boundary conditions are considered and theoretically substantiated.

Comparisons are made between model calculations and theoretical and experimental results obtained by other authors. The model realistically describes the effects of retardation and acceleration of wave fronts by the obstacle. A 2D version of a 3D non-hydrostatic finite-difference meteorological model is compared with a 2D finite-element model to simulate the effects of atmospheric front propagation over a 2D valley. The front surface is described in the models by an equation for advection of a scalar substance, which is solved with a third-order semi-lagrangian procedure. A leap-frog type scheme in a combination with an Asselin filter is used for the time discretization. Triangular elements are used in the finite-element model. The results of 2D model simulations have shown reasonable behavior of cold front propagation over the valley as calculated by both models.

This work was supported by the Russian Foundation for Basic Research under Grant 14-01-00125-a, the Presidium of RAS, Program 4, and the Department of Mathematical Sciences, Program 3.

Section 6. PROGRAMMING

Large data clustering based on MapReduce Hadoop

D. Akhmed-Zaki, M. Mansurova, A. Shomanov

The goal of this study is the implementation of parallel algorithms for clustering of hyperspectral images. In this study parallel clustering algorithms are based on MapReduce programming mode and are implemented on the platform Hadoop. Research results are compared with the results with different cluster settings and MPI model.

We have designed an experiment to gain data on working implementations of three Hadoop solutions for clustering problem: ISODATA without combiners, ISODATA with combiners and clustering using particle swarm optimization. The increasing of productivity is achieved by the process of data control. In this work the processed data are divided into two types: static, which are stored in the local file system, and states data that participate in the exchange between the Map and Reduce functions. Iterative algorithms use schemes that reduce the amount of data participating in the exchange of MapReduce processes. The results presented in this paper prove the effectiveness of MapReduce Hadoop technology for Remote Sensing data processing.

Specialized multiagent platform for semantic text processing

S.A. Anokhin, N.O. Garanina, E.A. Sidorova

One of the fundamental problems being solved within the framework of intellectual systems is automation of knowledge acquisition from heterogeneous sources, in particular from natural language texts. Under the proposed approach information is retrieved from a textual documents in the form of facts expressed in terms of a given subject area model. Information represented in such a way then could be stored and interpreted easily by an intellectual system, in which all knowledge and data are formally described by a domain-specific ontology. One of the key features of the proposed conception is an application of a multiagent paradigm for describing a process of facts extraction from a textual data.

The proposed agent model implemented by specialized multiagent platform defines agents of two basic kinds: information agents corresponding to some entities of a subject domain recognized in a text, and rule agents corresponding to patterns of fact representation that perform computation of requested characteristics of information agents. The platform possess sufficient flexibility within the proposed framework and provides a way to effectively parallelize computation.

Approaches addressing the problem of integration of ontology-based knowledge bases in the context of Linked Open Data

Z.V. Apanovich, A.G. Marchuk

Due to the fast progress of Semantic Web and its rapidly developing branch, Linked Open Data, large amounts of structured information from various fields are becoming available on the Web. Nowadays the Web of Data contains more than 28 billion RDF triples. New applications arise intended to use information from different data sources. This paper describes some problems of ontology alignment and identity resolution arising when employing the Linked Open Data datasets to enrich the content of a scientific knowledge base. The dataset of the Open Archive of the Russian Academy of Sciences, based on the BONE ontology, as well as various bibliographic datasets, structured by the AKT Reference ontology, are used as test examples. A template for SPARQL queries that establishes correspondence between groups of classes and relations of two ontologies is demonstrated. This template makes possible automatic generation of SPARQL queries based on the two ontologies visualization. The problem of identity resolution for bilingual identifiers of entities is discussed, and several approaches to its solution are proposed. All the experiments have been conducted with a toolkit developed at the IIS SB RAS. The experiments have shown that the datasets of the LOD cloud can be useful for the enrichment of the SB RAS Open Archive. In its turn, the content of the SB RAS Open Archive can be used for the refinement of information about researchers stored by many scholarly data repositories.

This work has been supported by the RFBR grant №14-07-00386-a.

Implementation of cellular simulation models on Supercomputers

O.L. Bandman (Invited talk)

Cellular Automata models of spatial dynamics are intensively studied and used for simulating nonlinear processes, in those cases when continuous mathematics is weak. After three decades of intensive development a scope of methods are created and a large arsenal of cellular automata models (diffusion, phase separation, wave propagation, chemical reactions) is accumulated, which allows to proceed to large-scale simulation tasks described by cellular automata systems and requiring supercomputer implementation. Hence, the problem arises to combine fine-grained parallelism of cellular automata with coarse grained parallelization methods, which is the subject of the report. So, an approach to parallel algorithm of a large-scale cellular automata model construction is proposed, which takes in consideration peculiarities of computational properties of CA. Special attention is paid to parallel implementation of asynchronous probabilistic CA models. Some techniques for CA-models transformation are proposed, which increase parallelization efficiency. The results are illustrated by simulation examples.

Realization of parallel calculations in the MCU-6 Monte Carlo software package

A.S. Bikeev, D.S. Oleynik, D.A. Shkarovsky, E.A. Sukhino-Khomenko

MCU (Monte Carlo Universal) is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in 3D-systems by means of the analog and non-analog Monte Carlo methods. Simulation is realized on estimated nuclear data basis.

MCU-6 is widely used for complex calculation related to reactor physics and reactor safety of various types of reactors, such as VVER and RBMK.

The MCU-6 package is parallelized using MPI. Multiprocessor code version is able to use all available processors to perform calculations. Three different modes are realized for multiprocessor calculations in which the unique random number sequence is used for each processor.

Internal architecture of modules was upgraded for calculations using a large processors number (1000). It significantly increased the efficiency of parallelization.

The MCU-6 code was verified by calculation of pin-by-pin power density in VVER-1000 core with feedbacks. The results were compared to the results obtained by means of the certified codes.

Movie-based programming: Principles, rules and components

R. Cortez, H. Tan, A. Vazhenin, D. Vazhenin

This paper deals with a visual programming platform named Movie-Based (MB) Programming. It is for creating algorithms and programs applying animation frames with computational and sensible operations. It facilitates the user's understanding and debugging of a program by coloring correlated areas of structures, introducing appropriate computational formulas, specifying algorithmic and logical behavior of those areas as well as ordering operations according to computational steps. This is supported by specific components called Control Lines and Structures referencing activity areas inside a structure. In this paper, features of MB-programming and the corresponding software are presented including semantic and syntactical rules of iconic programming language, GUI-interface and programmer's activities. We demonstrate a way of system adaptation to Service-oriented Architecture in order to organize a sharable storage and server-based execution of MB-programs and algorithms. The results of numerical experiments are also presented showing applicability of the proposed technique including implementation, usability, code generation, validity checking, and performance testing.

A local model of light interaction with translucent crystalline media

V.A. Debelov, D.S. Kozlov

Photorealistic rendering of virtual reality scenes requires specifications of geometry and materials of all scene objects. The latter characterizes particularities of light interaction with a surface and interior of an object. To develop a new material means to develop a new mathematical model, i.e. formulas and an algorithm that allow computing of mentioned interaction. Existing renderers calculate images of 3D scenes

that include only optically isotropic translucent objects and media. This work is devoted to a new material of optically anisotropic semitransparent (absorbing or colored) objects like crystals, crystalline aggregates. The study allows to extend the diversity of objects included into virtual reality scenes.

A new algorithm is developed to the following 2 statements.

1. Given: parameters of two optically anisotropic semitransparent media, parameters of light ray falling onto a boundary between the media. To compute: parameters of all reflected (up to 2) and refracted (up to 2) rays.

2. Given: parameters of an optically anisotropic semitransparent medium, parameters of light ray coming into a medium. As a rule, it is a reflected or refracted ray. To compute: parameters of this ray in an interior point.

Object-oriented data as prefix rewriting systems

A.E. Gutman

A new approach is suggested for representing and analysing object-oriented data by means of rewriting systems. A deterministic longest-prefix rewriting system is a rewriting system such that there are no rewriting rules $X \rightarrow Y$, $X \rightarrow Z$ with different Y, Z and only longest prefixes of words are subject to rewriting. Given such a system, analogs are defined and examined of some concepts related to object-oriented data systems: inheritance of classes and objects, instances of classes, class and instance attributes, conceptual dependence and consistency, conceptual scheme, types and subtypes, etc. A special attention is paid to the effective verification of various properties of the rewriting systems under consideration. In particular, algorithms are presented for answering the following questions: Are all words finitely rewritable? Do there exist recurrent words? Is the system conceptually consistent? Given two words X and Y , does X conceptually depend on Y ? Does the type of X coincide with that of Y ? Is the type of X a subtype of that of Y ? (See the following file for details: http://math.nsc.ru/LBRT/g2/files/OOD_as_PRS.pdf).

Information visualization based on hierarchical graph models

V.N. Kasyanov, E.V. Kasyanova, T.A. Zolotuhin (Invited talk)

Visualization is a process of transformation of large and complex abstract forms of information into visual form, strengthening user's cognitive abilities and allowing them to take the most optimal decisions. Graphs are the most common abstract structure encountered in computer science and are widely used for abstract information representation. Any system that consists of discrete states (or sites) and connections between them can be modeled by a graph. In the paper, we consider a practical and general graph formalism called hierarchical graphs and graph models. It is suited for visual processing and can be used in many areas where the strong structuring of information is needed. We present also the Higres and Visual Graph systems that are aimed at supporting of information visualization on the base hierarchical graph modes. Higres is a visualization tool and an editor for attributed hierarchical graphs and a platform for execution and animation of graph algorithms. Visual Graph was developed to visualize and explore large hierarchical graphs that present the internal structured information typically found in compilers.

The work was partially supported by the RFBR (№12-07-0091).

On some combinatorial optimization problems in a connection with the off-line analysis and recognition of sequences

A.V. Kel'manov

The research subject of the report includes discrete optimization problems induced by actual data analysis, pattern recognition and classification problems. In addition, the problems considered in the report are important and take place, in particular, in computational geometry, in approximation theory, in mathematical programming and in statistics. The purpose of this report is to review new results on the studying of computational complexity of these problems, and on the substantiating polynomial algorithms with performance guarantee for solution to these problems. The main results are following. Some new (previously not studied) and known (weakly studied) problems, and also generalizations and special cases

of classical partitioning problems, Euclidean vectors subsets and subsequences search are investigated. NP-hard and polynomial solvable cases of discrete optimization problems and corresponding NP-hard and polynomial solvable data analysis and pattern recognition problems are found. Exact polynomial and pseudo-polynomial algorithms and effective approximation algorithms with guaranteed accuracy bounds for these problems are constructed. The practical application our methods and algorithms in NASA (USA) space study center allowed discovering more than 100 new exoplanets.

Adaptation of data processing algorithms for GPU architecture

M.M. Lavrentiev, A.A. Romanenko (Invited talk)

Growing power of modern computer clusters offers the challenge to study more adequate models in geophysics. We speak first of all about the so-called hybrid architectures, where computational nodes are accompanied with Graphic Processing Units (GPU's). In a number of cases amazing performance could be achieved even with regular desk-top computer, provided that GPU is used properly. The authors discuss progress in GPU architecture, describe the differences in Nvidia product line and the corresponding software updates. Several examples are given in details. These range from modeling tsunami wave propagation to seismic cubes processing and selected problems of geo tomography. It was confidently shown that GPU allows one to speed up software application 10-100 times compare to the single core of CPU. So, algorithm of seismic data analysis was accelerated 150 times, tsunami wave propagation modeling was accelerated in 100 times, etc.

New approach to RDF-data processing technology

A.G. Marchuk, S.V. Leshtaev (Invited talk)

RDF (Resource Description Framework) is important structuring format mainly used for accumulation of data and meta-information. It was proposed in Semantic Web project with other standards such as OWL – language for ontology specifications, Sparql – query language for RDF, etc. Implementation of RDF-data processing is a key point for RDF-based information systems. The main difficulty of processing with RDF is very large volume of information to be processed. Billions of information pieces (so called triples) represent common information space and are already in use. There are several solutions for RDF-processing. Most complicated of them include Sparql as a query language. The goal of research work, which is presented in this report, is to propose new technology for RDF-data processing. Designed technology consists of triple store, Sparql-compiler and Sparql-engine. Advantages of proposed technology are: it can work using computers with small resources, even workstations, even using 32-bit OS; it is fast on middle scale data; data up to 1 billion of triples can be processed. Results of comparison with well-known solution OpenLink Virtuoso will be presented in the report.

IT-infrastructure for comprehensive energy research

L.V. Massel, A.N. Kopygorodsky

The approach to composition of IT-infrastructure for comprehensive energy research, which are used by experts for obtain complex solutions of energy system research, is presented. IT-infrastructure of systems research in energy consists of intelligent, information, computational and telecommunication infrastructures. Integration of information resources is performed on the basis of ontologies energy research through information infrastructure. The ontological space of energy system consist of energy system metaontology, metaontology of energy system research, which are defined a basic concepts, ontology of energy industry sector, problem ontologies, database ontologies and program ontologies. Specialized data and knowledge warehouse is suggested use to support the research individual energy industry sector. Ontology system, which are used to describe data sources, allows to perform integrate them into virtual database. Expert evaluations, models and research results are published in the knowledge warehouse. This article is described the suggested methodological approach, the architecture, the basic technologies and tools to implementation this proposed approach.

Comparison of different models for associative parallel computations

A.S. Nepomniashchaya

Associative processing is a completely different way of storing, manipulating and retrieving data as compared to traditional computation techniques. Of special interest is the class of associative (content addressable) parallel systems of the SIMD type with bit-serial (vertical) processing and simple processing elements. We first consider the STAR-machine that simulates the run of such systems. Then we analyze two generalizations of the STAR-machine: the associative graph machine (the AG-machine) and the multi-comparand associative machine (the MCA-machine). These models perform the bit-serial and the bit-parallel processing of binary data represented as matrices. To simulate the access data by contents, they use the typical operations for associative systems presented in the STAR-machine and some new operations to perform bit-parallel processing. The STAR-machine run is described by means of the language STAR that resembles Pascal but uses a few data types to perform the access data by contents. On the STAR-machine, algorithms are represented as procedures written in the language STAR. To perform bit-parallel processing, the AG-machine and the MCA-machine use two groups of new operations: one group is applied to a single matrix while another one is used for two matrices of the same size. Basic associative algorithms have been implemented on the STAR-machine and its generalizations. The main advantage of the AG-machine is the possibility of performing different parts of graph algorithms in parallel. The MCA-machine allows one to perform the relational algebra operations in parallel. Finally, we consider problem oriented shells that can be efficiently implemented on these models.

Construction of the intellectual control system of the interval-given object with delay on the basis of artificial neural networks

G.N. Pachshenko

Intellectual control systems are considered recently as one of the most perspective directions in scientific researches. Of particular interest are the principles of construction of intellectual control systems on the basis of various technologies, creation of modern intellectual technologies for control problems of complex dynamic objects. Complex technical objects, usually inherent qualities such as delay, high dimensionality of the control object, nonstationarity, nonlinearity and parameters can belong to some intervals. Therefore, developed control systems of complex objects should be such that their functioning was provided under any conditions with the given quality index. The algorithm for constructing of intellectual control systems of interval-given object with delay on the basis of artificial neural networks is developed. The intellectual control system of the interval-given object with delay on the basis of artificial neural networks is constructed.

On nonparametric statistical tests for the detection of craters in set of images

V.P. Pyatkin, G.I. Salov

Meteorite falling to Earth on its surface causes the formation, which in aerospace images often close to a circle or fuzzy ring structure may already dilapidated poorly visible, and hence hard to detect. Within this type of model problem of detection of craters actually refers to applied mathematics, namely the field of testing statistical hypotheses. Requires statistical test that would allow detection of the crater (if present in the studied area of the image) with the highest probability. The probability of detection by geometrically cooperative combination stochastically independent images obtained in different spectral ranges is obviously more than for one image. The report offers the first two efficient nonparametric statistical tests for detecting a set of images. These tests do not depend on unknown to the observer distribution laws of observed values of brightness in a single image.

A new nonparametric test for the problem of small object detection on a noisy image

G.I. Salov

There has been an increasing interest in the use of a nonparametric statistical test for the problem of object detection on a noisy image. Let X_1, \dots, X_m be set independent random variables obtained at m points

of domain of possible location object with continuous distribution function $F_1(x)$, for detecting this object in the case of its presence, two set observations Y_1, \dots, Y_n and Z_1, \dots, Z_m are additionally take on both sides of this domain.

The problem is to test the null $H_0 : F_1 = F_2 = F_3 = F$ hypothesis (the object is absence), against the alternative $H_1 : F_1(x) \leq F_k(x)$ ($k=2,3$), where strict inequality holds for some x (the object is presence). The purpose this report is to point a new nonparametric statistical test more efficiency than the well known Whitney test. The Whitney test is a particular (linear) case of the new test.

Generalized matrix fused multiply-and-add as a workhorse of scientific computing

S.G. Sedukhin, M. Paprzycki

Recent advances and observed development directions in high-performance hardware and software used in solution of large-scale scientific problems suggest the need to re-evaluate the role of dense matrix multiplication. The aim of this paper is to argue that, the same way as scalar fused multiply-and-add operation has changed computing in the last twenty years, the matrix fused multiply-and-add is going to influence the way we design computers and write cods for scientific computing in the future. Furthermore, we will show that a well-established general matrix multiply-and-add operation should be extended through the theory of algebraic semirings, to allow for unification of solvers for a large class of computational problems (within the scope of the discussed Algebraic Path Problem). We will also demonstrate that extended and generalized matrix multiply-and-add operation can be used not only for computing of the linear and multi-linear transforms but also for matrix data manipulations, such as reordering of matrix rows/columns, matrix rotation, transposition, etc. This data manipulation is an integral part of a large class of matrix algorithms, regardless of parallelism.

Visualization of polyhedral solution sets

I.A. Sharaya

The series IntLinInc of program packages is presented. These packages are intend to visualize various solution sets to interval systems of linear relations as well as the solution sets to point (i.e. noninterval) systems of relations with linear and absolute value operators. Algorithms are based on the Boundary Intervals Method proposed by the author. The package series IntLinInc is free software. Its codes are open and available from <http://interval.ict.nsc.ru/Programing> and <http://interval.ict.nsc.ru/sharaya>.

Equality-based alias calculus for iterative programs with dynamic memory

N.V. Shilov, A.K. Vorontsov

A very important research problem in program analysis is study of methods to determine whether two arbitrary address expressions can in program execution become aliased, that is to say, denote references to the same object in the dynamic memory. We study combination two different approaches to this problem: Alias Calculus (by Bertand Meyer) and Separation Logic (by John C. Reynolds). We define alias transformer `after` that computes alias distribution for programs written in language used in Separation Logic. This language comprises variable declarations, direct and indirect assignments, dereferencing, memory allocation and deallocation, sequential composition, while-loop and if-then-else conditional operator.

Theorem: Hoar triple $\{D\} \alpha \{aft(D, \alpha)\}$ is true for any program α and for any alias distribution [.

A method for solving mass figure-in-covering problems for arbitrary coverings using GPU

I.N. Skopin, D.Y. Tribis

Results of numerical experiments in solving mass problems of determining membership of a set of various figures in a set of arbitrary shapes covering a domain or intersecting with each other in a space of arbitrary dimension are discussed. The problems are solved using geometrical techniques on graphics processors.

The proposed solution can outperform the fastest classical algorithms by a factor from 6 to 700 in terms of speed. As an example, the construction of grids for computations within a geophysical model of the Earth is used. Such problems are typical for all the numerical computations involving geometric modeling where coverings or triangulations are used or rendering problems are solved.

Using distributed column indexes for query execution over very large databases

L.B. Sokolinsky, E.V. Ivanova

The special index structures called distributed column indexes are presented. These indexes are used for parallel processing of extremely large datasets. Column index of attribute B of relation R is a table that consists of two columns. First column is the inner primary key which is pointing the tuples in R, second column contains values of attribute B for corresponding tuples. Index is ordered by B and partitioned across computing nodes by domain-interval fragmentation. If two attributes belong to one domain, the elements of their column indexes having equal attribute values are placed on the same node. Distributed column indexes are compressed and stored in the main memory of cluster system. The relational operator is executed in parallel in all processor nodes as a set of parallel agents. Each agent processes the separate fragments of the column indexes by using Intel Xeon Phi coprocessor and generates partial resulting script. Each such resulting script includes all inner primary key values which are needed to construct resulting tuples. The partial resulting scripts are merged in the master node. Then DBMS constructs resulting relation using merged resulting script. This technology allows to eliminate data exchange during parallel execution of relational operators.

Technology of knowledge portal development oriented to experts in a subject domain

Yu. A Zagorulko

Recently, a great amount of scientific knowledge and information resources relating to various areas of knowledge has been accumulated in the Internet. However, the access to these resources is rather complicated as they are disembodied and ill-structured, or distributed over various Internet catalogues and sites. To solve this problem we have suggested the ontology-based architecture and technology of development of knowledge portals which provide systematization and integration of knowledge and information resources related to the modeled area of knowledge, as well as the content-based access to them. The methodology of ontology building, the main principle of which is to build the ontology of the knowledge portal by means of completion and evolution of the basic domain-independent ontologies was suggested. Based on this methodology, the technology of knowledge portal development oriented to experts in a subject domain was developed. It was successfully applied for creation of the scientific knowledge Internet portals on archeology and computational linguistics as well as an electronic Russian-English thesaurus on computational linguistics.

Section 7. INVERSE PROBLEMS

Fast stable parallel algorithms for solving gravimetry and magnetometry inverse problems

E. N. Akimova, A. F. Miniakhmetova, V. E. Misilov

The most important geophysical problems are the gravimetry and magnetometry inverse problems. Among them are the structural gravimetry and magnetometry problems of reconstructing interfaces between layers with different densities or magnetizations using known gravitational or magnetic data. The gravimetry and magnetometry problems are described by nonlinear integral Fredholm equations of the first kind, that is, they are ill-posed problems. On the discretization with iterative processes, the problems are reduced to systems of nonlinear equations with dense matrices.

For solving nonlinear Fredholm integral equations applied to the gravimetry and magnetometry inverse problems, fast stable iteratively regularized *modified* gradient methods and componentwise Newton's type method and efficient parallel are constructed. The parallel algorithms are implemented numerically on a parallel computing system "Uran" of the Institute of Mathematics and Mechanics of UrB RAS, NVIDIA graphics processors, and an Intel multicore CPU with some new computing technologies. Some *gravimetry and magnetometry* problems with "quasi-model" data are solved.

Inverse problems for evolution equations with parameter

Yu.E. Anikonov (Invited talk)

Some inverse problems for evolution equations with a parameter are investigated. We obtain and discuss some formulas for these problems. The formulas and equations for auxiliary equations apply for studying of problems of analytical pattern recognition in the case operators of evolution and source functions are unknown. This direction of investigation is one of the constructive approaches of studying multidimensional inverse and ill-posed problems of mathematical physics.

Numerical reconstructing of a function from its integral data on a family of segments

A.H. Begmatov, G. M. Djaykov

We study problems of reconstructing a function in a strip from its known integrals on a family of line segments with a given weight function. In the first case the weight is a power function, in the second case weight function of exponential type is considered. We present analytical representations of solution in the class of smooth finite functions. Results on uniqueness and existence for solution of the problem are proved. The stability estimates of solution in Sobolev spaces are obtained which implies weak instability of initial problem.

Next we use these theoretical results to the problem of recovery a function from tabular integral data. The method of solution is based on obtained analytical representations and application of finite difference methods and regularization. Analyzing results of numerical experiments we make a conclusion that applied algorithms are sufficiently effective.

Computational approach to weakly ill-posed problems of integral geometry

A.H. Begmatov, A.O. Pirimbetov, A.K. Seidullaev

We study problems of reconstruction of a function in a strip from their given integrals with known weight function along polygonal lines. We take into consideration cases when weights are piecewise constant functions. We obtained simply inversion formulas for the solutions to the problems in the class of smooth finite functions. Using these representations, we proved uniqueness and existence theorems to solutions in the class of twice-differentiable finite functions with support in a strip. We obtain stability estimates of solutions to the problems in Sobolev's spaces and thus show weak ill-posedness of these problems.

Using these theoretical results, we restore a function from given tabular integral data. We construct regularization procedures based on obtained analytical representations for considered problems with noisy data. Analyzing results of numerical experiments, we make a conclusion that applied algorithms are sufficiently effective.

Direct and inverse scattering problems: fast numerical method

O.V. Belai, L.L. Frumin, E.V. Podivilov, D.A. Shapiro (Invited talk)

The direct and inverse scattering problems are of interest in quantum physics, optics, electronics, acoustics, and geophysics. Calculation of reflection coefficient from given one-dimensional coordinate dependence of the scattering potential is the direct scattering problem. The inverse scattering problem consists of recovery of the scattering potential from given frequency dependence of the reflection coefficient. The inverse problem for coupled wave equations reduces to the system of Gel'fand–Levitan–Marchenko (GLM) integral equations. Recently an effective method of numerical solution of the inverse problem was presented, based on the Toeplitz symmetry in the discrete representation of the matrix of GLM equations. The method uses the fast inversion procedure of a Toeplitz–Hermitian matrix and special bordering technique. The method is highly competitive with the known discrete layer peeling method in speed and exceeds it noticeably in accuracy especially at high reflectance. The authors have successfully applied this method to the solution of inverse problems of optics for the one-dimensional wave equation. Surprisingly, this method can effectively solve not only inverse, but also the direct scattering problem. The results of testing this method with the help of an exactly solvable direct scattering problem are presented.

Direct and inverse problems of reservoir bottom sounding

V.S. Belonosov, A.V. Belonosova (Invited talk)

Acoustic waves in complex media formed by a horizontal water layer on the boundary of an elastic half-space are considered. The waves are generated by a point source on a free water surface. A direct initial-boundary value problem is formulated for the corresponding partial differential equations with kinematic and dynamic conditions on the boundary between liquid and solid phases. If the mechanical parameters of the elastic medium depend only on depth, the inverse dynamic problem of finding the acoustic impedance of the medium is solved when external action and corresponding response on the free surface are known.

This research was partially supported by the Presidium of the Russian Academy of Sciences (Programme of Fundamental Research no. 15, project no. 121) and the Siberian Branch of RAS (Integrating project no. 30).

Neural network approach for inverse fractional diffusion problem

A.N. Bondarenko, V.A. Dedok

This paper it is devoted to the numerical research of the inverse problem for a time fractional diffusion equation using Multilayer Perceptron Neural Networks. In this work the artificial network networks is applied to the numerical inverse problem where the goal is the determination of order of fractional derivative. We stress that this method of solving the problem has a high speed, but firstly we need to spend a sufficiently long time to train the neural network. Numerical results presented in this paper are based on study of noiseless and noisy data of system state. We show how the rate of noise affects on the solution of the problem.

The work was partially supported by RFBR, research project № 14-01-00208, 12-01-31436a, Interdisciplinary integration project of SB RAS № 14, Joint project of SB RAS and NAS, № 12 – 2013.

New algorithms for recovering coefficients of elliptic and hyperbolic equations

A.L. Bukhgeym (Invited talk)

In this talk we plan to discuss new algorithms for recovering coefficients of elliptic and hyperbolic equations from a theoretical and computational point of view.

Numerical modeling of direct and inverse pharmacokinetics problems with using of ChemPAK software package

I.G. Chernykh, D.A. Voronov (Invited talk)

Modeling of the drug diffusion in the human body is important for the development of new drugs. The currently available dual-chamber pharmacokinetics models do not meet the needs of the rapidly growing

pharmaceutical industry. Each multichamber pharmacokinetics problem can be represented by a system of ordinary differential equations. ChemPAK software package was adapted for solving these systems. There is a new modification of ChemPAK software package presented in this paper. Adapted version of ChemPAK has been tested on five chambers pharmacokinetics problem.

The numerical recovery of the boundary function for the tidal models

E.V. Dementyeva, E.D. Karepova

In this paper boundary function recovery in the problem of long-wave propagation in a large water area is considered. The mathematical model of the shallow water equations on a spherical surface is used. A boundary of a numerical domain consists of a coastline ("hard") part and an open-water ("liquid") part. In general case the influence of the ocean through an open-water part of a boundary is uncertain. Therefore at "liquid" part of a boundary the boundary conditions contain a special unknown function which should be determined together with velocity and free surface level. Thus, the ill-posed inverse problem of recovery of the boundary function is considered. To solve this problem we use additional information on a part of a "liquid" boundary. We investigate three different approaches to regularization of our ill-posed problem. For the numerical solving of the inverse problem the iterative algorithm is proposed which consists of alternate solutions of direct and adjoint equations and refinement equation of a boundary function.

The work was supported by Russian Foundation of Fundamental Researches (grant 14-01-00296-a) and by SB RAS (Project 130).

Differential approximation and identification on the uniform lattice

A.O Egorshin (Invited talk)

Mathematical modelling and prediction of the behavior of complicated dynamical processes in some fields of science (natural history, social science, biology, medicine) and technology (automatic control with an identifier, trajectory restoration, dynamical properties diagnostics, etc.) must often be realized rather efficiently at a high level of mistakes and on the sparse network data. Some problems related to approximated identification of some complicated dynamical objects that are efficient under specified conditions are considered here. It is feasible on finite intervals on the basis of "simple" models described by means of linear ordinary differential equations with constant coefficients. Corresponding variational problems are called piecewise linear dynamical approximation.

Such a piecewise linear approach for the problems of automatic control of complicated objects may become an alternative for applying complicated models whose identification and optimization control is not always feasible. For simple models there is a mathematical one and some constructive methods of automatic control (adaptive, optimal, etc.). Simple models suppose exact discretization, i.e. on the uniform ones they are accurately described by means of difference equations. This makes it possible to solve accurately problems of their identification in accordance with the network data. Finally, for simple models there are effective models of solving corresponding variational problems of identification on uniform lattices.

If the initial data are exact, the difference equations solved in this way, accomplish a uniform discretization the differential equations, and it is not expected to know their coefficients. An inverse problem is also studied: a differential approximation is a way of restoring differential equations coefficients on the basis of difference coefficients as a result of identifying differential equations on lattices, in particular.

The research was supported by the Russian Foundation for Basic Research (project no. 13-01-00329) and the Siberian Branch of the Russian Academy of Sciences (interdisciplinary project no. 80).

Identification of corrosion processes using morphology of metal surface

M.R. Enikeev, M.A. Maleeva, I.M. Gubaydullin

Many physical-chemical problems connected with the resolving of chemical technologies fundamental issues require considerable calculations. The subject of this paper is identification of corrosion processes using morphology of metal surface researches. A fractal dimension (FD) is a ratio providing a statistical

index of complexity comparing how detail in a pattern changes with the scale at which it is measured. FD is one of the most important features of images. Metal surface is scale-invariant as well as in the condition of corrosion process. FD in our experiments estimated by visual (optical microscopy) and electrochemical (impedance electrochemical spectroscopy and chronoamperometry) methods. In future it's useful to compare these approaches and suggest modified approach that is computationally attractive and gives accurate results.

The main objective of pilot phase was obtained different images of single sample during the reaction (these images were represented as a video file). The experimental work was done on the two control system. The first system is corrosion testing in solution, where in the metals is aluminium or copper. In this system the corrosion type is pitting model. Another system is corrosion cracking of stainless steels. It's necessary to estimate FD in both systems.

Information-analytical system of pre-experimental screening of potential anticancer compounds

L.V. Enikeeva, G.A. Tlyavsina

The problem of finding the biological activity of the compound prior to biological testing, the more expensive and complex compared with theoretical methods, and sometimes up to direct the synthesis of new compounds is relevant today. Predicting the probability of substance specific biological activities can significantly reduce the time and save precious research with natural experiments. The objective of this work is to develop a database of biologically active compounds, on this basis to create the training set using neural networks to analyze the SAR for substances from the training set and to construct the corresponding dependence, which would reveals many beneficial and adverse effects on early stages of the drug study. At present developed database stores substances in the SMILES chemical format. We convert them into the MNA-format, obtain descriptions of the first and second levels, which later will be used for developing the information-analytical system of pre-experimental screening of potential anticancer compounds.

Code generation as a mathematical programming task

V.A. Galatenko, S.V. Samborskij, N.I. Viukova

Code generation in the traditional compilation process is viewed as consisting of the three main tasks: instruction selection, scheduling, and register allocation. This approach while providing good code quality for universal processors may be unacceptable for DSP or other processors used in embedded systems. The work being presented is devoted to a method of code generation based on exact joint solution of the instruction selection and scheduling tasks. Both tasks are formulated as an integer linear programming (ILP) task. The solution of this task provides the optimal set of instructions and optimal schedule of their execution for a basic block. The ILP task includes restrictions on register usage, and the spill-code is generated automatically in case of register pressure; therefore register allocation is trivial for the output code.

The major benefits of the approach presented are full exploitation of instruction level parallelism, automatic use of specialized problem-oriented instructions supported by the target processor, use of optimizations based on mathematical equalities.

Analysis long-term of variation of air temperature for the purpose of energy reliability

E.V. Gubiy, V.I. Zorkaltsev, I.I. Khazheev

The results of researches of variation of air temperature in winter are presented for the purpose of energy reliability. Integrated temperature difference, duration of heating period, average daily difference between the temperature inside and the one outside, average temperature during heating period for long-term observations were used as the main long-term indicators for the research. Indicators of relative fuel demand variation for heating depending on the average value are analyzed, and the regularities that affect the reliability of power supply are defined. It was found out that variation range of fuel demand for heating in regions with cold climate and indicator of intensity of oscillations were significantly higher than ones

in areas with relatively warm climate. It is planned to bring estimation of rational reserves obtained with use of simulation models for analysis of reliability of fuel supply (based on the Monte Carlo method) and stocks' estimation of the fuel supply system including the fuel supply on the basis of biofuels with use of energy plantations

Multidimensional analogies of Gelfand – Levitan – Krein – Marchenko equations

S.I. Kabanikhin

We consider multidimensional analogies of equations of I.M. Gelfand and B.M. Levitan, equation of M.G. Krein and equation of V.A. Marchenko. This kind of equations arises in Geophysics when considering inverse problems of acoustics, elasticity and inverse scattering problems with the data in the half-plane. We discuss continuous and discrete versions of GLKM equations, conditions of their solvability and numerical algorithms.

Construction of fundamental solution of elasticity theory equations

S.I. Kabanikhin, K.S. Boboev, O.I. Krivorotko, N.Y. Zyatkov

Determining the elastic parameters of the Earth's internal structure is one of fundamental importance. It is well-known that for robust finding of the coefficients of hyperbolic equations and systems it is necessary to study the pulse response characteristic of the medium. We consider some numerical algorithms for constructing the pulse response characteristic of the medium. These are based on a study of the fundamental solution structure. For this, we consider the Riemann invariants derived from the system of equations of elasticity theory in terms of velocities and stresses for an isotropic elastic half-space. We construct a numerical algorithm for solving direct and inverse problems using a method of characteristics combined with interpolation at each time step.

Combined inverse problems for linear shallow water equations

S.I. Kabanikhin, O.I. Krivorotko

The most suitable physical models described tsunamis simulation are based on the shallow water equations. It is known that some of the parameters required for the direct simulation of tsunamis are the bottom relief characteristics and the initial perturbation data (a tsunami source). The seismic data about the source are usually obtained in a few tens of minutes after an event has occurred. A difference in the arrival times of seismic and tsunami waves can be used when operationally refining the tsunami source parameters (inverse problem) and modeling expected tsunami waves on the shore. We investigate two different inverse problems of determining a tsunami source using two different additional data: measurements of water free surface vertical displacement (1) at finite number of given points and (2) at fixed time. We investigate a gradient-type and Singular Value Decomposition of an inverse problem solution and show that using a combination of two different types of data allows one to increase the stability and convergence of numerical inverse problem solution. Results of numerical experiments of the tsunami source reconstruction are presented and discussed.

The sufficient condition for existence of constrained control

A.A. Kabidoldanova

Linear non-stationary control system described by ordinary differential equations with constraints on control values is considered. The sufficient condition for existence of two-sided constrained control is obtained. The control which satisfies given constraints is found in the set of all controls that transfer system trajectory from given initial state to desired final. It is formulated as convex combination of controls which ensure to reach the desired point for the fixed time interval and depends on initial data of the system and the functions defining constraints. The algorithm of control construction is developed for considered system.

Problem of "canister test" data interpretation for determination of coal bed diffusion and capacity parameters

A.L. Karchevsky, L.A. Nazarov, L.A. Nazarova (Invited talk)

The model is developed for gas emission from a coal placed in a sealed vessel "canister test". The experimental data (time variation of gas pressure in the vessel) interpretation procedure based on inverse problem solution allows finding initial coal bed gas content and diffusion parameters.

Reconstruction of images with triangular support

I.G. Kazantsev

It is known that the ridge functions with circular support are not reconstructed precisely from single projection, unless their directionality coincides with projection view. With forward projection operation, certain frequencies of the original image are lost. This is not the case when the image support has a simplex-wise shape. Forward projection keeps information on subtle behavior of image values within the corner areas. We show that a single ridge function with triangular support can be exactly reconstructed (under certain conditions) from a single parallel projection.

Tomographic reconstruction of mud volcano structure

I.G. Kazantsev, V.P. Pyatkin, V.V. Kovalevsky, L.P. Braginskaya, D.A. Karavayev (Invited talk)

In this work the vibro-acoustic data registered in the region of the Karabetov mud volcano are used to evaluate the volcano structure. The sources of acoustic waves and their detectors are arranged into the data registration system similar to that used in the problems formulated as the Radon transform on strip. However, because of small amount of overall data samples, it is not possible to apply analytical inversion methods. Instead, the algebraic iterative techniques are invoked for tomographic reconstruction of the volcano structure. We show that a priori knowledge embedded into the computational procedure can essentially improve the image reconstruction quality. The results are illustrated.

Kinematic-gravitational ionic model of geodynamo - the result of solving the inverse problem of global geomagnetic field IGRF-2005

V.A. Kochnev

Search for adequate geodynamo models is an important problem, and it is the subject of hundreds of scientific papers over the past decade. Special features of the approach in this paper are following.

1. There was posed and solved the inverse problem of magnetometry for the Earth's core from the main magnetic field of the Earth.

2. Integral Poisson equation was chosen as the basis of the mathematical model.

3. Numerical model of the core was represented by a set of vertical prisms. The unknowns are effective magnetizations of prisms. There were 460 unknowns and 2450 equations. By equivalence [1], each magnetized prism generates magnetic field equal to the magnetic field of the coil of the same shape, if the linear density of a current flowing around it is equal to the magnetization of the prism.

4. Program ADM-3D-earth, which implements adaptive iterative method [2], was used for the solution of the inverse problem.

The presented results gave a reason for the creation of kinematic-gravitational model of geodynamo, in which current is a positively charged core fluid moving under the action of tidal forces of the Moon and the Sun. The correctness of the model was verified with calculation of tidal forces and MP parameters and comparison with those observed on other planets of the solar system [3].

References

1. Альпин Л.М., Даев Д.С., Каринский А.Д. Теория полей, применяемых в разведочной геофизике. Учебник для вузов. М.: Недра, 1985. 407 с.
2. Кочнев В.А., Гоз И.В. Нераскрытые возможности магнитометрии // Геофизика. 2006. № 6. С. 51–55.
3. Кочнев В.А. Кинематико-гравитационная модель геодинамо // Геофизический журнал. 2013. Т. 35, № 4. С. 3–15.

Control of nonlinear object with the incomplete description on the basis of manifold

S.I. Kolesnikova

The problem of synthesis of a control system by nonlinear multidimensional objects with the incomplete description is considered. The technique of synthesis of a control system by such objects under the conditions of uncertainty on the basis of a sliding control on manifold is investigated. The comparative review of conditions of applicability of two methods of manifold is given: method of sliding control and method of analytical constructing of the aggregated regulators (ACAR). Theoretical justification of generalization of the ACAR method on a case of input perturbation of any nature in a problem of stabilization of nonlinear multidimensional object is given. Results of numerical modeling are given. The conceptual model of system of intellectual control on manifold is suggested. Results of approbation of system of intellectual control for a number of nonlinear objects are given.

The problem of irradiation doses minimization at maintenance service of an atomic power station

O.A. Lyakhov

It is shown, that the condition to visit each point one time in mathematical formalization of a trajectory optimization problem of maintenance crews moving in radiation-dangerous zones leads to loss of effective decisions. The weakened condition – "to visit each point not less than one time" promotes reduction of an atomic power station personnel irradiation. There are determined conditions, at which optimum solutions of problems in the standard formulation and with the weakened conditions coincide and differ. The method for searching the decision of the problem is considered. Numerical examples are resulted. The definition of a irradiation reduction problem at the service in radiation-dangerous zones as a several salesmen problem without Hamiltonian circles is proposed.

Solution of the inverse problem for n elliptic equations in cylindrical coordinates

B.G. Mukanova, S.D. Maussumbekova

General elliptic equation is a universal mathematical model to describe the set of natural and technological processes, including steady-state diffusion of the temperature field. In actual processes is the problem of determining the temperature at the inner boundary of the cylindrical layer if the researcher is available for observation only the outer boundary. Special case of a mathematical model for this problem is the Cauchy problem for the Laplace equation, which is a classic example of an ill-posed (Hadamard problem). Moreover, in the areas of simple form solution of the problem can be obtained in the form of a series [1], but this solution is exponentially unstable with respect to perturbation of the Cauchy data. This fact can be attributed to this problem greatly flawed, according to the classification of inverse problems [2].

Significant progress has been in the solution of inverse problems at over the past decade, namely, the method of quasisolution [3] and regularization [4]. They permit to solve the task with an acceptable accuracy. Minimization of the residual functional method based on gradient methods is standard method in the numerical solution of the inverse problem. However, analytical methods have an advantage over the numerical methods in accuracy and the analysis of results, depending on the problem parameters. At first time the analytical formulas were obtained in [5] for the regularized solution of the initial-boundary problem of the Laplace equation in a rectangle. The method is based on a system of necessary conditions of a minimum residual functional and constructing the solutions of this system in their final form. In this paper, we implement this approach to solving the inverse problem for three-dimensional steady equation conduction in cylindrical geometry. The inverse problem for the continuation of an elliptic equation with variable coefficient for steady-state diffusion models in the cylindrical layer is considered. We need to restore stationary field at the inner boundary of the cylinder by the Cauchy data on the outer shell of an inhomogeneous cylinder. The problem is reduced to solving three types of Cauchy problems for second-order ODE. The formulas are derived in the form of series for the regularized problem quasisolution on the basis of the necessary conditions for a minimum residual functional.

References

1. Lavrent'yev M.M. O zadache Koshi dlya lineynykh ellipticheskikh uravneniy vtorogo poryadka. DAN SSSR. 1957. T2. № 3.
2. Ivanov V.K., Vasin V.V., Tanana V.P. Teoriya lineynykh nekorrektnykh zadach i yeye prilozheniya. M:Nauka, 1978. 206 p.
3. Ivanov V.K. O nekorrektno postavlennykh zadachakh // Matem. sbornik. 1963. T. 61. № 2. C. 211-223.
4. Tikhonov A.N., Arsenin V.YA. Metody resheniya nekorrektnykh zadach. M.: Nauka, 1974. 224 p
5. Balgaisha Mukanova. Numerical reconstruction of unknown boundary data in the Cauchy problem for Laplace's equation. // Inverse Problems in Science and Engineering, 2012. V.21, Iss.8, P.1255-1267.

Numerical analysis of the regions of differential equations solutions with given properties

A.N. Rogalyov

Control theory and problems of stability of technical systems formed the direction in which we investigate dynamic systems with control or perturbation having restrictions on state variables and control. In such systems, we solve the problem of analysis of solutions, do not go beyond a given set in the phase space. This takes into account the various features of the dynamical system: the presence of controls, uncertainties, exit points, etc. The report describes the method of construction of the boundaries of solutions of dynamic systems. The method determines the symbolical formulas of solutions depending on the parameters of dynamic systems, bounds of global errors are computed.

The problem of qualitative analysis of such set is solved, the positions of the system are evaluated. The method was successfully applied to the study of nonlinear dynamical systems.

Practical examples of bounded trajectories to determine the periodic motions, stabilizing properties of the system, and the evaluation of the important transients in the system completes the report.

Calculation of thermophysical characteristics of the soil

B. Rysbaiuly

Convective heat transfer in the ground is carried out by water or air. Movement of moisture can be carried out in the ground or as a result of filtering (i.e., under the influence of gravitational forces), or as a result of migration (i.e., under the influence of the "internal" forces occurring in the soil at the surface of water section – mineral skeleton), or simultaneously by either methods. Martynov G.A., Globus A.M. /1, 2/ and other scientists have proved that the mechanism of motion in both cases is exactly the same, although the forces that cause it are different. In the works /3, 4/, an approximate formula is developed to calculate the thermal conductivity coefficient by taking into account the convective process. And the work /5/ develops an iterative method for calculating the thermal conductivity coefficient of the soil and proves its stability and convergence.

In this work, we develop an iterative method for finding the thermophysical parameters of the soil and conduct the following steps:

- Develop an iterative scheme for calculating the thermophysical parameters of the soil.
- Obtain a priori estimates of solutions of difference problems.
- Show the limitation of approximate values of thermophysical parameters of the soil and prove monotony of minimized functional.
- Demonstrate the convergence and stability of the developed scheme of calculation.
- Conduct numerical calculations.

References

1. Martynov G.A. Heat - and moisture transfer in the freezing and thawing soils. Fundamentals of Geocryology (Permafrost). Moscow: under Ed. of Tsytovich N.A., 1959, Chapter VI, 153-192 pp.
2. Globus A.M. Physics of nonisothermal subsurface moisture exchange. Leningrad: Gydrometizdat, 1983, 279 p.
3. Rysbaiuly B. & Birtaeva Z.B. An iterative method to determine the thermal conductivity coefficient by taking into account the moisture convection in a homogeneous medium // Herald KBTU, 2009, № 1, 13- 18 pp.
4. Rysbaiuly B. Birtaeva Z.B. Convergence of the iteration process to determine the thermal conductivity coefficient of multilayer soil by considering the moisture convection // DAN NAS RK, 2010, № 4, 37-41 pp.

5. Rysbaiuly B. Mathematical properties of the iterative method to calculate the coefficient of thermal conductivity of multilayer ground. Wulfenia Journal, Austria, 2014, Volume 20, Issue 12, 311-335 pp.

Distributed computing in intelligent systems of prediction and control on the based of approach of artificial immune systems

G.A. Samigulina, A.M. Abdenova, D.B. Akpan

The main directions of the modern world scientific progress and their relevance are defined by researches and development in the field of artificial intelligence and computer technologies. Recently, rapid development of intellectual technologies in various application areas and their real life application in many spheres of human activity makes great demands of quality of developed intellectual systems which have to work reliably in the conditions of indeterminacy of parameters, possess adaptation opportunities and function in real time. Intensive works are carried out around the world by development of nonconventional biological approaches of artificial intelligence, including on the basis of approach of artificial immune systems. Due to the feature of considered systems, bound to the intellectual analysis of larger data files in real time extremely actual is the parallelizing of calculations.

The inverse spectral problem for the Sturm-Liouville operator with piecewise continuous coefficients

A.A. Sedipkov

We study the inverse spectral problem for the Sturm-Liouville equation in the impedance form

$$-\sigma^{-1}(x)(\sigma(x)w_x)_x = \lambda w, \quad x > 0, \quad (1)$$

with the boundary condition

$$w_x|_{x=0} = 0, \quad (2)$$

which consists of finding the coefficient $\sigma(x)$ from the known spectral data of the problem.

We require that the functions w and $\sigma(x)w_x$ be continuous. The coefficient $\sigma(x)$ is piecewise continuous and has discontinuity points $x_n > \dots > x_1 > 0$ and jumps $\sigma_k = \sigma_k(x_x + 0)/\sigma_k(x_x - 0)$, $k = 1, \dots, n$. Also we suppose that $\sigma(x)$ is constant for $x \geq x_n > x_1$ and positive for $x > 0$.

Let us denote by $E(x, \omega)$, $\lambda = \omega^2$, the solution of (1) which coincides with $\exp(i\omega x)$ for $x \geq x_n$. By the scattering theory the function $E_x(0, \omega)$ called the Jost function of the system (1)-(2). The problem of finding piecewise continuous coefficient $\sigma(x)$ from the Jost function is still opened and its solution is obvious in the case when the discontinuity points x_1, \dots, x_n are incommensurable, i.e., none of its linear combinations with integer coefficients vanishes. Here we study this problem without the condition of incommensurability.

The continuation problem of the physical field from the part of the boundary

M.A. Shishlenin (Invited talk)

We investigate the continuation problem for the elliptic equation when the data is given on the part of the boundary. The continuation problem is formulated in operator form $Aq=f$. The singular values of the operator A are presented and analyzed for the continuation problem for the Helmholtz equation for simple geometry and homogeneous media. We describe and justify a gradient type algorithm for the continuation problem. The numerical results are presented and analyzed.

New methods for solving optimization problems with hidden nonconvex structures

A.S. Strelakovsky

We consider optimization problems with (d.c.) functions of A.D.Alexandrov, representable as a difference of two convex functions. We develop the Global Search Theory consisting of the following parts: 1) the local search methods special for each kind of nonconvex problems (d.c. minimization, convex

maximization, reverse-convex problems etc.); 2) the family of Global Optimality Conditions (GOC) special for each kind of nonconvex problems; 3) procedures of escaping local pits based on GOC; 4) Global Search Methods based on GOC and using the procedures from 1) and 3); 5) convergence theorems for methods from 1) and 4). The new technology as a whole opens the door for effective applications of convex optimization methods in nonconvex optimization. Applying the new technology we were successful to solve some problems: search for Nash equilibria in the bimatrix game, bilevel problems, linear complementarity problems with an indefinite matrix. These problems possess a so-called hidden nonconvexity and a rather large number of local solutions which are different from global ones. The work is partly supported by the interdisciplinary integration projects of basic researches of SB RAS No.141.

An approach to compare the accuracy of the approximate solving methods of a nonlinear inverse problem

E.V. Tabarintseva

We consider an ill-posed Cauchy problem for a semi-linear differential equation. We suggest a general scheme to construct stable approximate solutions to the unstable problem under study. Two-sided error estimates for the methods are obtained through the error estimates for the relevant methods of solving the linear problem on some natural uniform regularization classes. We use the value of the continuity modulus to compare the accuracy of different approximate solving methods and to state the order-optimality for the considered methods. We discuss the choice of the regularization parameter by the discrepancy principle and the adaptive choice of the regularization parameter in case when a priori information is insufficient to determine the uniform regularization class. The numerical examples are given to illustrate the theoretical outcomes.

The estimate of the precision for regularization of Tikhonov's method at the decision of the inverse problem of solid-state physics

V.P. Tanana, A.A. Ershova (Erygina) (Invited talk)

The problem of determining of the phonon spectrum of the crystal $n(\varepsilon)$ from its thermal capacity $C(\theta)$ that depends on temperature is described:

$$\int_0^{\infty} S\left(\frac{\varepsilon}{\theta}\right) \frac{\varepsilon}{\theta} n(\varepsilon) \frac{d\varepsilon}{\varepsilon} = \frac{C(\theta)}{\theta}; \quad 0 \leq \theta < \infty.$$

This problem was set in Lifshitz's work in 1954.

Numerical solution of this equation in natural spaces is unstable problem.

An additional difficulty of this problem lies in the fact that the phonon spectrum has several local max, which determine many of the physical properties of the crystal. At decision must be reconstructed.

In this work, the estimate of the accuracy of the regularization Tikhonov's method with the regularization parameter selected from the discrepancy principle in the space $L_2[0, \infty)$ with the weight of $1/\varepsilon$. A new method for solving this problem, which reproduces the "fine structure" of the solution, is showed.

Numerical algorithms for solution of identification problem for the lower coefficient of parabolic equation

P.N. Vabishchevich, V.I. Vasilyev, M.V. Vasilyeva (Invited talk)

Mathematical modeling of many applied problems of science and engineering, results in the numerical solution of inverse problems. In the theory and practice of inverse problems for partial differential equations (PDEs) much attention is paid to the problem of the identification of coefficients from some additional information.

In this work, we consider the problem of determining the lower coefficient of a parabolic equation of second order, where the coefficient depends on time only. As additional condition we have the specification of the solution at an interior point or the average value integrated over the whole domain.

For numerical solution we use standard finite elements approximation by space. A computational algorithm is based on explicit-implicit approximations in time which leads to solve linear problems at every time level. Linear problems at a particular time level are solved on the basis of a special decomposition into two standard elliptic problems. The numerical results for a model 2D inverse problem are demonstrate capabilities of the proposed computational algorithms for approximate solving of the inverse problems.

Implementation of the simplex method admitting vectorization

G.I. Zabinyako (Invited talk)

A software implementation of the dual simplex method admitting vectorization of calculations is considered. After LU factorization of the basic matrix at some iteration, it must be corrected at subsequent iterations. The Bartels, Golub algorithm provides numerically stable correction of the factors, but does not allow efficient vectorization. This algorithm makes it possible to perform up to 100 iterations, after which the LU factors for the current basic matrix must be recalculated. Here, an implementation without correction of the factors is used. The obtained solutions for direct and dual variables on the basis of fixed LU factorizations are corrected by using auxiliary matrices of small dimension. If k iterations are made after obtaining the last LU factorization, the dimension of the auxiliary matrix at this iteration is not greater than $k \times k$. The stability of the process for the variant of the method being considered is provided by using numerically stable algorithms of the LU factorization. In our case, pivotal elements are chosen from the solution to assignment problems, and the METIS package procedures are used to determine symmetrical permutations to provide sparseness.

Linear manifold and polyhedron points nearest to the origin

V.I. Zorkaltsev (Invited talk)

The results of researches of properties and interdependences of linear manifold and polyhedron points nearest to the origin are stated under the different definitions of the concept "proximity". Many mathematical problems and components of computational methods can be presented in the form of such geometric problem. There are several examples of such problems which are considered in the report:

- problems of construct of real and plan input-output balances;
- problems of factorization and prediction of time series;
- models of estimation of parameters of biological organisms life in the ecosystem of the lake Baikal;
- linearization based algorithms for solving of nonlinear systems;
- regularization methods for unstable and improper problems;
- interior point algorithms in the theory of optimization.

The next problems are considered for concretization of the concept "proximity":

- problems of minimization of the penalty functions from wide axiomatic defined class which includes Helder, octahedral and Chebyshev norms with variable weighted coefficients;
- Pareto optimal solutions of multicriterion problems;
- solutions with nonexpansible set of nonzero components.

The report is extension of researches which are published in V.I. Zorkal'tsev Octahedral and Euclidean Projections of a Point to a Linear Manifold // Proceedings of the Steklov Institute of Mathematics, 2014, Vol. 284, Suppl. 1, pp. S1 – S13.

The ways of improvement of the accuracy of reliability indexes of electric power systems

V.I. Zorkaltsev, S.M. Perzabinsky

The technique for evaluation of electric power systems (EPS) reliability is considered in the report. The given technique is based on the Monte Carlo method. We propose the approach for improvement of the accuracy of reliability indexes. The approach is relied on representation of the model for evaluation power shortage in the view of the parametric linear programming problem. The two-sided inequality constraints of variables depend on parameter β in the problem. Computations start from the worst state of EPS with minimal electric power generation and limited power line capacity, maximal load in the nodes. The volume

of power generation, power line capacity are increasing accordingly the given directions with the change of parameter β . In this case the load is reduced. The computations are finished if we'll get the EPS state with null shortage. The change directions are chosen for full cover of the set of EPS states. The special effective modification of simplex method is proposed to use for solving the given parametric linear programming problems.

The given approach increases the accuracy of reliability indexes due to growth of amount of analyzed states of EPS in the definite time and effective cover of the set of EPS states with no null shortage. In this case computational complexity of evaluation of one EPS state and solving of the parametric linear programming problem is comparable.

Section 8. INFORMATION AND COMPUTING SYSTEMS

An efficient block coding method of binary images

M.P. Bakulina

The problem of data compression for binary images transmission is considered. Such images are widely applied in digital cartography, geographic information systems and facsimile transmission. A new efficient block coding method of binary images is offered. The source is regarded as a model of first order Markov chain. The estimates of memory size and of average coding times have been obtained.

Computer social networks and their analysis

T.V. Batura, N.S. Kopylova, F.A. Murzin, A.V. Proskuryakov

The work focuses on the analysis of information flows and human behavior in the online social networks. We consider several formal definitions of various characteristics (numerical and structural) and introduce appropriate concepts, models and methods that could be useful for the analysis of information obtained from social networks. Preference analysis is proposed to be used to study interpersonal relations. Various modifications of Latané's dynamic social impact theory are proposed. The authors have studied techniques used to carry out psychological operations, and, as a result, have proposed several formal models. The paper briefly describes a software system that we have developed, which allows extracting, processing, analyzing and visualizing data from online social networking services. Our system has a data extraction module that can retrieve information from social networks such as Twitter, Facebook, and VKontakte.

Construction and research modular algorithms for creating a digital signature

R.G. Biyashev, S.E. Nyssanbayeva

Two systems of the digital signature (DS) are presented. The first one is DS scheme in a finite field (using the self-correcting (n,k) -codes of Lagrange) has been developed. These codes have parallel structure. In this algorithm cryptostrength of DS may not only depend on the length of DS, but also on complexity of hashing the electronic message block. Significant influence on DS cryptostrength magnification is also caused by choice of nonpositional polynomial notation (NPN) base systems (when encrypting the hash value). In this view, it is possible to generate more than one set of complete secret keys – in case of need to calculate a digital signature with given cryptostrength. The second system is ElGamal DS system based on NPNs. The algorithm for creating the DS is comprised of three stages: formation of NPN, hashing the message block of length N bits to the length Nk bits in this nonpositional system and computation of the digital signature for the obtained hash value based on ElGamal algorithm. Investigation of cryptostrength of the developed modular algorithm for creating the DS with a public key have been performed. The cryptostrength formula has been obtained.

Software modelling/simulation for cadastral appraisal on a real estatemarket (exemplification on appraisal flats in Omsk)

F.N. Boris, E.A. Boris

Cadastral (mass) appraisal on a real estatemarket is a field, where mathematic and software modelling are required. With the introduction of taxes to real estate the interest has been increased to this kind of appraisal, because cadastral value is the basis for taxation database. In the parameters of the research a methodology of mass appraisal and a corresponding software was developed.

Evaluation of multithreaded architecture supercomputers emulation on commodity clusters

V.S. Gorbunov, V.V. Korneev, L.K. Eisyomont

Concepts of multithreaded supercomputers emulation based on multisocket boards with many-core microprocessors, MVS-Express network with high message rate (especially for 8-32 byte messages),

special run-time system for OpenMP, q-threads and HPGAS parallel program models. Principle aspect of this run-time system - memory access to virtual global address space memory is executed by two-phase scheme and lightweight coroutines like in Grappa. This is the way to achieve memory access latency tolerance as in multithreaded architecture supercomputers like Cray XMT. In the article we have present some practical experimental results of our concept implementation. For example, we achieved 500 MRef/s memory access rate to socket DRAM using emulation by coroutine and prefetching on 8-core Sandy Bridge microprocessor. This is not far from 750 MRef/s rate achieved by hardware. This work have been done as a part of Russian Academy of Science exascale Hybrid SuperComputer Emulator (HSCE) research project.

Problems of stability "in the large" of multidimensional phase systems

M.N. Kalimoldayev, A.A. Abdildayeva, T. Duzbayev (Invited talk)

In this paper we solve the problem of evaluation of attraction domains of stable equilibria states, phase second order systems and isolated subsystems based on nonstandard Lyapunov function, which expands the area of stability of the system, in contrast to the well-known Lyapunov function of the type "kinetic energy plus potential energy". Let's consider the general model of multidimensional phase systems:

$$\frac{d\delta_i}{dt} = S_i, \quad \frac{dS_i}{dt} = w_i - D_i S_i - f_i(\delta_i) - \psi_i(\delta_{i*}), \quad w_i = C_i^* \chi_i. \quad (1)$$

$$\frac{dx_i}{dt} = A_i x_i + q_i S_i + b_i u_i, \quad i = \overline{1, l}, \quad (2)$$

where the function $\psi_i(\delta_{i*}) = \sum_{k=1, k \neq i}^l [P_{ik}(\delta_{ik})]$, $\delta_{ik} = \delta_i - \delta_k$ defines the relationship between subsystems

and $P_{ik}(\cdot)$ – the given continuously differentiable periodic function $D_i > 0$ – damping factor. δ_i – angular coordinate; S_i – angular velocity; $x_i - n_i$ – the state control vector; u_i – the feedback type control,

$f_i(\delta_i) = \frac{1}{T_i} [P_i \sin(\delta_{i0} + \delta_i) - P_i \sin \delta_i]$, $i = \overline{1, l}$. Investigation of stability "in the large" of the system (1),

(2) will be carried out in the band $G_{oi} = \{\delta_i, S_i, \chi_i \mid \delta_{-li} < \delta_i < \delta_{0i}, S_i \in R_i^1, x_i \in R_i^{n_i}\}$ using the method of Lyapunov. To investigate the stability "in the large", the feature $v_{oi}(\delta_{0i}, S_i)$ is offered which is defined in the band $\overline{G_{oi}}$ as follows:

$$\begin{aligned} v_{oi}(\delta_i, S_i) &= \frac{1}{2(S_i + a_i D_i \delta_i)^2} + \frac{1}{2} \alpha_i D_i (1 - \alpha_i) \delta_i^2 + F_i(\delta_i) + 2D_i \sqrt{\alpha_i (1 - \alpha_i)} \tilde{F}(\delta_i) = \\ &= \frac{1}{2(S_i + a_i D_i \delta_i)^2} + \int_0^{\delta_i} N_i(\delta_i) d\delta_i \end{aligned}$$

Non-stationary in connected structures

D.S. Legkiy, V.K. Popkov

Currently, the development of telecommunications networks is ever-increasing pace, while the overall situation has changed globally in infocommunications due to the ongoing transition from an industrial to an information society. As well changed and the basic approaches to the creation and development of telecommunication networks. The new technology are main reasons for the ongoing process, which rapidly begin to replace an existing and growing competition in the market of infocommunications services. The rapid growth of telecommunications networks is not only because of increasing needs for the increasing number and variety of services offered by providers, but also due to the unprecedented pace of change earlier network technologies.

Nowadays technological change is happening much faster than once every few decades, as it was in the last century. Often introduced into the existing network technologies have a significant impact on the very structure of the upgraded network. Thus there is not only a quantitative growth capacity and network bandwidth, but also qualitative changes, in most cases requiring revision of basic principles of

construction and design. The approach allows to describe and to optimize the process of dynamic change of the telecommunications network from the existing state of the introduction of several factors of non-stationarity, Parameters of non-stationarity require a fundamental change in the characteristics of the studied network, taking into account the spatial and temporal aspects. Describes the rules for constructing hypernet simulating the structure under consideration. Graphic simulation results are presented.

The Siberian Supercomputer center for collective use: current state and development trends

B.G. Mikhailenko, B.M. Glinskiy, N.V. Kuchin, I.G. Chernykh (Invited talk)

The Siberian Supercomputer Center (SSCC) was founded at the ICM&MG, SB RAS in 2001. The SSCC main objectives are development and using the supercomputer technologies for the numerical simulation, providing high performance computer resources to researchers from the institutes of SB RAS and Universities. A special attention is being given to training specialists of the SB RAS and university students in parallel scalable computing methods and algorithms on supercomputers as well as in methods of solving large-size problems. Currently there are two clusters in the SSCC that are exploited in the multi-access mode. One of the two clusters is based on the Intel Xeon processor (the MPP-architecture), its peak performance is 30TFlops, the MPI- and OpenMP-aided programming. The other cluster has a hybrid architecture with the GPU NVIDIA Tesla M2090 (the GPGPU-architecture), its peak performance is 85 TFlops, parallel programming in C/C++ CUDA and OpenCL. The seminars "Architecture, System and Application Software of Cluster Supercomputers" are regularly held on the basis of the SSCC, the Chair of Computer Systems of NSU and the Competence Center on High-Performance Computing of SB RAS - Intel.

Об одной математической модели транспортной сети мегаполиса

Д.А. Митченко, А.Т. Ахмедиярова

В докладе рассматриваются задачи оптимизации городского движения не только существующих транспортных систем, но и все возможные виды транспорта, которые разрабатываются или могут появиться в будущем [1-3].

Для этого необходимо рассмотреть:

1. Все виды транспорта, использующиеся в данный момент, и те, которые могут найти применение в будущем.
2. Классификацию транспортных систем, которые могут находиться в городе.
3. Собрать всю информацию о типах пассажиров и грузов, перемещающихся в городе, а также о маршрутах их следования.

Совокупность всех возможных видов транспорта представляет собой шестимерную таблицу, представляющую собой совокупность видов транспорта, разделенных на шесть категорий – место-положение движения, носитель, тип двигателя, источник энергии, тип движителя, тип топлива.

Транспортные системы включают в себя транспортные коридоры и транспортные узлы. В городских системах транспортными коридорами являются дороги, магистрали, виадуки, линии метро, трамвайные и троллейбусные пути, речные пути. Транспортными узлами являются: перекрестки, остановки общественного транспорта, автостоянки, парковки, а также вокзалы и аэропорты.

Evolutionary synthesis of families of circulant networks

O.G. Monakhov, E.A. Monakhova

A solution of an optimization problem of constructing families of optimal circulant networks having the minimum diameter for a given degree and number of nodes of a graph and families of circulant networks with a good ratio between order and diameter for a given degree is investigated. Circulant networks provide a practical interest as a graph theoretical model of reliable interconnection networks for the parallel supercomputer systems, and also as a basis of the structure in the model of small-world networks, as a base structure for discrete cellular neural networks and optical networks. We develop an approach

using evolutionary algorithms to automatically generate analytical (described by formulas) parametric descriptions of families of networks. An algorithm of evolutionary synthesis combines the advantages of genetic algorithms and genetic programming and is based on evolutionary computation, template (pattern, skeleton) of solution and a set of experimental data. Families of circulant networks, obtained by means of the evolutionary algorithm and improving earlier known in the literature results, are presented.

The synthesis of the proportional-integral regulators for optimal control problem

Z.N. Murzabekov

An optimal control problem for non-stationary linear systems with fixed ends of the trajectories taking into account external influences is considered. It is required to transfer the system from a given initial state to a desired final state for a fixed time interval. On the basis of optimal control problem solving by program control construction is maximum principle that reduces the solution to the corresponding two-point boundary-value problem. Solving of the same problem in the form of the synthesis of optimal feedback control is based on the dynamic programming method, where the problem is reduced to Bellman equation construction. Lagrange multipliers of a special form are used to solve the formulated problem in this work. The constructive proportional-integral regulator and corresponding algorithm of control based on feedback principle taking into account constraints on control values is developed. Minimized quadratic functional depends on the control, state vector and its integral.

Using modified and original genetic algorithms for reliability-based structural network optimization

K.A. Nechunaeva

Reliability-based structural network optimization problem is to maximize the network reliability subjected to some constraints such as the diameter of the network. Graphs were chosen for network modeling, because of their good applicability, wide facilities and profound elaborating. Graph optimization problems in conditions of constraints are NP-hard problems mostly. Genetic algorithms (GAs) are optimization technics based on natural evolution. It is applicable solution for network structure optimization and for obtaining good results within acceptable periods of time. This paper presents a strategy for using GAs and its modifications to solve NP-hard reliability-based structural network optimization problem. Some computational results are also presented which illustrate application of the method.

This research was supported by grant of the Russian Foundation for Basic Research (14-07-31069).

Моделирование систем "нарисованных" на системах

В.К. Понков (Invited talk)

В хорошо известной работе [1] автор, с методологической точки зрения, описал возможные отношения "ткань-рисунок", которые позволили выстроить взаимосвязи подсистем в виде многослойных структур, взаимодействующих в соответствующей системе.

В докладе рассмотрено несколько известных классов систем, которые адекватно моделируются с помощью аппарата теории S-гиперсетей [2].

В частности, приводятся примеры структурных моделей на языке теории нестационарных гиперсетей из следующих классов искусственных и естественных систем, формальные модели которых дают возможность решать различные задачи анализа и синтеза этих систем:

- транспортные системы [3],
- инфокоммуникационные системы и сети [4],
- коммунальные (трубопроводные) сети [5],
- задачи планирования и управления [6],
- социальные сети [7],
- структурные модели подсистем живых организмов [8],
- экосистемы и биосфера [9].

Список литературы

1. Лефевр В.А. Конфликтующие структуры. Издание второе, переработанное и дополненное. М.: Изд-во "Советское радио", 1973.168 с.
2. Попков В.К. Математические модели связности. Новосибирск: ИВМиМГ СО РАН, 2006. 490 с.
3. Попков В.К. О моделировании городских транспортных систем гиперсетями. "Автоматика и телемеханика". 2011. № 6.
4. Попков В.К. Попков Г. В. Величко В. В. Математические основы моделирования сетей связи. Учебное пособие для Вузов, Изд-во "Горячие линии Телеком", Москва, 2012г. 194 с
5. Попков В.К. Токтошов Г.Ы., Юргенсон А.Н. Об одном подходе к оптимизации инфраструктуры инженерных сетей. Вестник СибГУТИ № 3, 2012г.
6. Воронов Р.В., Воронова А.М., Пискунов М.А. Задача покрытия гиперсети взвешенным корневым деревом и ее приложение для оптимального проектирования схем волокон на лесосеках. Моделирование систем. 2012 г. №1 (31) стр. 56-64.
7. Попков В.К. Теория гиперсетей и ее применение Труды Международной конференции "Актуальные проблемы прикладной математики и информационных технологий – Аль-Хорезми 2009", 18-21 сентября 2009, Ташкент.
8. Попков В.К. Модель нейроэндокринной системы и ее применение в задачах управления и оптимизации 8-я Международная Азиатская школа-семинар "Проблемы оптимизации сложных систем" 2-12 июля 2012, Омск-Щучинск
9. Попков В.К., Правоторов Г.В. Об одной структурной модели биосферы Средней Азии. Материалы МНПК "Центральная Азия в исследованиях XIX-XXI ВВ". К 175 летию рождения Н.М. Пржевальского, Бишкек, г. Каракол 10-12. 04. 2014г. Стр.222-225.

About conception of modification of a transport communication network of the Russian federation

G.V. Popkov

Continuous growth of number of communications operators, continuous increase in a content, development and introduction of new systems of transfer at a limited spatial resource of settlements involve difficult solvable tasks of use of an urban area for placement of systems of transfer of various nature. Networks for a cable television and the Internet entangled houses and streets of the cities and villages. Development of new communication networks only aggravates this situation. Often unfair communications operators neglect norms of design and construction of networks, it also concerns also misuse of a transport network. It is obvious that such approach will not only worsen a present situation in branch, but also to reduce reliability and survivability of these communication networks. We will bring some arguments, into advantage above the provided statements. It is offered to consider eight levels of a such network: Level of consumers of communication services, level of communication channels, level of the environment of distribution of a signal, level of directing system (a cable, the communication air-line, a radio relay communication line (RRCL) trunk, etc.), level of channels (pipes) of the cable sewerage, systems of a suspension bracket of a cable, level of trenches, collectors or communication air-lines, level of routes of thoroughfares of communication networks, level of situational routes for possible realization of cable lines on streets of settlements or the rural territory. Thus, each level can put in compliance some count or the hyper count (the secondary S-gypernetwork) so that, formally it would be possible to describe an appropriate level of S-gypernetwork representing a transport network, communication networks of Russia.

Using structural peculiarities of random graphs for faster estimation of an average pairwise connectivity

A. S. Rodionov

The paper presents some algorithms and recommendations that enable increasing efficiency of calculating an average pairwise network connectivity (APNC) of a random graph and its cumulative updating for faster decision making about if a network is reliable. These methods are based on the well-known factoring method of calculating network reliability indexes and different ways of network decomposition and reducing its dimension.

Main income into speeding up of calculation is achieved by using so called "branching by a chain". Thorough experiments show that using this technique leads to speeding up exact calculation of the APNC by 1-2 decimal orders in average. At the same time speeding up of the decision making about a network's reliability based on cumulative update of its APNC is even higher.

Besides branching by chain, removing of dangling vertexes and special equations for some kinds of graphs that can be used for further speeding up of APNC calculation are discussed also.

Rules for choosing pivot edges and/or chains for factoring/branching are discussed also. Experiments show that choosing one incidental to a vertex with minimal degree increases efficiency of the algorithm by 15–20 % in average.

An efficient method for QoS parameter estimating

V.V. Shakhov

One of the most important performance measures of a modern network is the packet losses rate and the average delay required to deliver a packet from source to destination. Furthermore, consideration of the mentioned factors strongly influence the choice and performance of network protocols. For these reasons, it is important to investigate the nature and mechanism of packets blocking probability and packets delay, and the manner in which it depends on the characteristics of the network service. Teletraffic engineering is the primary methodological framework for analyzing quality of service. Its use requires simplifying assumptions since more realistic assumptions make meaningful analysis extremely difficult. For this reason, it is generally impossible to obtain accurate quantitative predictions for quality of service parameters. Nevertheless, these technique often provide a basis for adequate approximations of packets losses rate and packets delay, as well as valuable qualitative results and worthwhile insights. In this paper an efficient method, which is based on teletraffic engineering technique, for quality of service parameters estimating is offered.

Models and optimization algorithms for some modern networks problems

O.D. Sokolova

The paper describes some optimization problems in modern networks: broadcasting, intrusion detection, survivability estimation, monitoring and others. In order to develop algorithms for modern networks, appropriate models are required. Graphs, Unit Disk Graphs, hypergraphs and hypernets are using as models for various types of networks. Author gives some results of exploiting graph theory methods to investigate and solve various network problems, for example, reliable packet transmission. The minimum channel occupancy time is considering as the criterion of optimality.

Информационно-математические основы гиперспектрального ДЗЗ и супервычисления

Information and mathematical foundations of hyperspectral remote sensing and supercomputing

Т.А. Сушкевич, С.А. Стрелков, С.В. Максакова (Invited talk)

60 лет назад, в середине февраля 1954 года, в кабинете академика Мстислава Всеволодовича Келдыша состоялось ПЕРВОЕ совещание, на котором впервые обсуждался вопрос о создании и запуске в космическое пространство искусственного спутника Земли (ИСЗ). Работа посвящается 60-летию юбилею Института прикладной математики им. М.В. Келдыша Российской академии наук, 50-летию первого в мировой практике научного эксперимента по дистанционному зондированию Земли (ДЗЗ), проведенного человеком в космосе, на космических кораблях "Восток-5" В.Ф.Быковским (14-19 июня 1963 г.) и "Восток-6" В.В.Терешковой (16-19 июня 1963 г.), когда из космоса впервые были обнаружены стратосферные аэрозольные слои в атмосфере Земли.

Новые перспективные возможности математического моделирования атмосферной радиации Земли для решения прямых и обратных задач на основе кинетического уравнения переноса излу-

ния и гиперспектрального дистанционного зондирования атмосферы и поверхности Земли связаны не только с разработкой универсальной информационно-математической системы для широкой области приложений на суперкомпьютерах и кластерах с распараллеливанием супервычислений и распределением ресурсов, но и с созданием и развитием международных ГРИД-систем и тематических "облачных" систем.

Суперкомпьютеры очень высокой производительности помогут разобраться как именно и почему климат меняется. В результате природных процессов или воздействия человека? В настоящее время ответ на эти вопросы чрезвычайной важности определяется, по сути, "научным голосованием" совокупности специалистов, изучающих и моделирующих климат. Однако есть надежда, что с помощью спутниковых и наземных поляриметрических и гиперспектральных наблюдений и глобального космического мониторинга при поддержке "сценарного" математического моделирования точность и надежность таких прогнозов существенно возрастут. Радиационный форсинг на изменения климата составляет около 40 процентов!

Работа поддержана Российским фондом фундаментальных исследований (проекты № 12-01-00009, № 14-01-00197) и Российской академией наук (проект 3.5. ПФИ ОМН РАН)

Using the hypernets for synthesis of the optimal structure of engineering communications

G. Y. Toktoshov

The article is devoted to the questions of optimization of engineering communications in the given territory. Features of hypernet approach to the choice of the optimal structure of engineering communications, the essence of which consists in considering the "earth" and "engineering communications" in one hypernet model. At the same time as the primary network is understood mathematical or digital terrain model (DTM), taking into account the peculiarities specified territory, and as a secondary - configuration design communication. Thanks to the proposed approach, project engineer at the stage of design can determine the preliminary route for laying of engineering communications, which is important for the financial savings. In addition, hypernet approach to the design of engineering communications allows to take into account the interrelated set of primary and secondary networks, taking into account all structural parameters and economical characteristics of the designed communication.

Task pool implementation for effective utilization of CPU resources in the BioUML platform

T. F. Valeev, F. A. Kolpakov

The BioUML platform is a software platform written in Java and designed to perform research, experimental data processing, modeling and visualization in the fields of systems biology and bioinformatics. Being multiuser web-platform which allows running computationally-intensive tasks on the server side, BioUML needs an effective resource management including control over available processors utilization. When server has free resources, it's necessary to allow users to run analyses faster, performing parallelization if supported by analysis method. On the other hand users should not harm each other, so it should be possible to dynamically reduce number of threads available for each particular analysis. To reach this goal special task pool was implemented which controls all user threads and provides common tools for parallelization. It was successfully integrated into BioUML platform and proved its efficiency in public version of BioUML web edition 0.9.6 as well as in BioUML-based commercial platform geneXplain 2.4.

Some questions of the adapting the order filters to the signal form and character of noise

V.I. Znak

The objective of this paper is improvement of the quality of the vibroseismic research data under the condition of preservation of the form of a wave of a sounding signal. For this purpose, the weighted order statistics filters are offered. However, the given filters are nonlinear (an analytical estimation of their behavior is a complicated process), and the processing of periodic signals demands separate attention in this case (the filter response tends to zero when approaching the length of the filter to integer periods of a

signal). At the same time, the filters belong to the nonlinear ones. The result of signal processing (the filter response) depends both on the filter parameters (including the dependence on a sequence of operations) and properties of a signal and the kind of noise. Thus, analysis of their behavior is rather complicated. In this paper, the technique of order filters adaptation invoking a method of statistical trials and interactive graphical interface is offered.

Section 9. MATHEMATICAL MODELING

Investigation of spacecraft orbital stability using Ince – Strutt diagram

Sh.A. Aipanov

The planar circular restricted three-body problem is considered. It is supposed that two bodies with masses m_1 and m_2 move in circular orbits around the common center of masses, and the third body with mass m_3 ($m_3 < m_1$ and $m_3 < m_2$) moves in a circular orbit around the body m_1 . The motion equations for the body m_3 were reduced to Mathieu's equation, then orbital stability of the body m_3 was investigated using Ince – Strutt diagram. The problem of orbital stability for the spacecraft moving in circular orbit around the Earth in the Moon's orbit plane is considered as an example.

Design of multisection pressure tanks

S.N. Astrakov, S.K. Golushko

Pressure vessels, tanks and balloons are widely used in aviation and spacecraft applications. Minimum weight and geometric shape for convenient placement in the limited space are important requirements for such structures. The use of composite materials in the manufacture of such structures has opened additional opportunities to find their best form, providing a predetermined internal volume with minimal surface area. Authors W. Tam and I. Ballinger proposed design of tanks with baffles and nested tanks in the article "Conceptual Design of Space Efficient Tanks" (AIAA 2006-5058). In this paper we considered two and three sectional vessels with new form and gave the rationale for their use. In the simulation, we actively use isoperimetric properties of soap films and their interconnection rules.

The solution of some nonlinear problems of continuum mechanics

I.B. Badriev

We study the nonlinear problems of continuum mechanics, described by the operator equations and variational inequalities with monotone type operators in Hilbert and Banach spaces. Such problems arise when it is considered the steady filtration processes in inhomogeneous, including multilayer formations and anisotropic media, of an incompressible fluids, following the nonlinear filtration laws [1], nonlinear problems of the theory of shells, including the soft biological membranes in the presence of obstacles, multilayer shells with transverse fillers with constraints [2, 3].

Investigation of the solvability of these problems is based on the general theory of monotone operators. For this purpose, we establish the properties of the operators (monotony and coercivity) and functional (convexity and lower semicontinuity) entering in the considered equations and variational inequalities.

Approximate methods based on preliminary finite-dimensional approximation equations and variational inequalities by application of the finite element method, including the finite element method with numerical integration in the case of inhomogeneous media.

To solving the built finite-element schemes the iterative methods are used. The methods are implemented in software form complexes. For some model problems of filtration theory of shells the numerical experiments are performed.

The work was financially supported by the Russian Foundation for Basic Research (projects nos. 12-01-00955, 12-01-97022, 14-01-00755).

References

1. Badriev I.B., Nechaeva, L.A. Mathematical simulation of steady filtration with multivalued law // PNRPU Mechanics Bulletin. 2013. Is. 3. P. 37-65.
2. Abdusheva G.R., Badriev I.B., Banderov V.V., Zadvornov O.A., Tagirov R.R. Mathematical Simulation of the Equilibrium Problem for the Soft. Biological Shell. I. Generalized Statement. // Proceedings of Kazan University. Physics and Mathematics Series. 2012. V. 154, Is. 4. P. 57-73. (in Russian).
3. Paimushin V.N. Nonlinear theory of the central bending of three-layer shells with defects in the form of sections of bonding failure // Soviet Applied Mechanics. 1987. V. 23, Is. 11. P. 1038-1043.

Numerical solution of some problems of the theory of multilayer shells with transversely soft filler in the presence of the sections of bonding failure

I.B.Badriev, V.V. Banderov, M.V. Makarov, V.N. Paymushin

We consider the problem of determining the stress-strain state of sandwich shallow shells with a transversely soft filler having an average thickness. In constructing the basic relations we take in account the changing of the metric characteristics in the thickness of the filler direction. Its kinematic relations are derived by successive integration by the transverse coordinate of the original three-dimensional equations of elasticity theory, pre-simplified by the introduction of the assumption of the vanishing of the tangential stress components [1]. The presence of the sections of bonding failure is simulated by the restrictions on modules of the tangential stresses. To solve the problem, a continuation by the parameter method [2] is applied.

The work was financially supported by the Russian Foundation for Basic Research (projects nos. 12-01-00955, 13-08-90435, 13-08-97076, 14-01-00755).

References

1. Paimushin V.N. Nonlinear theory of the central bending of three-layer shells with defects in the form of sections of bonding failure // Soviet Applied Mechanics. – 1987. – V. 23, Is. 11. – P. 1038-1043.
2. Shalashilin V.I., Kuznetsov E.B. The method of the parameter continuation and best parameterization (in applied mathematics and mechanics). Moscow: Editorial URSS, 1999. 224 p (in Russian).

Numerical model of freeze-thawing permafrost

V. Belolipetskii, S. Genova (Invited talk)

Theoretical description of the temperature field in the soil when they are freezing or thawing is carried out using solutions of Stefan problems. Mathematical model based on the equations of heat conduction for frozen and thawed layers. Areas with lakes or swamps are discussed. You can select the following layers in the vertical structure of the permafrost zone: thawed soil, frozen soil, water, ice, snow. The approximate numerical algorithm for solving one-dimensional (in the vertical direction) heat conduction problems with moving boundaries of the phase transition with the formation of new and extinction of existing layers.

Efficient numerical modeling in applied problems of mathematical physics with a high computational complexity

A.M. Blokhin, S.K. Golushko, B.V. Semisalov

Currently, numerical simulation is an indispensable tool for solving a huge amount of applied problems in different areas of science and engineering. The practice of modeling of complex systems described by stiff nonlinear differential equations shows that the numerical algorithm should be designed on the basis of all known properties of the solution. This requirement enables one to create stable algorithms and find solutions of complex applied problem with sufficient accuracy and minimum computational costs.

The report presents adequate methods for numerically solving the problems of semiconductor physics and mechanics of composites accounting for a priori information about the smoothness of unknown functions. A new approach to design of spectral numerical methods based on the ideas of K. I. Babenko on approximations without saturation is proposed. Its advantages are discussed on the example of solving the problems of charge transport in semiconductor silicon devices and modeling of deformation and optimization of composite structures. The results of computations for silicon transistor DG-MOSFET and modeling of anisogrid carbon structure are performed.

Modeling of reactivity of organoaluminum compounds in olefin hydroalumination reactions

Yu. O. Bobreneva, A.V. Novichkova, I.M. Gubaydullin, K. F. Koledina

Modeling of reactivity is an important task in chemical kinetics. The maximum product yield can be predicted using the reactivity of the starting compounds. The most important characteristics of the

reactivity are rate of consumption of a substance, relative rate constants and activation energy. The kinetic models olefin hydroalumination reactions with triisobutylaluminum, diisobutylaluminum hydride and diisobutylaluminum chloride were constructed to determine the reactivity. The activation energy of stage of interaction between organoaluminum compounds and catalyst was analyzed using this models. The induction period olefin hydroalumination reactions with diisobutylaluminum chloride was investigated. Numerical parameters of the induction period and the rate-limiting step with the highest activation energy were defined, causing the induction period of the reaction. The graphs of consumption rate of organoaluminum compounds were constructed. In conclusion triisobutylaluminum is the most reactive compound.

Finite difference methods for nonlinear system of mathematical model of RF discharges

V.J. Chebakova, M.N. Schneider, V.S. Zheltukhin

RF discharge at low pressure $p=13.3-133$ Pa and inter-electrode distances of 20-30 cm is effectively applied to processing of different materials. One-dimensional model of non-stationary low pressure RF discharges with large-scale inter-electrode distances is constructed. The model is consist of 6 equations both parabolic and elliptic type with first and third boundary conditions. The problem is characterized by strong nonlinearity, a combination fast (electronic and field) and slow (nuclear and ionic) processes, convective members, strongly changing coefficients, oscillating boundary conditions depending on the direction of electric field.

For the solution of a task the special iterative process is constructed. The linearized problem is solved by means of implicitly finite difference scheme with uniform grid. For the solution of finite difference tasks the method of stream Thomas algorithm is modified. Results of calculations are showed that periodic solution is established during more than 10^3 periods of an electromagnetic field fluctuation. the received characteristics of the VCh-category well will be agreed with experimental data. Calculated characteristics of the RF discharge are agreed with experimental data.

Numerical models of some free turbulent flows

G.G. Chernykh, A.G. Demenkov, O.A. Druzhinin, A.V. Fomina, B.B. Ilyushin, N. P. Moshkin, O.F. Voropayeva (Invited talk)

Numerical simulation of the dynamics of axisymmetric turbulent jet flows with varied total excess momentum and angular momentum in homogeneous fluid is performed. Self-similar decay of a far turbulent swirling turbulent wake past self-propelled body was studied numerically (jointly with V.A. Kostomakha).

The dynamics of a passive admixture from an instantaneous localized source in the 2D turbulent mixing zone in a homogeneous and stably stratified fluid was modeled numerically (jointly with Yu.D. Chashechkin).

Based on hierarchy of modern semi-empirical models the numerical analysis of evolution of turbulent wakes and internal waves generated by them behind bodies of revolution in stably stratified media was executed. The description of anisotropic decay of turbulence in far wakes in stratified fluid was carried out. Comparison of DNS and RANS approaches to numerical modeling of turbulent wakes was executed.

The work was supported by the Russian Foundation for Basic Research (95-01-00910, 98-01-00736, 01-01-00783, 04-01-00209, 07-01-00363, 10-01-00435, 13-01-0246).

A numerical analysis of the spectrum of plane-parallel flows

T.G. Darmaev

In the linear theory of hydrodynamic stability research of development of small disturbances $v(y)e^{i(\alpha x - ct)}$ in plane-parallel flows of viscous liquid is reduced to Orr-Sommerfeld equation:

$$(D^2 - \alpha^2)^2 v = i\alpha Re \left[(U - c)(D^2 - \alpha^2)v - vD^2U \right] \quad (1)$$

where α – wave number, Re – Reynolds number, $c = c_r + ic_i$, $v = v_r + iv_i$ – required complex eigenvalue and eigenfunction, i – imaginary complex unit.

In this work the solution of equation (1) and a profile of basic flow U we seek in the form of decomposition on Chebyshev's polynoms. Further solving the received system of the algebraic equations with application of QZ algorithm we find a spectrum of eigenvalues at finite numbers of polynoms of Chebyshev.

Spectrums of plane Poiseuille and Couette flows, and also Blazius flow over a flat semi-infinite plate are received at different α and R values.

Usage of the energy method for mathematical simulation of the heat transfer in 2-D stream

V.V. Denisenko (Invited talk)

The problem of steady-state heat transfer in moving medium is transformed to minimization of a quadratic energy functional. Piece-wise functions are used to approximate the solution. Multigrid method by Fedorenko is applied to solve the system of linear algebraic equations for the values of the function at grid nodes. Temperature space distributions are calculated for Puaseil stream between parallel walls. Heat source space distributions are preliminary calculated as Joule dissipation due to electric currents which are created by voltage between two electrodes at opposite walls. The walls with given temperatures are studied as well as impenetrable for heat ones.

Mathematical simulation of the alive cells electrophoresis in moving liquid

V.V. Denisenko, V.A. Kolovskii

Puaseil stream between flat walls is analyzed. Electric field in the liquid conductor is created by two electrodes placed at opposite walls. The electric field space distribution is obtained numerically for the mixed boundary value problem for Poisson equation. Dirichlet principle and piece-wise linear functions are used to approximate the solution. The inhomogeneous electric field put a force on the cells because of their polarization. This force can be parallel or antiparallel to the gradient of the squared electric field. It depends on the cell composition, conductivity of the liquid, and on the voltage and frequency of the applied field. Spherically symmetrical cells are considered where we have simple formulae the force and cell's friction with liquid. The kinematic equations are numerically integrated for each cell separately. Initially cells are homogeneously distributed in the liquid. After passing between electrodes they are concentrated near one of the walls. Different geometries of the electrodes are analyzed to produce a higher concentration.

Method of integral averages in electromagnetic sounding problems

V.I. Dmitriev, M.S. Kruglyakov

New numerical method for 3d integral equations of electrodynamics was devised. The most challenging aspect of using these equations in forward problems of EM sounding is associated with a need to solve a high-order system of linear equations with a dense matrix. The main distinctive feature of the proposed method is a double integration of the electric Green's tensor in the process of algebraization of the original equation to decrease the condition number of the matrix. Another computational challenge arises from the fact that the Green's tensors elements are integrals containing the Bessel functions. In order to solve this problem we developed the new method motivated with W. Anderson's ideas on Hankel transforms calculations.

The method of integral averages was implemented as parallel program using both MPI and OpenMP technologies. The computational experiments were performed by Bluegene/P and "Lomonosov" supercomputers from MSU. These experiments showed the efficiency of the proposed method in high-contrast electromagnetic sounding problems.

Finite element modeling of time-harmonic electromagnetic field of arbitrary-oriented coil

P.A. Domnikov, Yu.I. Koshkina

We present the finite element scheme of 3D electromagnetic (EM) field modeling for an induction logging. Our scheme exploits the field separation technique, i.e. the total EM field is presented as a sum of a normal EM field in host horizontally layered media (HLM) and of an abnormal EM field in media containing

3D objects. The EM source is a coil with a time-harmonic current flow in it. Our scheme allows the axis of the coil to be oriented arbitrary relatively to the layers of HLM. It is performed through the summation of the EM fields of the horizontally and vertically oriented coils. We propose a new mathematical model for the vertically oriented coil with the time-harmonic current flow in it. This mathematical model consists of two relatively simple axisymmetrical problems. The computational efficiency of the finite element scheme proposed is analysed. Also we verify the correctness of the proposed mathematical model by comparing it with the full 3D finite element solution.

Тензор Коши как полная характеристика деформированного состояния

Т.Б. Дуйшеналиев, И. Козубай

Роль деформации в механике деформируемого тела подобна роли ускорения в механике твердого тела. В деформационном движении, т.е. в движении частиц тела относительно друг друга, соотношения между тензорами напряжения и деформации являются определяющими такое движение законами. В свете этого, вид выражения деформаций через градиенты перемещений имеет первостепенное значение. Если эти выражения не линейны, то решения задач становятся чрезвычайно сложными. В данной работе доказывается, что компоненты деформации линейно выражаются через градиенты перемещений при любых их величинах.

A Bayesian approach to simulate CO₂ emissions from natural fires

A.V. Eliseev, I.I. Mokhov, A.V. Chernokulsky (Invited talk)

The ensemble simulations for 850-2300 with the global climate model developed at the A.M. Obukhov Institute of Atmospheric Physics, Russian Academy of Sciences (IAP RAS CM) are presented. Different ensemble members were constructed by varying the governing parameters of the IAP RAS CM module simulating natural fires. These members are constrained by the GFED-3.1 observations and further subjected to Bayesian averaging. In our simulations, the present-day ensemble mean global area burnt due to natural fires S_g is $2.1 \cdot 10^6$ km²/yr, and the respective CO₂ emissions E_g in the atmosphere are $1.4 \cdot \text{PgC/yr}$. In the 21st century, the ensemble mean global burnt area is increased by 13-51% depending on scenario of anthropogenic forcing. The corresponding global emissions increase is 14-42%. In the 22nd-23rd centuries, under the mitigation scenario S_g and E_g decrease by 5% relative to their values in year 2100. Under other anthropogenic scenarios, these variables continue to increase: the ensemble mean burnt area in year 2300 is higher by 15-83% than its value in year 2100, and the ensemble mean CO₂ emissions are correspondingly higher by 9-31%. All changes of natural fire characteristics in the 21st-23rd centuries are associated mostly with the corresponding changes in boreal regions of Eurasia and North America.

Modeling of the electrochemical impedance using a genetic algorithm approach

A.R. Enikeev, M.A. Maleeva

In order to predict the general corrosion damage to metals and alloys, development of deterministic models and the acquisition of values for various model parameters are of paramount importance. Now it is generally accepted that elucidating an intricate reaction mechanism by means of steady-state techniques alone is a very difficult task. It was recently found that impedance diagrams reveal at least three time constants concerning the faradaic process in the iron-sulphate systems was proposed by Keddam.

The Faradaic impedance Z , can be calculated by Taylor expansion of equation limited to the first order:

$$\frac{1}{Z_f} = \frac{1}{R_t} - F \left\{ (K_1 - K_2 - K_3) \frac{d\theta_1}{dE} + (K_1 - 2K_4) \frac{d\theta_2}{dE} + (K_1 - (2-p)K_6 + K_{-5}) \frac{d\theta_3}{dE} + K_4 \frac{d\theta_4}{dE} \right\}$$

The reaction kinetic parameters was calculated by genetic algorithm. The experimental impedance diagrams showed one high-frequency capacitive arc and three time constant at lower frequencies appearing as inductive or capacitive loops.

Theoretical optimization of the tert-butylphenol oxidation reaction by the aqueous solution of hydrogen peroxide in presence of titanosilicates

L.V. Enikeeva, I.M. Gubaydullin, N.F. Murzaheva

At present the study of the processes of liquid-phase of the heterogeneous catalytic oxidation of organic compounds in presence of metal substituted silicate materials is actual and perspective problem. The titanosilicates among them are the most stable and active catalysts for the reaction of aromatic hydrocarbons and olefins oxidation as an oxidizing agent of different organic and inorganic peroxides. Institute of Petrochemistry and Catalysis, Russian Academy of Science conducts research in the synthesis of micro- and mesoporous titanosilicate materials and in the study of their catalytic activity in the reaction of the phenol and its derivatives oxidation by the aqueous solution of hydrogen peroxide.

The main objective of this work is to develop the kinetic model for the oxidation reaction of tert-butylphenol in presence of different titanosilicates as a catalysis and to optimize the model theoretically. For solving this optimization problem the simulated annealing algorithm, the genetic algorithm and their parallel realizations were used.

The medium with microinclusions: tensor effective characteristics of electrophysical properties

M.I. Epov, E.P. Shurina, N.V. Shtabel, E.I. Mikhailova (Invited talk)

The approach of calculating the effective characteristics of electrophysical properties for medium with microinclusions as a dense tensor of the second rank is proposed. This coefficient is considered as the complex-valued tensor $Z=Z(\varepsilon, \sigma, \omega)$ that depends on the dielectric permittivity and the conductivity of the medium and inclusions as well as a excitation frequency. The solution of the Helmholtz equation for electric field in an area with inclusions is used to determine the elements of the effective tensor. The Helmholtz equation is solved by using the vector finite element method on tetrahedral unstructured meshes. The finite element modeling of the electromagnetic field in anisotropic medium with calculated effective coefficient is held out. The proposed approach is verified on the series of problems in homogeneous medium. The obtained tensors for homogeneous medium are diagonal ones. All nonzero elements are equal to dielectric permittivity and conductivity of the medium. The effective tensors for media with microinclusions are computed. The admitted region of the approach with respect to the contrast of inclusions, their number and distribution is investigated.

Mathematical modeling of propagation opinions in society

A.M. Fedotov, S.G. Lomakin (Invited talk)

Ideas have enormous potential to influence public opinion. Study the dynamics of competition of ideas is extremely important for many areas. To study the dynamics of propagation of the new information (memes) in society (on the set of interacting agents modeled by cellular automata) was chosen simple visual model Naming Game, considering expansion of opinions (memes) in the graph of social interactions.

For modeling the propagation of ideas selected dual model agreement. Shown as the predominant opinion of the majority can be reversed small part of distributed agents who distribute their opinion and are immune to the influence of others opinions. The existence of a tipping point, after which the community has promoted the idea.

From the point of view of the influence of ideas on the population of automata (society), the most important property is the competition of ideas. In the presence of competition steady state becomes unstable structures may occur in the form of traveling waves or periodic solutions. Possible and structurally stable scenarios (eg, multiple periodic modes). It is interesting that "patchiness": the emergence of a new idea - it EXTENDED not uniformly on the set of agents, and agents are grouped.

Hierarchy of models of long wave hydrodynamics

Z.I. Fedotova, G.S. Khakimzyanov

Hydrodynamics of surface waves is characterized by the wave processes of different scales. The corresponding boundary value problem for the Euler equations in the case of a complex geometry is a

difficult task. When dealing with practical problems it is profitably to use approximate models aimed at the description of waves in certain ranges. In the long-wave hydrodynamics for the construction of approximate models is advisable to use a hierarchical approach of step by step modifications of the original differential problem. Several hierarchies are traced, to wit on geometry (plane, sphere), on the nonlinearity (linear models, nonlinear shallow water equations, weakly nonlinear Boussinesq equation, the full nonlinear dispersive equations), on the dispersion and others. This paper presents a uniform derivation of the full hierarchical chain of nonlinear dispersive equations taking into account a movable bottom both in Cartesian coordinates on the plane, and on the rotating sphere. Derivation is based on the using of small parameters. Here it was important to retrace that the most significant properties should be inherited, for example, the conservation laws. The resulting equations have been recorded in the universal form on a plane and on the sphere. The developed approach is transferred to the numerical algorithms for the entire chain models.

Солитоны и волны огибающих в многорезонансных средах Лоренца с квадратичной и кубической нелинейностью

В.Г. Гасенко

В работе численными и аналитическими методами исследуется полидисперсное уравнение КдВ (ПКдВ), полученное для многорезонансных сред Лоренца с квадратичной (полидисперсные газожидкостные смеси) и кубической нелинейностью (диэлектрики и ферромагнетики с конечной индукцией насыщения) и являющееся обобщением уравнений КдВ и нелинейного уравнения Шредингера (НУШ). На низкочастотной ветви дисперсионной кривой ПКдВ имеет солитонные и бризерные решения и переходит в уравнение КдВ, на последующих ветвях его решениями являются солитоны огибающих, и ПКдВ в случае кубической нелинейности переходит в НУШ. ПКдВ с квадратичной нелинейностью разрешено методами ОЗТР аналитически: найдена пара Лакса, безотражательные потенциалы и т.д. В общем случае разнообразные нестационарные решения ПКдВ находились численно высокоточными Фурье методами с периодическими граничными условиями. Показано, в частности, что начальный сигнал может распадаться на последовательность солитонов, бризеров, солитонов огибающих и новых типов уединенных волн, присущих только уравнению ПКдВ, которые одновременно существуют и не взаимодействуют между собой.

GPU computing in the Vortex element method for numerical simulation of the flow around an airfoil

S.R. Grechkin-Pogrebnyakov, I.K. Marchevsky

The vortex element method is a meshless lagrangian method which allows to simulate the flow around arbitrary airfoils and also to solve coupled hydroelastic problems effectively. The Viscous vortex domains method is used for dynamics simulation of the vortex wake. The procedure of computing convective and diffusive velocities of vortex elements (VE) has the greatest computational cost.

All pair-influences of VEs should be taken into account so the computational cost of this operation is $O(n^2)$. GPU computing usage allows to reduce time of computation manifold and to perform simulations of unsteady viscous vortex flows around airfoils on personal computers instead of computer clusters. Using CUDA technology the algorithm and the corresponding computer program are developed for numerical simulation of flows around airfoils. For some model problems speedup is more than 100 times, the number of VE can be brought up to 100,000 or even more at a reasonable time of the calculation on a personal computer with GPU accelerator.

On the stability for a class of 1–D states of dynamical equilibrium of the Vlasov – Poisson plasma

Yu.G. Gubarev, A.A. Gubkin

The Vlasov – Poisson plasma model continues to be one of basic mathematical models of modern plasma physics. This is due to its simplicity, clarity and obvious usefulness for solving of the problem of controlled thermonuclear fusion. The Vlasov – Poisson plasma model is intensively studied for a long time.

However, only sufficient conditions of the theoretical stability for a number of dynamic equilibrium states with respect to both small and finite perturbations of adjective subclasses were established. In this report, it is proved by the direct Lyapunov method that 1–D states of dynamic equilibrium of the Vlasov – Poisson plasma are absolutely unstable in the theoretical sense (at semi–infinite time intervals) in relation to the same 1–D small perturbations. At that, the known sufficient condition of the theoretical linear stability for these states is turned, and the range of its applicability is strictly described. In addition, we obtained sufficient conditions of the practical linear instability (on finite time intervals), constructed a priori exponential lower estimate and characterized the initial data for growing small perturbations. According to authors, these results may be useful in the process of mathematical modeling of various physical phenomena in plasma.

Analytical technique in the boundary element method for 3D electron optics problems

V. Ivanov

The analytical technique was developed for 3D boundary problems described by Poisson's equation. It includes the analytical integration over triangle elements represent the boundary surfaces, and over hexahedral space elements represent the space charge distribution with linear approximation for surface and space source distributions. Analytical integration removes the kernel singularities inherent to the original Green's function which corresponds to the integral representation for the single-layer potential. Special notice was attended to the analysis of the edge singularity problem for the field gradients. The complete set of equations for self-consistent problems of electron optics includes the field equation, the motion equation for relativistic particle in electromagnetic field, and the continuity equation for space charge and current density. This non linear problem was solving by iteration procedure with charge and current relaxation. The accuracy of numerical solution was demonstrated as for the test problems as for the computer design of electron gun for 75MW X-band sheet-beam klystron by comparison with experimental data.

Development of mathematical models for the efficient management of economic systems

M.N. Kalimoldayev, G.A. Amirkhanova

In this paper the mathematical models of economic growth processes and development of methods for optimal stabilization of economic systems are investigated. In modern conditions of economy transformation and transition to market relations, functioning and development of production systems are characterized by instability, non-linearity and dynamics of key indicators and parameters. Therefore, it is necessary to have the effective management and operational decision-making system. The actual direction of solving this problem is to develop the flexible intelligent control system which allows to quickly diagnose the adverse condition of the financial - production system and to timely actuate the mechanisms which return the system to equilibrium. In this connection, the models of optimal control of diversified economy were developed on the finite planning horizon, taking into account the scientific and technological progress: the economy model dependent on export of natural resources was constructed; the one-sector and the multi-sector economic models were analyzed for developing the optimal macroeconomic policy during the integration of the country economy.

Direct numerical simulation of transition to turbulence in supersonic flat plate boundary layers

D.V. Khotyanovsky, A.N. Kudryavtsev

Direct Numerical Simulation (DNS) of the transition to turbulence in a supersonic boundary layer over a flat plate is performed using the fifth order WENO (Weighted Essentially Non Oscillatory) shock capturing scheme. The computations are conducted at moderate supersonic (Mach number $M = 2$) as well as hypersonic ($M = 6$) speeds. All stages of the transition starting from the linear instability up to emergence of small scale 3D chaotic pulsations are simulated. At $M = 2$ the study is focused on the oblique breakdown mechanism of the transition while at $M = 6$ the main attention is paid to the nonlinear interaction of the first and second modes of hydrodynamic instability. The numerical results are compared, where is possible, with available experimental data.

This study was supported by the Russian Foundation for Basic Research (Grant 12-01-00840) and by the Russian Government Grant 14.Z50.31.0019 for the promotion of research directed by leading scientists.

The research of mathematical model for the thermal conductivity of a continuous medium with a nonlocality in space

V.N. Korchagova, I.K. Marchevsky, I.Yu. Savelyeva

Modern structural and functional materials produced using nanotechnology have micro-or nanostructure. Such materials are often used as covers. Microscopic elements of such materials are subject to influence of other surrounding elements of structure, i.e. so-called nonlocality of media takes place. Thereof materials can possess the unique heatphysical properties allowing effectively of them to use in designs, subject to high-intensity thermomechanical influence. However such materials don't submit to classical model of heat conductivity.

The goal is to study non-classical mathematical model that consider the energy transfer processes at the micro level, and to calculate the temperature field of the material by the finite element method. Practical and theoretical value of this model is the ability for predicting the properties of advanced materials and creating the framework for constructing the thermodynamic behavior of advanced materials.

Modeling of the factors of production using Navier – Stokes equations

S.B. Kuznetsov

Equation of Navier-Stokes type was obtained through the study of development of production factors of the economy. A new index called the economic numbers was build based on the equation. In order to calculate the economic number statistical data on the main factors of production of national economies were used. It is proved that the economic number is not random, but it is an objective characteristic of the economic condition of the state. The economic number proposed in the study allows any economics with different scales to be compared. Calculations of the economic numbers made for several countries in Europe and America are well correlated with existing economic ratings, such as rating of the global competitiveness, business rating, and rating of the most competitive country in the world.

Numerical modelling of oscillatory processes in the model two-stage centrifugal pump

V.Ya. Modorsky, P.V. Pisarev

In this work authors are given results of numerical experiments on modeling of oscillatory processes, with use of the three-dimensional hydrodynamic model considering characteristics of oscillatory system "the free volume of the pump of the first step - the connecting channel - the free volume of the pump of the second step". Features of emergence and strengthening of fluctuations in model channels are revealed at a variation of parameters of a stream and channel geometry. Authors examined the influence the phase angle φ on the characteristics of oscillatory processes in the connecting channel and adjacent volumes of the two-stage centrifugal pump model. Diagnosed growth intensity oscillation processes in the area of the second stage of increasing the phase angle φ from 90 to 180 degrees.

Parallel calculation of the large-size fan of the cooler

V.Ya. Modorsky, A.F. Shmakov

In power cooling tower are widely applied for cooling the working fluid. At present in the world a large number of such devices of various standard sizes is used. One of elements of the cooling tower is the fan. In this work, within numerical modeling, for set productivities (10 million m³/h) and power consumption (450 kW), the fan with a diameter of 20 m is designed. Various designs of blades are considered, the analysis of influence of angles of attack blades, width, a gap between the diffuser and the fan, an entrance confusor on productivity and power consumption is carried out. Aerodynamic calculation was carried out in the program ANSYS CFX complex. In total about 10 options from which the design of the fan providing the set expense and power consumption was chosen are calculated. Two designs were developed for the chosen option accepted from the point of view of aerodynamics. For the selected options with use of the program ANSYS complex the analysis intense the deformed state was carried out. As a result of calculations the

design of the fan providing the set expense and consumption of energy is revealed accepted from the point of view of durability and costs of production.

Sensitivity analysis of kinetic model parameters of the gas-phase ethane pyrolysis reactions

L.F. Nurislamova, O.P. Stoyanovskaya, N.M. Bainazarova, O.A. Stadnichenko, I.M. Gubaydullin, V.N. Snytnikov

Kinetic models of chemical reactions are systems of nonlinear ODE with parameters defined experimentally with a level of uncertainty. The process of kinetic model developing and coupling with computational fluid dynamics requires sensitivity analysis of the solution to variation of model parameters. We applied local and global sensitivity analysis to an autocatalytic scheme of ethane pyrolysis. It was shown that the steps involving ethylene biradical, which were introduced into conventional scheme of the radical chain mechanism of ethane pyrolysis, represent the main mechanism of methyl radicals generation. Admissible ranges of preexponential factors and activation energies for reactions in the scheme were found using the Monte Carlo statistical method. For the studied reaction we reduced the scheme and demonstrated its further irreducibility and validity for the temperature range of 750-900 °C.

The work was financially supported by RFBR 120831095, UNIHEAT Project of Skolkovo Foundation (A64), President RF Grant Y.PhD 2737.2013.3.

Simulation of technological processes in coal mining

V.V. Okolnishnikov, S.V. Rudometov, S.S. Zhuravlev

The paper describes the new visual interactive simulation system of technological processes intended for the development and execution of simulation models for process control systems. A set of simulation models was developed with the help of this simulation system. These models were developed with the goal to be used as a quality assurance tool for new process control systems of coal mining. Simulation models of various subsystems of coal mining were united to create simulation environment of coal mining. Simulation environment is visually interactive, include emulation models of technological equipment and allow to simulate complex situations in mines and working faces visually as well as to check the response of process control system developed for these situations. Simulation environment was used for testing of algorithms of programmable logic controllers as a part of process control systems prior to commissioning. Simulation environment can be used not only for existing coal mining techniques but also for perspective (robotized) techniques.

Performing 3D inversions adjusted to medium anisotropy for marine electrical survey technologies

M.G. Persova, Y.G. Soloveichik, D.V. Vagin, T.B. Epanchintseva, O.S. Trubacheva

This work is devoted to the results obtained when applying the 3D inversion software for solving electromagnetic survey tasks of searching for oil and gas deposits. The mathematical apparatus allowing the recovery of 3D geometrical characteristics together with their anisotropic conductivity is considered. The results of 3D inversions of the synthesized data of marine electrical survey in the media containing isotropic and anisotropic 3D objects are demonstrated. The results obtained through analyzing the possibilities of marine electrical survey technologies both when revealing low conductivity 3D heterogeneities and when defining their possible anisotropy are presented.

Mathematical model study of different types of microelectromechanical resonators

D.O. Pimanov, S.I. Fadeev, E.G. Kostsov

Microelectromechanical SHF-resonators, developed on basis of current MEMS (MicroelectroMechanical Systems) technology relevant to principally new type of devices with a wide range of applications, in particular as micrometer-sized SHF-filters in the GHz frequency range. We consider the results of the numerical study of forced and natural oscillations in the initial boundary value problems simulating

oscillations of a movable electrode. We consider different types of the movable electrode: a metallized film with fixed ends, a elastic beam with rigidly fixed ends, a cantilever beam and a spring-mounted rigid platform. Oscillations appear because of the intensity of the electrostatic field in a microgap between the movable and fixed electrodes and then continue as natural oscillations. Conditions of the appearance of oscillations are determined numerically as the relationship between the parameters of launching and the parameters of natural oscillations.

The software package for the numerical simulation of the airfoils' motion in the viscous incompressible flow by using the LS-STAG method

V.V. Puzikova, I.K. Marchevsky

The LS-STAG immersed boundary / level-set method are useful for numerical simulation in coupled aeroelastic problems, since it doesn't require a coincidence of cell edges and boundaries of the computational domain, and allows to solve problems when domain shape is irregular or it changes in the simulation process due to aeroelastic body motion on the Cartesian mesh.

A software package is developed for the numerical simulation of the bodies' motion in the viscous incompressible flow by using the LS-STAG method. The C++ language and the paradigm of object-oriented programming are used. It allows to modify and to develop the package (for example, by including a mesh for non-Newtonian and turbulent stresses in addition to the staggered meshes "velocity-pressure") much easier in comparison with procedure-oriented programming paradigm.

To verify the software package test problems of flow past various non-moving and moving airfoils have been solved. The Taneda's effect (stabilization of the wake past a rotary circular cylinder), circular airfoil wind resonance phenomenon and wind turbine rotors autorotation were simulated.

A shape optimization method for 3D nonlinear magnetostatics using a coupling of finite and boundary elements

M.E. Royak, I.M. Stupakov

This report is devoted to a method for a shape optimization of an electromagnet. The geometry of the magnet is set parametrically and parameter values are required to minimize the given magnetic field B dependent functional. To determine the magnetic field in the magnet a 3D nonlinear magnetostatics problem is solved. Finite elements are used to approximate a total scalar magnetic potential within the ferromagnetic domain and Galerkin boundary elements are applied to simulate the reduced scalar magnetic potential within the exterior air domain. A nonlinear problem is solved using Newton method. The constrained optimization problem is solved using gradient method, where gradients are calculated by semi-analytic approach. The effectiveness of the proposed approach is demonstrated on dipole electromagnet shape optimization examples.

The comparison of finite volume schemes for electrical impedance tomography problem

E.S. Sherina

This research is focused on electrical impedance tomography (EIT) problem that estimates the conductivity distribution of an object employing boundary measurements. Static EIT image reconstruction suffers of sensitivity to a measurement noise and approximation error. In this work a special consideration has been given to reducing the latter. Two numerical approaches for solving EIT forward problem are presented. The finite volume method (FVM) on unstructured triangular mesh is introduced on different finite volumes. The finite element (FEM) based forward solver was implemented, which has gained the most popularity among researchers in EIT. In order to assess approaches, they have been compared to the analytical solution of a test Neumann boundary problem.

Reconstruction of the conductivity distribution is an ill-posed problem, typically requiring a large amount of computation and resolved by minimization techniques. The objective function to be minimized is constructed of measured voltage and calculated boundary voltage on the electrodes. A classical modified Newton type iterative method with regularization was employed. A software package has been developed for the problem under investigation. Numerical tests were conducted on simulated data.

Plasma instability simulation with hybrid supercomputers

A.V. Snytnikov

A 3D kinetic study of the plasma relaxation processes caused by the propagation of an electron beam in high-temperature plasma was carried out. The mathematical model is based on the Particle-In-Cell method. The beam plasma instability was simulated in three different modes: the hydrodynamical mode, the transit mode and the kinetic mode.

The values of the instability increment are in good agreement with the theoretical predictions. The simulations are performed with hybrid (GPU-based) supercomputers. Thus the computation is done by the order of magnitude faster than with ordinary supercomputers.

Modeling of semiconductor artificial graphene

O. A. Tkachenko, V. A. Tkachenko

We model artificial graphene-like systems which are created in a two-dimensional electron gas confined in a high-mobility semiconductor heterostructure. A two-layered system of metal gates form a hexagonal antidot lattice. Three-dimensional electrostatics of such structures is calculated including technological errors (deviations from ideal position of antidots and spread in antidot sizes). An optimization of the heterostructure has been carried out to reduce the impact of disorder. Calculation of two-dimensional quantum transport shows that in the absence of disorder the proposed structure should exhibit physical properties characteristic for graphene, with associated magnetic fields several orders of magnitude lower. Calculations were performed on Intel Xeon Phi coprocessors (MVS-10P, Joint Super Computer Center RAS, Moscow).

Numerical simulation of electromagnetic processes based on a new two-potential formalism for the Maxwell equations

S.I. Trashkeev, R.V. Galev, A.N. Kudryavtsev (Invited talk)

A new formulation of electromagnetic field equations based on the use of two vector potentials and two scalar potentials is proposed. This formulation allows the Maxwell equations both in vacuum and in a material medium to be written in the form of a hyperbolic system consisting only of evolutionary equations and not including any differential constraints similar to the divergence-free conditions for electric and magnetic fields. Numerical methods for solving the new system of equations including a properly modified FDTD (Finite Difference Time Domain) scheme and a high-resolution WENO (Weighted Essentially Non Oscillatory) scheme are discussed, analyzed and compared. Examples of numerical simulations of propagation of electromagnetic waves by solving the equations in the new formulation are given.

This work was supported by the Siberian Branch of the Russian Academy of Sciences within the framework of Interdisciplinary Integration Projects of Basic Research No. 129 (2012-2014).

Numerical solution of dynamic elastic problems of deformable solids

Yu.M. Volchkov, I.O. Bogulskii (Invited talk)

The report contains results of investigations in the area of numerical solution of dynamic problems of solids. The method of construction of numerical algorithms was developed based upon the several local approximations by linear polynomials for every sought-for function of problem. An arbitrariness resulting from several local approximations allows in each step time to split the two- and three-dimensional problems in one-dimensional those with the simultaneous formation of artificial dissipation sufficient for monotony of numerical solution. The developed algorithms are applied to research of unsteady processes in a mechanics of solids.

Some algorithms for solving the problem of oscillations of the soil particles

T. Yuldashev

In the article for the boundary value problem fluctuations of soil particles use a variational principle of Hamilton – Ostrogradskii. On the basis of Hooke's law and Navier, a system of canonical equations. To solve the system of canonical equations using finite difference method. System of canonical equations can be used in the design of soil structures based on a variety of dynamic effects, including seismic.

POSTERS

CA-model of populations' dynamic of Baikal organisms. Verification and investigation of pollution influence

I.V. Afanasyev

CA-model of populations' dynamics of three kinds of Baikal organisms is proposed. Each kind is divided onto age groups, total eight groups of organisms. Prey-predator and demographic relationships are defined between groups. Model allows taking into account organisms' spatial distribution, seasonal dependency of birthrate, individuals' movement, water streams and influence of the possible pollution. Computational experiments show that simulating process tends to stable annual oscillation and final individuals' distribution is not uniform and defined by water streams map. Model verification within production-to-biomass and quantity-to-quantity criteria is done. Results differ from assessments of physical values in about 20%. Investigation of the possible pollution influence on the populations' dynamics was done. Assessments of the critical pollution that leads to death of all organisms and pollution which influence is not observable within natural population dynamics are found and presented.

Toroidal decomposition of magnetic field vector potential and its applications

V.V. Aksenov

This paper justifies the necessity to toroidally decompose the vector potential of a magnetic field. The electrodynamics equations originating from the toroidal decomposition of the vector potential have been formulated. The following applications of the decomposition in question are discussed: substantiation of generating the poloidal magnetic field by the toroidal magnetic field and vice versa; substantiation of twicemodality of the Earth's electromagnetic field; substantiation of existence of non-force electromagnetic fields; substantiation of generalized electromagnetic equations of toroidal and poloidal electromagnetic fields; substantiation of earthquake prediction; explanation of the Aharonov – Bohm effect; studying the electrodynamics inside a tokamac.

Calculation of the limiting current of electron beam injected into multi-mirror trap GOL-3

V.T. Astrelin, I.V. Kandaurov, V.M. Sveshnikov

Numerical simulation of the electron beam motion in the transport channel of multi-mirror trap GOL-3 is carried out. The geometry of computational domain is characterized by a large different scales. The beam moves in a sharply converging nonuniform magnetic field. Angular spread of the electrons at the inlet boundary and the heterogeneity of the current density along the radius are taken into account. Relativistic equations of motion are integrated over balanced schemes. An algorithm for choosing the numerical integration step is developed. Examples of numerical calculations are given.

Matrix formulas for a system of the second order equations

N.B. Ayupova

We consider an inverse problem for system of the second order equations: to determine vector-functions $W(x,t)$, $\lambda(x)$, $\mu(x)$ such that

$$\frac{\partial^2 W}{\partial t^2}(x,t) + (AW)(x,t) = F(x,t)\lambda(x) + \Phi(x,t)\mu(x),$$

$$W|_{t=a} = W_a(x), \quad W|_{t=b} = W_b(x), \quad \frac{\partial W}{\partial t}\Big|_{t=a} = W'_a, \quad \frac{\partial W}{\partial t}\Big|_{t=b} = W'_b.$$

We obtain and discuss formulas for this problem.

Компьютерное моделирование переноса загрязняющих веществ с использованием вариационного усвоения данных

С.А. Бельгинова, С.Ж. Рахметуллина, А.Т. Кусаинова

Одной из основных задач прогнозирования состояния атмосферного воздуха является моделирование распространения загрязняющих веществ в атмосфере с целью оценки и прогноза загрязнения в условиях неопределенности. Одним из подходов решения этой задачи является использование в системе мониторинга алгоритмов усвоения данных. Основной задачей рассматриваемого метода является наилучшим образом совместить результаты численного и аналитического моделирования и полученные независимо от модели данные наблюдений.

Внедрение алгоритма усвоения данных для моделирования и прогнозирования загрязнения атмосферы позволит оценивать состояние атмосферного воздуха в режиме реального времени, моделировать состояние атмосферного воздуха в каждой точке г. Усть-Каменогорска, определять зоны повышенного экологического риска. Анализ этих результатов позволит своевременно подготавливать предложения для принятия управленческих решений природоохранного характера для предотвращения отрицательных последствий неблагоприятных и, особенно, чрезвычайных ситуаций.

Работа поддержана программой грантового финансирования Министерства образования и науки Республики Казахстан.

Numerical simulation of the ion dynamics in a magnetic trap

Е.А. Berendeev, А.А. Efimova

In this work the problem of a plasma losses calculation from open type magnetic traps is considered. As an example the trap developed in INP SB RAS is considered. The authors have developed an algorithm of calculation of the plasma losses through multipolar walls and end faces of the trap. This algorithm is based on the PIC/Monte Carlo method with the cylindrical coordinates. The dynamic time step is used to increase the accuracy of calculation of particles trajectories in areas of a strong magnetic field. By the reason of complexity of processes under study, and by the requirement of calculation of trajectories of billions particles the scalable parallel algorithm was developed. For uniform loading of computing knots the modification of Euler – Lagrangian decomposition of area taking into account essential heterogeneity of size of a magnetic field and, therefore, a time step is offered. High scalability of the offered parallel algorithm was shown by means of computing experiments on the supercomputer, and also it was succeeded to install the areas of plasma exit on the surface of the trap and the qualitative evaluation of the volume of plasma losses was make.

The work supported by the RFBR under Grant № 14-01-31220 and 14-01-00392

Paralle algorithm for solution of problems of charged particle dynamics in ultrarelativistic case

М.А. Boronina, V.D. Korneev, V.A. Vshivkov

We present a three-dimensional parallel algorithm for simulation of particle beam dynamics in supercolliders, where colliding beams have superhigh densities and high relativistic factors and the charge density distribution is significantly non-linear. The physical effect can be described by the three-dimensional set of Maxwell equations and the Vlasov – Liouville equation for the distribution function of beam particles. We use particle-in-cell method with leap-grog scheme. The parallel code is based on the mixed Euler – Lagrangian domain decomposition along the transversal direction: every processor group gets its own part of the subdomain grid and all the particles of the subdomain, within the group every processor gets its own set of particles. This method allows to overcome the high restrictions on number of particles in cell and demonstrates good speed-up and scalability. With advances of the code and with the advent of its parallel supercomputer version it will be possible to apply it for beam-beam simulations for supercritical parameters.

The work was supported by RFBR grants № 14-01-31088, 14-01-00392, 14-07-00241.

Complex information support of scientific research in active seismology

L.P. Braginskaya, A.P. Grigoruk, S.V. Kratov

The paper presents a web-oriented Scientific Information System (SIS) for the complex information support of theoretical and experimental investigations of the seismic and acoustic wave fields in active seismology, including the monitoring of natural seismic and volcanic processes. SIS covers all major stages of research: experiment, modeling, bibliography, publication of results and their discussion. At present the informational system can be found at <http://opg.sssc.ru>.

The automatic classification of the Earth Remote Sensing Data

A.A. Buchnev, V.P. Pyatkin

The effectiveness of Earth remote studies is determined by the methods used to process the Earth Remote Sensing Data (ERSD). The system of classification is undoubtedly the main in thematic processing. Some algorithms of automatic classification (which are known as the clustering algorithms too) of multispectral ERSD are included into the pattern recognition system of the software complex for ERSD processing, which is developed in ICM&MG. One of these algorithms is K-means algorithm, whose result is the hard clustering. The hard clustering assigns each feature vector (pattern) strictly to one cluster. In ERSD feature vectors there are mixed vectors, which are the results of registration of more than one natural category. For such data, it is more appropriate to use the fuzzy classification, which allows to share a feature vector between many clusters. Our system includes two algorithms of fuzzy clustering – fuzzy C-means, which is known as probabilistic fuzzy clustering, the second is fuzzy C-means with regularization, which is known as possibilistic fuzzy clustering. The developed clustering system provides the map of classification that fits best true thematic classes in the dataset.

Thermal motion of a gas in three-dimensional space

Yu. A. Chirkunov, E. O. Pikmullina

For obtained by means of specially selected mass Lagrangian variables reduced system of differential equations equivalent to the system describing thermal motion of a gas in three-dimensional space, the simplest representatives of all significantly different (not connected by point transformations) invariant submodels of rank 0 and 1 are found. Some boundary value problems for the system are studied by means of these invariant submodels and production solution formulas. Thus, it is obtained a description of gas particle trajectories under its, generally speaking, not invariant thermal motion.

Almost orthogonal quasi-isometric grids

G.A. Chumakov

A special class of canonical domains is discussed for the generation of quasi-isometric grids. The base computational strategy of our approach is that the physical domain is decomposed into five non-overlapping blocks, which are automatically generated by solving a variational problem. Four of these blocks – the ones that contain the corners – are conformally equivalent to geodesic quadrangles on surfaces of constant curvature, while the fifth block is a conformal image of a non-convex polygon composed of five planar rectangles (or a large rectangle with four small rectangles cut out of its corners). To ensure that the angles of the physical and canonical domains coincide and the conformal modules are the same, the four corner blocks are taken to be geodesic quadrangles on surfaces of constant curvature, namely, spherical, planar or Lobachevsky plane, depending on the angles of the physical domain.

Within each of these blocks a quasi-isometric grid is generated. Orthogonality of coordinate lines holds in the fifth, central block.

We present an algorithm for automated construction of one-parameter family of such canonical domains. The parameter δ is defined in such a way that, according to a theorem that we have proved, for any physical domain there exists a unique value of δ for which the mapping from the canonical domain onto physical region is conformal and its derivative is bounded. Application of such a mapping results in a

grid inside the physical region that is orthogonal far from the corners. This strategy ensures the existence of such canonical domain (the possibility to generate the grid) and the uniqueness of the mapping, i.e., our algorithm cannot converge to two different solutions. Note that the grid lines are the images of the geodesics in corresponding metrics.

Nonlinear dynamics of heterogeneous catalytic reactions

N.A. Chumakova, G.A. Chumakov

Discovery of self-oscillations in the some heterogeneous catalytic reactions in 1972-1973 initiated the application of the theory of nonlinear dynamics in catalysis. The report is devoted to studying different types of generation of complex and chaotic behavior in the small-dimensional dynamical systems with a hierarchy of characteristic times (i.e., with fast, intermediate and slow variables). An attractor Λ was found in the phase space of a 3-D kinetic model such that chaotic dynamics is observed on Λ . Squeezing and stretching are the necessary properties for existence of some saddle periodic solutions (called *Möbius orbits*) which constitute a "skeleton" of Λ . The attractor includes infinitely many Möbius orbits, but there are no steady states. Extremely high parametric sensitivity on Λ is due to existence of the trajectory bundles of "shower" and "tunnel" type that are generated by transversal homoclinic trajectories to the Möbius orbit. The Kaplan –Yorke formula gives the lower estimate of the Lyapunov dimension of Λ : $D_L(\Lambda) \geq 2.075838$. To be sure in the computational results, we developed some special procedures for a posteriori estimation of the global error of numerical integration. The approach is shown to be rather efficient for studying catalytic reactions with complex dynamics.

The authors were partially supported by the Siberian Branch of the Russian Academy of Sciences (Interdisciplinary project no. 80 (2012-2014)).

The Cauchy problem for the Stokes equations

G. Dairbayeva

In the given work the Cauchy problem is considered for the Stokes equations, which is an ill-posed problem. The initial problem is reduced to the inverse problem relative to some well-posed direct problem. It is shown that the inverse problem can be stated as an operator equation. The inverse problem is numerical solved using the optimization method and the finite element method. The estimation of the rate of algorithm's convergence with respect to the functional is given.

Step-by-step method of the Laguerre transform with respect to time for solving the 2D dynamic problems of elasticity theory

G.V. Demidov, B.G. Mikhailenko, V.N. Martynov

Application of the Laguerre transform with respect to time results in solving a problem for a system of differential equations independent of the separation parameter. After application of finite difference approximations in spatial variables the solution to the original problem reduces to solving a system of linear algebraic equations with many rights-hand sides, and we can solve them using different modern approaches to solving linear systems. The main idea of the approach proposed is in that the Laguerre transform with respect to time is used on a sequence of finite time intervals. The solution obtained at the end of one time interval is used as initial data for solving the problem at the next time interval. When using the approach proposed, there arises a necessity in selecting the four parameters: the number of projections of the Laguerre transform, the scaling factor that is needed for approximating the solution by the Laguerre functions, the exponential coefficient of the weight function, which is used for finding the solution on a finite time interval and the duration of this interval. We propose and substantiate the method of selecting the above-mentioned parameters. The approach is question is implemented for the numerical solution of the problem of the elastic wave propagation from the point source.

2D magnetic field calculation using tree-cotree method

P.A. Domnikov

The applications of a vector finite element method to a magnetostatic problem implies solving the differential equation with the rot-rot operator. The resulting finite element system of linear algebraic equations (SLAE) is singular due to the kernel of the rot-rot operator which consists of gradient functions. This singularity causes obstacles when solving the SLAE. It is known that the so-called tree-cotree method allows avoiding the singularity but may deteriorate the spectral properties of the finite element matrix. In this paper the tree-cotree method is applied not to improve the spectral properties of the matrix but to make the matrix as close to a diagonal matrix as it possible. Thus, a direct method becomes suitable for the SLAE solution. It is shown that the tree-cotree method proposed allows us to obtain a strictly tridiagonal matrix on a regular rectangular mesh with edge basis functions. When using a nonstructured triangular mesh, it is not possible to obtain a tridiagonal matrix but the speedup achieved remains considerable. The study was performed with the financial support from the Ministry of Education and Science of the Russian Federation.

Implementation of the solver for the magnetotelluric finite element systems on GPU

P.A. Domnikov, N.V. Kondratyev

A set of large complex systems of linear algebraic equations (SLAE) arises when the vector finite element method is used for the 3D-modelling of the magnetotelluric field. The real parts of all matrices from this set are equal and the imaginary parts differ by a scale factor (which is equal to a frequency of the electromagnetic field). We implemented the COCR method on the graphical processor unit (GPU) to speed up the SLAE solution process. As the sparse matrix-vector multiplication procedure shows low performance on GPU, we developed a special matrix-vector multiplication scheme for this SLAE set arising in 3D magnetotellurics. This scheme consists of the multiplication of the real and the imaginary parts of the matrix on multiple vectors to exploit sparse BLAS3 level operations. With the use of the scheme proposed, the total computational time was reduced more than 25 times. The study was performed with the financial support from the Government of Novosibirsk Region.

Versions of conservative collocations and least residuals method for solving convection-diffusion equation

G.M. Drozdov, V.P. Shapeev

The boundary-value problem with Dirichlet conditions for convection-diffusion equation with small parameter

$$\begin{cases} \left(k \frac{\partial u}{\partial x} + (x-a)u \right)_x + \left(k \frac{\partial u}{\partial y} + (y-b)u \right)_y = f(x,y), \\ u|_{\partial\Omega} = v(x,y). \end{cases}$$

in domain $\Omega = [0, 1] \times [0, 1]$ is considered:

Formulae of different versions of conservative collocations and least residuals (CLR) method with second and fourth order polynomials as basis functions were constructed. Influence of the method parameters on the solution properties was studied. Numerical experiments for solving boundary-value problem with boundary conditions taken from exact solution at small parameter $k = 10^{-2} \div 10^{-4}$ on a sequence of refining grids were conducted. Results obtained by proposed conservative CLR method and results obtained by finite-difference and nonconservative CLR methods were compared. It was demonstrated that on smooth solutions, high-accuracy methods have significant advantages over low-accuracy ones and allow one to solve problems with high accuracy at relatively moderate grid step, even at small values of parameter k .

Numerical simulation of the nonlinear evolution scenario of a beam-plasma system in the case of low density beam

A.A. Efimova, E.A. Berendeev

The task of relaxation of an electron beam in plasma is a classical problem of the plasma physics, and there are numerous theoretical models describing various regimes of the beam-plasma interaction, but the

research into this area remains actual. Studying the influence of the beam nonlinearities on the behavior of instability in the conditions of the developed turbulence requires numerical modeling which, on the one hand, is capable of tracing turbulence evolution raised by the beam at long time periods, and on the other, provides rather a detailed description of the kinetic effects related to capture of a beam. The two-dimensional numerical model based on the particles-in-cell method is developed. By means of numerical modeling it appeared possible to reproduce various scenarios of excitement of plasma turbulence with an electron beam. The numerical convergence of the solution depending on calculating parameters was investigated, good compliance with available analytical decisions is obtained. Calculations are performed on the supercomputers NKS-30T and the "Lomonosov".

Supported by the RFBR under Grant № 14-01-31220 and 14-01-00392.

Computation of eigenvalues and eigenvectors

A.A. Eleuov

Scientific work is devoted to the development of stable algorithms for finding approximate numerical eigenvalues and eigenvectors of finite matrices. In this paper a new proof of the existence of eigenvectors and eigenvalues of self-adjoint matrices, based on which the proposed specific algorithms for finding the eigenvalues of these matrices. Approximate methods for finding approximate numerical eigenvalues and eigenvectors of matrices based on a variational principle, according to which it is necessary to build a functional target. In a scientific paper, the choice of such functional extremes which coincide with the eigenvalues of the matrix.

These algorithms have been applied in the case of self-adjoint and positive definite matrices and then extended to the case of matrices of arbitrary type.

References

1. Godunov SK Modern aspects of linear algebra. Novosibirsk Academic Book, 1997. 390.
2. Eleuov AA Otelbaev MO Akzhalova AZ, Rysbaiuly B. Calculation of eigenvalues and eigenvectors of matrices // Eurasian Mathematical Journal ENU. LN Gumilev and MSU. MV University. 2005. № 1. S. 57-78.
3. Eleuov AA algorithms account eigenvalues and eigenvectors of matrices // Herald KazNPU. Abai. Series of physics, mathematics, computer science. 2007. № 1 (17). P.23-28.

Nonstandard finite difference multisymplectic variational integrators for the Korteweg-de Vries equation

N.I. Gorbenko

We suggest some geometric integrators based on the discrete Hamilton's principle for the Korteweg-de Vries equation with use of the idea of nonstandard difference methods especially with regard to their robustness for large steps in space and time and over long times. The discrete Euler –Lagrange equation is produced in the discrete variational principle ; meanwhile, the discrete multisymplectic structure is also generated. In the other words, the discrete variational integrators are multisymplectic automatically. Their discrete multisymplectic structures are presented by the multisymplectic form formulas. The convergence of the discretization schemes is discussed. The effectiveness and efficiency of the proposed methods are verified by the numerical experiments

Application programming interface of HPC Community Cloud

M. Gorodnichev, S. Vaycel

The HPC Community Cloud (HPC2C) solves the problem of aggregation of heterogeneous computing systems into a single resource with a high lever user interface and automatic provision of high performance computing service to external program systems via an application programming interface. The HPC2C software system consists of a managing server and a web-application. The HPC2C server implements an application programming interface (API) that includes functions to manage user accounts, the registry of attached computing resources, file storage, to specify, run and monitor jobs. Different computing systems can be attached to the HPC2C managing system and run jobs. The HPC2C web-application is a user

interface system that allows users to develop batch or GUI interactive programs in different programming systems, submit and control jobs, manage their files, exchange their results with other users. The web-application calls the HPC2C API to process user requests. With the HPC2C, users can create, accumulate and share content such as software components, tutorials, and numerical simulation codes. User-developed applications with interactive interfaces extend functionality of the system.

On the language for basic learning of parallel programming

L.V. Gorodnyaya

During last twenty years the world of computer science and its technical basis underwent considerable changes. The urgency of studying parallel programming is increasing thus demanding the development of language and information support of introduction to programming. In the mid 1970s active research on parallel programming methods was considered leading direction to overcome crisis in programming technologies. Nowadays growth of interest in parallel programming is related to transition to mass production of multi-core architectures. First of all one should mention rapid development of supercomputers and distributed data systems as well as transition to multi-core processors and wide spread of graphic processors. To train expert in the field of parallel programming the study course needs a flexible tool and language support with different models of parallelism. However many high-level languages usually have one parallelism model in their semantics. Thus the task of making a language for basic parallel programming training having principal parallelism models for allowing natural parallelism in solving difficult problems becomes urgent.

Numerical modeling of multicomponent plasma-chemical kinetics in CF_4/H_2 mixture

Yu.N. Grigoryev, A.G. Gorobchuk

In the frame of hydrodynamic approach the plasma-chemical etching technology of silicon in CF_4/H_2 mixture was simulated. The calculations were carried out based on 2D mathematical model of plasma-chemical etching reactor. The gas flow of the mixture was described by the equations of multicomponent physical-chemical hydrodynamics. The chemical kinetic model contained 28 gas-phase reactions of dissociation and recombination processes and 6 heterogeneous reactions on the wafer, which included the products - F, F_2 , CF_2 , CF_3 , CF_4 , C_2F_6 , H, H_2 , HF, CHF_3 , CH_2F_2 . The concentrations of chemical components were calculated from the system of conservation equations included the mentioned gas-phase reactions. The governing equations were numerically solved by iterative finite difference splitting-up method. It is shown that the CF_4/H_2 system is characterized by lower fluorine concentrations and higher CF_2 , CF_3 coverage of silicon surface compared to the CF_4/O_2 system.

Concorrelational and singular spectrum analysis of seismic signals

V.V. Gubarev, M.S. Khairtdinov, N.V. Abalov, O.K. Alsova, T.V. Tairov, G.A. Melnikov

We propose and investigate following three hypotheses concerning the seismic signals.

1st hypothesis: Not all of seismic signals belong to the class of signals described by models of stationary random signals with linear regression. As a consequence, traditional methods and means of correlational and spectral analysis cannot be correctly applied to all of seismic signals (in terms of interpretation of results).

2nd hypothesis: The 1st hypothesis can be tested on the specific realizations of signals in terms of applied problem being solved.

3rd hypothesis: Some solutions for applied problems do exist under the conditions of validity of 1st hypothesis.

In the report a validity of these hypotheses is proved. Methods and means that were used for proving are described. Examples of applied calculations for real-world signals are given. Among them: methods of detection and accounting for non-stationarity, application of concorrelational transformations, which are invariant to one-to-one transformations, and singular transformations and characteristics.

Simulation of tsunami wave generation by submarine landslide using the fully nonlinear dispersive equations

O.I. Gusev

Unlike earthquakes landslides generate waves with shorter length, so one has to take into consideration the frequency dispersion for its accurate simulation. Calculations of surface waves using complete hydrodynamic models require much computation time. Therefore, approximate nonlinear dispersive (NLD) shallow water models should be employed, which are difficult to solve directly. In recent work the partitioning of the full NLD system with a movable bottom on elliptic and hyperbolic parts is proposed. On the model problems of tsunami wave generation by submarine landslide numerical solutions of the presented model are compared with experimental data and the other author's computations by different models. On the base of the comparisons the importance of dispersion and the influence of the landslide parameters are discussed.

On the numerical solution of non-linear Schroedinger equation

V.P. Ilin, N.V. Panchenko

The aim of the paper is the comparative experimental analysis of the various numerical methods for the solution of boundary value problems for non-linear complex Schroedinger equation which describes dynamic wave processes. Different space finite difference and discontinuous Galerkin schemes are considered. The computational stability and the order of accuracy are the main topics of investigations. The approximations in time by implicit Runge –Kutta methods are applied. The conservation properties of symplectic algorithms are demonstrated numerically. The set of represented computational results for the model problems are presented

Numerical solution of inverse problems of pharmacokinetics. Identifiability of compartmental models

A.I. Ilyin, S.I. Kabanikhin, D.A. Voronov

Pharmacokinetics deals with kinetics of absorption, distribution, metabolism and excretion of drugs responses in man and animals. We can visualize this whole process as a dynamic system described by a system of ordinary differential equations of the form: $C'(t) = AC(t) + u(t)$, where $C(t)$ is a vector of concentrations in different compartments. Parameter identifiability analysis for dynamic system ODE models addresses the question of which unknown parameters can be quantifies from given input-output data. In this report we consider scaling reparametrization. Inverse problem states as following: it is required to find rate constants knowing concentration of a drug at the given moments of a time in one compartment – $(C_1(t_1), \dots, C_1(t_M))$. Inverse problem is solved by different algorithms. The question of choosing initial approximations is covered in this report. It is shown that physical properties of initial approximations strongly affect on obtained solutions. The results of numerical experiments are presented. Also an algorithm for solving inverse problem in case of n-compartment is covered in this report.

Numerical modeling of propagation of seismic fields in porous media for irreversible case

Kh.Kh. Imomnazarov, A. A. Mikhailov

The paper presents the algorithm, based on the application of the spectral Laguerre method for approximation of temporal derivatives as applied to the problem of seismic wave propagation in the porous media in the presence of dissipation of energy. The initial system of equations as first order hyperbolic system in terms of velocities, stresses and pore pressure. For the numerical solution of the task in question, the method of combination of analytical Laguerre transformation and a finite difference method is used. The proposed method of the solution can be considered as analogue to the known spectral method on the basis of Fourier transform. However, unlike Fourier transform, application of integral Laguerre transform with respect time allows us to reduce the initial problem to solving a system of equations in which the parameter of division is present only on the right-hand side of equations and has a recurrent dependence.

As compared to time-domain method, with the help of an analytical transformation in the spectral method it is possible to reduce an original problem to solving the system of differential equations, in which there are only derivatives with respect to spatial coordinates. This allows us to apply a known stable difference scheme for recurrent solutions to similar systems. Such an approach is effective when solving dynamic problems for porous media. Thus, because of the presence of the second longitudinal wave with a low velocity, the use of difference schemes in all coordinates for stable solutions requires a consistent small step both in time and in space, which inevitably results in an increase of computer costs.

This work was supported in part by grant the President of the Russian Federation for support of leading scientific schools of the Russian Federation No NSh-5666.2014.5 and the Russian Foundation of Fundamental Research under grant No 13-01-00689.

Discontinuous Galerkin numerical schemes for singular perturbation elliptic problems

N.B. Itkina, S.I. Markov

Two numerical schemes IP (Interior Penalty Method) and NIPG (The Nonsymmetric Interior Penalty Method) discontinuous Galerkin method are analyzed. Special numerical lifting operators are presented in the bilinear form for IP and NIPG methods. The numerical lifting operator increases the consistent of schemes. Numerical schemes are investigated on the model singular perturbation two dimension elliptic problems. The finite element space consists of linear interpolation functions. Error estimate analysis on structured quadrilateral meshes is presented. Numerical continuous and discontinuous Galerkin schemes are compared.

Анализ влияния случайных шумов на течение автоколебательных химических реакций методом Монте-Карло на суперкомпьютерах

A.A. Ivanov

In this paper study the question of influence of random noise on stochastic differential equations (SDE) describing the behavior of chemical reactions on the Belousov Zhabotinsky model and the hydrogen oxidation reaction on nickel. In this case the random noise can be both external (additive noise in the SDE and internal parametric (multiplicative noise), causing the amplitude of oscillation is growing.

For numerical analysis using Monte Carlo method solutions SDE generalized Euler method is used as the least time-consuming compared with other numerical methods. In modeling of oscillatory solutions using a fixed step size of integration, which is determined by the oscillation period of the highest frequency component solutions.

Extremely small dimension of the integration step and very large volume simulation of trajectories of solutions of multidimensional SDE systems requires the use of supercomputers for the calculations in a reasonable time (up to day 256 processors). Note that the algorithms of the Monte – Carlo naturally are parallelized due to the independence of the simulated trajectories, which facilitates preparation of problem to solving.

This paper investigates the moments of component solutions SDE, frequency phase portrait, the frequency integral curve.

The review of mathematical models for precision solving of electron optical problems

V. Ivanov, Yu. Kulikov

The review is devoted to the analysis of status of art and to the prospects of development for the mathematical models and computational algorithms in computer aided design of electron optical instruments and physical electronic devices. The set of decided and subject to decide fundamental static and dynamic problems in scanning microscopy, high-current electronics and image electron optics is noted. First of all we focused on the development of new theoretical approaches and numerical methods for simulation of self-consistent interaction of charge particles with the external electromagnetic fields in static and dynamic work modes. One of the most topical problems in scanning microscopy is the problem of precision computation of charged particle trajectories, when the ratio for device dimension to the beam cross-section is about

10^6 - 10^7 . The other challenge problem is the development of computational scheme for reconstruction of electron image in the devices with ultrahigh spatial and temporal resolution. One need to develop those precision algorithms in 3D, which combine the high accuracy and computational efficiency. The provided analysis is based on many-years experience of the authors in solving of theoretical and applied problems in electron optics.

Discrete stochastic modification of algorithm for calculating the angular distribution of the directions of departure from plane scattering layer

E.G. Kablukova, B.A. Kargin

Probability of departure from plane scattering layer in given subspace of directions $\omega \in \Omega$ can be represented as a collision estimate $I_{h_\omega} = (\varphi, h_\omega)$ of Monte Carlo methods from a solution $\varphi(x)$ of the integral equation of radiative transfer $\varphi = K\varphi + f$. In our case the solution is represented as a convergent Neumann series. The function $h_\omega(x)$ is an integral of the probability of departure from the layer at point x in a direction ω during single straight-line run over directions $\omega \in \Omega$. If a collision point lies below the horizontal plane $z = z_1$ the considered integral is estimated for one random direction, which coincides with photon scattering direction after the collision. If a collision point x lies upper the plane the considered integral is estimated for K random directions. Density distribution of the cosine μ of departure angle is chosen as a piecewise linear approximation of the integrand. The modification of algorithm may be used for horizontally homogeneous scattering layer.

The effect of system software on parallel program performance

K.V. Kalgin

Impact of system interrupts to performance of *parallel reduction* is investigated by different authors, for example see paper [1]. In this work the impact of system interrupts to performance of *parallel stencil* computations is investigated. The model of interrupts effect is constructed and verified on NKS-30T and MVS-100K. The performance impact is varied from 1 to 50 % depending on size of domain, version of Linux, hardware, communication functions (blocking or non-blocking). To reduce the impact of interrupts one has to install modern Linux with better implementation of interrupt handling or quiet at all and use non-blocking communication functions.

The author was supported by the Grant of the President of the Russian Federation for Young Russian Researchers (project no. MK-3644.2014.9).

References

1. P. Beckman, K. Iskra, K. Yoshii, S. Coghlan, A. Nataraj. Benchmarking the effects of operating system interference on extreme-scale parallel machines. //Cluster Computing, Vol. 11 N 1, pp.3-16, 2008.

Simulation of multiphase flow in deforming porous media on clusters with GPU and Xeon Phi

K.V. Kalgin, S.E. Kireev

In [1] a software "Porodynamics" for simulation of multiphase flow in deforming porous media has been developed. A WENO –Runge –Kutta algorithm used for the solution of equations of continuous medium dynamics allows efficient parallel implementation on modern supercomputers, ordinary and hybrid. The work presents a performance comparison and analysis for three different parallel implementations: using CPUs only, using nodes accelerated by NVIDIA GPUs and nodes accelerated by Intel Xeon Phi coprocessors.

This work was supported by the Government Contract № 07.514.11.4156.

References

1. Yu. V. Perepechko, E. I. Romensky, G. V. Reshetova, L. N. Perepechko, V. E. Malyshkin, K. V. Kalgin, S. E. Kireev, M. B. Ostapkevich Supercomputer Simulation of Multiphase Flow in Deforming Porous Media // Collected articles "Supercomputer technologies in science, education and industry ", № 5, 2013.

Parallel numerical simulation of stochastic ion motion in an optical lattice

L.P. Kamenshchikov, I.V. Krasnov

Ion traps have been intensively studied over the last two decades. This interest is explained by their numerous important physical applications which are associated with the possibility of forming ion Coulomb clusters in such traps [1-3]. Our simulation of the ion motion in the optical lattice is based on the numerical solution of stochastic differential equations [3-4]. Use was made of 256–512 processing cores of the MVS-100K supercomputer and 262144 independent realizations. The uniform random number generator well-adapted for parallel computations [5] was used. An existence of long-lived all-optical ion cluster was shown.

References

1. Schneider C., et al. Optical trapping of an ion. *Nature Photonics*. 4, 772 (2010).
2. Krasnov I.V. *Phys. Lett. A*, 375, 2471 (2011).
3. I.V.Krasnov, L.P.Kamenshchikov. All-optical trapping of strongly coupled ions. *Optics Comm.*, 312, 192 (2014).
4. R. Mannella. Integration of stochastic differential equations on a computer. *Int. J. Mod. Phys. C* 13, 1177 (2002).
5. G.A. Mikhailov, M.A. Marchenko. Parallel realization of statistical simulation and random number generators. *Russ. J. Num. Anal. Math. Model.*, 17, 113 (2002).

Researches of parallel algorithm work for 3D seismic field simulation on hybrid clusters

D.A. Karavaev

This paper describes researches of program work for simulation on hybrid clusters with Nvidia GPU and Intel Xeon Phi coprocessors nodes. A 3D seismic field simulation problem is considered. A difference method is used for problem solving. Parallel program realization is made with use of 3D schema of calculation area decomposition. All the computations is held on GPU and Xeon Phi. CPU is used for interconnection between computational devices. The combination of MPI, CUDA and tools for programming on Intel MIC architecture are used. The results of algorithm work on NKS-30T+GPU cluster of the Siberian Supercomputer Center and on MVS-10P cluster of the Joint Supercomputer Center of RAS are presented.

Work is supported by RFBR grants No. 12-05-00786, 13-07-00589, 14-07-00832, 14-05-00867, IP SB RAS No. 54, 39, 130.

The parallel implementation of semi-lagrangian method of continuity equation

E.D. Karepova, A.A. Efremov, A.V. Vyatkin

The finite difference scheme presented in our work is one of modifications of semi-lagrangian approach (the modified trajectories method). The absence of algebraic condition for a time step makes this approach convenient for problems with large value of velocities. Fulfillment of conservation law is another advantage of semi-lagrangian approach. The theorem which permits to take in to account volume of substance passed through a boundary is considered. Furthermore, the theorem on the first order of convergence is proved.

The theoretical convergence estimates are confirmed by our numerical experiments.

Some of parallel implementations of modified semi-lagrangian method are investigated. We discuss the design subtleties of parallel implementations of the algorithm by OpenMP technology for shared memory computational systems and by CUDA technology for general-purpose GPU programming. Inter alia, the influence of Hyper Threading technology to performance of our OpenMP code is investigated. Moreover, the difficulties of the algorithm implementation and performance for hybrid architecture computation systems are discussed for our CUDA codes.

The boundary value problems for div-curl system in a ball

S.G. Kazantsev

We study the div-curl problem in the unit ball under the different boundary conditions. At first the orthogonal basis in the relevant functional spaces of vector fields are constructed and then the solutions of these problems are described.

Parallel implementation of polymer chains conformation enumeration for crystal engineering

S.E. Kireev, V.Yu. Komarov

Solution of both theoretical and practical problems concerning clathrate hydrates requires atomic models of crystal structure to be obtained. One of the challenging problems of this field of science is crystal structure determination of tetraalkylammonium polyacrylate clathrate hydrates. Complexity of the crystal structures of these compounds makes applying of usual experimental investigation using X-ray diffraction almost uninformative. Application of the modern computational methods (molecular mechanics or molecular dynamics simulations) may give only a restricted number of solutions, defined by the initial model. Presently there are no developed approaches of systematic conformation enumerations of polyacrylate anions which may be embedded into the water host framework. To obtain reliable structural models simple simulation methods combined with effective selection of promising polyacrylate chain conformations are required.

A "brute force" enumeration algorithm of polyacrylate anion conformation enumeration with a number of geometrical restraints was implemented and parallelized. The promising results, including a number of plausible models of embedding of polyacrylate chains into water framework, were obtained. The prospects of further development of more sophisticated algorithms based on this approach were shown.

Cellular automata model of catalytic CO oxidation reaction considering surface temperature changes

A.E. Kireeva

Double-layer cellular automata (CA) model of carbon monoxide (CO) oxidation reaction on the platinum (Pt) is developed and investigated. This reaction in non-equilibrium conditions can be accompanied by the various spatio-temporal patterns such as surface waves, spirals and turbulences. Catalytic reactions are complex nonlinear systems. Powerful method of simulation and studying such systems is CA. Double-layer CA is a parallel composition of two CA: the main CA simulating oxidation reaction, and the second layer CA simulating temperature spatio-temporal distribution on the catalyst surface. Cells states of the main CA are calculated depending on cells states of the second layer. Double-layer CA allows to take into account changes of catalyst adsorption properties when temperature changes. During the CA evolution different spatial patterns on the catalyst surface with different temperature are obtained and studied. Oxidation reaction dynamics during the cooling and heating of the Pt surface is investigated.

Supported by Presidium of Russian Academy of Sciences, Project 14-01-31425.

On the preconditioned biconjugate direction stabilized methods

E.O. Kondrashkin

An experimental investigation of various versions of the parallel biconjugate direction stabilized methods is presented. These algorithms include biconjugate gradient and biconjugate residual for solving non-symmetric systems of linear algebraic equations (SLAEs) with sparse very large matrices which are presented in compressed sparse row format. Two kinds of preconditioners are considered. The first one is Eisenstadt modification of incomplete factorization and the second one is based on the smoothed aggregation approach. The results of numerical experiments are given for representative set of the model problems.

Mathematical modeling for studying underground seismic array characteristics

D.V. Kononova, V.V. Kovalevsky, A.S. Belonosov

The paper presents the results of studies using mathematical modeling directional characteristics of underground seismic array of 6 seismic records with areal aperture 2.5 km by 0.5 km, deployed in a tunnel BNO INR in Elbrus region. Emphasis is placed on the definition of the error in determining hypocenters of local seismic events depending on the distance and azimuth relative to the axis of the seismic array and errors in determining the arrival times of the waves. Examples of processing real records of local seismic events are presented

Parallel technology of 3D boundary value problems on parallelepipedal quasistructured grids

V.D. Korneev, V.M. Sveshnikov, I.A. Klimonov

Some technological issues of application domain decomposition method for solving three-dimensional boundary value problems on quasi-structured grids are considered. Iterations on subdomains in decomposition method are based on direct approximation of the Poincare –Steklov equation. Data structures for economical information storage are presented and evaluates of the parallelization effectiveness on examples of methodological problems are stated.

Kelvin problem on partitioning bounded figures

L.A. Korolenko, S.N. Astrakov

The classical Kelvin problem is to find partition of space into cells of equal volume such that the area of the partition walls is minimal. Kelvin suggested splitting into the truncated octahedron (polyhedron with 6 square faces and 8 hexagonal faces). Similarly, we can consider the problem of partitioning plane into the tiles the same area with a minimum boundary length. The planar case was resolved in 2001 by Thomas

Hales. The solution is a honeycomb structure. Such a structure in the $\sqrt{3}$ times better then partitioning plane into squares in terms of ratio of area to perimeter. In this paper we consider the partition of plane bounded figures on a predetermined number of regions the same area with the least boundary length between them. Such problems have not been studied previously, even for the simplest geometric shapes. In our research we found the best partition of the circle and the square into three or four parts. For some figures we obtained interesting partitioning on another number of pieces. In the calculations we used the principle structure of soap films that describes by the Plateau's laws.

Some acceleration methods for the result calculations in the boundary element modeling

N.S. Kosminova, I.M. Stupakov

One of the problems that complicate the application of the boundary element method is the computational cost in calculating the characteristics of the field based on the obtained solution. This report is devoted to the research of acceleration possibility for such calculations via parallelization and vectorization and using the fast multipole method. Standard features of .NET 4.0 Framework are used for parallelization. Vectorization is implemented using SSE and AVX SIMD instruction sets. The implementation of the fast multipole method is based on real harmonics, uses Wigner rotation matrices and includes adaptive clustering according to boundary element mesh. Another way to speed-up the calculation is solving the problem of field interpolation using auxiliary mesh in the subregion of the computational domain which is also discussed in the report. The effectiveness of the proposed methods is investigated on the example of calculating charged particles trajectories in the field of the dipole magnet.

Calculation of intensive charged particle beams on locally modified rectangular quasistructured grids

A.N. Kozyrev, V.M. Sveshnikov

Some algorithmic and technological issues of building a locally modified rectangular quasistructured grids and based on their calculation of intensive charged particle beams are considered. Numerical error estimation of the electric field potential calculation in domains with curvilinear boundary with local modification of the grid is given. When solving the self-consistent problem the near cathode singularity is isolated. A system of nonlinear operator equations on the interface between the near cathode and base subdomains is build. It is solved by the Broyden method.

Solving 2D nonlinear vorticity equation with the help of mixed finite element and splitting methods

V.V. Kravtchenko, V.I. Kuzin

Based on the splitting in terms of physical processes and with respect to time and on a finite element method (FEM) as applied to a 2D nonlinear vorticity equation, a scheme with two splitting steps is obtained. For constructing FEM operators at the steps of splitting in terms of physical processes, different types of finite elements are used. Hence, it appears possible to essentially reduce the number of grid points in a numerical scheme when passing from one splitting step to another. At the first step, corresponding to the vorticity advection and diffusion, the non-conforming finite elements are used. At the second step, for solving the linear stream function equation, the conforming piecewise linear finite elements are used. The efficiency of the scheme was proved with numerical tests. The EOF analysis and the Fourier analysis of the solution were performed.

Abstract finite element method for solving a saddle point problems, the theory and examples

I.A. Kremer

This article explores the finite element method for the numerical solution of the saddle point problems. Let V and Q are Hilbert spaces, $A : V \rightarrow V'$ and $B : V \rightarrow Q'$ ($\text{Ker } B^\tau \neq \{0\}$) are linear and bounded operators, $F \in V'$. The problem is formulated as follows: need to define a pair of functions $u \in V, p \in Q$ that satisfy the equations

$$\begin{cases} Au + B^\tau p = F, \\ Bu = 0. \end{cases} \quad (1)$$

Sufficient conditions for the solvability of this problem are given in the book [1]. We consider the special case when

$$V = \text{Ker } A \oplus \text{Ker } B.$$

This condition allows to obtain separate problems for the unknown functions u and p . Existence and uniqueness of solutions to these problems are established. Application of the finite element method for the numerical solution of these problems is justified. The paper presents three examples of these problems: a degenerate Neumann problem for the diffusion equation, Maxwell stationary problem with natural boundary conditions, grad – div problem with restrictions on the circulation of solutions.

References

1. Brezzi F., Fortin M. Mixed and Hybrid Finite Element Methods. Springer – Verlag, New-York, 1991.

Signal processing in program system for vocal training

A.I. Kulikov, A.A. Alyabushev, S.G. Levin

Given work presents program system intended for training those who is going to learn the basis of vocal techniques. This problem is important today because learning by instruction is still the most efficient way to train, but often there is no possibility to use professional vocal trainer's service. The target is to develop a feedback system to evaluate the vocal exercises using the digital signal processing. For solving this problem, a model of melodic signals was developed. This model is based on regular structures in the Fourier-spectrum named "acoustic cores". Based on this model, the problem of audio source separation can be resolved, including the distinction of voice. The acoustic core parameters are used to evaluate execution characteristics. Pitch detection, short-time transforms and edge effects compensation problems are also considered. The proposed algorithms are built as stages of the program pipeline. Other components of the system perform exercises, scenarios of training, gathering statistics and interaction functionality.

AstroPhi vs GPUPEGAS: two hydrodynamic codes for numerical simulation of galaxy formation by means hybrid supercomputers

I.M. Kulikov

In these paper new two hydrodynamic codes AstroPhi and GPUPEGAS is proposed. The codes are designed for simulation of astrophysical objects dynamics on hybrid supercomputers. In this code was implemented a two-phase MHD hydrodynamic model. These codes are optimized for use with Intel Xeon Phi computation accelerators and for use NVIDIA GPU-accelerators. The Numerical codes are based on combination of Godunov method as well as on the original implementation of Fluid-In-Cells method. The codes were tested on gas dynamics test problems, classical gravitational gas dynamics problems. The scalability of AstroPhi and GPUPEGAS codes is compared and shown.

The research work was supported by the Grant of the President of Russian Federation for the support of young scientists number MK – 4183.2013.9, RFBR grants 13-07-00589 and 14-01-31199.

A variational algorithm of real-time data assimilation for the convection-diffusion substances model in the atmosphere for the non-stationary two-layered discrete-analytical numerical scheme

A.T. Kussainova, A.V. Penenko

In this work, we have developed an algorithm for combining time two-layered discrete-analytical numerical schemes for convection-diffusion substances models in the atmosphere, algorithms for sequential data assimilation of contact measurements of substance concentration. We use the split-step method for solving forward modeling problems and two-dimensional data assimilation problems. Convergence of discrete analytic schemes is numerically verified by comparison with known analytical solutions.

This work was supported by the Committee on Science and by the Ministry of Education and Science of the Republic of Kazakhstan under Project 594 (86-421-13) "Development of informational technology for real-time ecological monitoring data assimilation".

Radial inflow model in the bottom zone of exploitation wells

G.G. Lazareva

The model, in its simplest form is a vertical well placed at the centre of a cylindrical drainage volume of constant thickness. It derives its simplicity from the assumption of homogeneity which implies that the flow from the reservoir at any radial azimuth into the well will be constant and hence easily integrated around the circumference of the circular drainage area. The model will apply Darcy's law to this geometrical system.

Radial propagation in porous media of several substances emitting energy and gas is considered. Obtaining the distribution of total pressure is the objective of the simulation. Considered the motion of the following Newtonian fluids in a porous medium along the axis r : oil, binary composition, acid, water and gas. Compressible substances model is used. Accounting of chemical reactions occurs at the stage of calculation of saturation. Saturation is determined from the equation Buckley –Leveretta for the porosity. The gas emitted is taken into account in the calculation of saturation, the law of conservation of mass is performed.

In engineering design of the oil production technology, it is vital to get the low pressure on the well head. We obtained pressure on the well head, hole bottom and the bottomhole zone. Inspection of these results shows that the pressure does not exceed permissible values.

A study of (m,k)-methods with inexact Jacobean for solving differential-algebraic systems of index 1

A.I. Levykin

A class (m,k)-methods with inexact Jacobean is discussed for the numerical solution of the initial value problems for implicit systems of ordinary differential equations. The order conditions and convergence of the numerical solution in the case of implementation of the scheme with the time-lagging of matrices

derivatives for systems of index 1 are received. At $k \leq 4$ the order conditions are studied and schemes optimally computing cost are obtained.

Numerical analysis of long-term substance fallout observation for a high-altitude source

A.A. Lezhenin, V.F. Raputa, V.A. Shlychkov, T.V. Yaroslavtseva

A vertical wind distribution is considered to design chimneys of several hundred meters in height. The wind tends to flow to the right in the atmospheric boundary layer due to the Coriolis effect. The rotation angle is about 30° . These factors are taken into account to study the distributions of aerosol smoke produced by a high-altitude source. A model based on a substance transport equation for the reconstruction of polydisperse substance fallout from a continuous high – altitude source is proposed. The model is put to an evaluation test with field and laboratory data on benzoperin pollution of snow cover in the vicinity of Power Station -3 in the city of Barnaul. The effects of wind direction changes in the atmospheric boundary layer on the formation of long-term aerosol substance fallout are estimated. A reasonable agreement is found between the observed and computed data.

Numerical simulation of the evolution of a Bose – Einstein condensate with the two-dimensional Gross – Pitaevskii equation

Y. Likhanova, S.B. Medvedev, M.P. Fedoruk, P.L. Chapovsky

A Bose – Einstein condensate (BEC) is a state of matter of a dilute gas of bosons cooled to very cold temperatures. Under such conditions, a large number of atoms occupy ground state of the system, and quantum effects become apparent on a macroscopic scale.

This report presents the results of numerical modeling of BEC behavior using by the two-dimensional Gross –Pitaevskii equation with a harmonic potential.

The variational and finite-difference models have built. A stationary state for weakly and strongly interacting condensates have numerical simulated by using ones. The use of these models in conjunction has allowed us not only to verify the algorithms, but also to optimize the process of finding the stationary solution corresponding to the ground state.

Also results on modeling of the condensate behavior after holding off the trap demonstrates. The experiments show - whether agreement on both building models and qualitative agreement with the physical experiments.

Particle-in-cell simulation of laser-matter interaction

T. Liseykina, D. Bauer, G. Dudnikova

Using three-dimensional, relativistic particle-in-cell simulations with ionization included we study the interplay between ionization and pulse propagation in intense laser-matter interaction. Of particular interest is the laser intensity and frequency regime for which initially transparent, wavelength-sized targets are not homogeneously ionized and the charge distribution, instead, changes both in space and in time on a sub-cycle scale. We find that a strong near-infrared or optical laser pulse interacting with an initially neutral, wavelength-sized He-droplet may generate a charge density distribution that neither is homogeneous throughout the droplet nor created only within a thin skin layer at the surface. Instead, oscillating electric fields may penetrate into the droplet interior under a certain angle, ionize, and propagate further in the just generated plasma [1]. We studied, moreover, the interaction of the laser light with small initially homogeneous and neutral H-droplets for the range of parameters relevant to the corresponding parameters in the recent FLASH TS experiments. We found that the field enhancement at the droplet surface gets clearly imprinted in the structure of the surface ion density at the time scale of 100 fs. Our preliminary study indicates that it might be possible to identify this structure by scattering experiments at FLASH. Numerical simulations were performed on JUROPA Supercomputer (NIC, Juelich, Germany).

References

1. T. Liseykina and D. Bauer, Phys. Rev. Lett. 110, 145003 (2013).

Estimates of the Monte Carlo method for the first eigenvalue of the Laplace operator with mixed boundary conditions

V.L. Lukinov

New statistical estimation algorithms of eigenvalues and eigen functions of the Laplace operator with mixed complex-boundary conditions were constructed. Equations are considered in the triangular areas. To construct the required estimates, the initial differential problem is reduced to a system of linear equations by replacing differential operators by finite-difference. To solve corresponding system of linear equations, an adjoint algorithm "walk on a lattice" is used, whose trajectories are realizations of the corresponding Markov chain. To construct implemented algorithm, randomization of obtained equations is used and is taken into account in the auxiliary multiplicative weights. Account boundary conditions occur in a small neighborhood of the boundary by their approximation to the desired order of accuracy. In constructed algorithms, a choice between breakage of trajectories and theirs rebound into the domain is implemented.

Nonstandard approximation of functions

O. A. Makhotkin

The next problem investigates: approximate a probability density $p(x)$, $x \in X = (0, 1)$ by the "simpler" density of the form

$$\hat{p}(x) = \sum_{i=1}^M c_i \phi_i(x), \quad c_i \geq 0, \quad \phi_i(x) \geq 0,$$

where $W_i = \int_0^1 \phi_i(x) dx < \infty$, $\sum_{i=1}^M c_i W_i = 1$. The norm $L = \|\hat{p}(x) - p(x)\| = \int_0^1 |\hat{p}(x) - p(x)| dx$ is the suitable measure of the approximation error. It is possible to find the approximation by minimization of $L(c_1, \dots, c_M)$, but this algorithm is too complicated. The computer experiments shows that the two-stage approximation algorithm gives the value of L not too far from the optimal one.

For the piecewise approximation this algorithm has the next representation:

- 1) Find the standard approximation $\tilde{p}(x) = \sum_{i=1}^m p(x_{i-1/2}) \chi(x | \Delta_i)$,
- 2) Calculate $S_0 = h \sum_{i=1}^m p(x_{i-1/2})$ and then norm $\tilde{p}(x)$: $\hat{p}(x) = \tilde{p}(x) / S_0$.

Here $\chi(x | \Delta_i) = 1$ for $x \in \Delta_i = (x_{i-1}, x_i)$ and $= 0$ otherwise.

The piecewise constant and piecewise linear approximations of the test densities $p_s(x) = (s+1)x^s$, $s > -1$ on the grid $X_m = \{h \cdot i, h = 1/m, i = 0, \dots, m\}$ were investigated in details. Next asymptotic expressions for $L(h)$ were obtained:

- for the piecewise constant approximations $L(h) \approx O(h^r)$, $r = \min(1, 1+s)$,
- for the piecewise linear approximations $L(h) \approx O(h^r)$, $r = \min(2, 1+s)$.

Particle in cell method implementation in LuNA fragmented programming system

V.E. Malyshkin, V.A. Perepelkin

The Particle-In-Cell (PIC) method is a powerful tool for modeling on supercomputers the behavior of complex non-linear phenomena in plasmas, astrophysics, and other application domains. This method is hard to implement for distributed memory due to necessity of provision of such dynamic properties of the program's execution as dynamic load balancing. In order to reduce the complexity of PIC implementation automation can be employed. The LuNA (Language for Numerical Algorithms) language and programming system are developed in the Institute of Computational Mathematics and Mathematical Geophysics. The main purpose of LuNA is to automate implementation of large-scale numerical models for supercomputers. In LuNA one describes an application algorithm in LuNA language, and the program to implement the algorithm is constructed automatically. The dynamic load balancing and other properties of program execution are provided automatically by the LuNA system. Using LuNA the PIC method for modeling self-

gravitating dust cloud evolution was implemented. It is shown in the work, that the dynamic load balancing is implemented automatically.

The fast method for approximate tsunami amplitude estimation

An. G. Marchuk, G. S. Vasiliev

The method for estimating a tsunami height using the wave front kinematics computation has been developed and tested. This method is based on an orthogonal advance of computational points located along a moving tsunami wave front line. Precise algorithms for determining these points movement direction and an addition of new ones have been proposed. This method was tested in an area with a constant depth. Then in the areas with parabolic and sloping bottom topography the obtained result of wave front propagation was compared to exact analytical solutions, which are delivered for such depth models. The method proposed makes possible to compute not only tsunami travel times but wave rays as well. Tsunami amplitudes can be estimated by the wave-ray divergence and a change in depth along the wave route. The wave amplitude estimation was tested against the results of the shallow-water numerical modeling of tsunami propagation using the MOST software. A difference in results between the two methods on the model (slope-like) bathymetry does not exceed a few percent. The advantage of the method proposed is its rapidness and low computer costs.

Identification of the development of different types of gravitational instability in the gas-dust massive and medium massive circumstellar disks

T.V. Markelova, O.P. Stoyanovskaya, V.N. Snytnikov

Formation of planetesimals and planets in the circumstellar disks can go via development of gravitational instabilities as a whole disk (global) and in separate areas of the disk (local). Numerical simulation dynamic massive and medium massive circumstellar disk reproduces the formation of structures involving gravitational instabilities of different types. It is not clear how identifying key mechanism of formation and existence structures in tow-phase self-gravitation systems. This is due to the fact that the simulated times on the background dynamics of the system may develop several types of instabilities and to reproduce affects numerical method. We make an attempt to identify different types of unstable solutions, expanding the total gravitational energy of the disk on the components and separating them in increments of instability. Analytic dependence of the instability increment on the parameters of the medium is known as gravitational instabilities for global (Toomre parameter, spyral number) and for local (Jeans length). Changing the parameters of the medium is also seen in an inelastic collision particle swarms in disk.

The work was financially supported by RFBR 140131516, RAS Presidium programmes No 21, 28; SB RAS Integration Project No. 130, and Russian Federation President Grant for the Leading Scientific Schools NSH 524.2012.3

Modeling of electromagnetic waves using Laguerre spectral method

A.F. Mastryukov

A spectral simulation method for modeling high-frequency electromagnetic waves is proposed. The method is based on expansion of the solution of Maxwell's equations in Laguerre functions in the time region. The spectral method is used to solve Maxwell's equations both for 2-dimensional medium, and stratified media. The effectiveness of the spectral and finite-difference methods are compared. Harmonic solutions and solitary solutions by Laguerre method are considered and the dynamics of monochromatic and broadband electromagnetic pulses are examined.

Дивергентные формулы и законы сохранения в дифференциальной геометрии и их приложения в математической физике

А.Г. Меграбов

Найдены дифференциальные законы сохранения (тождества вида $\operatorname{div} \mathbf{F} = 0$) для семейств произвольных гладких кривых и поверхностей и равносильные им формулы векторного анализа для

произвольных гладких векторных полей. Векторное поле \mathbf{F} выражается соответственно через характеристики кривых – их базис Френе, кривизну и кручение; через характеристики поверхностей – их нормаль, главные направления, главные кривизны, гауссову и среднюю кривизны; через направление и модуль векторного поля. Получены формулы связи между характеристиками кривых и поверхностей таких семейств в случае их взаимной ортогональности. Найдены дивергентные представления для гауссовой и средней кривизны семейства поверхностей. С помощью этих общих геометрических формул получены дифференциальные законы сохранения в трехмерном случае для решений уравнения эйконала (для поля времен в кинематической сейсмике (геометрической оптике)), уравнения Пуассона и гидродинамических уравнений Эйлера. Систематически исследована группа Ли, являющаяся расширением группы конформных преобразований трехмерного пространства на пространство шести переменных и одновременно – группой эквивалентности трехмерного уравнения эйконала и других уравнений математической физики. Найдена связь ее дифференциальных инвариантов с вышеупомянутыми формулами и другими полученными ранее тождествами векторного анализа, связывающими модуль и направление векторного поля. В двумерном случае найденные формулы переходят в результаты, полученные автором в статьях в ДАН: 1984. Т. 275, № 3; 2004. Т. 395, № 2; 2009. Т. 424, № 5; 2010. Т. 433, № 3, 4; 2011. Т. 441, № 3.

Particle-in-Cell simulation of low density electron beam kinetic instability in plasma

E.A. Mesyats, A.V. Snytnikov

A three-dimensional numerical model is created on the basis of Particle-In-Cell method. The model is designed for simulation of relaxation processes of the warm low density electron beam in plasma. Growth saturation of a separate unstable mode is studied in three different regimes. Solution accuracy of the created three-dimensional parallel numerical code based on the Particle-In-Cell method is investigated. In particle-In-Cell method the discreteness of model particles can bring the energy loss, self-heating and self-force occurrence and other non-physical effects. Therefore it is necessary to define sufficient number of particles for this model.

The results accuracy dependence on model particle number is determined. Minimal model particle number for correct instability increment calculation in weak electron beam-plasma interaction is defined. The results of 3D PIC simulation are in good agreement with theoretical predictions. It is shown by instability increment values computation and also by phase plane analysis for both cold and warm beam relaxation.

A parallel method for network probabilistic connectivity calculation

D.A. Migov

Networks with unreliable communication links and perfectly reliable nodes are considered in the present report. The most commonly used reliability measure for such networks is network probabilistic connectivity. Network probabilistic connectivity is defined as the probability of all the terminal nodes in a network can keep connected together, given the reliability of each network node and communication link in the network. We propose the parallel method for calculating the network probabilistic connectivity which is based on the well-known sequential factoring method. The proposed method is designed for supercomputers with distributed memory. The scalability of the proposed algorithm was examined. The analysis of the numerical experiments results allowed us to optimize some important parameters of the algorithm which further increase its speedup.

This research was supported by grants of the Russian Foundation for Basic Research (13-07-00589, 14-07-31069)

Mathematical modeling of acoustic-gravity waves in a heterogeneous earth – atmosphere model with wind in the atmosphere

B.G. Mikhailenko, A.A. Mikhailov

In this paper, we consider an efficient algorithm for the numerical modeling the propagation of seismic and acoustic-gravity waves for heterogeneous earth – atmosphere model with wind in the Atmosphere.

Seismic wave propagation in an elastic half-space is described by a system of first order dynamic equations of the elastic theory for the 3D Cartesian system of coordinates. Propagation of acoustic-gravity waves in the non-ionized isothermal atmosphere is described by the linearized Navier – Stokes equations. The algorithm proposed is based on combining integral transformations with a finite difference method. A characteristic feature of this algorithm is the use of the Laguerre transform along the temporal coordinate. As opposed to the Fourier transform, the application of the Laguerre integral transform with respect to time makes possible to reduce the original problem to solving a system of equations, in which a parameter of separation is present only in the right-hand sides of equations. As a result, the matrix of the reduced system is well-conditioned, thus making possible to use fast techniques of solving systems of linear algebraic equations. This paper presents numerical results of the simulation of wave fields for test medium models that were obtained by carrying out calculations on the multi-processor computer.

This work supported by the Russian Foundation of Fundamental Research under grant No 14-05-00867.

Construction of adaptive meshes using neural network models

A.V. Molchanov

As a result of real 3D objects scanning the large unstructured point clouds are obtained. It is necessary to process these data to create a digital CAD-model. A development of new algorithms for unstructured adaptive 3D meshes construction is important problem for laser scanning data processing. Unlike classic algorithms the approach based on neural network algorithms of self-organization allows to use clouds of points instead of geometry shapes as input data.

The "Growing triangulation" algorithm was developed and successfully tested on the real laser scanning data. This algorithm is based on Growing Neural Gas model of the self-organizing neural network which reconstructs the surface of 3D objects by the cloud of points. The reconstructed surface is called an unstructured triangulated mesh adapted to the given point cloud. Before mesh construction the algorithm selects points with geometric features, for example belonging to edges, which are necessary for the following surface specification. The algorithm does not require additional information about the surface and can be applied to noisy point clouds or to the clouds with low density.

Surface chemical reactions in DSMC computations

A.N. Molchanova, A.V. Kashkovsky, Ye.A. Bondar

At the initial stages of the development of prospective space vehicles, it is necessary to study their aerothermo-dynamic characteristics along the reentry trajectory. Experimental modeling of such conditions is difficult from the technical viewpoint; therefore, numerical simulation is the main tool for studying high-altitude aerothermodynamics of space vehicles. The continuum approach to numerical simulation of flows is inapplicable at high flight altitudes because of rarefaction and thermal non-equilibrium effects, therefore the kinetic approach, such as Direct Simulation Monte Carlo (DSMC) method, should be used. One of the important problems of numerical simulation of such flows is the allowance for chemical reactions on the vehicle surface, which can severalfold increase the heat flux to the vehicle. This work is aimed at developing different molecular surface chemistry models for DSMC computations and investigation of surface catalycity effects on aerothermodynamics of blunted bodies in high-enthalpy flows.

This work was supported by the Russian Government under grant "Measures to Attract Leading Scientists to Russian Educational Institutions" (contract No. 14.Z50.31.0019)

Numerical methods for solving Gel'fand – Levitan – Krein equation

N.S. Novikov

The report considers acoustic inverse problem. The problem consists in determining density and wave's velocity of the medium, using the acoustic data on the surface. In order for solving this problem, the approach of I.M. Gel'fand, B.M. Levitan and M.G. Krein was applied. The GLK-method reduces nonlinear inverse problem to a one-parameter set of linear Fredholm integral equation. Then Monte Carlo method

was applied for solving this set of integral equation. Monte Carlo method based on a representation of the solution as a mathematical expectation of a certain random variable.

The numerical experiments for solving GLK-equation with different levels of data's error will be represented. In addition, the comparative analysis of Monte Carlo method and other numerical methods will be made.

Simulus/V, a visualization tool for physical models

M.B. Ostapkevich, A.N. Herega

A description of Simulus/V visualization tool is presented in the work. Simulus/V is primarily oriented to the visualization of percolation models [1] and cellular automata models of gas dynamics. The distinguishing features of such models are the complexity of their structure and huge dimensions of data objects. In order to support the required diversity of kinds of visualization, Simulus/V has an extensible set of visual modes that are either implemented as subroutines in C or composed of other existing visual modes. Simulus/V provides an easy to use interface to computational programs as well as a transparent access to clusters. Simulus/V can be used as a stand-alone system or as component embedded into simulating systems, such as ODNO.

This work is supported by RAS project 14.6.

References

1. A.N. Herega. Simulation of cluster structures in material: force fields and descriptors // Physical Mesomechanics. 2013. Vol. 16, iss. 5. P. 87-93. (in Russian)

Universal technology of numerical simulation of dynamic and stationary boundary value problems with the decomposition of areas

V. I. Paasonen

The report describes methods of calculating boundary problems in areas composed of a finite number of rectangles the same way oriented. The technology is based on a transformation of the source area to the cellular structure with the real and fictitious borders section. On the fictitious borders written soft boundary conditions of smoothness in the form of equality left and right derivatives. Such conditions are quite similar to balance flows conditions. This technology can be applied to traditional difference schemes and the schemes of high order accuracy. It is proved that the technology can be applied to solve different types of equations. This technique is demonstrated on the fourth-order accurate schemes for the heat equation, Poisson equation for the equation of oscillations, as well as for Navier – Stokes equations are solved using the method of decomposition areas. Tests demonstrate the efficiency and wide applicability of the method, and also confirm that the accuracy of the method corresponds to the theoretical order of accuracy.

Variational source function estimation algorithms in city atmosphere monitoring technologies

A.V. Penenko, S.J. Rakhmetullina

The work is devoted to the implementation and evaluation of atmospheric pollutant source estimation algorithms to be used in the monitoring system of the city. The monitoring system consist of several automatic measurement devices providing point-wise concentration measurement data. Considered algorithms are based on variational approach with the use of adjoint equations for the convection-diffusion models with source-term uncertainty. Adjoint equations allows to formulate the problem as an underdetermined system of equations connecting unknown source function with measurement data. The excess of unknowns is treated in two ways: representing sources as a weighted sum of illumination-corrected [Issartel,2003] adjoint functions and as a weighted sum of point-wise sources. The algorithms are tested on a realistic scenario resembling the city monitoring system.

Special features of software for 3D modeling and 3D inversions of data of electrical survey with circular electrical dipole in the Arctic

M.G. Persova, Y.G. Soloveichik, D.V. Vagin, V.O. Demina

The software for 3D modeling and 3D inversions of data obtained using the source in the form of a circular electrical dipole (CED) which is located on drifting ice when investigating the geoelectrical structure of the deep-water area in the Arctic basin is proposed in the work. Computational aspects of calculation of the stationary and non-stationary electromagnetic field of CED in the receivers which are closely located to the source and removed at big distances are considered. The algorithms for investigated medium geoelectrical characteristics recovery considering the possible unbalance of currents in CED beams are proposed. The data processing technology based on the use of 3D inversions algorithms for radial observation systems is proposed. The developed software performance is shown by the example of the synthesized data obtained with 3D modeling for geoelectrical conditions in the deep-water part of the Arctic basin.

Performing 3D inversions for surface electrical survey technologies using a loop source

M.G. Persova, Y.G. Soloveichik, D.V. Vagin, D.S. Kiselev, Yu.I. Koshkina, N.V. Simankovich

This work is devoted to the technology features of software and the results of its application for 3D inversions of electromagnetic survey data received with the loop source in the time domain. The 3D inversions are performed in the form of successive (multistep) recovery of geoelectric section: from reconstructing the conductivity of heterogeneities of the section upper part at the initial stages to searching the conductivity of the deep target bodies at the final stages. The results of the 3D inversions, which are based on accurate and linearizational mathematical models for calculating parameter derivatives, and the corresponding computational costs are compared. The possibility to differentiate the impacts of the section upper part heterogeneities located at the side of the area to be measured, and deep heterogeneities located below this area, which is based on the 3D inversion, is analyzed.

The results of 3D inversions obtained when solving the problems of East Siberian oil reservoirs exploration and the definition of their characteristics are demonstrated.

Stochastic simulation of wind turbines operating in atmospheric turbulence

K.K. Sabelfeld, S.A. Efremov

We suggest a stochastic model for the stand-alone wind turbines in atmospheric turbulence, and consider the effect of the stratification of the atmospheric boundary layer on the capacity. Simulations are also made to calculate the distribution density function of the capacity.

We study also the case of a set of turbines in a farm and analyze the cases of the velocity deficit, which is directly associated with power losses in wind farms, and the wake turbulence, which affects the flow-induced dynamic loads on downwind turbines. The results may be useful for optimizing the wind farms, i.e., to maximize the power output and minimize the maintenance costs.

Neumann problem for a sphere, solution on the surface

A.O. Savchenko

The solution to the Neumann problem for a sphere is the surface integral of the given normal derivative multiplied by the known function. Due to the presence of singularity in integrand, the application of simple quadratures to calculate the integral is inefficient.

The idea of the proposed method is that the sought function is represented in the form of a double integral such that the integral of the singular multiplier in the inner integrand can be evaluated analytically. The inner integral is approximated by a quadrature for the product of functions of which one can be calculated analytically. As a result, the integrand obtained before the next integration has only a weak logarithmic singularity. This singularity can be taken into account by changing variables in the subsequent integration.

To illustrate the proposed method numerical experiments are carried out. The average and maximum errors of calculation of the values of the function on the surface have the order of a thousandth of a percent from the precise values of the function.

Design of efficient numerical methods for problems with smooth and piecewise smooth solutions

B. V. Semisalov

The requirement of adequacy of a computational model to the original formulation of problem is essential for stable, sufficiently rapid and accurate solving the problems with a high computational complexity including the problems of small parameters, large scales, optimization and many others. In order to make a full-fledged use of a priori information about the smoothness of the desired solutions the concept of localization and local approximation method is introduced. On the example of solving of nonlinear boundary value problems for the Poisson equation we propose a new class of numerical methods based on nonlocal approximations and ideas of schemes without saturation of K. I. Babenko. It is worth noting the advantage of the proposed methods.

1. Efficiency in solving nonlinear problems with small parameters, steep gradients, smooth and piecewise-smooth solutions.
2. Natural generalization of the proposed ideas in case of arbitrary dimension providing the possibility of effective parallelizing.
3. Significant flexibility associated with the possibility of applying different kinds of interpolations with consideration of different boundary conditions.

To development of the computational exploration

V.A. Sergeev

Computational exploration (CE) as a scientific direction developed in the Computing Center of the USSR Academy of Sciences (later on - ICMMG). Founder of the CE, its leading methodologist, theorist and the algorithmist was Yuri A. Voronin (1925-2005). Since 1970, he moved with the staff to the Computing Center at the invitation of G.I. Marchuk. Created and developed new disciplines of mathematics and nonclassical geokibernetiks: search theory, classification, algorithmic description, pattern recognition, similarity measures, zoning and others.

Currently, colleges and followers of Y.A. Voronin continue this work in the top ten cities of the former USSR. In aspects of development of algorithms and computer-programs among them the leader is Moscow. In ICMMG brought me to be the sole successor of these works and the keeper of the archive of scientific school Y.A. Voronin. Experience works on formalization and mathematization of geology has allowed me to receive and publish after the year 2005 a number of research results not only in computational exploration, but also geokatastrofik, on data, knowledge and ontologies, on important social problems.

Semi-lagrangian approach in finite element method for Navier – Stokes equations of viscous heat-conducting gas

V.V. Shaydurov, G.I. Shchepanovskaya, M.V. Yakubovich

The algorithm is proposed for numerical solving the Navier – Stokes equations for two-dimensional motion of viscous heat-conducting gas. The discretization of equations is performed by a combination of a special semi-lagrangian method for transport derivatives and the finite element method with piecewise linear basis functions for other terms. The results of numerical studies of the structure of a supersonic flow around an obstacle for a wide range of Mach numbers and Reynolds numbers will be presented. Velocity and pressure fields and the vortex structure of flow are studied in the circulation area of the obstacle.

Mathematic modeling and optimization of transport streams of the city

A.F. Shaykhnurova, G.R.Karamutdinova, I.I. Bakirov

Today, the number of vehicles in the cities of Russia increases, and this leads to occurrence of traffic jams, awkward movement, worsening conditions for the normal development of the city. To solve the above problems the mathematic models are used. In this paper we consider the entropy model, which let us to calculate the matrix of correspondences. To calculate the matrix we apply algorithm, based on the method

of balancing: at each step alternately relative balance of rows or columns is performed, and after a number of steps, this procedure leads to a matrix of correspondences. Thus, on the basis of the matrix we can make the most accurate schedule of public transport, determine load elements of the road network, estimate the number of passengers carried by type of passengers, by mode of transport, by the routes and directions, assess the intensity of passenger traffic between different items

DNS of shear flows on hybrid CPU-GPU clusters

A.A. Shershnev, A.V. Kashkovsky, A.N. Kudryavtsev

Direct numerical simulation of turbulent flows even at moderate Reynolds numbers requires computational meshes consisting of hundreds of million of points and accurate high-resolution methods. One of the reasonable ways to increase efficiency and significantly reduce computational wall-clock time is to employ modern general-purpose graphics processing units (GPGPU) with high computational and data throughput. In the present work a parallel numerical code for direct numerical simulation of laminar-turbulent transition in supersonic flows is developed. It solves 3D unsteady compressible Navier – Stokes equations in general curvilinear coordinates using modern high-resolution shock-capturing numerical schemes. Supersonic mixing layer flow was taken as a test problem to demonstrate features of numerical code and measure the efficiency of parallelization and speed-up as compared to parallel CPU version of the code.

This work was supported by the Russian Government under grant "Measures to Attract Leading Scientists to Russian Educational Institutions" (contract No. 14.Z50.31.0019)

Rarefied flow computations using relaxation-type kinetic equations

A.A. Shershnev, A.N. Kudryavtsev

A high resolution finite difference method for solving nonlinear model kinetic equations is presented. The approach based on relaxation-type kinetic equations does not suffer from statistical scattering inherent in stochastic approaches similar to the DSMC (Direct Simulation Monte Carlo) method and is equally accurate when simulating both steady and unsteady flows. At the same time, it is not so prohibitively resource consuming as deterministic solving of the Boltzmann equation. Thus, it can be a useful and powerful tool for rarefied flow computations in high-altitude aerodynamics and microfluidics. The presented numerical method is used to simulate some classical problems of rarefied gas dynamics as well as microflows of practical interest such as shock wave propagation in a microchannel and flows in supersonic micronozzles and jets.

The work was supported by Grant of Russian Government (Agreement No. 14.Z50.31.0019) and by Russian Foundation for Basic Research (Project No. 12-01-00776).

Contextual clustering multispectral data of remote sensing the Earth

V.S. Sidorova

There are several contextual classification methods for the data of remote sensing the Earth. For example, a number of statistical measures can be employed to obtain spatial features. Or there have been a variety of stochastic models proposed for modeling pixel neighborhoods. The alternative approach is considered here. The focus of this approach is doing not use statistical measures calculated on collected statistics, but statistics themselves. Within each pixel window, one can obtain an occurrence-frequency table containing all possible gray-level vectors of multispectral image. The advantages of this approach: tables can be quickly computed, directly compared, tables contain more spatial information than the statistical parameters, disk storage is not required. The number of gray-level vectors in multispectral space was reduced using a special data-reduction algorithm through rotation multispectral space into eigen space. Due to this, the multispectral data were reduced to image of one feature dimension with the loss of relatively little information. The results of clustering the multispectral data of remote sensing the Earth were illustrated.

Anisotropic and directed window functions with shearlet transform

K.V. Simonov, S.V. Kirillova, L. Cadena

In the framework of solving spatial data analysis considered the principles of constructing a fast algorithm of discrete shearlet transform observational data which is based on the implementation of the algorithms are Fast Fourier transform. Following describes the continuous shearlet transform and then through the sampling parameters discrete shearlet transform. Shearlet considered on a cone this approach provides a good separation of the horizontal and vertical directions shearlet in the frequency domain.

Note that the problem of separation an image into morphologically different constituents recently received much attention due to its importance for critical applications. Successful computational techniques for efficient and accurate solution of this problem can be applied to a wide range of areas including the problems of spatial data visualization for diagnosis of complex phenomena.

Relatively recently introduced a system of representation of spatial signals (images) called shearlet system. Shearlet system is generated by the parabolic scaling, shear and translation parallel operators to the initial spatial observations. These are the same wavelet systems with binary scaling and translation functions but also includes profiles of focus, with an extra "The shear" operation (anisotropic scaling). This operation is, in fact, gives a more convenient approach for the analysis of trends. Thus, shearlet is a function that is similar to the wavelet along one axis and bump function on the other axis.

Consequently, shearlet transform requires a combination of the following operators: the operator to scale to create items in different scales; orthogonal operator to change direction, and the operator to translate of these elements in the 2D plane. Most important features of multi-dimensional problems of the studied data are concentrated in the varieties of small dimension. For example, in image processing, the edge is a one-size curve on which the image intensity changes dramatically.

Recently, a new approach shearlet system provided effective tools for the analysis of geometric features of the internal spatial signal using anisotropic and directed window functions. In this approach the orientation is achieved by using integer powers of matrices shear and these operations preserve the structure of the integer lattice which is crucial for a digital implementation. The algorithm of discrete shearlet transform effectively implemented using fast Fourier transform algorithms. In the Matlab environment based on the considered algorithm the possibility shearlet transform for analysis in particular medical images.

New frequency characteristics of solutions to stochastic differential equations

D.D. Smirnov

Modern development of supercomputers highlights Monte Carlo methods, the most well-adapted to parallel computation in terms of ease of parallelization algorithms. The most difficult for all methods of investigation of the properties of solutions of systems of stochastic differential equations (SDE) are nonlinear stochastic fluctuations. Calculations showed that the moment functions and density distributions of SDE solutions do not provide complete information about the nonlinear stochastic fluctuations. More informative are the frequency of generalized integral curve "frequency integral curve (FIC)" and the phase trajectory "frequency phase portrait (FPP)", which take into account all the statistics of the simulated ensemble of trajectories. FIC at a fixed time is an approximation of density distribution, ie, evaluates solution of the Fokker – Planck – Kolmogorov. For one simulated trajectory solutions SDE schedule FPP gives one implementation phase portrait. Similar calculations can be carried out overnight only on supercomputers, especially for parametric analysis, when one and the same system of SDE repeatedly statistically modeled for different sets of real parameters.

Parallel algorithm for solving Vlasov – Poisson equations on CPU/GPU hybrid supercomputers

N.V. Snytnikov

One of the commonly used methods for solving equations of stellar dynamics, consisting of Vlasov equation and Poisson equation, is particle-in-cell (PIC) method. It requires to compute individual movements of a large number of particles and to calculate self-consistent gravitational field using a finite-difference

method. To develop a scalable parallelization for thousands and millions cores one needs to redistribute dynamically particles among processors to avoid non-uniform loading, and provide efficient domain decomposition for Poisson equation.

We present a new parallel numerical algorithm, aimed to run on hybrid CPU/GPU supercomputers. First, we use a special domain decomposition technique for solving Poisson equation [2]. It is based on a partial pre-computation of Green's function and calculation of a single-layer potential in a spirit of [3]. Second, it is reasonable to calculate independent movements of particles (which is the most computationally intensive procedure), using a huge number of light-weight GPU cores. A proof-of-concept tests with several billions of particles and 1024^3 grid nodes have been conducted at Siberian Supercomputer Center (Novosibirsk, Russia).

The work is supported by RFBR grants No. 14-01-31088, No. 14-07-00241, Integration project of SB RAS No. 130.

References

1. Berezin Yu.A. Vshivkov V.A. Particle-in-cell method in the plasma dynamics // Nauka. 1980.
2. N. Snytnikov. Scalable Parallel Algorithm for Solving the – Collisionless Boltzmann – Poisson System of Equations // Astronomical Society of the Pacific Conference Series. 2012. V. 453. P. 393.
3. Huang J., Greengard L. A Fast Direct Solver for Elliptic Partial Differential Equations On Adaptively Refined Meshes // SIAM J. Sci. Comput. 2000. Vol.21. P.1551-1566.

Modification of PIC method with adaptive mass: results for 2D problems

T.V. Snytnikova, G.I. Dudnikova, V. A. Vshivkov

Particle-based simulations are widely used, for example to study fluid flows or plasmas. The physical particles of interest are often not simulated individually, but as groups of particles, called super-particles or macro-particles. Most systems contain so many particles that simulating them individually would be very slow or impossible. On the other hand, a sufficient number of particles is required to limit stochastic fluctuations. Traditionally, super-particles had a fixed weight. But the simulation can run faster or give more accurate results if the weight of these super-particles is controlled adaptively.

The methods of adaptive particle management can be divided into two classes: pairwise merging and group merging. The first class can not provide for execution of the conservation laws accurately. Our modification belongs into second class. It accurately executes the conservation laws and does not make unphysical effects.

The method is tested on problem of interactions of laser impulse with plasma. The work is supported by the Russian Foundation for Basic Research (project 14-01-00392).

Construction and substantiation of convergence of discrete analogues conjugate-operator models

S.B.Sorokin

The study includes the construction and justification of the discrete analogue of the conjugate-operator model heat conduction problem. To construct a discrete analogue of the following procedure:

1. As a support operator is selected operator from the defining relations;
2. Built its approximation;
3. Approximation of the adjoint operator (the law of conservation) is constructed as the adjoint of built in the preceding paragraph.

Difference scheme built on an arbitrary irregular grid for the variables (including discontinuous) parameters in the constitutive relations and has second order accuracy. Convergence of difference scheme is performed to recorded in the conjugate-operator form (rather than the consequences of it) and is carried out by proving the stability and study its approximation properties. The study begins with the approximation of the discrete analogue of the support operator and approximation properties of the discrete analogue of the operator of the conservation law (uniquely defined by discrete analog reference operator) are derived from the obtained results for the support operator. Of particular note is an important circumstance inherent

in the difference scheme: All components are discrete analogs of vector quantities are defined in the same grid nodes.

Computer simulation of ethane pyrolysis in a tube reactor with laser radiation

O.A. Stadnichenko, V.N. Snytnikov, V.I. Snytnikov

Mathematical models of a laboratory and experimental-demonstrational tube reactors of C₂-alkanes pyrolysis were developed. Gas dynamics describes a three-dimensional laminar flow with the pyrolysis reaction and thermal effects of heating by heat transfer from the walls and by laser radiation. Ethane dehydrogenation in the gaseous phase described as a radical chain mechanism. Laser radiation is taken into account phenomenologically as a constant source of energy with complex configuration dependent of ethylene distribution and parameters of laser beam.

Mutual verification of experimental data and simulation results for laboratory reactor has shown performance of the created models. It was numerically and experimentally shown that ethane pyrolysis could be controlled by using laser radiation. Usage of a phenomenological approach for accounting of the energy absorption of laser radiation allowed to estimate the impact of the radiation power density on the conversion of ethane with the analysis of thermal and energy regimes of pyrolysis tubular reactor.

The developed model was used for large-scale transition to an experimental-demonstration reactor. Set of simulations for experimental-demonstrational reactor was made to find the optimum geometry and physical parameters in case of laminar flow of gas. According to the results new reactor was created.

For calculations package ANSYS FLUENT (license SSCC SB RAS) was used with user's external UDF- modules created by the authors of the report.

RFBR 120800871A, RFBR 120831095, RFBR 140131516, UNIHEAT Project of Skolkovo Foundation (A64), President RF Grant Y.PhD 2737.2013.3

Supercomputer simulation of laser-catalytic reactor of C₂-C₃ alkane pyrolysis

O.P. Stoyanovskaya, P.V. Snytnikov

To develop the laser-catalytic approach of olefins production from C₂-C₃ alkanes we designed a reactor where the zone of homogeneous endothermic pyrolysis of C₂-C₃ alkanes (gas zone) is surrounded by the zone of catalyst (porous zone) where methane and hydrogen are oxidized with energy release. This energy goes into the zone of gaseous pyrolysis by means of thermo conductivity of products of deep oxidation: CO₂ and H₂O. The energy of CO₂ laser that is effectively absorbed by the mixture components is introduced into the same zone to increase the rate of methyl radical generation.

Using ANSYS FLUENT software package we developed numerical model of such laser-catalytic reactor, where the transient 3D flow of gas mixture in gas and porous media is reproduced. We used specially defined coefficients of diffusivity to model the multi-component gas flow and Zimont approach to introduce the radiation into gas. The aim of simulation is to verify whether the higher diffusivity of hydrogen compared to the other components of the mixture can influence the selectivity of the pyrolysis.

The work was financially supported by RFBR 120831095, UNIHEAT Project of Skolkovo Foundation (A64), President RF Grant Y.PhD 2737.2013.3

Full parallel GPU solvers for well resistivity and high-frequency induction logging applications

I.V. Surodina, I.B. Labutin

Fast direct solver is a corner stone for the number of inverse geophysical problems. Modern and promising approach to implement fast solver is to use parallel GPU computations. In order to obtain maximum speed-up by utilizing maximum GPU resources it is better to implement fully parallel solver designed specifically for GPU architecture.

Direct problems in well resistivity logging or high-frequency induction logging applications lead to large sparse linear systems arising after finite-difference or finite-element approximations. These systems

are typically solved with conjugate directions methods which suits well for parallelization. However in order to increase convergence of these methods you should choose a right preconditioner.

In this work an algorithm for constructing parallel sparse approximate inverse preconditioner with very good properties is proposed. Implementations of parallel solvers with NVIDIA GPU technology are given. Comparisons and speed-up over CPU solvers and other competitors using real geophysical data are presented. Obtained speed-up varies from 10 to 50 times depending on discretization level and geophysical properties of the medium.

Accuracy evaluation of regularizing algorithm based on the method of M.M. Lavrent'ev

V.P. Tanana, A. I. Sidikova

Considers the operator equation of the first kind with the error in the operator and in the right part of the equation. For the method M.M. Lavrent'ev made his discrete approximations and obtained error estimation of this approximations.

Let H is Hilbert space. Consider operator equation of the first kind

$$Au = f, u \in M_r, \quad (1)$$

where M_r is compact, A -linear completely continuous operator, $A: H \rightarrow H$. The method of M.M. Lavrent'ev consists in replacement of the operator equation of the first kind by the equation of the second kind

$$Au + \alpha u = f, \alpha > 0. \quad (2)$$

As $M_r = B\bar{S}_r$, where $B = A^p$, $p > 1$. Assume that for $f = f_0$ there exists an exact solution $u_0 \in M_r$ and $f_0 = Au_0$. Instead of f_0 such $f_\delta \in H$ is given that $\|f_\delta - f_0\| \leq \delta$. Number $\delta > 0$ is given. It is required by $A_h, f_\delta, h, \delta, M_r$ to find an approximate solution $u_{\delta h}$ of equation (1) and to evaluate $\|u_{\delta h} - u_0\|$ on the class M_r . The operator A replaces by finite-dimensional operator A_h , where the level of error $h > 0$ will be considered known, $\|A_h - A\| \leq h$. Thus the equation (2) reduce to $A_h u + \alpha u = f_\delta$. The regularization

parameter $\alpha(\delta, h, r) = \sqrt{\frac{r\|B\|h + \delta}{r\|A\|^{p-1}}}$. For approximate solution $u_{\delta h} = (A_h + \alpha(\delta, h, r)E)^{-1} f_\delta$ of equation (1) the estimate $\Delta[P_{\alpha(\delta, h, r)}(A)] \leq 3\sqrt{r\|A\|^{p-1}(r\|B\|h + \delta)}$ was derived.

One method of cellular automata generalization

A.B. Terentev, S.A. Savikhin, S.A. Zolotov, D.E. Borisov, A.A. Pankratov, A.A. Nosov, A.O. Muzychenko

Cellular automaton model is known to be one of the best paradigm to construct parallel HPC applications in very different scientific domains using very different mathematical methods. However, traditionally CA are used for modeling in a regular manner: all the cells are the same — same size, same set of states, same set of rules. To widen applicability of the CA paradigm for modeling of very complex systems, we constructed the CUMPS solver platform which implements several unusual extensions to the classical CA. These extensions allow to construct irregular models while keeping the regularity of the computing process, thus providing highest scalability of the application. We'll present several applications performed with our solver to show its applicability to process really big and complex models.

A way to define the control flow of the fragmented program

A.A. Tkacheva

Nowadays in the Institute of Computational Mathematics and Mathematical Geophysics of the Siberian Branch of the Russian Academy of Sciences the LuNA (Language for Numerical Algorithm) fragmented

programming system (FP) is under development. The system is oriented to the implementation of the large scale numerical models on supercomputers. In FP an application program is assembled out of fragments of computation (FC) and data fragments (DF). The fragmented structure of an application program is kept in the course of its execution. This approach allows automatically to provide different dynamic properties of fragmented program execution, such as dynamic processors load balancing.

Efficient execution of a fragmented program faces the control problem, i.e. choice of ready FCs for execution. The choice is performed dynamically by the LuNA runtime system, based on information dependencies among FCs. Due to nondeterminism of fragmented program execution, solution of the control problem implies high overhead and is hard to automation. Thus, additional means to define the control flow are proposed for the fragmented programming system. The means allow defining the desired order of FCs execution. When the order is defined, the complexity of control problem decreases significantly. The proposed means are based on Petri net. In this case the choice of ready FCs for execution is based on execution Petri net. Applicability of the means for a class of numerical models is studied.

The proposed means were implemented as RuSh program module for LuNA programming system. The objective of this work was research applicability of RuSh module. Applicability of the means was studied for solution of Poisson's equation (explicit finite-difference scheme). For this a comparative performance testing with alternative MPI implementation and alternative LuNA implementation without using RuSh module was performed.

Convergence of finite element method for stationary linear elasticity equation

M.V. Urev, M.O. Shimonaeva

We consider stationary linear elasticity problem into a three-dimensional cylindrical domain Ω :

$$\begin{aligned} -\operatorname{div} \sigma(\mathbf{u}) &= \mathbf{f} \text{ in } \Omega, \\ \mathbf{u} &= 0 \text{ on } \partial\Omega. \end{aligned}$$

Here $\sigma(\mathbf{u})$ is a stress tensor.

In axisymmetric case a weak formulation of the problem mentioned above has the next presentation:

Find $\mathbf{u} \in \mathbf{V}_0(\omega)$ such that for all $\mathbf{v} \in \mathbf{V}_0(\omega)$ $\frac{\partial v_z}{\partial z}$, where ω is a half section of domain Ω in cylindrical coordi-

nates (r, z) and space $\mathbf{V}_0(\omega)$ can be presented as $\mathbf{V}_0(\omega) = \mathbf{V}_0(\omega) = V_{1/z,0}^1(\omega) \times H_{r,0}^1(\omega)$. Spaces $V_\alpha^k(\omega)$ and

$H_r^k(\omega)$ used for consideration of this problem were examined by S. Nikolsky and P. Lizorkin. In these spaces we obtain estimation of convergence which has the same order as convergence for problems without degeneration. Multiplicative allocation of singularity technique proposed by M. Timerbaev is used as well. Also some numerical results which illustrate convergence are presented.

Computer simulation of self-organization in the bacterial MinCDE system by cellular automata

A.A. Vitvitsky

Exact theoretical description of self-organization processes in biological systems is a hard task because of the difficulty to obtain information about spatiotemporal dynamics of individual particles from bulk biochemical assays. Hence, computer simulation in this area plays an important role and helps to confirm (or to disprove) the proposed hypotheses. A bright example of self-organization in biology is MinCDE system. The MinCDE system is a bacterial proteins system that properly positions the septum in the middle of the cell in *Escherichia coli*. Currently, there are several articles devoted to detailed experimental studies of protein dynamics MinCDE *in vitro*. In this paper, we propose the Cellular Automaton model of self-organization MinCDE system and its implementation in C++. The results of this computer simulation can be effectively compared with those obtained from experiments *in vitro*, and as a result help to confirm (or to disprove) some existing MinCDE theoretical propositions.

Framework for development of parallel programs implementing particle-in-cell method*A. S. Volkov*

The framework for development of parallel programs implementing particle-in-cell (PIC) method of numerical simulation is developed in the ICM&MG, RAS. The PIC method computes the movement of model particles with given characteristics such as mass and charge. Initial velocities and positions in a simulation domain are set for the particles, and the simulation advances in time steps as the particles move under the forces determined by external fields and particle interaction. The structure of the method does not depend on the nature of the particles and can be implemented once and reused in particular applications.

The framework defines concepts of a simulation domain and fragments. The fragments are the parts of simulation domain, data units that can be automatically moved between processes for the purposes of inter-process communications and workload balancing. A fragment contains a list of particles and a set of meshes on which the values of density, forces, potentials, and so on are represented. A user through a GUI tool has to define initial distribution of the particles, their velocities and the subroutines to compute forces that should act on the particles.

A new approach to constructing vector splitting schemes in Mixed FEM for heat transfer problems*K.V. Voronin, Y.M. Laevsky*

A new approach to constructing vector splitting schemes for heat transfer problems is proposed. Heat transfer problem is considered in the mixed formulation in terms of temperature and heat flux. For space discretization mixed finite element method with Raviar – Thomas elements of lowest order on quadrilateral meshes is used. In order to obtain efficient algorithms of solving the arising vector equation for the heat flux one has to develop splitting schemes for the time variable. The crucial idea of the proposed approach is to construct splitting schemes for the flux using well-known scalar splitting schemes for the flux divergence. The properties of the scalar splitting scheme for the divergence can be also used for analyzing accuracy and stability of the vector scheme for the flux and computation of the temperature.

Using the proposed approach several splitting schemes in 2D and 3D cases are developed. Numerical results of studying accuracy of these schemes in comparison with Crank – Nicolson scheme are presented. Several theoretical results on stability of these schemes as well as numerical behaviour in case of nonuniform meshes and nonconstant coefficients are discussed. The developed splitting schemes were used for numerical modeling of accretionary-collisional processes in the lithosphere.

Fractal analysis in the problem of the seismic waves selection*G.M. Voskoboynikova*

The a posteriori algorithms for joint detection and estimation of arrival times of wave pulses quasiperiodic sequences are considered. The high precision of the waveforms selection and measurements of their arrival times in the noise applied to the problems of geophysical monitoring on the basis of numerical experiments are shown. The fractal approach for better noise immunity and reliability of a posteriori algorithms is proposed and analyzed. Approach is based on the waves mapping on two-dimensional plane "time–frequency" using a two-dimensional Fourier transform. Numerical experiments show that this approach significantly improves the accuracy of the solution as a whole. In some cases, the error decreases on order.

Modeling of the bubble fluid dynamics*V.A. Vshivkov, V.K. Kedrinsky*

The problem to model wave processes in the fluid with gas bubbles, dissolved in it, is considered. As a mathematical model the gas dynamics model, where the equation of state consists of the ordinary differential equation for a bubble concentration, has been taken. The numerical model based on the Harlow particle in cell method is presented. Also, there are given the computational results for different initial conditions.

Numerical simulation of ion acceleration by electrostatic shock wave

L.V. Vshivkova, G.I. Dudnikova, T.V. Liseykina

Electrostatic collisionless shock wave can accelerate ions to high energies, and the study of the mechanism of such kind of acceleration is very important in wide range of phenomena in laboratory and space plasma, especially in acceleration of cosmic rays to ultrahigh energies. The details of the acceleration physics process are not fully understood yet, and computer simulation is necessary to study this phenomenon. We present a numerical model for simulation of electrostatic shock wave formation on the base of a kinetic plasma model. Plasma consists of hot electrons and cold ions ($T_e \gg T_i$). Initially plasma propagates through a simulation box in the -x direction, and reflects from the right boundary. The speed of plasma flow can be smaller or comparable with the electron thermal velocity. The development of two stream instability depending on Mach number of counter-propagating flows, soliton formation and shock wave formation is investigated. Ion acceleration by reflection from the front of shock occurs for the critical Mach number. One-dimensional PIC method for the purpose of high numerical resolution is used to solve Vlasov equations for electrons and ions with the real mass ratio.

Supported by RFBR under Grant 14-01-31304.

Advantages and problems of using GPU implementation permutation test

A.A. Yakimenko

This paper proposes an algorithmic approach and the parallel and serial versions of programs for solving search problems statistically significant over- the biological characteristics of a given set of genes. The problem is connected with the implementation of well-known in biology permutation (randomization) test. By taking into account the potential parallelism permutation test developed in parallel with the implementation of the program on GPUs. Provides estimates of the acceleration of parallel programs developed with respect to its serial counterpart.

Analysis of the accuracy of estimates of the moments of solution to scalar linear SDE with Wiener and Poisson components using the statistical modeling method

M.A. Yakunin

The numerical solution scheme on a uniform time grid based on the generalized Euler method is proposed for the SDE system with Wiener and Poisson components. The formulas for exact solution to scalar linear SDE and for moments of this solution are presented. The dependences of the accuracy of estimates of the expectation and the dispersion of SDE solution on SDE parameters, the size of the integration step, and the size of an ensemble of simulated trajectories are investigated on the base of the analytical expressions and the statistical modeling method. The obtained results show a loss of the accuracy of estimates with the increase of the dispersion of SDE solution. This requires the considerable increase of the number of simulated trajectories.

Model and algorithm optimization, forecasting and management of changes in the main parameters influencing underground leaching system under the condominium development

T.M. Zhuraev, K.D. Ismanova

Development of mineral resources in underground leaching (UL) has a vital economic importance. This article presents the results of development of methods and algorithms for determining the parameters to ensure better management of UL processes in the conditions of use of horizon mining.

CONTENTS

INVITED PLENARY TALKS

<i>P.E. Bjørstad</i>	4
<i>C. Carstensen</i>	4
<i>N.T. Danaev</i>	4
<i>V.P. Dymnikov, V.N. Lykosov, V.B. Zalesny,</i> <i>V.Ya. Galin, E.M. Volodin, A.V. Glazunov,</i> <i>A.S. Gritsun, N.A. Dianski, M.A. Tolstykh,</i> <i>N.G. Iakovlev, A.V. Gusev, S.V. Kostykin,</i> <i>D.V. Kulyamin, R. Yu. Fadeev, V.V. Shashkin</i>	5
<i>С.К. Годунов</i>	5
<i>G. Mauri</i>	6
<i>B.G. Mikhailenko, S.I. Kabanikhin</i>	6
<i>G.A. Mikhailov, G.Z. Lotova</i>	6
<i>M.A. Olshanskii</i>	7
<i>V.G. Romanov</i>	7
<i>V.V. Shaydurov, G.I. Shchepanovskaya,</i> <i>M.V. Yakubovich</i>	7
<i>R.M. Shagaliev, A.S. Kozelkov</i>	7
<i>E.E. Tyrtysnikov</i>	8
<i>Yu. V. Vassilevski</i>	8
<i>V. V. Voevodin</i>	8

Section 1. NUMERICAL METHODS OF SOLVING DIFFERENTIAL AND INTEGRAL EQUATIONS

<i>A.A. Belozеров, E.I. Romenski, I.M. Peshkov</i>	10
<i>I.A. Blatov, U.I. Shustikova</i>	10
<i>V.V. Churuksaeva, A.V. Starchenko</i>	10
<i>S.V. Gaidomak</i>	10
<i>V.N. Grebenev, A.N. Grishkov, M. Oberlack</i>	11
<i>G.M. Kenenbaeva</i>	11
<i>V. M. Kovenya</i>	11
<i>O.A. Kovyrykina, A.N. Kudryavtsev,</i> <i>V.V. Ostapenko</i>	12
<i>N.G. Marchuk</i>	12
<i>S.B. Medvedev</i>	12
<i>G. V. Muratova, L. A. Krukier, E.M. Andreeva</i>	12
<i>E. A. Novikov, A. E. Novikov</i>	12
<i>V.A. Rukavishnikov, S.G. Nikolaev</i>	13
<i>G.I. Shishkin (Invited talk)</i>	13
<i>T.A. Сушкевич (Invited talk)</i>	13
<i>L.P. Shishkina, G.I. Shishkin</i>	14
<i>S.V. Tikhovskaya, A.I. Zadorin</i>	14
<i>V.V. Uchaikin (Invited talk)</i>	15
<i>P.N. Vabishchevich (Invited talk)</i>	15

<i>A.V. Vyatkin, V.V. Shaydurov</i>	15
<i>V.P. Zhitnikov, N.M. Sherykhalina,</i> <i>R.R. Muksimova</i>	16

Section 2. ALGEBRA AND APPROXIMATION

<i>D.S. Butyugin, Y.L. Gurieva, V.P. Il'in,</i> <i>A.V. Petukhov, D.V. Perevozkin (Invited talk)</i>	17
<i>V. Druskin, S. Güttel, L. Knizhnerman</i> (Invited talk)	17
<i>В.Г. Гасенко</i>	17
<i>V.P. Golubyatnikov</i>	18
<i>Y.L. Gurieva</i>	18
<i>A. Kalinkin, A.Anders, R. Anders</i>	18
<i>A. Kalinkin, N.Shustrov, A.Anders, R. Anders</i>	19
<i>A.I. Kulikov</i>	19
<i>A.I. Kulikov, A.A. Kopylov</i>	19
<i>S.V. Kuznetsov, N. Mozartova</i>	20
<i>B. I. Kvasov</i>	20
<i>V.L. Miroshnichenko (Invited talk)</i>	20
<i>P.V. Mokshin, A.I. Rozhenko</i>	20
<i>N.S. Mozartova, A.A. Zotkevich</i>	21
<i>E.I. Pak, V.P. Ilin</i>	21
<i>D.V. Perevozkin</i>	21
<i>A.V. Petukhov</i>	21
<i>A.S. Popov</i>	22
<i>S.S. Primakov</i>	22
<i>S. G.Pudov</i>	22
<i>S.P. Shary</i>	22
<i>B.M. Shumilov (Invited talk)</i>	23
<i>S.A. Solovyev</i>	23
<i>S.A. Solovyev, S.Tordeux</i>	23
<i>S.I. Solov'ev</i>	23
<i>N.A. Strelkov</i>	24
<i>Yu.N. Subbotin</i>	24
<i>Yu.S. Volkov (Invited talk)</i>	24
<i>A.I. Zadorin, N.A. Zadorin (Invited talk)</i>	25
<i>V. G. Cherednichenko</i>	25

Section 3. MONTE CARLO METHODS

<i>A.Yu. Ambos</i>	26
<i>V.S. Antyufeev</i>	26
<i>S.S.Artemiev, V.D.Korneev (Invited talk)</i>	26
<i>T.A. Averina</i>	26
<i>A.V. Burmistrov, M.A. Korotchenko</i>	27
<i>S.A. Gusev</i>	27
<i>E. G. Kablukova, B. A. Kargin, A. A. Lisenko</i>	27
<i>N.A. Kargapolova</i>	27
<i>B.Yu. Lemeshko (Invited talk)</i>	28

<i>E. N. Akimova, A. F. Miniakhmetova,</i>		<i>R.G. Biyashev, S.E. Nyssanbayeva</i>	65
<i>V. E. Misilov</i>	53	<i>F.N. Boris, E.A. Boris</i>	65
<i>Yu.E. Anikonov (Invited talk)</i>	53	<i>V.S. Gorbunov, V.V. Korneev., L.K. Eismont</i>	65
<i>A.H. Begmatov, G. M. Djaykov</i>	53	<i>M.N. Kalimoldayev, A.A. Abdildayeva,</i>	
<i>A.H. Begmatov, A.O. Pirimbetov,</i>		<i>T. Duzbayev (Invited talk)</i>	66
<i>A.K. Seidullaev</i>	53	<i>D.S. Legkiy, V.K. Popkov</i>	66
<i>O.V. Belai, L.L. Frumin, E.V. Podivilov,</i>		<i>B.G. Mikhailenko, B.M. Glinskiy, N.V. Kuchin,</i>	
<i>D.A. Shapiro (Invited talk)</i>	54	<i>I.G. Chernykh (Invited talk)</i>	67
<i>V.S. Belonosov, A.V. Belonosova (Invited talk)</i>	54	<i>Д.А. Митченко, А.Т. Ахмедиярова</i>	67
<i>A.N. Bondarenko, V.A. Dedok</i>	54	<i>O.G. Monakhov, E.A. Monakhova</i>	67
<i>A.L. Bukhgeym (Invited talk)</i>	54	<i>Z.N. Murzabekov</i>	68
<i>I.G. Chernykh, D.A. Voronov (Invited talk)</i>	54	<i>K.A. Nechupaeva</i>	68
<i>E.V. Dementyeva, E.D. Karepova</i>	55	<i>B.K. Попков (Invited talk)</i>	68
<i>A.O. Egorshin (Invited talk)</i>	55	<i>G.V. Popkov</i>	69
<i>M.R. Enikeev, M.A. Maleeva, I.M. Gubaydullin</i>	55	<i>A.S. Rodionov</i>	69
<i>L.V. Enikeeva, G.A. Tlyavsina</i>	56	<i>V.V. Shakhov</i>	70
<i>V.A. Galatenko, S.V. Samborskij, N.I. Viukova</i>	56	<i>O.D. Sokolova</i>	70
<i>E.V. Gubiy, V.I. Zorkaltsev, I.I. Khazheev</i>	56	<i>T.A. Сушкевич, С.А. Стрелков, С.В. Максакова</i>	
<i>S.I. Kabanikhin</i>	57	<i>(Invited talk)</i>	70
<i>S.I. Kabanikhin, K.S. Boboev, O.I. Krivorotko,</i>		<i>G.Y. Toktoshov</i>	71
<i>N.Y. Zyatkov</i>	57	<i>T.F. Valeev, F.A. Kolpakov</i>	71
<i>S.I. Kabanikhin, O.I. Krivorotko</i>	57	<i>V.I. Znak</i>	71
<i>A.A. Kabidoldanova</i>	57		
<i>A.L. Karchevsky, L.A. Nazarov, L.A. Nazarova</i>		Section 9. MATHEMATICAL MODELING	
<i>(Invited talk)</i>	58	<i>Sh.A. Aiparov</i>	73
<i>I.G. Kazantsev</i>	58	<i>S.N. Astrakov, S.K. Golushko</i>	73
<i>I.G. Kazantsev, V.P. Pyatkin, V.V. Kovalevsky,</i>		<i>I.B. Badriev</i>	73
<i>L.P. Braginskaya, D.A. Karavayev (Invited talk)</i>	58	<i>I.B. Badriev, V.V. Banderov, M.V. Makarov,</i>	
<i>V.A. Kochnev</i>	58	<i>V.N. Paymushin</i>	74
<i>S.I. Kolesnikova</i>	59	<i>V. Belolipetskii, S. Genova (Invited talk)</i>	74
<i>O.A. Lyakhov</i>	59	<i>A.M. Blokhin, S.K. Golushko, B.V. Semisalov</i>	74
<i>B.G. Mukanova, S.D. Maussumbekova</i>	59	<i>Yu. O. Bobreneva, A.V. Novichkova,</i>	
<i>A.N. Rogalyov</i>	60	<i>I.M. Gubaydullin, K. F. Koledina</i>	74
<i>B. Rysbaiuly</i>	60	<i>V.J. Chebakova, M.N. Schneider,</i>	
<i>G.A. Samigulina, A.M. Abdenova, D.B. Akpan</i>	61	<i>V.S. Zheltukhin</i>	75
<i>A.A. Sedipkov</i>	61	<i>G.G. Chernykh, A.G. Demenkov, O.A. Druzhinin,</i>	
<i>M.A. Shishlenin (Invited talk)</i>	61	<i>A.V. Fomina, B.B. Ilyushin, N. P. Moshkin,</i>	
<i>A.S. Strekalovsky</i>	61	<i>O.F. Voropayeva (Invited talk)</i>	75
<i>E.V. Tabarintseva</i>	62	<i>T.G. Darmaev</i>	75
<i>V.P. Tanana, A.A. Ershova (Erygina)</i>		<i>V.V. Denisenko (Invited talk)</i>	76
<i>(Invited talk)</i>	62	<i>V.V. Denisenko, V.A. Kolovskii</i>	76
<i>P.N. Vabishchevich, V.I. Vasilyev, M.V. Vasilyeva</i>		<i>V.I. Dmitriev, M.S. Kruglyakov</i>	76
<i>(Invited talk)</i>	62	<i>P.A. Domnikov, Yu.I. Koshkina</i>	76
<i>G.I. Zabinyako (Invited talk)</i>	63	<i>T.Б. Дүйшеналиев, И. Козубай</i>	77
<i>V.I. Zorkaltsev (Invited talk)</i>	63	<i>A.V. Eliseev, I.I. Mokhov, A.V. Chernokulsky</i>	
<i>V.I. Zorkaltsev, S.M. Perzabinsky</i>	63	<i>(Invited talk)</i>	77
		<i>A.R. Enikeev, M.A. Maleeva</i>	77
Section 8. INFORMATION		<i>L.V. Enikeeva, I.M. Gubaydullin,</i>	
AND COMPUTING SYSTEMS		<i>N.F. Murzaheva</i>	78
<i>M.P. Bakulina</i>	65	<i>M.I. Eпов, E.P. Shurina, N.V. Shtabel,</i>	
<i>T.V. Batura, N.S. Kopylova, F.A. Murzin,</i>		<i>E.I. Mikhailova (Invited talk)</i>	78
<i>A.V. Proskuryakov</i>	65	<i>A.M. Fedotov, S.G. Lomakin (Invited talk)</i>	78

<i>Z.I. Fedotova, G.S. Khakimzyanov</i>	78	<i>N.I. Gorbenko</i>	90
<i>В.Г. Гасенко</i>	79	<i>M. Gorodnichev, S. Vaycel</i>	90
<i>S.R. Grechkin-Pogrebnyakov, I.K. Marchevsky</i>	79	<i>L.V. Gorodnyaya</i>	91
<i>Yu.G. Gubarev, A.A. Gubkin</i>	79	<i>Yu.N. Grigoryev, A.G. Gorobchuk</i>	91
<i>V. Ivanov</i>	80	<i>V.V. Gubarev, M.S. Khairtdinov, N.V. Abalov,</i>	
<i>M.N. Kalimoldayev, G.A. Amir Khanova</i>	80	<i>O.K. Alsova, T.V. Tairov, G.A. Melnikov</i>	91
<i>D.V. Khotyanovsky, A.N. Kudryavtsev</i>	80	<i>O.I. Gusev</i>	92
<i>V.N. Korchagova, I.K. Marchevsky,</i>		<i>V.P. Ilin, N.V. Panchenko</i>	92
<i>I.Yu. Savelyeva</i>	81	<i>A.I. Ilyin, S.I. Kabanikhin, D.A. Voronov</i>	92
<i>S.B. Kuznetsov</i>	81	<i>Kh.Kh. Imomnazarov, A. A. Mikhailov</i>	92
<i>V.Ya. Modorsky, P.V. Pisarev</i>	81	<i>N.B. Itkina, S.I. Markov</i>	93
<i>V.Ya. Modorsky, A.F. Shmakov</i>	81	<i>A.A. Ivanov</i>	93
<i>L.F. Nurislamova, O.P. Stoyanovskaya,</i>		<i>V. Ivanov, Yu. Kulikov</i>	93
<i>N.M. Bainazarova, O.A. Stadnichenko,</i>		<i>E.G. Kablukova, B.A. Kargin</i>	94
<i>I.M. Gubaydullin, V.N. Snytnikov</i>	82	<i>K.V. Kalgin</i>	94
<i>V.V. Okolnishnikov, S.V. Rudometov,</i>		<i>K.V. Kalgin, S.E. Kireev</i>	94
<i>S.S. Zhuravlev</i>	82	<i>L.P. Kamenshchikov, I.V. Krasnov</i>	95
<i>M.G. Persova, Y.G. Soloveichik, D.V. Vagin,</i>		<i>D.A. Karavaev</i>	95
<i>T.B. Epanchintseva, O.S. Trubacheva</i>	82	<i>E.D. Karepova, A.A. Efremov, A.V. Vyatkin</i>	95
<i>D.O. Pimanov, S.I. Fadeev, E.G. Kostsov</i>	82	<i>S.G. Kazantsev</i>	95
<i>V.V. Puzikova, I.K. Marchevsky</i>	83	<i>S.E. Kireev, V.Yu. Komarov</i>	96
<i>M.E. Royak, I.M. Stupakov</i>	83	<i>A.E. Kireeva</i>	96
<i>E.S. Sherina</i>	83	<i>E.O. Kondrashkin</i>	96
<i>A.V. Snytnikov</i>	84	<i>V.D.V. Konovalova, V.V. Kovalevsky, A.S.</i>	
<i>O. A. Tkachenko, V. A. Tkachenko</i>	84	<i>Belonosov</i>	96
<i>S.I. Trashkeev, R.V. Galev, A.N. Kudryavtsev</i>		<i>D. Korneev, V.M. Sveshnikov, I.A. Klimonov</i>	97
(Invited talk)	84	<i>L.A. Korolenko, S.N. Astrakov</i>	97
<i>Yu.M. Volchkov, I.O. Bogulskii</i> (Invited talk)	84	<i>N.S. Kosminova, I.M. Stupakov</i>	97
<i>T. Yuldashev</i>	84	<i>A.N. Kozyrev, V.M. Sveshnikov</i>	97
		<i>V.V. Kravtchenko, V.I. Kuzin</i>	98
POSTERS		<i>I.A. Kremer</i>	98
<i>I.V. Afanasyev</i>	85	<i>A.I. Kulikov, A.A. Alyabushev, S.G. Levin</i>	98
<i>V.V. Aksenov</i>	85	<i>I.M. Kulikov</i>	99
<i>V.T. Astrelin, I.V. Kandaurov, V.M. Sveshnikov</i>	85	<i>A.T. Kussainova, A.V. Penenko</i>	99
<i>N.B. Аурова</i>	85	<i>G.G. Lazareva</i>	99
<i>C.A. Бельгинова, С.Ж. Рахметуллина,</i>		<i>A.I. Levykin</i>	99
<i>A.T. Кусаинова</i>	86	<i>A.A. Lezhenin, V.F. Raputa, V.A. Shlychkov,</i>	
<i>E.A. Berendeev, A.A. Efimova</i>	86	<i>T.V. Yaroslavtseva</i>	100
<i>M.A. Boronina, V.D. Korneev, V.A. Vshivkov</i>	86	<i>Y. Likhanova, S.B. Medvedev, M.P. Fedoruk,</i>	
<i>L.P. Braginskaya, A.P. Grigoruk, S.V. Kratov</i>	87	<i>P.L. Chapovsky</i>	100
<i>A.A. Buchnev, V.P. Pyatkin</i>	87	<i>T. Liseykina, D. Bauer, G. Dudnikova</i>	100
<i>Yu. A. Chirkunov, E. O. Pikmullina</i>	87	<i>V.L. Lukinov</i>	101
<i>G.A. Chumakov</i>	87	<i>O. A. Makhotkin</i>	101
<i>N.A. Chumakova, G.A. Chumakov</i>	88	<i>V.E. Malyshkin, V.A. Perepelkin</i>	101
<i>G. Dairbayeva</i>	88	<i>An. G. Marchuk, G. S. Vasiliev</i>	102
<i>G.V. Demidov, B.G. Mikhailenko,</i>		<i>T.V. Markelova, O.P. Stoyanovskaya,</i>	
<i>V.N. Martynov</i>	88	<i>V.N. Snytnikov</i>	102
<i>P.A. Domnikov</i>	89	<i>A.F. Mastryukov</i>	102
<i>P.A. Domnikov, N.V. Kondratyev</i>	89	<i>A.Г. Мезрабов</i>	102
<i>G.M. Drozdov, V.P. Shapeev</i>	89	<i>E.A. Mesyats, A.V. Snytnikov</i>	103
<i>A.A. Efimova, E.A. Berendeev</i>	89	<i>D.A. Migov</i>	103
<i>A.A. Eleuov</i>	90	<i>B.G. Mikhailenko, A.A. Mikhailov</i>	103

<i>A.V. Molchanov</i>	104	<i>V.S. Sidorova</i>	108
<i>A.N. Molchanova, A.V. Kashkovsky,</i>		<i>K.V. Simonov, S.V. Kirillova, L. Cadena</i>	109
<i>Ye.A. Bondar</i>	104	<i>D.D. Smirnov</i>	109
<i>N.S. Novikov</i>	104	<i>N.V. Snytnikov</i>	109
<i>M.B. Ostapkevich, A.N. Herega</i>	105	<i>T.V. Snytnikova, G.I. Dudnikova,</i>	
<i>V. I. Paasonen</i>	105	<i>V. A. Vshivkov</i>	110
<i>A.V. Penenko, S.J. Rakhmetullina</i>	105	<i>S.B.Sorokin</i>	110
<i>M.G. Persova, Y.G. Soloveichik, D.V. Vagin,</i>		<i>O.A. Stadnichenko, V.N. Snytnikov,</i>	
<i>V.O. Demina</i>	106	<i>Vl.N. Snytnikov</i>	111
<i>M.G. Persova, Y.G. Soloveichik, D.V. Vagin,</i>		<i>O.P. Stoyanovskaya, P.V. Snytnikov</i>	111
<i>D.S. Kiselev, Yu.I. Koshkina,</i>		<i>I.V. Surodina, I.B. Labutin</i>	111
<i>N.V. Simankovich</i>	106	<i>V.P. Tanana, A. I. Sidikova</i>	112
<i>K.K. Sabelfeld, S.A. Efremov</i>	106	<i>A.B. Terentev, S.A. Savikhin, S.A. Zolotov,</i>	
<i>A.O. Savchenko</i>	106	<i>D.E. Borisov, A.A. Pankratov, A.A. Nosov,</i>	
<i>B. V. Semisalov</i>	107	<i>A.O. Muzychenko</i>	112
<i>V.A. Sergeev</i>	107	<i>A.A. Tkacheva</i>	112
<i>V.V. Shaydurov, G.I. Shchepanovskaya,</i>		<i>M.V. Urev, M.O. Shimonaeva</i>	113
<i>M.V. Yakubovich</i>	107	<i>A.A. Vitvitsky</i>	113
<i>A.F. Shaykhnurova, G.R.Karamutdinova,</i>		<i>A. S. Volkov</i>	114
<i>I.I. Bakirov</i>	107	<i>K.V. Voronin, Y.M. Laevsky</i>	114
<i>A.A. Shershnev, A.V. Kashkovsky,</i>		<i>G.M. Voskoboynikova</i>	114
<i>A.N. Kudryavtsev</i>	108	<i>V.A. Vshivkov, V.K. Kedrinsky</i>	114
<i>A.A. Shershnev, A.N. Kudryavtsev</i>	108	<i>L.V. Vshivkova, G.I. Dudnikova, T.V. Liseykina</i>	115
		<i>A.A. Yakimenko</i>	115
		<i>M.A. Yakunin</i>	115
		<i>T.M. Zhuraev, K.D. Ismanova</i>	115

Abstracts

International conference
ADVANCED MATHEMATICS, COMPUTATIONS
AND APPLICATIONS – 2014

Тезисы Международной конференции
"Актуальные проблемы вычислительной
и прикладной математики – 2014"

Ответственные за выпуск:

В. П. Ильин, М. А. Боронина, Л. В. Вишкова

Компьютерная верстка *О. Г. Заварзина*

Подписано к печати 28.05.2014. Формат 60×84, 1/8.
Усл. печ. л. 16,8. Уч. изд. л. 14,2. Тираж 450 экз. Заказ № 137.

Отпечатано в типографии «Академиздат», 630090, Новосибирск, просп. Акад. Лаврентьева,
д. 6/1, оф. 622; тел. +7 (383) 380 65 20.