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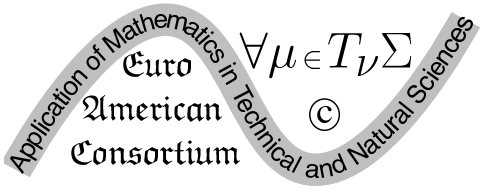
BOOK OF ABSTRACTS



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Numerical Solution of the Thermal Influence of Oil Well Cluster on Permafrost

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Currently, in the development of oil fields the cluster drilling is widely used to increase oil recovery. The exploitation of oil wells in areas of permafrost soils leads to thawing around wellbores, which could lead to serious consequences: violation of the stability of wells, subsidence of soil around wells. The cluster drilling means that wellbores are located relatively close to each other, which leads to increase of thawing area.

In this work, we study the thermal effects around the oil well cluster on permafrost using numerical modeling. We use the mathematical model of heat transfer with phase transitions. To take into account the arrangement of wells in a cluster, three-dimensional domains with complex geometry are employed, which leads to the use of finite element approximation in space. For time approximation we use fully implicit scheme with linearization of nonlinear coefficients.

Numerical implementations are performed using open-source libraries and programs for scientific and engineering computations. On the supercomputer of the North-Eastern Federal University large-scale computational experiments are conducted to predict the temperature field and formation of thawing area around wells with different sets of input parameters (construction of wells, their count, thermal properties of reservoir and oil, etc.).

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Fitted Difference Method for a Singularly Perturbed Delay Integro-Differential Equation

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In this paper we consider the singularly perturbed initial-value problem for a linear first-order Volterra integro-differential equation with delay. Our purpose is to construct and analyse a numerical method with uniform convergence in the perturbation parameter. The numerical solution of this problem is discretised using an implicit difference rules for differential part and the composite numerical quadrature rules for integral part. On a layer-adapted mesh error estimations for the approximate solution are established. Numerical examples supporting the theory are presented.

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Asymmetric Metric: Application to Dealing with Uncertainty

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The uncertainty in mathematical models often manifests as set-valued data, parameters or solutions. We propose a new approach for dealing with such uncertainty, which combines features of validated computing (wrapping the set by a set of computer representable type, e.g., intervals, zonotopes, ellipsoids) and point approximation accompanied by error analysis. More precisely, we consider approximation by a set which is not necessarily an enclosure. The mathematical theory is based on asymmetric metric, where the metric gives an estimation of the error, while the order induced by the metric provides means for estimating the size of the approximating set.

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Molecular Dynamics Simulation of the Structure and Dynamics of 5-HT3 Serotonin Receptor

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Membrane proteins play crucial role in functioning of nervous systems, which makes them an interesting object for study. Experimental study of such objects is a significant challenge, and one of possible approaches here can be using methods of computational physics for studying such objects.

In this work we focused of structure, dynamics and ion transportation in transmembrane domain of 5-HT3 Serotonin Receptor. High resolution structure (0.35 nm) structure of the 5-HT3 receptor in complex with stabilizing nanobodies was determined by protein crystallography in 2014 (PDB code 4PIR). Transmembrane domain of the structure was prepared in complex with explicit membrane environment (POPC) and solvent (water model TIP3P). Chain breaks were capped with ACE/NME residues with fixed spatial positions. Gromacs 6.3 software with Gromos-96 forcefield was used for MD simulations.

Molecular dynamics protocols for simulation and stabilization of the transmembrane domain of 5-HT3 receptor model were developed and 60 ns simulation of the structure were conducted in order to explore structural parameters of the system. We estimate the mean force profile for Na+ and K+ ions using umbrella sampling method and compare resulting profiles for various initial conditions of the system.

Acknowledgements: All simulations were performed using "Arian Kuzmin" supercomputer center of M.K.Ammosov North-Eastern Federal University, the work was supported by the Sakha Scientific Educational Support Foundation for the Junior Scientists (Grant 2014-01-0008) and the Ministry of Education and Science of Russian Federation.

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A Comparative Analysis of Goodwin's Business Cycle Models with Continuously Distributed Lags

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The well-known Goodwin nonlinear models of business cycle [1], can be represented in the form of integral-differential equation

$$\varepsilon\dot{Y}(t) + (1-\alpha)Y(t) = \langle\varphi(\dot{Y}(t))\rangle + \mathrm{I}_a(t). \tag{1}$$

Here $Y(t)$ is income, $\mathrm{I}_a(t)$ is autonomous investment, $\varphi(\dot{Y}(t))$ is nonlinear Goodwin's accelerator, t is time, $\varepsilon > 0$ and $\theta > 0$ are the time-lag of the dynamic multiplier delay and the time-lag between the investment decisions and the resulting outlays, α is the marginal propensity to consume, $0 \le \alpha \le 1$,

$$\langle g\rangle = \int\limits_{-\infty}^{\infty} w(s,t)g(s)ds$$

and $w(s,t$ is the weighting function,

$$w(s,t) \ge 0, \quad \int\limits_{-\infty}^{\infty} w(s,t)ds = 1.$$

Matsumoto ([2], [3]) consider the another form of Goodwin's business cycle model

$$\varepsilon\dot{Y}(t) + (1-\alpha)Y(t) = \varphi(\langle\dot{Y}(t)\rangle) + \mathrm{I}_a(t). \tag{2}$$

It can be shown, that for

$$w(t,s) = \theta^{-1}\exp\left(-\frac{t-s}{\theta}\right),$$

both models (1) and (2) reduce to the second-order ODE systems and they have a limit cycles if $\varphi'(0) > \varepsilon + (1-\alpha)\theta$.

But the parameters of these limit cycles can differ greatly. In this paper, we compares in detail the time behavior of income $Y(t)$ for the business cycle models (1) and (2).

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Hierarchy of Bases for Serendipity Finite Element with the Biquadratic Interpolation

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Recently the interpolation bases of the hierarchical type have been used for the problem solving of the approximation of multiple arguments functions (such as in the finite-element method). The bases of the hierarchical type are effectively used in the adaptive refinement procedures, which are based on the posteriori error estimates for the finite-element solution. When using hierarchical finite-elements (FE), it is easy to add a multiple element locally, in order to make an adjustment in the area, where the searched function changes very quickly; and the approximation can produce great errors. Nowadays the mostly developed questions are the ones of the building of hierarchical bases on one-dimensional and three-angled FEs. But there is very little information about the hierarchy of the models on serendipity finite elements (SFE) in the famous monographs; and only the standard type bases are given. The great interest is aroused in learning of the possibility of increasing

of the degree of serendipity polynomials by means of introducing of new terms by the fixed number of nodes of the interpolation. It is clear that the common method of the inverse matrix does not fit in this case, and the new innovative approaches are needed.

In this work the cognitive graphical method of constructing of the hierarchical form bases on the serendipity finite elements is suggested, which allowed to get the alternative bases on a biquadratic finite element from the serendipity family without internal knots' including. The modified bases on SFE-8 have nine parameters in the interpolation polynomial: one "hidden" parameter is added to the standard polynomial, whose presence provides the endless number of infinite bases on this item. The cognitive-graphic method allowed to improve the known interpolation procedure of Taylor and to get the modified elements with irregular arrangement of knots.

The study of the influence of the "hidden"parameters on the quality of the approximation arouses the interest itself, that is why the tests of the alternative bases of the biquadratic serendipity finite element were performed while solving problems of the elliptic type. It was proved that on the biquadratic SFEs the best computational abilities belong to the basis, by which the stiffness matrix has a minimum trace. The proposed procedures are universal and are spread in the area of FE.

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Super-Solitons and Mixed Solutions for Defocusing Super-Gardner Equation

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Applying the Hirota super-bilinear formalism we discuss the supersymmetric version of defocusing Gardner equation. After constructing the super-solitons, we notice that in some conditions the equation under consideration admits super-shock wave solutions. We also build a mixed solution containing one super-soliton and one super-shock and analyse its dynamics. The integrability of defocusing super-Gardner equation is also discussed.

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A New Alignment-Free Method of Comparison of DNA Sequences

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A new alignment-free method of comparison of DNA sequences called by us 2D-dynamic Representation of DNA Sequences is presented [1-4]. 2D-dynamic representation is based on a method known in the literature as Nandy plots but it removes the degeneracy (non-uniqueness) of the Nandy Plots. The method is computationally not demanding and there are no limitations on the lengths of the DNA sequences. In this presentation the way of construction of the 2Ddynamic graphs and their numerical representations are shown. Some numerical examples are also presented.

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Computer Technologies of Mathematical Modeling of Complex Hydrogeological Environment

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Information modeling of complex ecological condition of geological environment is actual task for today. The aim is designing and theoretical foundation of computer technology based on high-resistant integral-approximation algorithms for simulation of dynamic processes in heterogeneous environments.

The feature is the construction of information and mathematical models that possess optimal properties for the accuracy, information complexity and non-saturation, the class of algorithms that can be attributed to the predictive modeling and computational intelligence. It is important to avoid the phenomenon of "explosion of errors" in solving problems in heterogeneous environments in large and endless fields. Developed algorithmic application software support information analysis and forecasting of heofiltration environments, based on a mathematical model based on a system of equations that describe the routine transient groundwater flow in interconnected aquifers. The algorithm of modeling hydrogeological processes are applied in the use of the monitoring of the ecological state of groundwater, determine the regime of flooding and contamination areas and anthropogenic processes optimization to maintain the ecological balance of aquatic ecosystems.

A software-modeling system for forecasting hydrological regime of industrial and industrial areas, including processes of hazard removal of contaminated water into the geological environment.

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Finding Discrete Structures via Problem Dependent Optimization

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Various discrete structures such as Designs, Packings, Coverings and Partitions are studied as both pure mathematical objects with certain extremal properties, and also as objects having applications in areas such as Computer Science, Statistics,

Coding Theory and Cryptography. In this presentation I talk about the exploitation of a recently published optimization method, Problem Dependent Optimization (PDO), in finding such objects.

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Advanced Numerical Methods in Finance for Black-Scholes Model

Z. Bučkova, M. Ehrhardt, M. Günther

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The talk focuses on advanced numerical methods for linear and nonlinear Black-Scholes models. We point out challenges posed by nonlinear and higher-dimensional models and suggest novel methods for efficient numerical solutions. We focus on implementation and numerical analysis of finite difference methods for parabolic partial differential equations. We deal with the Alternating direction explicit methods.

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Traditional vs. Trefftz Difference Schemes for the Black-Scholes Equation

Z. Bučkova, M. Ehrhardt, I. Tsukerman

University of Wuppertal, Germany

We explore applications of Trefftz finite difference (FD) schemes to the linear Black-Scholes model. This model involves a parabolic partial differential equation, which is used in finance applications for option pricing. The solution of this equation is the price of the European call/put option for each asset price as a function of time. The initial condition is the payoff of the option. Trefftz schemes, also known as FLAME (the Flexible Local Approximation Method), have previously been applied to problems in wave propagation, electro- and magnetostatics, for generating absorbing boundary conditions - but not to computational finance. FLAME relies on accurate local approximations of the underlying equation – typically, by Trefftz functions, which by definition satisfy this equation exactly in

a (small) subdomain around FD stencil nodes. Examples of such functions are the exponential discount factor or functions expressed via the Black-Scholes formula. We compare FLAME with more traditional explicit and implicit FD schemes – FD methods, such as Alternating direction explicit (ADE) schemes and Crank-Nicolson.

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Stability of Vortex Filaments

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The Vortex Filament Equation (VFE), a model for the self-induced motion of a vortex filament in an ideal fluid, is a simple but important example of integrable geometric evolution equation for space curves. Its connection with the cubing focusing Nonlinear Schrödinger (NLS) equation through the well-known Hasimoto map allows the use of tools of integrable systems to construct and investigate finite-gap and soliton solutions. I will discuss linear and nonlinear stability properties of some of these solutions, including filaments in the shape of torus knots and solitons on vortex filaments.

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Analysis of Oscillation Processes in a Blocky Medium by Means of Discrete and Continuous models

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Oscillation processes in a blocky medium are investigated. A discrete model of transverse-rotational oscillations in the monoatomic Bravais lattice with different boundary conditions is considered. Using this model, the analysis of resonant frequencies is conducted. To study the behavior of the system in the resonant frequency neighborhood and to examine amplitude vector alteration, spectral portraits are constructed. It is shown that there is one specific frequency of rotational motion that does not depend on the amount of particles in the chain. This result

corresponds with resonant properties of the Cosserat continuum, where a similar frequency exists; it is related to rotational motion of elements, too, and does not depend on the area size and type of boundary conditions.

Further analysis of oscillatory processes is fulfilled using the models of a blocky medium, where elastic blocks interact via interlayers with different properties. To describe these processes, three different models are applied. First is the Hook model, which consider elastic interaction between blocks, second one is the viscoelastic Pointing-Thomson model, that combines both the Maxwell and Kelvin-Voigt models, and third one is the model with rigid contact, which excludes a possibility of blocks interpenetration. The dissipationless Ivanov scheme is applied in interlayers, while in blocks the Godunov gap decay scheme is used. It is shown that additional enclosing equations, which guarantee absence of energy dissipation in the Ivanov scheme, provide thermodynamic consistency of the model. It means that the difference analogue of energy conservation law for blocky structures is performed. Using MPI technology, a parallel software is designed for the imitation of elastic waves in two-dimensional blocky medium with interlayers, related to the mentioned models.

Acknowledgement: This work was supported by the Complex Fundamental Research Program no. 18 of the Presidium of RAS and the Russian Foundation for Basic Research (grant no. 14-01-00130).

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On-axis Electromagnetic Scattering from a Sub-Wavelength Aperture on a Conducting Screen

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Closed-form analytic expressions for the on-axis scattered fields by a sub-wavelength circular aperture on an infinite perfectly conducting plane were derived using a vector potential formulation and the equivalence principle. The obtained expressions are valid and accurate for the near-field, intermediate-field, and far-field zones. An electromagnetic plane wave of arbitrary polarization is incident on the aperture at an angle with respect to the normal and the observation is taken along the axis of the aperture. The underlined formulation begins with the equivalent quasi-static magnetic current distributions in the aperture, which were

derived by Bethe and Bouwkamp in the mid 40's and early 50's. By implementing the equivalence principle and image theory, the on-axis scattered electric and magnetic fields by the aperture were formulated in terms of the electric vector potential to derive expressions in the form of a double integral over the surface of the aperture. These integrals, which involve the free-space Green's function, were evaluated analytically after introducing Taylor series expansion and using a series of transformations. The final closed-form expressions of the scattered fields are given in terms of a recursion formula. Obtained results based on these closed-form expressions are compared with data generated by a numerical integration scheme. The two sets of data are in excellent agreement, thus validating the formulation and obtained closed-form expressions.

Keywords: Electromagnetic scattering, sub-wavelength aperture, wave diffraction, electric vector potential formulation

PACS: 41.20.Jb, 42.25.Bs, 42.25.Fx

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Thermo-Acoustic Waves in Rarefied Gas between Two Coaxial Cylinders in the Temperature Suddenly Change of the Outer Cylinder

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The heat transfer in a monatomic rarefied gas between two stationary concentric cylinders in the case of suddenly change outer wall temperature is studied. Based on the developed in previous publications Navier-Stokes-Fourier (NSF) model and Direct Simulation Monte Carlo (DSMC) method and their numerical solutions, are considered non-stationary transients process in the gas phase. Different cases were calculated for a set of radius and temperatures of outer cylinder. On the wall of the inner cylinder are used two types of thermal boundary conditions - constant temperature and adiabatic isolated inner cylinder. The study aims to determine effect of arising waves on the gas macro characteristics (density, temperature and pressure) and in the case of adiabatic isolated case the inner wall temperature variation.

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The Inexact Uzawa – Conjugate Gradient Method for the Stokes Problem for Incompressible Fluid

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In the present talk the two-dimensional Stokes equations are considered for a viscous incompressible fluid in a channel. At the inlet boundary a flow is assumed to be given, besides, we impose the no-slip condition at the rigid boundary and the modified "do nothing" boundary condition at the outlet boundary.

To construct a discrete problem, we use the Taylor-Hood finite elements on rectangles: the biquadratic elements for the velocity components and the bilinear elements for the pressure. These elements satisfy the Ladyzhenskaya-Babuska-Brezzi condition that ensures the pressure stability.

As a result, we obtain a system of linear algebraic equations that corresponds to a classical saddle point problem. A solution of this system is calculated by a modified inexact Uzawa - conjugate gradient method which is widely used in numerical analysis for a saddle point system. Usually the method is considered with respect to velocity-pressure unknowns. In our modification we formulate the problem in terms of velocity-pressure deviations from the desired saddle point of the discrete problem. This substitution does not affect on the result provided that we use a linear iterative process. However, the numerical efficiency is considerably improved when we use the non-linear conjugate gradient method for the calculation of the Shur operator and its image. The number of external iteration steps as well as of internal ones (with respect to the Shur operator and its image, respectively) is a parameter of the iterative process. In the case that both these parameters equal one, the iterative process becomes the gradient descent method. With exact calculations, the approach gives the exact solution provided that the number of internal iteration steps and the number of external ones coincide with the dimension of the velocity and of the pressure, respectively.

Numerical experiments show convergence and good efficiency of the method.

Acknowledgement: The work was supported by Russian Science Foundation (grant 14-11-00147).

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Numerical Approach of an Optimal Control Problem for a Diffusive Ecosystem with Two Competing Preys and One Predator

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In this work, we consider the numerical approach of an optimal control problem introduced in [2], related to a diffusive ecosystem composed of one predator population of density y_2, and two competing prey populations, whose densities are y_1 and y_3. The three densities y_1, y_2, y_3 depend on the time $t \in [0,T]$ and on the spatial position $x \in \Omega$. Here Ω is a bounded domain in $\mathbb{R}^p$ $(p \geq 1)$ with the boundary $\partial\Omega$ smooth enough. The interaction of the two competing prey species are of Lotka-Volterra type, while the predator functional response is of Beddington De Angelis type. A similar optimal control problem involving the classical functional responses (such as Holling type I-IV) was analyzed both theoretically and numerically in [1].

A control u is introduced in this ecosystem, which can be interpreted as a stimulant for the prey populations by enhancing their densities. Assume that this enhancement is proportional to the density of each prey population. The proportionality factor u can be seen as a control variable and it is supposed to vary inside a finite interval $[0,1]$. Denoting $Q_T = \Omega \times (0,T)$, the admissible control set is defined as

$$\mathcal{U} = \left\{ u \in L^2(Q_T) \,:\, 0 \leq u(x,t) \leq 1 \quad \text{a.e. in } Q_T \right\}.$$

Our goal is to maximize a certain weighted density of the three populations on Q_T and a weighted density on Ω at the end of the time interval $[0,T]$. More exactly, the optimal control problem can be formulated as

$$\min_{u \in \mathcal{U}} \Phi(y,u) \quad \text{with} \quad \Phi(y,u) = -\int_{Q_T} (k_1 y_1 + k_2 y_2 + k_3 y_3)(x,t)\, dx\, dt, \\ -\int_{\Omega} (\ell_1 y_1 + \ell_2 y_2 + \ell_3 y_3)(x,T)\, dx$$

where $k_i, \ell_i > 0$ are given weights $(i = 1,2,3)$, while $y = (y_1, y_2, y_3)$ is the solution

of the controlled system:

$$\begin{cases} \dfrac{\partial y_1}{\partial t} = \alpha_1 \Delta y_1 + y_1 \left(u + a_1 - y_1 - b_1 y_3 - \dfrac{c_1 y_2}{1 + y_1 + d_1 y_2} \right), & \text{in } Q_T, \\ \dfrac{\partial y_2}{\partial t} = \alpha_2 \Delta y_2 + y_2 \left(\dfrac{e_1 y_1}{1 + y_1 + d_1 y_2} + \dfrac{e_2 y_3}{1 + y_3 + d_2 y_2} - d \right), & \text{in } Q_T, \\ \dfrac{\partial y_3}{\partial t} = \alpha_3 \Delta y_3 + y_3 \left(u + a_2 - b_2 y_1 - y_3 - \dfrac{c_2 y_2}{1 + y_3 + d_2 y_2} \right), & \text{in } Q_T, \end{cases}$$

for $(x,t) \in Q_T$, subject to homogeneous Neumann boundary conditions (i.e., the environment is isolated)

$$\frac{\partial y_i}{\partial \nu} = 0 \text{ on } \Sigma_T = \partial\Omega \times [0,T],\ i = 1,2,3$$

and to the initial conditions

$$y_i(x,0) = y_i^0(x) > 0, \quad x \in \Omega,\ i = 1,2,3.$$

The parameters α_i $(i = 1,2,3)$, a_j, b_j, c_j, d_j, e_j $(j = 1,2)$ and d are all positive constants. Using the theoretical results established in [2] – optimality conditions, bang-bang form of the optimal control – we construct and implement the optimization algorithm. Results of the numerical simulations are presented.

Acknowledgement: This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS–UEFISCDI, project number PN-II-ID-PCE-2011-3-0563, contract no. 343/5.10.2011 "Models from medicine and biology: mathematical and numerical insights".

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Functional Analysis of Recoverability from Discrete Presented Continuous Dependence

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There is discussed the recovery conditions of continuous image from a discrete representation. Discrete representation is in a network of model elements located on Riemannian differentiable manifold.

Method is applied similar to "functional stability analysis" method, which is applied to detect instability in numerical algorithms. This method has several key definitions. In the common theory of sensibility for computing problems are used valuations for precision. If the data in X are with permissible relative error ε and the data in Y are with permissible absolute error δ, then if norm of gradient function F, multiplied by the ε not exceed δ, the continuous function F discrete presenting with model elements can be recovered.

For optimal evaluation of the dependencies represented differentiable manifold, the symmetry group is determined.

Keywords: Optimal modeling, recoverability of image, local density of model elements, half-logarithmic derivative function

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Numerical Solution of The PTC Thermistor Problem with a Modified Electrical Conductivity

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This paper presents the numerical solution of the one-dimensional PTC thermistor with a modified electrical conductivity. The partial differential equation model is solved using the method of lines. Results are presented to show temperature evolutions and time dependent temperature response in all the phases. Results obtained when compared with exact steady state solution indicate that the method is suitable for the solution of the PTC thermistor problem.

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Numerical Models of Ion-acoustic Collisionless Shock

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The self-consistent evolution of an ion-acoustic collisionless shock with shock-reflected ions is studied numerically with kinetic simulations.

The results of one-dimensional fully kinetic simulations for both plasma component with the real ion-to-electron mass ratio are compared with those obtained for two different forms of electron density distribution in terms of the wave electrostatic potential. One distribution corresponds to the Boltzmannian electrons, the other – to the adiabatically trapped electrons.

Acknowledgement: The research was supported by the Russian Science Foundation (RSF) under Grant 16-11-10028.

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Stochastic Generation of Spatial Patterns in Brusselator

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Spatial-temporal model of Brusselator under stochastic disturbances is considered. In the deterministic case, spatial patterns in the zone of Turing instability in dependence on boundary conditions are investigated. For the quantitative analysis of these structures, a dispersion is used. Zones of multistability in which spatial-temporal patterns depend on initial conditions are found. In the stochastic case, a phenomenon of patterns generation in the zone of stable homogeneous steady state are studied. Application to population models are discussed.

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A Universal Framework for Non-deteriorating Time-domain Numerical Algorithms in Maxwell's Electrodynamics

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We present the implementation of the Lacuna method, that removes a key difficulty that currently hampers many existing methods for computing unsteady electromagnetic waves on unbounded regions. Numerical accuracy and/or stability may deteriorate over long times due to the treatment of artificial outer boundaries. We describe a developed universal algorithm and software that correct this problem by employing the Huygens' principle and lacunae of Maxwell's equations.

The algorithm provides a temporally uniform guaranteed error bound (no deterioration at all), and the software will enable robust electromagnetic simulations in a high-performance computing environment. The methodology applies to any geometry, any scheme, and any boundary condition. It eliminates the long-time deterioration regardless of its origin and how it manifests itself. In restrospect, the lacunae method was first proposed by V. Ryaben'kii and subsequently developed by S. Tsynkov.

We have completed development of an innovative numerical methodology for high fidelity error-controlled modeling of a broad variety of electromagnetic and other wave phenomena. Proof-of-concept 3D computations have been conducted that convincingly demonstrate the feasibility and efficiency of the proposed approach. Our algorithms are being implemented as robust commercial software tools in a standalone module to be combined with existing numerical schemes in several widely used computational electromagnetic codes.

Acknowledgement: Work supported by the US Army Phase II STTR contract W911NF-14-C-0161; Program manager Dr. Joe Myers.

Subject Terms: Unsteady electromagnetic waves; Maxwell's equations; unbounded regions; (grid) truncation; artificial outer boundaries; artificial boundary conditions (ABCs); non-reflecting boundaries; perfectly matched layer (PML); long-time deterioration; loss of accuracy, loss of stability, error build-up; the Huygens' principle, aft fronts of the waves; lacunae of the solutions; quasi-lacunae; accumulation of charge; guaranteed accuracy; temporally uniform error bounds

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Characterization of Perfluorinated Cation-Exchange Membranes MF-4SC Surface Modified with Halloysite Nanotubes

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The electro-conductivity and diffusion permeability through perfluorinated cation-exchange membranes MF-4SC (Russian analogue of Nafion-type membrane), whose surface is modified by nanotubes of halloysite using short exposures of a low temperature microwave plasma, is theoretically investigated using the Nernst-Planck approach. The method of quantitative evaluation of physicochemical parameters (individual and averaged diffusion coefficients and averaged distribution coefficients of ion pairs in the membrane) of the systems 'electrolyte solution – bi-layer ion-exchange membrane – water/electrolyte solution', which was proposed by us earlier, is further developed. The mentioned parameters of modified membranes on the base of MF-4SC and nanotubes of halloysite are obtained from both experimental data on electroconductivity and diffusion permeability for different concentration of NaCl and HCl solutions using theoretical calculations by the help of least squares method. New model of bi-layer membrane system can be used for refining calculated results with taking into account both diffusive layers. It is shown that grafting the layer of halloysite nanotubes onto the membrane surface noticeably affects exchange capacity as well as structural and transport characteristics of the original perfluorinated membrane. In particular, such a membrane possesses a feature of asymmetry of diffusion permeability when changing its position inside a measuring cell. Hybrid MF-4SC/halloysite membranes can be productively used in fuel cells and catalysis.

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Estimates of Reachable Sets of Impulsive Control Problems with Special Nonlinearity

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The problem of estimating reachable sets of nonlinear dynamical control systems with quadratic or bilinear nonlinearity and with uncertainty in initial states is studied. We assume that the uncertainty is of a set-membership kind when we know only the bounding set for unknown items and any additional statistical information on their behavior is not available. The motivation to consider the set-membership approach is that in traditional formulations the characterization of parameter uncertainties requires assumptions on mean, variances or probability density function of errors. However in many applied areas ranged from engineering problems in physics to economics as well as to biological and ecological modeling it occurs that a stochastic nature of the error sequence is questionable. For instance, in case of limited data or after some non-linear transformation of the data, the presumed stochastic characterization is not always valid. Hence, as an alternative to a stochastic characterization a so-called bounded-error characterization, also called set-membership approach, has been proposed and intensively developed in the last decades. The solution of many control and estimation problems under uncertainty involves constructing reachable sets and their analogs. For models with linear dynamics under such set-membership uncertainty there are several constructive approaches which allow finding effective estimates of reachable sets. Many applied problems are however mostly nonlinear in their parameters and the set of feasible system states is usually non-convex or even non-connected. The key issue in nonlinear set-membership estimation is to find suitable techniques, which produce related bounds for the set of unknown system states without being too computationally demanding. We present here approaches that allow finding ellipsoidal estimates of reachable sets which use the special quadratic or bilinear structure of nonlinearity of studied control system. The algorithms of constructing such ellipsoidal set-valued estimates and numerical simulation results are given in two cases, first, for control systems with classical controls and second, for measure driven (impulsive) control systems.

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Numerical Study of an Error Model for a Strap-down INS

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Today, many navigation applications are based on the miniaturised inertial navigators (INS) which include MEMS (micro-electro-mechanical systems) and NEMS (nano-electro-mechanical systems) sensors in their Inertial Measurements Units. Such navigators are more and more used near the GPS in many aerospace navigation applications, in various integrated INS/GPS configurations, due especially on the low size and low cost advantages brought by the miniaturisation. In these applications the Kalman filter, used to fuse the GPS and INS data, has degraded estimation accuracy and even divergence problems because it processes low-quality inertial data. To defeat these problems researchers proposed few solutions, one of them supposing the incorporation of artificial intelligence algorithms in the INS/GPS integration structures. In this context, our research team started a research project related to "High precision low-cost INS/GPS integrated navigation systems, based on intelligent data fusion algorithms." Currently, the team develops the navigation algorithms and their associated error models in order to be further integrated in the intelligent data fusion algorithms.

The paper exposes the validation of an error model associated with an inertial navigation system. As a start point, the navigator mechanization and its error model are highlighted, both from the mathematical point of view, as well as from their Matlab/Simulink software implementation point of view. To validate the error model a software procedure is developed. It implies the using of few standardized errors affecting the miniaturized inertial sensors, software modeled and interfaced in order to allow the user to run various testing scenarios. The numerical and graphical results obtained by applying this procedure prove the validity of the error model. In the same time, are created the premises to use the developed testing procedure to evaluate the performance limits of an inertial navigation system when the sensors in the detection unit are affected by certain errors.

Keywords: Mathematical modeling, strap-down inertial navigation systems, error model, software implementation, testing procedure, numerical validation

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Manakov Soliton Trains: External Potentials and Cross-Modulation Effects

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It is well known that the Complex Toda chain (CTC) models the N-soliton train dynamics for the Manakov solitons for several of its perturbed versions [1, 2]. In this report we will review the derivation of the relevant perturbed CTC for two classes of perturbed Manakov models. In the first one the perturbation is due to external potentials:

$$i\vec{u}_t + \tfrac{1}{2}\vec{u}_{xx} + (\vec{u}^{\,\dagger}, \vec{u})\vec{u} = V(x)\vec{u}(x,t). \tag{3}$$

for several important choices of $V(x)$: a) harmonic potentials $V(x) = v_2x^2 + v_1x + v_0$, b) periodic potentials $V(x) = A\cos(\Omega x + \Omega_0)$ and c) shallow potential wells $V(x) = c_0(\tanh(x - x_{\rm f}) - \tanh(x - x_{\rm in}))$, $c_0 \ll 1$ and $x_{\rm in} < x_{\rm f}$. The second type of perturbation is due to the cross-modulation with parameter α_2:

$$\begin{aligned} i\frac{\partial u_1}{\partial t} + \frac{1}{2}\frac{\partial^2 u_1}{\partial x^2} + \left[(1-\alpha_2)|u_1|^2 + (1+\alpha_2)|u_2|^2\right] u_1(x,t) = 0, \\ i\frac{\partial u_2}{\partial t} + \frac{1}{2}\frac{\partial^2 u_2}{\partial x^2} + \left[(1+\alpha_2)|u_1|^2 + (1-\alpha_2)|u_2|^2\right] u_2(x,t) = 0, \end{aligned} \tag{4}$$

Both perturbed Manakov models are non-integrable. Using analytical methods we derive the relevant perturbed CTC which also come out to be non-integrable. However we propose a criterium which ensures that the combination of initial potential and the initial state of the soliton train comply with the adiabatic approximation. We demonstrate that the perturbed CTC adequately models the soliton train dynamics providing our criterium holds true [1, 2, 3].

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Stochastic Univariate and Multivariate Time Series Analysis of PM2.5 and PM10 Air Pollution: a Comparative Case Study for Plovdiv and Asenovgrad, Bulgaria

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Fine particulate matter PM2.5 and PM10 air pollutants are a serious problem in many urban areas affecting both the health of the population and the environment as a whole. The availability of large data arrays for the levels of these pollutants makes it possible to perform statistical analysis for various time horizons, to obtain relevant information, and to find patterns within the data. Research in this field is particularly topical for a number of Bulgarian cities, an European country, where in recent years regulatory air pollution health limits are constantly being exceeded. This paper examines average daily data for air pollution with PM2.5 and PM10, collected by 4 monitoring stations in the cities of Plovdiv and Asenovgrad between 2011 and 2016. The goal is to find and analyze actual relationships between data time series, to build adequate mathematical models, and to develop short-term forecasts. Modeling is carried out by stochastic univariate and multivariate TS analysis, based on Box-Jenkins methodology. The best models are selected following initial transformation of the data and using a set of standard and robust statistical criteria. The Mathematica software is used to perform calculations. This examination showed measured concentrations of PM2.5 and PM10 in the region of Plovdiv and Asenovgrad regularly exceed permissible international and national health and safety thresholds with a seasonal component being observed. We obtained adequate stochastic models with high statistical fit with the data and good quality forecasting when compared against actual measurements. The mathematical approach applied provides an independent alternative to standard official monitoring and control means for air pollution in urban areas.

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EMcorrProbit R Package

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Correlated probit models (CPMs) are widely used for modeling of ordinal data or joint analyses of ordinal and continuous data which are common outcomes in medical studies. When we have clustered or longitudinal data CPMs with random effects are used to take into account the dependence between clustered measurements. When the dimension of the random effects is large, finding of the maximum likelihood estimates (MLEs) of the model parameters via standard numerical approximations is computationally cumbersome or in some cases impossible. EM algorithms for one ordinal longitudinal variable and for one ordinal and one continuous longitudinal variable are recently developed. The methods developed set the foundations of the *EMcorrProbit R* package (https://github.com/ninard/EMcorrProbit) which is going to offer also MLEs of CPM for two longitudinal ordinal variables via recently developed ECM algorithm. An application of the algorithm is presented to CPM for the longitudinal ordinal outcomes self-rated health and categorized body mass index from the Health and Retirement Study. We will report results from fitting the model and also some simulation studies.

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Estimating Population Size of the Bulgarian Brown Bear Population

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One of the best habitats of brown bears (Ursus arctos) in Europe are located in Bulgaria. They are situated in the mountain massifs – The Rhodopes, Balkan Mountains, Rila, Pirin, Vitosha. The species is a strict protected and the Nature protection act declared areas for conservation of its habitats. That is why it is important to estimate the population size of brown bear and how this population is changed in the country during the years.

In this work we apply statistical methods for assessment of the brown bear population based on statistical data from the National Monitorings which were carried out in the last 3 years. We also describe a framework of computing model that can be used for automatic estimation of brown bear population in the country.

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Application of Penalty Function Method to Computation of Reachable Sets for Control Systems with State Constraints

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We study a penalty function type method for computing the reachable sets of nonlinear control systems with state constraints. The state constraints are given by a finite system of smooth inequalities. The proposed method is based on removing

the state constraints by replacing the original system with an auxiliary system without constraints. This auxiliary system is obtained by modifying the set of velocities of the original system around the boundary of constraints. The right-hand side of the system depends on a small penalty parameter. We prove that the reachable sets of the auxiliary system approximate in the Hausdorff metric the reachable set of the original system with state constraints as the small parameter tends to zero and give the estimates of the rate of convergence. The numerical algorithms for computing the reachable sets, based on Pontryagin's maximum principle, are also considered.

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Free Surface Fluid Flows Modeling

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Study of fluid flows in the presence of the free surface is both scientific and practical interest. The theoretical and laboratory researches are performed. With the creation of supercomputers, it became possible to mathematical modeling of the studied processes. Bearing in mind that such flows there are areas with large gradients of hydrodynamic parameters required methods possess such properties as a high order of accuracy, minimum scheme dissipation and dispersion, as well as monotony. This paper will provide a brief description of the method SMIF (Splitting on physical factors Method for Incompressible Fluid flow) possessing the properties mentioned above. The foundation of the problem on the water layer going over the barrier will be given. The test calculations and comparison with some theoretical, experimental data and calculations of other authors will be demonstrated.

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Exploitation of Statistical Tools to Determine the Law Behavior of Materials by Nanoindentation

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The determination of the performance of materials requires the characterization of materials at scales: macro, micro and nanoscale. Among the most common experimental methods, the instrumented indentation test for determining the contact stiffness and contact depth, analyzing the characteristic curve by nanoindentation load on the penetration of the indentor. When statistical processing of the experimental results, we expressed the rigidity of contact on the contact depth, depending on the indentation load, to bronze, brass and copper. A mathematical model is adopted to describe the polynomial regression by the method of least squares growth rigidity with one or more geometric parameters representative of the size of the footprint. This study allows us to identify factors that influence the rigidity of the materials examined and sensitivity of the used indenters.

Keywords: Nanoindentation, modeling, power law, contact stiffness, contact depth

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Hybrid Segmentation of 3D CT Data, Incorporating Various Physical Characteristics of the Scanned Object

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Voxel data processing based on 3D Computed Tomography (CT) images of microstructures is of great importance nowadays and has numerous applications such as virtual material design, quality control of technological processes and nondestructive defectoscopy, high-tech innovations in biomedical engineering, etc. In the case of porous media, accurate 3D CT reconstruction of the material/object is not only crucial for future realistic numerical simulations of its macro characteristics, but also a quite complicated task, due to the highly irregular structure of the pores and the presence of noise in the image. Classical 2-phase segmentation methods are not reliable and standard algorithms may differ drastically (even on up to 50% of the voxel data).

Therefore, we incorporate various physical properties of the scanned specimen, such as volume and connectivity preservation of the solid (material) phase, into

the segmentation process in order to improve its quality. The mathematical model takes into account a weighted combination of different segmentation vectors as data fidelity term in the optimization function. By changing the weights, we change the impact of the corresponding material's characteristics on the output segmentation, thus its accuracy.

In this paper, we test our hybrid segmentation approach on CT images of various types of porous and composite materials. We collect experimental data for different weighted combinations of the input segmentation vectors and study the effect of the weight values on the quality of the output material phase.

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The Solution of the Volterra Integral Equations of the Second Kind and Their Discrete Analogues on the Basis of Equation Linking the Kernel and the Resolvent

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There is proposed a generalization of the methods of analytical solutions of some types of the Volterra integral equations of the second kind on the basis of finding the solutions of the corresponding equations linking the kernel and the resolvent. The statements, determining the analytical form of resolvent at a given kernel for a number of important special cases, namely, at the kernel of a separable form, are proved.

The discrete analogues of Volterra integral equations of the second kind are analyzed. The equations, linking the kernel and the resolvent in the class of discrete functions, was obtained. The methods of analytical solutions of these equations on the basis of finding the solutions of the corresponding discrete equations, linking the kernel and the resolvent, are proposed. There are considered the equivalent conversions of the proposed mathematical models to linear difference equations, including the kernel and resolvent of difference form. There was established the possibility of using the operational method for solution of discrete analogues of the Volterra integral equations of the second kind with the kernel of difference form.

We propose an approach to the solution of applied problems of simulating the dynamic processes and measuring channels with transcendent or irrational transfer functions. An equivalent representation of these mathematical models we offer to find in the form of Volterra operator. The known methods of solution of the Volterra integral equations of the second kind relatively to the residual between inputs and outputs of measuring channels are used at simulation.

The proposed approach can be used for solving the Volterra integral equations of the second kind, in which the kernels are approximated or submitted in a separable form. It also can be used for finding the fractional integro-differential transformations and solving the corresponding equations with fractional integral and differential operators.

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Are There Folding Pathways in the Functional Stages of Intrinsically Disordered Proteins?

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We proceed from the description of protein folding in terms of all-atom MD force field, with folding pathways interpreted in terms of soliton structures, to identify possible systematic dynamical patterns of self-organisation that govern protein folding process. In the case of a protein, a soliton describes a collective, coherent structure of several peptide planes and residues. Our approach thus provides certain conceptual advantages in protein folding studies. More specifically, we have revealed the particular soliton efficiency in addressing the properties of intrinsically disordered proteins. For proteins with an ordered native state (so, with a well-defined secondary structure), this very state is actually a representative of an ensemble of structurally closely related conformational substates with a highly localized statistical distribution. The fold is a local minimum of the low-temperature thermodynamic free energy. Contrary to this, for intrinsically disordered proteins, the low temperature limit produces a scattered statistical distribution of structurally disparate but energetically comparable ensembles of conformational substates. These proteins are believed to fulfill their biological functions while constantly varying their form.

We question this assumption for an intrinsically unstructured antimicrobial peptide (AMP) the 13-residue long indolicidin. Indolicidin is a short antimicrobial and cytolytic peptide, cationic and rich in tryptophan and proline. Also upon binding (e.g., to calmodulin), indolicidin does not adopt helical conformation. Its microbicidal activities in vitro are thought to be related to the membrane-disruptive properties of the peptide. We perform in silico investigation of the conformational transformations indolicidin undergoes in the process of membrane penetrations, resp. pore formation. We discuss the emergence of soliton-mediated secondary motifs in the context of the functional activity of the peptide. We hypothesize that soliton-like quasi-ordered conformations appear as an important intermediate stage in this process.

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Hydrodynamic Instability of a Convective Flow in an Annulus Generated by Heat Sources in a Chemically Reacting Fluid

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In this paper we analyze convective instability of a flow of viscous incompressible fluid in an annulus under the assumption that heat sources are distributed in the fluid in accordance with the Arrhenius' law. The annulus is assumed to be infinitely long and closed. The problem is described by the system of the Navier-Stokes equations under the Boussinesq approximation. The base flow solution is found numerically solving a nonlinear boundary value problem. The linearized system of equations for small perturbations is solved numerically by the Chebyshev collocation method. Asymmetric perturbations with the azimuthal wave number $n = 1$ are investigated (experimentally this mode is found to be the most unstable for uniform heat sources generated in a pipe).

It is found that for small Prandtl numbers shear instability takes place due to interaction of two fluid streams moving in the opposite directions. The second branch of the marginal stability curve appears for large Prandtl numbers and it is associated with thermal running waves moving along the axis of the annulus. The critical wave numbers in this case have a jump (thermal instability is associated with perturbations which have smaller wave numbers). Critical Grasshof numbers are calculated for different values of the parameters of the problem. It is found

that the flow becomes less stable as the Prandtl number and Frank-Kamenetsky parameter increase.

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Radial Basis Functions: Accomplishments and Challenges

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Traditional mesh-based finite difference, element, and volume methods were first developed on primitive computers that lack memory and execution speed. As computers evolved, single precision word-lengths became the norm and sparse low order polynomial schemes became the accepted standard world-wide. To obtain sufficient scientific accuracy, successively finer meshing was required that even the sparse finite element method yielded ill-conditioned systems of equations requiring both pre-conditioners and domain decomposition.

C^∞ radial basis functions(RBFs) are a generalized spectral method that does not require meshing, is valid in any dimensional space, and is exponentially convergent, and is global or very broad banded in nature.

Such systems of equations, especially pushing the average shape parameter to increasingly larger values become very ill-conditioned in double precision arithmetic. It is counter-intuitive, but extended precision arithmetic is fast. If properly implemented, and is many orders of magnitude faster than linear finite elements, and C^∞ RBFs appear at present the only viable method to address multi-dimensional problems in plasma fusion, molecular quantum mechanics, semi-conductors, etc.

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On the Parallelization Approaches for Intel MIC Architecture

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The Intel MIC architecture is one of the main processor architectures used for the production of computational accelerators. The increased energy and cost-efficiency of accelerators is one important option for building new HPC systems.

However, the effective use of accelerators requires careful optimization on all stages of the algorithm and use of appropriate parallelization approaches. In the domain of statistical methods the quasi-Monte Carlo methods present distinct challenges when thousands of computational cores are to be involved in a computation. In this paper we compare several approaches for parallelization of quasi-Monte Carlo methods on devices with Intel MIC architecture and obtain important conclusions about the relative merits of these approaches on such kinds of algorithms, based on numerical and timing results as well as energy efficiency observations.

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New Hermitian Finite Elements on Rectangles with Useful Properties for Spectral and Parabolic Problems

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In the report, new types of Hermitian finite elements in two- and three-dimensional rectangles will be proposed. Recall that the Hermitian finite elements of the same polynomial degree as the Lagrangian ones usually produce less number of unknowns and equations in the system of the finite element method [1].

First we discuss biquadratic finite element on a rectangle with 8 degrees of freedom (the values of a function and its second-order derivatives at the vertices of a rectangle). From the standard point of view, it provides the third order of accuracy in the L2-norm. But the use of symmetry on a uniform grid provides the fourth order of accuracy in the discrete analogue of the L2-norm calculated at the nodes of the elements.

Then the bicubic finite element on a rectangle with 12 degrees of freedom is considered (also with the values of a function and its second-order derivatives at the vertices of a rectangle). From the standard point of view, it provides the fourth order of accuracy for the functions in L2-norm, and the third order for its first-order derivatives. But the use of symmetry on a uniform grid again provides the fourth order of accuracy for the first-order derivatives.

These conclusions are confirmed by numerical experiments.

Another useful feature of these elements is the ability to use degrees of freedom as the values in a quadrature rule. Moreover, this choice provides the diagonalization of the mass matrix that simplifies the assembly of discrete systems for the finite element method for spectral problems. This is especially useful in the semi-Lagrangian approximation for time-dependent parabolic problems.

This reasoning is generalized in the three-dimensional case to the cubic cell. As a result, the triquadratic and tricubic finite elements on the cubic cell are proposed

with 20 and 32 degrees of freedom, respectively, with the values of a function and its second-order derivatives at the vertices of a cell. They also have useful properties similar to those of the two-dimensional finite elements both in terms of superconvergence and diagonalization of the mass matrix by choosing a quadrature rule with the values of degrees of freedom.

Acknowledgement: This work is supported by Project 14-11-00147 of Russian Scientific Foundation.

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Methods for Solving Inverse Nonlocal Problems for Parabolic Equations

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In this paper, a general mathematical model of the high-temperature thermodiffusion that occurs in a limited environment is considered. Based on this model formulation of inverse problems for homogeneous and inhomogeneous parabolic equations are proposed. In the problems existing in the closed area of internal and external sources of heat (substance) are reflected. The inverse problem aims at identifying one or several unknown parameters of the mathematical model. These parameters allow to maintain the required temperature distribution and concentration distribution of substance in whole or part of the area.

Depending on the type of the inverse problem and the known parameters of the process that describes the mathematical model, the appropriate method of its solution is proposed. In particular the problem of restoration the right side of a parabolic equation is considered. Cases when the right part of the non-homogeneous equation, or one of its parameters depend on the time, on the spatial coordinates and time, or only on the spatial coordinates are considered. It is shown that the problem of finding the temperature field and concentration distribution of both internal and with external heat source can be reduced to extremal and solved by one algorithm. Integral energy balance condition or substance which is allocated in the closed area used for the construction of functional of the quadratic residual of

an extremal problem. The conjugate gradient method is used to find the unknown function (control) of the source, the difference scheme with weights used for solving boundary value problems. It is shown that the problem of heat conduction with the external heat source can also be represented as a boundary inverse heat conduction problem. Direct numerical method for solving such problems is proposed. The inverse problem for the heat equation with impulse functions in the equation and the boundary conditions is considered. Features of solving such problems are investigated. Numerous calculations are made and the comparative analysis of the results carried out.

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Dynamics of High-intensity Ultrashort Light Pulses at Some Basic Propagation Regimes

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The propagation dynamics of high-intensity ultrashort light pulses at some basic propagation regimes in bulk nonlinear medium is presented. The pulse propagation behavior is studied by numerical simulations of physical models at realistic physical conditions. The spatiotemporal dynamics of ultrashort light pulses within (3+1)D nonlinear Schrödinger equation and (3+1)D nonlinear envelope equations as propagation equations as well as at ionization free and ionization regimes is revealed and summarized.

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Modifications of PCPT Method for HJB Equation

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Many problems in computational finance involve some optimization part. In such cases, Hamilton-Jacobi-Bellman (HJB) equation is often an effective way to solve the problem. As the HJB PDE is highly nonlinear, analytical solutions are rarely feasible and numerical methods are used. Most often monotone implicit schemes with policy iteration are used. Piecewise constant policy timestepping (PCPT) method is simple alternative to classic implicit scheme for HJB equation. In contrast to the implicit method, the PCPT method does not need policy iteration. In our talk we will present some useful modifications of PCPT method, leading to decrease in computational time in many cases.

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On Estimating Reachable Sets for Multi-Agent Motion: Discrete-Time Dynamic Systems

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The reachability problem is an essential theme in control theory. Since the practical construction of trajectory tubes (reachable tubes) and reachable sets, which are cross-sections of the mentioned tubes, may be cumbersome, especially for high dimensional systems, different numerical methods were devised over the last decades. Among them the techniques were developed for estimating reachable sets by domains of some fixed shape such as ellipsoids, parallelepipeds, zonotopes. Such techniques are designed to produce the approximations for the investigated tubes and sets without being too computationally demanding.

Here we consider the reachability problem for linear discrete-time control systems which describe so called multi-agent motion. Namely, we consider a finite set of control subsystems under condition that the trajectories of the subsystems should be pairwise not very close to and not very far away from each other. It is also assumed that the initial states and the controls of the subsystems are subjected to given parallelepiped-valued constraints. Some properties of the reachable sets of such systems are indicated. In particular, the mentioned reachable sets can be

non-convex and even disconnected. The reachable tubes may be presented in the form of branching trajectory tubes whose cross-sections are convex polytopes. Some algorithms for constructing external and internal polyhedral estimates for reachable sets using parallelepipeds as basic sets are proposed.

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Central Schemes: A Powerful Black-Box Solver for Nonlinear Hyperbolic PDEs

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The talk will be focused on non-oscillatory central schemes, which are simple, efficient, highly accurate and robust Godunov-type finite-volume methods for general hyperbolic systems of conservation laws. I will first show their derivation and then several recent applications.

I will first give a brief description of Godunov-type finite-volume methods for general hyperbolic systems of conservation laws. These methods consist of two types of schemes: upwind and central. My lecture will focus on the second type – non-oscillatory central schemes.

Godunov-type schemes are projection-evolution methods. In these methods, the solution, at each time step, is interpolated by a (generically discontinuous) piecewise polynomial interpolant, which is then evolved to the next time level using the integral form of conservation laws. Therefore, in order to design an upwind scheme, (generalized) Riemann problems have to be (approximately) solved at each cell interface. This however may be hard or even impossible.

The main idea in the derivation of central schemes is to avoid solving Riemann problems by averaging over the wave fans generated at cell interfaces. This strategy leads to a family of universal numerical methods that can be applied as a black-box-solver to a wide variety of hyperbolic PDEs and related problems. At the same time, central schemes suffer from (relatively) high numerical viscosity, which can be reduced by incorporating of some upwinding information into the scheme derivation – this leads to central-upwind schemes, which will be presented in the lecture.

During the talk, I will show a number of recent applications of the central schemes.

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PDE Models for Pulses in Binary Wave Guide Arrays

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Binary waveguide arrays are linear arrays of optical waveguides with binary alternation of parameters, and have been of recent interest. They can be modeled by systems of nonlinear ODE's with forms related to the discrete nonlinear Schrödinger equation. Such equations can also arise in semi-classical molecular models of polymers with excitable states in each monomer, and coupling between these.

An important class of solutions arises from an initially highly localized signal, such as a single element of the array. Simulations show that for a wide array of parameter values and of such initial data, a pulse is generated that travels approximately as a traveling wave. After a suitable phase shift in the variables, this pulse quickly develops a slow spatial variation, leading to a long-wave approximation by a system of coupled third order PDE's; one each for nodes of even and odd indices.

This system of PDE's is presented, and verified to quite accurately reproduce the pulse propagation seen in the ODE system; further there is a strong tendency for the behavior of the two PDE components to converge, with a corresponding convergence of the even and odd index parts of the ODE system solution. The PDE model gives some indication of why this occurs.

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Semi-rigidity vs. Flexibility in Collective Variables Preselection for Metadynamics Studies of Large Proteins

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Molecular dynamics (MD) simulations have enabled in silico investigations of versatile biomolecular events. However, many important biological processes involve transitions with higher free energy barriers on long time-scales due to large-scale molecular rearrangements that despite modern computational power and

algorithms are still difficult to sample adequately with standard MD approaches. Advanced sampling techniques such as metadynamics [1] now allow these phenomena to be studied more efficiently. Metadynamics is based on computation of the free energy of the system as a function of a small set of collective variables (CVs) that are assumed to be able to adequately describe the investigated process.

The reliability of metadynamics strongly depends on the choice of the CVs. The set of CVs should be able to clearly distinguish between the initial state and the final state and preferably the intermediates. Ideally, the CVs should describe all the slow events that are relevant to the investigated process, but in the same time their number should be small. There is no a priori recipe for identification of a suitable set of CVs and most often a trial and error approach is the only way.

The purpose of our work is to develop a CV selection protocol based on the conformational steadiness of the protein in the most sensitive for the investigated process domains. The structure identification is performed using the spatiotemporal multistage consensus clustering [2], with adequate selection of the cluster size and rigidity parameters.

Acknowledgement: Financial support under the Young Scientist's Programme of BAS (Grant DFNP-99/04.05.2016) is acknowledged.

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Numerical Models of Ion-acoustic Collisionless Shock

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An analysis of the general problem of wastewater transport and removal of pollutants in porous media is presented. A numerical simulation of available experimental data, by using the Visual MODFLOW computer code, is realized. Emphasis is given to the simulation of the removal of an non-absorbable pollutant (Biochemical Oxygen Demand-BOD), in horizontal subsurface flow constructed wetlands (HSF CW). Further computational investigation is made on the one hand to select the optimal type of the chemical reaction for BOD removal and on the other hand to obtain upper and lower solution bounds. These bounds can be used for aposteriori checking numerical simulations or/and for draft design purposes to overcome the uncertainties concerning some problem input parameters.

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Mathematical Models of Thermal Processes in the Spherical Area

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Modeling of the temperature field $U = U(r, \theta, \varphi, t)$ in the rotating sphere, which has radius $r \leq R$, with an angular velocity of $\omega(\varphi)$, when the direction of a

heat transfer $q(\varphi, t)$ orthogonal to the axis of rotation is one of the most important problem in astrophysics and geophysics. Such problems arise during the study of the heat flows from the surface of stars, in particular pulsating stars, from the surface of planets that have an atmosphere, and from the surface of space objects that are exposed to radiation. In the first approximation using a continual approach to solve problems, each of these objects can be considered in the form of a sphere with homogeneous physical conditions. The solution of the nonlinear problem of determining the temperature field in a rotating sphere, which has a radius $r \leq R$ is considered in this paper. The angular velocity of the sphere and the heat flow are constant values. The heat flow is orthogonal to the axis of rotation. Mathematical models are presented in the form of non-stationary boundary value problems for homogeneous and inhomogeneous heat conduction equations in a spherical area with 2nd and 3rd kind boundary conditions.The solution of the problem for the homogeneous equation is reduced to solving the equivalent integral equation of Fredholm type by the angular coordinates, and the solution of problem is reduced to solving integral equation of Volterra type by the time coordinate. Green's function and the second Green's formula were used for the solution of the problem. Green's function is obtained by solving the conjugate problem in the area of research. In this case the Dirac delta function in a spherical coordinate system was involved. As a result of transformation, the solution to the inhomogeneous equation is obtained in the form of an integral equation of Hammerstein type with Green's function type kernel.The temperature distribution on the surface of a sphere is constructed with the use of numerical methods and computer mathematics methods

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A Simple Low Computation Intensity Model for Approximating the Distribution Function of a Sum of Non-Identical Lognormals for Financial Applications

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The distribution function of a sum of non-identical lognormal random variables (RVs) is almost as ubiquitous as that of a sum of normal random variables. However, it has no known closed form. Such distribution function is required in many fields of science and specifically in finance for portfolio management and exotic options valuations (e.g. basket, Asian options and the like). Most of the approximations of the sum of lognormal RVs are complicated, difficult to implement as well as

computation intensive. Via a novel approach that is based on a finite version of the central limit theorem I present a new, simple and easy to implement approximation method for financial applications that is both intuitive and highly efficient computation-wise. This paper presents a moment matching method as well as rational functions correction (Pade approximation) for the distribution function of a finite sum of non-identical lognormal RVs. The accuracy of the method is compared against the results of Monte Carlo simulations as well as the popular Markowitz' model portfolio equations.

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Measurement of Similarity Users and Items by Feedbacks and Tags for Recommendation System

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The idea of recommendation is optimize what we know about users and items and maximize utility function. If we have not enough value of similarity to calculate relevant prediction we can use association rule approach. It means we have enough quantity data to say it may be a rule to use it in similar cases. Moreover we can add the order to actions to follow more correctly and use sequential analysis. One of the nuances is what if we have a small number of actions at all, it is not a new user or item to use cold start approaches like content or knowledge approaches, we just have not enough quantity to say it may be interpreted like regularity. But at the same time our prediction should has a low value of root mean square error and we should stay care about sparsity level of current matrix. That is why these is a point how to calculate similarity measure in this case. Explicit and implicit feedbacks are not older day by day, opposite they are growing day by day as long as user use some tool and we pick up the knowledge about his behavior. In proposed way we create an algorithm using as explicit and as implicit feedbacks from users and evaluate tags by Jaccard distance to resolve this issue.

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Mathematical Models of Magnetite Desliming for Automated Quality Control Systems

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The article deals with construction of mathematical models of the process of magnetite desliming. Built models should be suitable for use in automated systems for process control. The results of the study are models of the motion of two-phase slurry in the case of an axisymmetric two-dimensional and three-dimensional vortex flow of the pulp. To calculate the three-dimensional flow and particle trajectories the applications Flow Simulation was used from package SolidWorks. We also developed a method of imitating the numerical experiment to determine the dependence of the enrichment's quality from the process parameters and the shape of the desliming machine. The results of calculations allow us to estimate the impact of technological and structural factors on the quality of the magnetite enrichment. The practical value of the results is the possibility of direct use of models in the automated control systems enrichment processes.

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Analytic Approximation of Periodic Ateb Functions via Elementary Functions in Nonlinear Dynamics

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We consider the problem of analytic approximation of periodic Ateb functions, which are widely used in nonlinear dynamics. Ateb functions are the result of the following procedure. Initial ODE contains only the inertial and non-linear terms. Its integration leads to an implicit solution. To obtain explicit solutions one needs to invert incomplete Beta functions. As a result of this inversion we obtain the special Ateb functions. Their properties are well known, but the use of Ateb functions is difficult on practice. In this regard, the problem arises of approximation of Ateb functions with the help of smooth elementary functions. For this purpose in the present article the asymptotic method is used with a small parameter which is inverted to the exponent of nonlinearity. We also investigated the analytical approximation of Ateb functions' period. Comparison of simulation results, obtained by the approximate expression, with the results of numerical solution of the corresponding Cauchy problem shows their sufficient accuracy for practical purposes, even for the exponent of nonlinearity equal to unity.

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On the Monotonicity of Multidimensional Difference Schemes

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The concept of monotonicity is introduced to multidimensional linear difference schemes. Necessary and sufficient monotonicity conditions are obtained. The constraints on the numerical viscosity are given that ensure the monotonicity of a difference

scheme in the multidimensional case. It is shown that the monotonicity of a scheme in each spatial variable does not generally imply its monotonicity as a multidimensional scheme.

Recently, a two-time-level representation of the CABARET scheme has been widely used for the numerical simulation of multidimensional gasdynamic and hydraulic flows. The monotonicity of this scheme in the one dimensional case was examined earlier. In this work we analyze its monotonicity in the multidimensional case. In the case of standard correction of flux variables, it is shown that this scheme does not preserve the monotonicity of one-dimensional difference solutions, which results in noticeable oscillations occurring in the computation of two- dimensional discontinuous solutions. We propose a modification of the two-time-level multidimensional CABARET scheme that preserves the monotonicity of one-dimensional difference solutions and, as a result, ensures higher smoothness in the computation of multidimensional discontinuous solutions. The results of two-dimensional test computations illustrating the advantages of the modified scheme are presented.

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Modeling of Web Services Flow for Distributed Systems

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Web services technology can be used to provide different kind of services, such as selecting, updating, deleting any type of data. Web services infrastructure includes standards, such as JSON and XML on HTTP protocol. In this paper we developed a program to determine a combination of web services from different systems, according to server distance, system types and data quality. In this work we present distributed Web services by modeling the flow of different types of data and methods in a Web service transaction. Specifications of the design are modeled in UML (Unified Modeling Language). In development process we used MySQL database, PHP and Google MAP API's.

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A Note On Fundamental Units in Some Type of Real Quadratic Fields

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Let $k = Q(\sqrt{d})$ be a real quadratic number field where $d > 0$ is a positive square-free integer. The map $d \to Q(\sqrt{d})$ is a bijection from the set off all square-free integers $d \neq 0, 1$ to the set of all quadratic fields

$$Q(\sqrt{d}) = \{x + y\sqrt{d} | \, x, y \in Q\}.$$

Furthermore, integral basis element of algebraic integer's ring in real quadratic fields is determined by either $w_d = \sqrt{d} = [a_0; \overline{a_1, a_2, ..., a_{l(d)-1}, 2a_0}]$ in the case of $d \equiv 2, 3 (\mathrm{mod}\, 4)$ or $w_d = \frac{1+\sqrt{d}}{2} = [a_0; a_1, a_2, ..., a_{l(d)-1}, 2a_0 - 1]$ in the case of $d \equiv 1 (\mathrm{mod}\, 4)$ where $l(d)$ is the period length of continued fraction expansion.

The primary purpose of this paper is to classify some type of real quadratic fields $Q(\sqrt{d})$, which include the specific form of continued fraction expansion of integral basis element w_d for which has all partial quotient elements are written same as ξ?s (except the last digit of the period) for arbitrary ξ positive even integer where period length $l = l(d)$ and $d \equiv 2, 3 (\mathrm{mod}\, 4)$ is a square free positive integer.

Also, the present paper deals with determining new certain parametric formula of fundamental unit $\varepsilon = (t_d + u_d\sqrt{d})/2 \rangle 2$ for such real quadratic fields. All supported results are given in numerical tables.

Keywords: Quadratic field, continued fraction, fundamental unit

AMS Subject Classification: 11R11, 11A55, 11R27

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Common Fixed Point Theorems in C^*-Algebra Valued b-Metric Spaces

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In this talking, we establish some common fixed point theorems for self maps in C^*-algebra valued b-metric spaces (see [1]-[14]. Besides, we give examples to illustrate our theorems.

Keyword: Fixed point theory, b-metric spaces, C^*-algebras

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A Discontinuous Galerkin Finite Element Method for High-Prandtl Number Non-Fourier Convection

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Despite its success for many applications, Fourier's heat conduction law violates the principle of causality. One of the first solutions to this problem is the Maxwell-Cattaneo law which introduces a thermal relaxation time to the constitutive relationship between the heat flux and temperature. The resulting heat conduction equation however is not Galilean-invariant. This was resolved by Christov in [1] who proposed a frame-indifferent version of this law. Here, we examine the effects of these two approaches on the stability of the two-dimensional in space natural convective flow in a vertical cavity, including the case of fluids with large Prandtl number.

It is a well-established fact that stability problems require a robust numerical scheme with very high accuracy, especially for computations near the neutral stability curve. Furthermore, the large value of the Prandtl number leads to issues similar to the cell Reynolds number constraint. To this end a High-Order Discontinuous Galerkin Finite Element Method is developed and tested. The scheme follows the explicit time-stepping process proposed by Liu in [2] meaning that is both efficient and suitable for high Prandtl numbers.

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$\rightarrow \infty \diamond \infty \leftarrow$

On Some Questions in Computer Modeling of the Reachability Sets Constructing Problems

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The research considers the problem of constructing the reachability sets of nonlinear dynamical system in n-dimensional Euclidean space on the fixed time interval. The reachability sets constructing problem is one of the most important problems in the control theory. The effective analytical solution of this problem is available only for limited number of the simplest classes of the systems, thus the approximate solution methods of the reachability sets constructing are considered in this research as well as the accuracy estimations for this methods are given. The research contains the computational experiments on computer modeling of described reachability sets constructing methods, which use the algorithms implemented for using on CPU as well as the algorithms implemented for GPU based on CUDA technology. In this research the description and comparison of approaches to the computer modeling of the problem are presented. Furthermore, the CPU-based computer modeling result comparison with the result obtained on GPU based on CUDA technology are presented. In addition, this research discusses the side issues caused by the rapid growth of the number of point during computer modeling, the issues raised during the computer algorithms implementation, as well as the ways to eliminate these issues or reduce their impact. This research was supported by Russian Science Foundation (Projects 15-11-10018)

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Some Mathematical Models for the World Population

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Scientists believe that the world population plateau of 9.2 billion. In this paper, some mathematical models are presented to predict the year that the world population will reach 9.2 billion. Three of these models are the kind of simple iterative ordinary differential equation which M. Podisuk proved the existence and uniqueness in [1]. Four of these models predict that the year of 2039, the world population will reach 9.2 billion.

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Derivative Pricing in Markets with Transaction Costs

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The pricing of financial derivatives with transaction costs is one of the most important extensions of the traditional Black-Scholes model. Utility indifference pricing can be used to price financial derivatives in these conditions and it leads to a free-boundary problem whose solution can be found numerically. We present several numerical results and analysis of the prices obtained with this approach and compare different utility functions.

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Recognizing Food through Deep Learning and Egocentric Vision

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The analysis of people's nutrition habits is one of the most important mechanisms for applying a thorough monitorisation of several medical conditions (e.g., diabetes, obesity, etc.) that affect a high percentage of the global population. Methods for automatically logging one's meals could not only make the process easier, but also make it objective to the user's point of view and interpretability. One of the solutions adopted recently that could ease the automatic construction of nutrition diaries is to ask individuals to take photos with their mobile phones. An alternative technique is visual lifelogging that consists of using a wearable camera that automatically captures pictures from the user point of view (egocentric point of view) with the aim to analyse different patterns of his/her daily life and extract highly relevant information like nutritional habits. In this talk we will show how deep learning applied to the food detection and food recognition problems can help to automatically infer the user's eating pattern.

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On Analogs of Number π in q–Calculus

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Since the number π was introduced like quotient of circle circumference and diameter, it occupies attention of whole scientific world. It is an interesting fact that q–calculus, like a complete analogy of the standard calculus, did not recognize importance of q-version of number π during the whole twentieth century. A lot of classes of special q–numbers were introduced and investigated in details, such as: q–Fibonaccci, q–Stirling numbers and so on. Also, q-exponential functions and the numbers $e_q(1)$ and $E_q(1)$ are in usage for a long time.

But, at the beginning of this century, there were a few papers by R. Diaz, S. Suslov and W.S. Chung with coauthors, dealing with trials do define the number $\pi(q)$.

In this paper we will compare their results, suggest a few new possible definitions and discuss their advantages and lacks in order to find the optimal one.

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Mathematics Subject Classification: 33D05, 11A67.

Keywords: q–calculus, number sequences, number π

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Magnetohydrodynamic (MHD) Flow of Cu-water Nanofluid Due to a Rotating Disk with Partial Slip

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This paper investigates MHD steady flow of viscous nanofluid due to a rotating disk. Water is treated as a base fluid and copper as nanoparticle. Nanofluid fills the porous medium. Effects of partial slip, viscous dissipation and thermal radiation are also considered. Similarity transformations reduce the nonlinear partial differential equations to ordinary differential equations. Flow and heat transfer characteristics are computed by HAM solutions. Also computations for skin friction coefficient and Nusselt number are presented and examined for pertinent parameters. It is noted that higher velocity slip parameter decreases the radial and azimuthal velocities

while temperature decreases for larger values of the thermal slip parameter. Also the rate of heat transfer enhances when the nanoparticle volume fraction increases.

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Dynamical Systems Approach to the Platforms Dynamics

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I will discuss a dynamical system, which models a two-sided platform. The model estimates the volume of users from each side of the platform as a function of time. I will discuss theorems describing the long-term behavior and tendency of the platform. Even though I consider generic attachment functions, I obtain a concrete result, formulated in terms of local properties of attachment functions. These generic results will be followed by examples (defined by the popular in economics attachment functions), which illustrate behavior of the two-sided platform. I will also present simulations of some two-sided platform scenarios, showing how adjustments of attachment functions can influence the users' dynamics.

The dynamical system's approach to the study of two-sided problem allows natural generalization to multi-sided platforms (MSP), where one can utilize the same technique and obtain similar results in higher dimensions.

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Pricing and Hedging Correlation Swaps with a 2-Factor Model

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We introduce a new model to price and hedge correlation swaps. The model is based on an approximation for the realized correlation payoff, written as the ratio between two quantities, which can be replicated from traded assets in the variance swap markets. The model allows us to derive simple analytical formulas

for the price of a correlation swap. Finally, numerical evaluations of correlation swap prices are presented.

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The Distributed Control Network Resources Problem as a generalized Kolkata Restaurant Problem

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The network control plays a key role while optimizing the allocation of resources among users applications and maximizing the utility function. There is weakness into a centralized control system when we are increasing the number of users during short time. It requires more time to consideration of control problem. For this reason, there is one efficient way to reduce a solved time of the resource allocation problems is using the decentralized methods. The multi-agent approach is used for simulation of decentralized control process. For each data flow is allocated certain resources. The data flow is received a rejection of service in case of there is no enough resources. Interaction of the agents in the process of resource allocation can be represented as a game with successive repetitions. This game could be reduced to the solution of the Kolkata Restaurant Problem. This paper presents an analysis of efficient for different strategies of agents while solving problems of resource allocation, and supplemented there is an investigation of effective for different models of the training agents.

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Applying Transormations for Accelerating the Convergence of Trigonometric Series

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This paper examines the generalized transformation of trigonometric series through a generalized operator of Euler type. Through this operator is achieved

that the trigonometric convergent series to be transformed in a series that converges faster that the initial series. In the paper are also given the algorithms for accelerating the convergence of trigonometric series.

Keywords: trigonometric series, convergence, accelerating, generalized operator

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Method of Superposition of Dislocations for Finding Stress-Strain State around Fan-Shaped Structure in a Brittle Rock

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Recent researches by Prof. Boris Tarasov from the University of Western Australia have resulted in the identification of a hitherto unknown shear rupture mechanism, which is responsible for extreme dynamics and violence of shear rupture development in hard rocks at stress conditions corresponding to seismogenic depths. The key feature of this mechanism is a fan-shaped microstructure of the rupture head, formed on the basis of an echelon of microcracks and intercrack blocks generated in the rupture interface. Under the action of applied shear stresses the fan-shaped rupture head travels as a wave of high velocity due to extremely low shear resistance.

For computation of the stress-strain state of a rock near the equilibrium fan-structure the original method is constructed. The fault is modeled as a narrow elongated layer, filled with the domino-blocks, between two elastic half-spaces. Displacements and stresses around the fan are represented in the integral form as a superposition of edge dislocations with an unknown function of distribution of the Burgers vector. To take into account the stresses of lateral thrust, the solution of plane problem of the elasticity is used for a tensile crack, on the surfaces of which the previously unknown normal stresses are distributed. The exact formulation of the problem leads to a system of two nonlinear singular integral equations, which is solved numerically by the method of successive approximations. The obtained solution is used, when setting the initial data in computations of the dynamics of the Tarasov fan-shaped mechanism. With the help of this solution the discontinuous nature of shear ruptures, observed in natural and laboratory experiments, is explained.

Acknowledgements: This work was supported by the Centre for Offshore Foundation Systems (COFS UWA), the Complex Fundamental Research Program

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Modeling of Fan Formation in a Shear Rupture Head on the Basis of Singular Solutions of Plane Elasticity

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Shear rupture is a universal form of rock failure under confined compression. It is generally accepted today that the rupture front moves through the rock due to the creation of an echelon of micro-tensile cracks in the rupture tip with formation of intercrack (domino-like) blocks inclined at an initial angle to the rupture plane. These blocks are subjected to rotation and collapse at shear displacement of the rupture faces creating friction in the rupture head. It was recently established that in hard rocks at high confining stresses corresponding to seismogenic depths the domino-blocks can withstand the rotation without collapse forming a fan-shaped structure in the rupture head. In this case the domino-blocks behave as hinges by rotating between the moving rupture faces decreasing dramatically friction in propagating rupture head.

The mathematical model of the equilibrium fan-structure formation between two elastic half-planes is constructed, simulating a shear rupture at stress conditions of seismogenic depths. The stress-strain state far from the fan-structure is analyzed with the help of solution of the problem on the Volterra edge dislocation resulted in estimation of the fan length. The model of formation of two differently directed fans due to the localized action of tangential stress, which pushes two edge dislocations with the antiparallel Burgers vectors, is proposed. Singular solutions of the plane elastic problem with stepwise pressure profile at the boundary of a half-plane, as well as the problem on the action of concentrated normal stress and concentrated couple stress at the boundary are applied to the analysis of mechanisms of the fan-structure formation.

Acknowledgements: This work was supported by the Centre for Offshore Foundation Systems (COFS UWA), the Complex Fundamental Research Program no. 18 of the Presidium of RAS and the Russian Foundation for Basic Research (grant no. 14-01-00130).

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Mathematical Modeling of Wastewater Treatment from Multicomponent Pollution by Using Microporous Particles

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The mathematical model of singularly perturbed process of multicomponent convection-diffusion mass transfer in microporous heterogeneous media is proposed.

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Urysohn Measure Driven Integral Equations in the Space of Bounded Variation Functions

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Motivated by the fact that bounded variation (often discontinuous) functions frequently appear when studying integral equations that describe physical phenomena, we focus on the Urysohn-Stieltjes integral equation

$$x(t) = g(t) + \int_0^1 f\left(t, s, x(s)\right) \mathrm{d}_s u(t, s) \tag{5}$$

driven by a function $u : [0,1] \times [0,1] \to \mathbb{R}$.

Due to numerous applications of Urysohn integral equations in mathematical physics, in electrical engineering, economics or mathematical biology ([3]), problems

of this kind have been extensively studied in literature, under more restrictive assumptions. Our approach concerns the very comprehensive framework of Kurzweil-Stieltjes integration, which is necessary whenever f and u are both discontinuous (when the Riemann-Stieltjes integral may not exist) or the function f is not absolutely integrable with respect to u (in such a case, the Lebesgue-Stieltjes integral is not well defined). Note that this integration theory allows the occurrence of high oscillatory features on the right hand side of the equation.

Applying a Leray-Schauder alternative, we get the existence of bounded variation solutions.

A discussion about interesting consequences of our main result (given by particular cases of the measure driving the equation) is presented. Thus, our results cover usual integral equations (when working with absolutely continuous functions), difference equations (when the function with respect to which we integrate is a series of Heaviside functions) and impulsive integral equations (when the continuous and the discrete parts are both involved).

Finally, inspiring ourselves from the practical problems presented in [3], we show the generality of our results by investigating (by theoretical and numerical points of view) two examples of impulsive type problems for which existing theories (such as, [1] or [2]) do not apply.

Acknowledgement: This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-RU-TE-2012-3-0336.

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A Free-Form Surface Modeler

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Free-form surface modelers in Computer Aided Geometric Design are usually based on the representation of a surface as a construction of rectangular patches

because of the relatively simple structures involved in their use. Unfortunately, it is sometimes impossible to model a surface as a mapping from a regular rectangular grid. Many surfaces require the insertion of patches which do not have four sides. A considerable amount of effort has been devoted to developing schemes for solving the problem of branching. These schemes can handle arbitrary topological meshes and are useful for precise surface modeling as in industrial design. However, they are computationally expensive or require complex constraints to maintain the continuity between two patches. Therefore, these methods are not suitable for interactive manipulation.

To date there does not exist a completely satisfactory method which generates surfaces of arbitrary topology and at the same time is able to produce fine detail on the surface. Most modeling is done by some combination of methods to produce the desired result, which is time consuming and can also be very complex.

This paper presents a method which constructs, at different steps, a new set of points with more vertices and smaller faces than the original set of points. After a number of iterations, this results in a smooth surface. The new points generated are divided into three categories: *new face points* – new points lying in the middle of the squares of the original mesh, *new vertex points* – new points corresponding to old control points, and *new edge points* – new points lying near the edges connecting original control points. Each kind of new point is divided into different sub-categories. In fact in the case of curves there are two kinds of new vertex points and two kinds of new edge points, whereas in the case of surfaces there are three kinds of new face points, three kinds of new vertex points and four kinds of new edge points.

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The Method of Kinematic Elements in Geotechnics – New Developments and Applications

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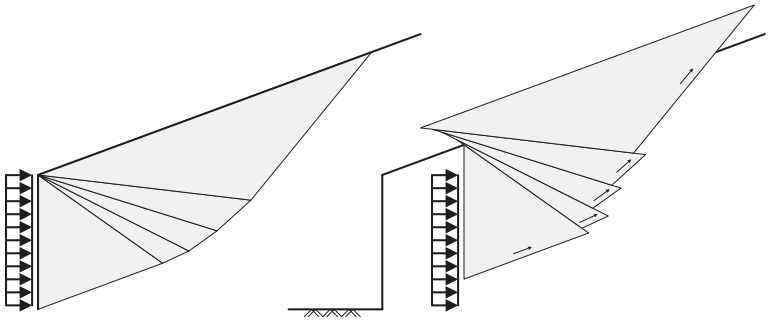
The prediction of limit states in soils and rocks is a classical task in foundation engineering. An efficient and adaptable tool to solve such problems is the kinematical element method (KEM), which has been presented by Gussmann nearly 30 years ago. This method has been improved continuously and has been applied to a more and more broad field of problems. Following a short introduction to the basic principles of the method a number of applications of KEM to complex topics is presented and discussed. Bearing capacity of deep footings and of two adjacent interfering footings, the trap door problem and the ultimate load of plate anchors

are studied. The potential of optimizing the geometry of a slope is demonstrated and approaches to take into account unsaturated soil conditions as well as three dimensional effects are shown.



Calculation of the passive earth pressure on a vertical wall.

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JONSWAP Rogue Waves Over Non-Constant Backgrounds

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JONSWAP rogue waves are large amplitude waves on a non-constant background that are distinct from prior analytical models, including spatially periodic breathers and rational solutions of the Nonlinear Schrödinger (NLS) equation, which are all constructed over a constant background. In this talk we classify JONSWAP rogue waves using the inverse spectral theory of the NLS equation and construct NLS solutions that model JONSWAP rogue waves. The associated spectral configurations are more complex that those of prior models, but also in these cases proximity to instabilities is the main indicator of rogue wave occurrence. To support this claim, we correlate the maximum wave strength as well as the higher statistical moments with elements of the nonlinear spectrum.

The result is a diagnostic tool widely applicable to both model and field data for predicting the likelihood of rogue waves. Finally, we show that NLS solutions

with JONSWAP initial data are described by non-Gaussian statistics, in agreement with the TOPLEX field studies of sea surface height variability.

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The Numerical Solving of the Navier-Stokes Equations for Real Gas

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In the present talk, the numerical algorithms are proposed for modeling the heat-pressure phenomena that accompany the body motion at supersonic velocity in the atmosphere consisting of oxygen and nitrogen. The proposed algorithms are constructed on the basis of the Navier-Stokes equations for viscous heat-conducting gas and include two state equations for a pressure and a viscosity depending on temperature for real (not perfect) air. The mathematical model also involves the relation between 3 types of energy for air consisting of N_2 and O_2 molecules in correspondent ratio. The first type is the energy of translational degrees of freedom. It defines the thermodynamic temperature and the pressure in the Navier-Stokes equations. The second one is the energy of rotational degrees of freedom by diatomic molecules. For moderate temperature and pressure, these two types of energy are proportional to one another because of equilibrium between different degrees of freedom like in a perfect gas. But this is not the case for high temperature and pressure. Moreover, the third type of energy is the vibration of atoms in molecules which begins to play a great role in the heat-pressure phenomena only at high temperature. The last two types of energy do not directly define the thermodynamic temperature and the pressure.Nevertheless, under changes of temperature and pressure, redistribution of all three types of energy begins attended by increasing or decreasing the translational energy. Therefore, the system of equations is supplemented by the additional algebraic equation of state relating the specific internal energy with temperature and pressure. It is assumed that the relaxation time for the transition of these three types of energy to the most probable state (the state with maximum entropy) is much less than a time step in the computational algorithm. Therefore, at a given pressure and an internal energy, the temperature is determined by this state with maximal entropy. For numerical computations, we use the table of thermodynamic states of the atmosphere for a given pressure and temperature. A numerical algorithm is proposed for the initial-boundary problem for the extended Navier-Stokes equations on the basis of the combination of the semi-Lagrangian approximation and the conforming finite element method [1].

A numerical experiment illustrates the proposed mathematical model and the numerical algorithm.

Acknowledgement: This work is supported by Project 14-11-00147 of Russian Scientific Foundation.

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Modeling of Josephson Junctions and Structures under External Electromagnetic Radiation

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We present results of numerical simulations of physical features of Josephson junctions, shunted Josephson junctions and coupled system of Josephson junction and magnetic moment. Investigation of phase dynamics and IV-characteristics of these systems under external radiation demonstrate a series of novel effects which might be important for superconducting electronics and quantum computation.

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The Numerical Solving of the Navier-Stokes Equations for Real Gas

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The Numerical Solution of Thermo-poro-elastoplasticity Problems

Before constructing buildings in permafrost areas the careful study of stress-strain state of soils and building foundations must be performed in order to estimate their bearing capacity and stability to avoid issues with maintenance. To determine stress-strain state of frozen soils the numerical modeling of thermo-poro-elastoplasticity problems is used. The mathematical model of considered problems includes the elasto-plasticity equations and equations of heat and mass transfer with phase transition.

The computational algorithm is based on the finite element approximation in space and the finite difference approximation in time. As the model problem we consider the deformation of pile foundations and surrounding soils. Special attention is given to thawing of frozen soils, which can cause additional deformations and lead to loss of stability.

The results of numerical simulation of the three-dimensional problem in the complex geometric area are presented. Calculations are performed using the North-Eastern Federal University computational cluster Arian Kuzmin.

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Noise-Induced Bursting in Rulkov Model

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A problem of mathematical modeling and analysis of the stochastic phenomena in neuronal activity is considered. As a basic example, we use the nonlinear Rulkov map-based neuron model with random disturbances. In the deterministic case, this one-dimensional model demonstrates quiescence, tonic and chaotic spiking regimes. We show that due to presence of random disturbances, a new regime of noise-induced bursting is generated not only in bistability zones, but also in monostability zones. To estimate noise intensity corresponding to the onset of bursting, the stochastic sensitivity technique and confidence domains method are applied.

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Analysis of Stochastic Phenomena in 2D Hindmarsh-Rose Neuron Model

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In mathematical research of neuronal activity, conceptual models play an important role. We consider 2D Hindmarsh-Rose model, which exhibits the fundamental property of neuron, the excitability. The aim of our work is to study how random disturbances affect this property. The effects of noise are analysed in various parametric zones of the model. We show that under random disturbances, the new complex dynamic regimes form in the system. For the analysis of the stochastic phenomena, we apply the stochastic sensitivity technique and confidence domains method.

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On the Stability and Control Strategies for Impulsive Lotka-Volterra Systems of Fractional Order

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The goal of the present work is to develop an impulsive fractional Lotka-Volterra model that bring together the advantages of using of fractional-order derivatives whose nonlocal property makes the fractional calculus a suitable tool for modeling actual population dynamics systems and the control power of some impulsive perturbations.

The first main objective of this research is to provide asymptotic stability criteria for the model's equilibrium. To extend the application of fractional calculus to impulsive Lotka-Volterra systems, the Mittag-Leffler stability concept and Lyapunov-like functions will be used. The second objective is elaborating of impulsive control strategies to the equilibrium states.

Developing of stability and control strategies for fractional-order systems would have many applications. In particular, it will play an important role in understanding the control power of some instantaneous perturbations and experiences abrupt changes at certain instants which can be used to compensate the deviating trend in fractional Lotka-Volterra models.

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Numerical Simulation of the Convective Heat Transfer on High-Performance Computing Systems

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In this work, we consider a coupled system of equations for the convective transport and flow problems. which describes the processes of the natural or forced convection in some bounded area. Mathematical model include the Navier-Stokes equation for flow and the transport equation for the heat transfer. Numerical implementation is based on the finite element method, which allows to take into account the complex geometry of the modeled objects. For numerical stabilization of the convective transport equation for high Peclet numbers, we use streamline upwinding Petrov-Galerkin (SUPG) method.

The results of the numerical simulations are presented for the 2D and 3D formulations. As the test problems, we consider the flow and transport problems in technical construction under the conditions of heat sources and boundary conditions. We couple this formulation with heat transfer problem in the surrounding grounds and investigate the influence of the technical construction to the ground in condition of the permafrost and the influence of the grounds to the temperature distribution in the construction. Numerical computation are performed on the computational cluster of the North-Eastern Federal University.

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Nonlinear Dynamical Analysis of Plates by Efficient Parallel Algorithms

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Parallel implementation of the numerical methods used for analyzing the nonlinear vibrations of elastic plates is developed and presented. The equation of motion of the plate is derived by Hamilton's principle. Mindlin–Reissner's plate theory is assumed and geometrical type of nonlinearity is considered. The equation of motion is discretized into a system of ordinary differential equations by the finite element method.

The dynamical analysis is performed in the frequency domain due to external harmonic excitations. The variation of the periodic steady-state response of the plate with the excitation frequency is investigated. Shooting method is used to compute the periodic solution and prediction for the next point from the frequency-response curve is defined by the continuation method.

Often due to accuracy requirements of plates with complex geometries, the discretization scheme leads to large-scale models. The computation of periodic responses of large-scale systems becomes computationally burdensome and time consuming process. The parallel realization of the numerical methods used to compute the frequency-response curves becomes essential part for the future usage of the nonlinear dynamical analysis of real-life engineering applications.

Parallel realization of the shooting method is developed for distributed memory machines. Its scalability and speedup are investigated. The method consists of several matrix-matrix computations, solutions of sparse and dense systems and solutions of eigenvalue problems. The proposed parallel implementation efficiently spreads the computations and memory among multiple processors. In addition, the computation of the Jacobian is another time consuming process, which is necessary for solving the nonlinear equation of motion. Parallel computation of the Jacobian is presented and implemented within the shooting method. The potential of the the proposed parallel realization of the numerical methods is demonstrated by computing the nonlinear frequency response curve of plate with complex geometry

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Description of Data Reanalysis of Discharge and Gauge Height for the Amazon River Basin

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The Amazon River is the world's largest, discharging more water to the ocean than any other river. Study of the world's freshwater resources becomes more significant with increasing awareness of global climate change and its potential effect on those resources. In this talk, we present a method of reanalyzing the daily

discharge and gauge height data for active gauge stations throughout the Amazon River Basin. The data was originally obtained from the web site maintained by ANEEL – Brazilian Electricity Regulatory Agency. We describe the problems encountered in the original data and the assumptions applied in the reanalysis procedure. The reanalysis consisted of changing the decimal notation, filtering inconsistencies, and filling in missing data, by using Stochastic Models. The reanalyzed data is fundamental for future modeling of the river network, and prediction of the water's budget applied to Large Scale Climate Models.

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Velocity and Shear Rate Estimates of Some Non-Newtonian Oslillatory Flows in Tubes

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The two-dimensional Newtonian and non-Newtonian (Carreau viscosity model used) oscillatory flows in straight tubes are studied theoretically and numerically. The corresponding analytical solution of the Newtonian flow and numerical solution of the Carreau viscosity model flow show differences in velocity and shear rate, which occur to be the largest at low Womersley numbers. This result is estimated as well theoretically for the velocity and shear rate differences between the two models. As numerical examples the blood flow in different type of arteries and the polymer flow in pipes are considered.

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Towards Efficient Nonlinear Option Pricing with GPU

Computing

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Nonlinear option pricing is a new approach for traders, hedge funds, or banks to obtain more accurate option price and to do fast model calibration using huge market data. Numerically the main problem is to solve fully nonlinear PDEs and strategies like Newton's method and ADI scheme are employed. Batch operations are used as well for calculating different option pricing problems together at the same time. In this presentation, we will introduce how to use OpenACC and CUDA libraries to accelerate the whole computation. The complexity analysis will be shown first. We can obtain around 2X speedup by using OpenACC, and around 5X speedup by using libraries from cuSPARSE for solving tridiagonal systems and cuBLAS for computing level-2 functions.

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Spatial Nonlinear Absorption of Alfven Waves by the Dissipative Plasma

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In the report, we study numerically the nonlinear absorption of a plane Alfven wave incident on the stationary boundary dissipative plasma caused by the magnetic viscosity, hydrodynamic viscosity and thermal conductivity of electrons and ions, bremsstrahlungand and the energy exchange between plasma components. Relevance of the proposed research is caused by a number of workers in 2011, the heating mechanism of solar corona and solar wind generation as a result of the absorption of plasma Alfven waves generated in the lower significantly colder layers of the sun. Since, as shown by calculations, the absorption of Alfven waves occurs at wavelengths order of the skin depth, in which the equations of classical MHD clearly inapplicable, the research is based on equations of two-fluid magnetohydrodynamics taking into account the inertia of the electrons. The proposed implicit difference scheme for calculating the plane-parallel flows of two-fluid plasma revealed a number of important patterns of absorption, in particular to study the dependence the absorption on Alfven wave frequency and electron thermal conductivity and viscosity,

as well as the depth and the velocity of plasma heating during the penetration of Alfven waves interacting with the dissipative plasma.

Acknowledgement: The study was performed by the grant from the Russian Science Foundation (project No.16-11-10278).

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Solitons in Two-Fluid MHD with Electron Inertia

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In the report, the interaction of solitary waves in a model of two-fluid MHD with view of the inertia of the electrons is studied analytically and numerically. We consider the wave in linearly polarized magnetic field. The main difference of this work is the use of "exact" equations, and is not use of approximate approach (model equation). Numerically it shows that solitary waves really are solitons, i.e. their interaction similar to the interaction of the colliding particles.

Acknowledgement: This work is supported by the Russian Foundation for Basic Research (grant No.15-01-03085, No.16-31-00302).

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Polynomial Interpolation of the Function of Two Variables with Large Gradients in the Parabolic and Exponential Boundary Layers

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The problem of interpolation of the function of two variables with large gradients in the parabolic and exponential boundary layers is investigated. The case of the exponential boundary layers is considered in [1]. It is assumed that the function has large gradients near the boundaries of a rectangular domain. Such function corresponds to the solution of the convection-diffusion problem with dominant

convection. It is known that the error of polynomial interpolation on a uniform grid for such function can be of the order of O(1). It is suggested to use the two-dimensional polynomial interpolation on the piecewise uniform Shishkin. The uniform with respect to the singular perturbation parameter error estimate is obtained. Some numerical results are discussed.

Acknowledgement: Research has been partially supported by the Russian Foundation for Basic Research grant No.15-01-06584.

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Monte Carlo methods for Numerical Integration for European Option Pricing

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The pricing of options is a very important problem encountered in financial markets today. The famous Black-Scholes model provides explicit closed form solutions for the values of European style call and put options. In this paper, we illustrate examples of highly accurate Monte Carlo and/or quasi-Monte Carlo methods for multiple integrals related to the evaluation of European style options. We compare four very effective Monte Carlo algorithms for multidimensional integrals. It is known that as long as the integral is sufficiently regular, lattice rules generally outperform not only basic Monte Carlo but also other types of low discrepancy sequences. On the other hand, the adaptive Monte Carlo algorithm is another widely used method for evaluation of integrals, which gives good results regardless of the integral's smoothness. We make a comparison with quasi Monte Carlo method with Sobol sequence which is another highly accurate method for solving multidimensional integrals which gives superior results to crude Monte Carlo method.

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Effective Medium Theories from the 19th to the 21st Century: Finite Samples, Interface Boundaries, Non-Asymptotic and Nonlocal Approximations

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We explore a broad range of effective medium theories, starting with an overview of the classical ones (Maxwell Garnett, Clausius-Mossotti,Bruggemanand others) and leading to non-asymptotic homogenization of electromagnetic metamaterials with nontrivial magnetic effects at high frequencies. Our key points are as follows:

- Several aspects of the homogenization problem are often passed over in the literature and yet are essential: the finite size of the sample and the role of interface boundaries;non-asymptotic and nonlocal approximations.
- Westrive to unify classical theories with the new ones we developed. One unification framework involves Dirichlet-to-Neumann maps for finite samples.

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Numerical Statistics for Estimation of Initial Meteoroid Form from Empirical Mass Distribution of Recovered Fragments

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This paper is concerned with a numerical technique for meteoroid shape estimation based on empirical statistics of fragment mass distributions. The idea is generalized from the experiments on brittle fracturing. Each experiment produces multiple fragments of size lesser than or equal to the least dimension of the body. The common assumption states that the amount of fragments depends on fragment

masses as a power law with exponential cutoff. The scaling exponent essentially indicates the initial form of the fragmented body. We apply the technique of scaling analysis to the empirical data on the mass distributions for Kosice, AlmahataSitta and Bassikounoumeteorites. These mass distributions manifest undersampling for small fragments and exponential cutoff due to finite size effect. We apply methods of numerical optimization to estimate best values for the scaling exponent,the lower and upper constraints as well as the dimensionless shape parameter. Next, the shape parameter is translated into the triad of relative sizes along respective cartesian axes. Therefore, the obtained triad yields one of three distinct options of the estimated shape: rod-like, plate-like and sphere-like.

Acknowledgement: The work was supported by the Russian Foundation for Basic Research, Project 16-07-01072

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Numerical Simulation of the Stress–Strain State of the Dental System

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We present mathematical models, computational algorithms and software, which can be used for prediction of results of orthopedic treatment. More interest issue is biomechanics of the periodontal complex because any prosthesis is accompanied by a risk of overloading the supporting elements. Such risk can be avoided by the proper load distribution and prediction of stresses that occur during the use of dentures.

In this regard, we developed the mathematical model of the periodontal complex and its software implementation. This model is based on linear elasticity theory and allows to calculate the stress tensor and displacement fields in periodont and jaw bone.

The input parameters for the developed model can be divided into two groups. The first group of parameters describes the mechanical properties of periodont, teeth and jaw (for example, elasticity of periodontal ligament etc.). The second group characterized the geometric properties of objects: the size of the teeth, their spatial coordinates, the size of periodont etc.

The mechanical properties are the same for almost all, but the input of geometrical data is complicated because of their individual characteristics. In this connection, we develop algorithms and software for processing of images obtained by computed tomography scan and for constructing individual digital model of the tooth-perio-dont-jaw system of the patient.

Integration of models and algorithms described allows to carry out biomechanical analysis on three-dimensional digital model and to select denture design.

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Numerical Modeling of Wave Propagation Processes in Micropolar Rods and Thin Plates

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Thin-walled structures such as rods, plates and shells are widely used in civil engineering, aero-space industry, medical and biological fields. To describe microstructure of a material the theory of micropolar (Cosserat, nonsymmetric) media with independent rotational degrees of freedom of particles is applied. Mathematical models of the processes of wave propagation in micropolar rods and thin plates are the reduction of the three-dimensional Cosserat continuum equations to the one- and two-dimensional equations. The system of equations can be written in the form of thermodynamically self-consistent conservation laws suitable for the numerical computations.

Numerical algorithms for the solution of dynamic problems in micropolar media are based on two-cyclic decomposition method in combination with explicit monotone finite-difference schemes of the "predictor-corrector" type. The results of numerical computations of dynamic problems on wave propagation under the action of distributed and concentrated periodic and impulse loads are shown.

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Solution of the Neutronics Code Dynamic Benchmark by Finite Element Method

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The objective is to analyze the dynamic benchmark developed by Atomic Energy Research for the verification of best-estimate neutronics codes. The benchmark scenario includes asymmetrical ejection of a control rod in a water-type hexagonal reactor at hot zero power. A simple Doppler feedback mechanism assuming adiabatic fuel temperature heating is proposed. The finite element method on triangular calculation grids is used to solve the three-dimensional neutron kinetics problem. The software has been developed using the engineering and scientific calculation library FEniCS. The matrix spectral problem is solved using a scalable and flexible toolkit SLEPc. The solution accuracy of the dynamic benchmark is analyzed by condensing calculation grid and varying degree of finite elements.

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Generalized Multiscale Finite Element Method (GMsFEM) for Non-Newtonian Fluid Flow in Perforated Domains

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In this work, we consider a non-newtonian fluid flow in perforated domains. In many applications, these problems have a multiscale nature arising because of the perforations, their geometries, the sizes of the perforations, and configurations. The solution techniques for these problems require high resolution. In particular, the discretization needs to honor the irregular boundaries of perforations. This gives rise to a fine-scale problems with many degrees of freedom which can be very expensive to solve. We develop a multiscale approach that attempt to solve such problems on a coarse grid by constructing multiscale basis functions. In particular, we are interested in cases when there is no scale separation and the perforations can have different sizes. In this work, we follow Generalized Multiscale Finite Element Method (GMsFEM) and develop a multiscale procedure where we identify multiscale basis functions in each coarse block using snapshot space and local spectral problems. We show that with a few basis functions in each coarse block, one can accurately approximate the solution, where each coarse block can contain many small inclusions.

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On the Numerical Solution of the Boundary Inverse Problem for a Parabolic Equation

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Boundary inverse problems have quite important applications among mathematical physics inverse problems. They are associated with diagnostic problems when additional measurements inside the computational domain is necessary to restore the boundary regime. The boundary inverse problems belong to the class of conditionally correct problems, and therefore for their numerical solution requires the development of special computational algorithms. One of the common approaches to solving unstable problems for partial differential equations is the method of quasi-inversion. It is based on such a perturbation of the original equation that perturbed problem becomes correct and parameter perturbations act as a regularization parameter.

The paper deals with a different approach solving a boundary inverse problem for one-dimensional parabolic second-order equations, which consists in restoring the boundary regime according to measurements inside the computational domain. For the numerical solution of the inverse problem it is proposed to use an analog computational algorithm, proposed and developed to meet the challenges of identification the right side of the parabolic equations in the papers cite [1,2], based on the decomposition of a special task at each of time step. Results of the numerical calculations are presented and discussed.

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Numerical Simulation of Meteoroid Dark Flight Trajectory

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This paper is concerned with numerical simulation of meteoroid dynamics. Bolide ballistics is approximated via a system of differential equations for movement and heat transfer, using hard sphere approximation for meteoroid fragments. This system of equations is solved in Lagrange variables via Runge-Kutta methods. We obtain fragment trajectories with respect to the reference ellipsoid WGS-84. The drag force of atmospheric air is computed via Henderson formula valid for wide ranges of Reynolds and Mach numbers.

The parameters of surrounding gas are obtained from the COSPAR International Reference Atmosphere (CIRA-86), which includes monthly zonal wind chart. The impact pressure is computed taking into account entropy jump through a bow head shockwave and consequent isentropic deceleration of the ow in the vicinity of streamlined sphere. Meteoroid fragmentation is modeled as sequential division of parent body into two parts using random weighting coefficient for parent mass. The fragmentation event is triggered when the hemisphere-averaged value of impact pressure exceeds the threshold of relative body strength, which nonlinearly depends on ration of initial meteoroid mass to current mass of considered fragment. To compute trajectory divergence for newly-formed splinters we introduce the repulsive force, dependent on impact pressure, cross sectional areas of mutually repulsing bodies and distances between them. The set of mathematical models is implemented as the program complex. Preliminary computational results show that fragmentation altitude, terminal velocities and maximum splinter masses are in good agreement with corresponding observations and measurements.

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Risks Assessment Concept as a Factor for Managerial or Investment Decisions

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Risks assessment concept has been more often included into the list of factors upon which managerial or investment decisions are taken. Quantitative risk assessment can significantly improve its management. Nowadays Markowitz risk assessment methods have already become classical, they are based on standard deviation of financial instruments' profitability. Further development of financial technologies resulted in additional risk assessment methods, including Value-at-Risk (VaR), Shortfall, beta-analysis of CAPM theory, Maximum Loss, ART, Capital at-Risk, and others.

Practical use of standard deviation, beta-analysis and variation coefficient showed completely opposite results in some cases (based on Ukrainian stock market data). Therefore, there is a need to learn the reasons of differences and develop an optimization model. This model should help uniting the diverse indicators and provide a more comprehensive stock risk assessment; as a result, it should identify attractive stock for different strategies. The study found out that standard deviation is deeply dependent on trade activity, and investment decisions in most cases are taken within a single market. In other words, investors have limited choice of instruments. The basis of standard deviation method is profitability, but it does not fit all investment strategies. As a result, the use of standard deviation without combining it with another metrics will give incorrect conclusions.

Diversity of the chosen risk assessment tools is driven by different calculation methods and different risks interpretation. For example, standard deviation when characterizing profitability volatility, includes only historical factors that influenced on the stock price. Beta-coefficient method in addition takes into account the general tendencies of a particular financial market. Finally, variation coefficient allows to compare the risk with expected income.

As a result, we believe that the developed model, based on standard deviation, beta coefficient, and variation coefficient, will provide investors with a comprehensive risk assessment tool while they develop their investment strategies.

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Hybrid Numerical Model of Shock Waves in Collisionless Plasma

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We present a 2D hybrid numerical plasma model of generation and structure of collisionless shock waves in plasma and ion acceleration on their front considering physical processes in supernova remnant shock precursor. In modeling a shock wave is generated by sending a supersonic flow against a reflecting wall. The following interaction between incoming and reflected plasma flows lead to formation of waves, the structure of which depends on a flow velocity. The hybrid approach reduces the computational expenses relative to a fully kinetic one, and from other hand, permits to model ions with a greater accuracy than the MHD allows. Also, another important advantage of the hybrid approach is the possibility to study the important instabilities on an ion time scale, neglecting the modes associated with electrons. In the current work a new computational scheme where stability condition allows carry out computations on more wide set of computational and physical parameters is presented.

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The Conservative Semi-Lagrangian Method for the Advection Problem with the Bogner-Fox-Schmit Elements on Rectangles

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Nowadays a semi-Lagrangian approach to the approximation of the advection terms is intensively developed in the fluid dynamics applications, the fiber dynamics, the heat-conduction and shallow water equations, the equations describing atmospheric flows. The main feature of several semi-Lagrangian approaches consists in the approximation of the advection terms as the whole "directional" (Lagrangian) derivative in the motion direction.

In the present talk an initial-boundary value problem is considered for the two-dimensional advection equation defined by a scalar time-dependent hyperbolic conservation law. To construct a discrete problem, a uniform rectangular grid is considered. At each time level we find an approximate solution by the finite element method with the application of the Bogner-Fox-Schmit elements on rectangles. These elements provide the C1-continuity of an approximate solution. Moreover, a discrete analogue of the integral balance equation is valid between two neighboring time levels. We describe the technique of the approximation of each integral in this balance equality. Numerical experiments show that the method preserves the shape of the solution in the neighborhood of strong gradients. Besides, the algorithm is resource-intensive and well-parallelizable (because of data independence in the general space loop). We discuss parallel implementations of the method for modern high-performance architectures.

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Risks Assessment Concept as a Factor for Managerial or Investment Decisions

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Agent in Grids Extended to Clouds

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The presented work is an attempt to extend considerations from Agents in Grid (AiG) project into Clouds. The AiG project is aimed at development of an agent-semantic infrastructure for AiG efficient resource management in the Grid. Decision support within the AIG system helps the user without in-depth knowledge to choose optimal algorithm and/or resource to solve a problem from a given domain, and later to choose the best contract defining terms of collaboration with the provider of a resource used to solve the problem. It is relatively easy to notice that solutions considered in the context of AiG system can be easily extended to computational clouds that evolved from computational grids.

Cloud computing refers to an architecture in which groups of remote servers are networked to allow online access to computer services or resources. The general vision is the same as in case of computational grids i.e. to reduce cost of computing, as well as to increase flexibility and reliability of the infrastructure. However, there are also important differences. It can be observed that grids are designed with bottom-up approach i.e. heterogenous resources are combined and offered to the

end-users. On the other hand, clouds follow the top-down design approach in order to serve a specific use cases (functionalities). Clouds may be composed from grids with services and interfaces superimposed on them, offering limited set of exposed features. In grid systems clients look for resources that match their needs, in cloud systems they look for services.

In the cloud computing model we can distinguish three roles: infrastructure provider (leases resources on demand), service provider (rents resources to one or more infrastructure providers) and service client (final consumer). Despite some differences, problems for grids and clouds are mostly the same, i.e., (i) to define methods by which consumer discovers, requests and uses services (and related resources), (ii) to support negotiations between service provider and resource provider, as well as client and service provider. Both grid and cloud computing require SLA-oriented service negotiation, distributed resource management and scheduling. In this context, it will be shown that knowledge representation based on ontologies can enable common understanding of cloud architecture (as in case of grids), and can give possibility to, for instance, compare SLA received from different cloud providers. As it was shown in the case of grids, integrating software agents, semantics and cloud computing could enable highly efficient, intelligent systems making clouds more flexible and autonomic, and on the other hand, providing agent systems with reliable and scalable computing infrastructure.

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A New Method in Graphical Bioinformatics

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A new method which belongs to the class of methods called Graphical Bioinformatics, 3Ddynamic Representation of DNA Sequences, [1,2] is proposed. The DNA sequences can be compared both graphically and numerically. This approach removes the graphical degeneracy present in our previous method, 2D-dynamic Representation of DNA Sequences. The descriptors, i.e., the numerical values characterizing the sequences, are composed using the ideas of classical mechanics. For example, moments of inertia of the graphs are used as descriptors. In this approach,

the accuracy of description is very high: a pair of sequences which differ by only one base can be recognized.

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Numerical Study of a Model of Stacked Long Josephson Junctions

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A system of stacked long Josephson junctions (LJJs) with inductive and capacitive coupling is studied. Mathematical formulation of problem is considered as well as a procedure of calculation of physical characteristics of the LJJ system. Numerical approach and MPI-based parallel implementation is presented for solution of respective system of nonlinear partial differential equations. Results of numerical simulation are discussed.

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Atmospheric Characteristics Statistic Study of Ruse Region, Bulgaria

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Ruse region is situated in the north-eastern part of Bulgaria and is one of the medium sized regions in the country, concerning territory and population Ruse is located 320 km from the capital of Bulgaria – Sofia and 70 km from the capital of Romania – Bucharest. The city stretches some 11 km along the banks of the Danube River. The northern boundary of Ruse region goes along the Danube river valley and coincides with the state boundary of the Republic of Bulgaria and the Republic of Romania.

The climate of the region of Ruse is temperate continental, characterized by cold winters and dry, warm summers. Danubian terrace, including the region of Rousse district, is open to northeasterly winds. Spring and autumn are short.

Regular meteorological measurements for temperature, air humidity and atmospheric pressure exist since 1874 in Bulgaria. We studied information from 40 years period measurements of temperature, air humidity and atmospheric pressure in Ruse region, Bulgaria. Descriptive statistics and graphics are presented and commented in this paper. So far absolute minimum temperature is $-27°C$ and absolute maximum temperature is $+44.0°C$ for Ruse region. Some data for Ruse region are also compared with official basic data for Bulgaria.

It is shown that mean values of the temperature in Ruse region are slightly go up for last 10 years and they are bigger than the mean temperature for Bulgaria. This could be a proof for climate change in Ruse region of Bulgaria.

The most variable atmospheric parameter is air humidity during the spring seasons. The hardest change of temperature and atmospheric pressure is during January. Temperature has biggest change in January and smallest – in July. Humidity has biggest change in April and smallest – in October .Atmospheric pressure has biggest change in January and smallest – in July.

Characteristics temperature and atmospheric pressure of spring (April) and autumn (October) are very similar. Summer temperatures and atmospheric pressure (July) have smallest change.

It is well known that there are different points of view regarding the causes of climate change. The highest percentage of authors, however, insists that the influence of anthropogenic factors is too serious and it cannot be ignored. Thus the change of temperature and humidity may be correlated with atmosphere pollution for example with fine dust particles. In Ruse region it is observed that water of river Danube and the air pollution increased. Especially strong is the air pollution during the autumn-winter season with particulate matter and oxides of sulfur, nitrogen and carbon in the last decade. The reasons for this are not only transportation, but the use of solid fuel heating. Also it is known that the valleys and places along

the rivers are polluted stronger than the plains and slopes. All this in our opinion may be a reason for the increase in average temperatures for the period examined. Air pollution maybe affects temperature, atmospheric pressure and humidity and this influence has to be studied and analyzed in greater depth.

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