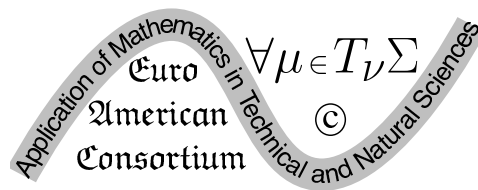


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# BOOK OF ABSTRACTS



Euro-American Consortium for Promoting the Application  
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**Edited by Michail Todorov**

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## The Dynamics in the In-Plane Oscillations of a Geometrically Nonlinear Lattice

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In this work we investigate the in-plane damped oscillations of a finite lattice of particles coupled by linear springs and viscous dampers under distributed harmonic excitation. Employing a Melnikov analysis we study the existence and persistence of localized traveling waves and study their linear stability. We find conditions under which the homoclinic orbits persist using the homoclinic Melnikov Method. Our analytical results are found to be in good agreement with direct numerical computations.

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## Numerical Simulation of the Transport and Flow Problems in Perforated Domains Using Generalized Multiscale Finite Element Method

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Many processes in real applications have multiscale nature. These include flow and transport in porous media, deformation in composite materials, filtration processes and so on. In these physical processes, the transport of the material can be described by the convection-diffusion equation. The convection term in the transport equation is governed by a flow velocity field. The flow can be described by Darcy equation or the steady-state Stokes equation. Numerical solutions for flow and transport equations are expensive and require resolving fine-scale details. For

this reason, some type of model reduction is necessary. In this work, we consider transport and flow processes in perforated domains. For coarse grid approximation, we use Generalized Multiscale Finite Element method (GmSFEM) and construct local multiscale basis functions. We present numerical results for model problem in two dimensional perforated domain.

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## Estimation Problems for Impulsive Systems

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In this talk, we consider estimation problems for linear  $n$ -dimensional systems  $\dot{x} = A(t)x + B(t)\dot{v}$ ,  $t \in [0, T]$ , with an observation equation  $y(t) = G(t)x + w(t)$ . Here  $v(\cdot) \in \text{BV}(0, T)$  is an uncertain function of bounded variation and a disturbance function  $w(\cdot) \in L_2^n(0, T)$ . Impulse impacts arise, for example, in space maneuvering, where the mass of the ship changes intermittently because of fuel consumption on each operation of rocket engines. The function from  $\text{BV}(0, T)$  is a sum of an absolutely continuous function, a saltus function, and a singular function. We use the approach from [1] and suppose that functions  $v(\cdot)$  have no singularities, the absolutely component has the derivative from  $L_2^p(0, T)$ , and the saltus function has jumps only in prescribed instants  $0t_1 \dots T_N T$ . We deal with two kind of problems. Introduce a Hilbert space  $\text{DS}(0, T)$  consisting of functions of the form  $v(t) = v(0) + \int_0^t z(s)ds + \sum_{k=1}^N \chi_{[t_k, T]}(t)\Delta y(t_k)$  and suppose that all the uncertain functions  $v(\cdot) \in \mathcal{V} \subset \text{DS}(0, T)$ , where  $\mathcal{V}$  is a convex compact set. Here  $\chi_A$  is a characteristic function of the set  $A$  and  $\Delta y(t_k) = y(t_k) - y(t_k-)$ . First, let the function  $w = 0$  in the observation equation. We seek for an operation  $\phi(\cdot)$  with bounded norm solving the problem

$$\max_{v(\cdot) \in \mathcal{V}} \left| \int_0^T \phi(t)y(t)dt - l'x(T) \right| \rightarrow \min_{\phi(\cdot)}$$

under condition  $\int_0^T \phi(t)y(t)dt = l'x(T)$  with  $v(\cdot) = 0$ . We investigate the existence of the solution and formulate the dual control problem. In the second problem under investigation we suppose that uncertain functions  $v(\cdot)$  along with disturbances  $w(\cdot)$  in observation equations form an infinite-dimensional ellipsoid in the Cartesian product  $\text{DS}(0, T) \times L_2^m(0, T)$ . We define the information set for our system, give the defining relations, and describe the evolution of this set. Some examples are considered.

**Acknowledgement.** The work is supported by the Russian Fund for Basic Research, Project No. 18-01-00544-a.

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## Estimation Problems for Impulsive Systems

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The long term properties, like co-existence and extinction, are usually determined by the demographics of the competing species as well as competition advantages. Here we consider the special case of the competing species with the same demographics and where their interaction has the same impact on each one. We show co-existence of all species can be destabilized by sufficient level of conspecific support.

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## Model of the Formation of the Multiphase Zone between the Inclusion and the Matrix during the Composite Synthesis

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Liquid-phase methods of preparation of composite materials allow producing of complex shape products with minimal further processing. The process of forming a composite by casting with crystallization under pressure is used to increase density of casting and improve uniformity of particle distribution in the metal matrix. During the crystallization process the transition layer with a new chemical compound is formed between the matrix and the inclusion. The inclusions are

coated previously to improve the interphase bonds. Of particular interest is represented the processes at the phase boundary, defining the physical and mechanical properties and performance characteristics of the product. In this work we analyzed numerically the spherically-symmetric problem about formation of the transition zone between the coated particle and the matrix. In the general case in a spherical coordinate system, the model includes diffusion equations for moving elements and kinetic equations for chemical compounds. To solve the diffusion equations, implicit difference scheme and double sweep method are used. The kinetic equations are solved by the Euler method. The model takes into account diffusion and formation of the phase in the transition zone. The aim is to study the influence of technological parameters on the thickness and composition of this zone.

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## **Inverse Problems in Industry: Theory and Methods**

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Inverse problems arise in a number of important practical applications, ranging from biomedical imaging to seismic prospecting. This work sheds light on both the underlying mathematics and the computational methods used to solve inverse problems. It also addresses specialized topics like image reconstruction, parameter identification, total variation methods, nonnegativity constraints, maximum likelihood estimation, Bayesian estimation and regularization parameter selection methods. Physical theories allow us to make predictions: given a complete description of a physical system, we can predict the outcome of some measurements. This problem of predicting the result of measurements is called the forward problem. The inverse problem consists of using the actual result of some measurements to infer the values of the parameters that characterize the system. While the forward problem has (in deterministic physics) a unique solution, the inverse problem does not. As an example, consider measurements of the gravity field around a planet: given the distribution of mass inside the planet, we can uniquely predict the values of the gravity field around the planet (forward problem), but there are different distributions of mass that give exactly the same gravity field in the space outside the planet. Therefore, the inverse problem of inferring the mass distribution from observations of the gravity field has multiple solutions. A collection of MATLAB m-files used to generate many of the examples and figures are available in this work. These resources enable scholars to conduct their own computational experiments in order to gain insight. Finally, we provide templates for the implementation of

regularization methods and numerical solution techniques for industrial inverse problems like the determination of the depth dependence of the director field in a liquid crystal cell from polarized light measurements, capacitance tomography for monitoring flow in pipes, and a problem in which the ocean current is estimated from the position of a cable towed behind a geophysical survey ship.

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## Stochastic Dynamics in the Bistable Goldbeter Model

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Problems of the mathematical modeling and analysis of the enzymatic reactions in presence of random disturbances are considered on the example of the conceptual dynamical model suggested by Goldbeter. This model comprises two variables, namely, the substrate and product concentrations. It possesses mono- and bistable regimes with equilibria and self-sustained oscillations. The random disturbances can induce complex multimodal oscillations. We study mechanisms of the generation of such stochastic oscillations. For the parametric analysis of noise-induced phenomena in Goldbeter model, we use stochastic sensitivity functions technique and the method of confidence domains. Peculiarities of the stochastic dynamics near the critical bifurcation points (sub- and supercritical Andronov-Hopf, saddle-node) are analyzed.

**Acknowledgements.** The work was supported by Russian Science Foundation (No 16-11-10098).

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## Impact of the Parametric Noise on Map-Based Dynamic Systems

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Discrete-time nonlinear dynamical systems with general parametric stochastic disturbances are considered. For such systems, a problem of the probabilistic analysis of the random states dispersion around attractors is studied. For the constructive approximation of probabilistic distributions, the method of the stochastic sensitivity is developed. Matrix equations for the asymptotics of moments of deviations from attractors are derived. An application of the suggested mathematical theory to the analysis of noise-induced phenomena in nonlinear population models is discussed.

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## Fuzzy Method of Identification the Results of Electrolytic Impedance Spectroscopy

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Electrochemical impedance spectroscopy is a widely used method for determining the characteristics and structure of the systems under study, both in general and their individual constituents. The essence of the method is to obtain and analyze the dependence of the reactance of the system under study on the active resistance in a large frequency range of alternating current. The values of the



resistances for each frequency are determined from the magnitude and phase shift of the induced current sine wave  $I = f_1(t)$  upon imposing a sinusoidal varying voltage  $U = f_2(t)$  on the system. The method has a number of drawbacks that do not allow it to be applied with sufficient accuracy to some practically important systems. So, the overwhelming majority of the systems studied have a nonlinear dependence  $I = f_1(U)$  and their analyzed dependence in coordinates  $(U, I)$  is theoretically represented as an ellipse, which is very different from the ideal shape. As a consequence, the impedance results have an unaccounted error. Moreover, the standard 20-point data per decade of the signal frequency with an unaccounted error is not enough for a full analysis of the impedance curve. There are cases when, for this reason, in a certain frequency range, the data calculated using an equivalent circuit have a significant deviation from the actual values. The increasing of the number of analyzed points and determination of their error can be made by using oscilloscopes with a wide-frequency oscillator. However, when modulating signals of complex shapes, the relationship between the data being set and received remains unclear.

In the present paper, it is proposed to use previously proposed methods of fuzzy identification of experimental results [1] and a modified method for determining the frequencies of systems with deviations [2]. The application of these methods to the interpretation of the results of experimental data obtained in the spectroscopy of electrolytic impedance makes it possible to take into account the uncertainty of the data and to draw valid conclusions about the nature and structure of the system under study.

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## Parallel Algorithm for Numerical Modeling of Colliding Ultrarelativistic Beams with Crossing Angle

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We present a new algorithm for mathematical modeling of colliding beams dynamics in supercolliders. A single-pass collision of the high-energy beams makes

possible their strong deformation or even disruption, and the study of the beam stability is needed. We consider the motion of the charged particle beams with the high relativistic factors of the particles and large crossing angles in self-consistent electromagnetic fields. The standard numerical models and algorithms are quasi-three-dimensional and have difficulties with taking into account large crossing angles (20mrad). We present a fully three-dimensional algorithm, based on solution of the Vlasov equation and set of Maxwell equations with particle-in-cell method. In the 3D modelling the problem is not only the computational speed, but also the insufficient memory of one processor to keep the data for the beams with highly nonuniform density distribution. The presence of the high value of the relativistic particle factor is a fundamental feature of the non-linear problem and leads to high gradients. The particle and domain parallelization helped us to perform numerical simulations with  $10^9$  particles on  $200^3$  grid. We present the computational results and analysis of the beam evolution for the case of two focused colliding beams. The computations were performed on the supercomputer Lomonosov (MSU, Moscow), Polytechnic (SPBSTU, Saint Petersburg) and SSCC cluster (ICM&MG SB RAS, Novosibirsk).

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## Method of Network Modeling as a Criterion for Optimization the Process of Business Planning

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This article discusses the problem of multi-criteria optimization of business project control in the presence of several technologies for their implementation. On the basis of network modeling in this article, an economic-mathematical model and a method for solving the problem of multicriteria optimization of the control of the process of implementing business projects in the presence of several technologies are proposed. The practical example shows the formation of network models, the calculation of their parameters, the critical paths and the optimal time for implementing the selected technologies of the business project. Also shown is the choice of the optimal technology from a set of possible technologies for the implementation of the project, taking into account the time and cost of performing the work. Network economic and mathematical modeling is a tool to increase the company's

competitiveness. The proposed model and method of solving the problem of control business projects can serve as a basis for the development, creation and application of appropriate computer information systems to support the adoption of control decisions by businessmen.

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## Special Discontinuities in Models of Continuum Mechanics

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Solutions of a problem about an arbitrary discontinuity disintegration for the generalized Hopf equation are under investigation. The solution is constructed from a sequence of the non-overtaking Riemann waves and discontinuities having the stable stationary and non-stationary structure. The influence of small-scale effects of dissipation and dispersion are analyzed. Small-scale processes determine a discontinuity structure and a set of discontinuities with stationary structures. Among discontinuities with stationary structures there are special ones on which (in addition to relations following from conservation laws) some additional relations should be satisfied which follow from the requirement for the discontinuity structure to exist. The existence of special discontinuities leads to non-unique way to construct self-similar solutions to the problem of arbitrary discontinuity disintegration.

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## Thermoacoustic Waves in Pulsed Pirani Gauge MEMS. Frequency Analysis

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The transient heat transfer process is studied in rarefied gas confined between two stationary concentric cylinders. The inner cylinder (filament) is subjected to a periodically heating-cooling cycle. The energy transfer is modeled with continuous model based on Navier-Sokes Fourier equations of motion and energy transfer and with a statistical DSMC model.

Numerically is analyzed the operation of the MEMS pulsating Pirani gauge at the real-time frequencies obtained by other authors. The actual read pressure (pressure difference) variation is studied. The results can be used to analyze the pulsating Pirani gauge sensitivity, i.e. the time to reach sustained oscillations as well as to adjust the pressure reading to the actual value.

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## Application of the Dynamic Mode Decomposition Method in Epidemiology for Malaria Disease

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Modeling the spread of infectious diseases is extremely challenging due to the lack of a single set of physics-based governing equations. Besides, the underlying disease system can be mathematically defined by several methods, including deterministic ordinary differential equations, partial differential equations and stochastic differential equations. Many current infectious diseases models tend to be based on historic data.

Originally introduced in the fluid mechanics the Dynamic Mode Decomposition (DMD) is an equation-free, data-driven matrix decomposition that can provide accurate reconstructions of spatio-temporal coherent structures arising in nonlinear dynamical systems. The equation-free aspect of operating solely on data snapshots of DMD, can help in the analysis of infectious disease data.

In this study, the Dynamic Mode Decomposition method is applied to malaria infectious disease using historical data from World Health Organization (WHO)

and Institute of Health Metrics and Evaluation (IHME), Global Burden of Disease (GBD). Several cases are analysed by using snapshots of infectious disease data concerning malaria death by region, incidence of malaria, and malaria death rates at different space locations. The examples show how DMD can extract the relevant spatio-temporal patterns from the data. Each location's time series is normalized in mean and variance, allowing for a better visual comparison.

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## A Meshless Method of Lines for the Solution of the One-Dimensional PTC Thermistor

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In this paper a meshless method of lines is presented for the numerical solution of the one dimensional PTC thermistor with a modified electrical conductivity. Contrary to the mesh oriented method of lines which uses the finite-difference method to approximate spatial derivatives, this new technique approximates the problem using some radial basis functions. Results obtained are compared with exact steady state solution and with the results in relevant literatures to show the efficiency of the method.

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## Simulation of Open Beam-Plasma Systems by the Particle-In-Cell (PIC) Method

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The beam injection into plasma is one of the important problems in the beam-plasma interaction simulation. It is usually assumed that the beam is already in the plasma and the beam injection itself is not described in formulation with the periodic boundary conditions. However, the beam loses energy quickly in this formulation, which limits the applicability of the model. This paper is devoted to the construction of open boundary conditions, when a beam is injected through the boundary of the plasma region. The problem is considered in the following formulation. There is the plasma held by a longitudinal magnetic field in the rectangle region. The dynamics of the plasma is described by the system of the Vlasov-Maxwell equations, which are solved by the particle-in-cell (PIC) method. Beams with set parameters (density, velocity) can be injected through the left and right boundaries of the region. Plasma may also freely penetrate these boundaries. However, it is required to ensure both the continuity of the particle distribution function at the boundaries, and the natural counterflow that occurs when the beam is injected. The paper considers several boundary conditions on particles and electromagnetic fields at the left and right boundaries (it is assumed that the plasma does not reach the boundaries in the  $y$ -direction). Comparison of this model and the model with periodic boundary conditions is fulfilled. The numerical simulation of the generation of the electromagnetic radiation by beam-plasma interaction is carried out under conditions of continuous beam injection on the basis of the created model.

**Acknowledgements.** The work was supported by the Russian Science Foundation, project no. 16-11-10028.

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## Representation of Solutions of Initial Boundary Value Problems for Nonlinear Equations of Mathematical Physics by Special Series

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An analytical method is used to represent solutions of nonlinear partial differential equations. This method is called a method of special series. The essence of this method is in the expansion of solutions of nonlinear partial differential equations into series by the powers of special basic functions, which can also contain an arbitrary function. Such a choice of basic functions makes it possible to find the coefficients of series from a sequence of linear ordinary differential equations and to investigate convergence of these series. A class of boundary conditions that can be satisfied with the help of the proposed series is determined and a theorem on the series convergence to the solution of the initial-boundary value problem for a certain class of initial conditions on the example of a nonlinear filtration equation is proved. The proposed method of constructing solutions can be used to find solutions for a wider class of nonlinear equations of mathematical physics.

**Acknowledgements.** The work was supported by Russian Foundation for Basic Research 16-01-00401.

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## Numerical Study of the Influence of the Heater Position upon the Heat Transfer during Pyrolysis Process used for End-of-Life Tires Treatment

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One of the most dangerous waste in the world are the End-of-Life tires (EOLT). They are waste that does not practically decompose in nature. Because of this their

sound treatment is needed for environment protection. Pyrolysis process is one of the possible methods for such a treatment. Globally, around 23% of all EOLT are processed through pyrolysis, whereas in the Republic of Bulgaria only 5% are processed by pyrolysis. It is clear that for Bulgaria this method still has a good potential for usage, development and further research. The pyrolysis process, used for EOLT treatment, usually is 3D and non-stationary. Thus it is very complicated for modeling and studying.

An adequate mathematical model of the heat transfer during the pyrolysis process used for the treatment of the End-of-Life tires (EOLT) has been presented in our previous paper [1]. There a numerical algorithm for solving the respective mathematical initial and boundary value problems has been also developed in the frame of MATLAB software. Some results for the temperature field for several characteristic periods of operation of pyrolysis station are presented and commented in this paper [1]. In our next paper [2] we have examined the influence of the heating upon the heat transfer during the pyrolysis process used for EOLT treatment.

This paper deals with studying the influence of the heater position upon the heat transfer during EOLT treatment by pyrolysis process. The results for temperature fields, temperature isolines and gradients at some specific moments of time and for two different initial heating functions are graphically presented and commented. Results from this modeling can be used in the real pyrolysis station for more precise displacement of heaters and measurement devices and for designing of automated management of the process.

**Keywords:** End-of-Life tires, Pyrolysis, Heat transfer modeling, Influence of the heater position

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## Numerical Homogenization for Wave Propagation in Fractured Porous Media

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Wave propagation through fractures plays an important role in seismology and has a significant influence in the fluid flow in the hydrocarbon and geothermal reservoirs. For modeling fractures, a suitable interface model should be used for describing the dynamic response of the fracture. Frequency dependent models on the fracture interface based on the displacement discontinuity model, where stress components are proportional to the displacement. Knowledge of the orientation and spatial distribution of fractures in rocks is also highly important in simulations. Seismic wave propagation through fractured media can be characterized by multiple scales. For small scale fractures whose sizes are much smaller than the seismic wavelength, the effective medium approach can be applied and leads to seismic anisotropy. The effective compliance tensor of the fractured rock can be expressed as the sum of the compliance tensor of the background medium or by direct computational simulations of the local problems (numerical homogenization technique). In this work, we consider a homogenization methods to solve the Helmholtz problem related to elastic wave propagation in fractured media in the frequency domain. For numerical solution, we use a symmetric interior penalty discontinuous Galerkin (IPDG) method with linear-slip model to represent the fractures. We solve local problems for calculation of the effective elastic properties and use them for coarse grid approximation. We present numerical solution of the model problems in fractured porous media.

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## 3D-PIC Model of the Electromagnetic Radiation Generation by the Counter-Streaming Electron Beams

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One of the perspective directions in the terahertz radiation obtaining is the generation of electromagnetic radiation near the plasma frequency when the electron beam interacts with the plasma. Experiments on GOL-3 facility [1] showed the

electromagnetic radiation efficiency increase ( $\sim 1\%$ ) in the regime when the transverse dimension of the system comparable with the length of the emitted waves. Theoretical estimation predicts obtaining up to 5% efficiency in the continuous injection of a beam into a plasma channel with a previously created longitudinal density modulation. But the radiation with the plasma frequency is hampered by the effect of plasma screening. However, it is known that the counter injection of electron beams into a plasma results in enhanced electromagnetic emission near the second harmonic of plasma frequency and it is not sensitive to plasma screening. The determination of the most suitable for radiation generation plasma and beams parameters is a very difficult task. That is why a numerical modeling is needed. Nowadays the particle-in-cell method is considered as a convenient tool for the simulation of complex nonlinear processes in plasma physics [2]. In this report a three-dimensional parallel numerical model based on Particle-In-Cell method for simulation of beam-plasma interaction is presented. The problem of continuous beam injection is considered. It requires the establishment of a special open boundary condition that holds the plasma in the region and allows the beams to be injected across the boundaries. The first results of the three dimensional counter-streaming electron beams simulation are presented.

**Acknowledgements.** This work was supported by the Russian Science Foundation (project 16-11-10028). Simulations are performed at the Siberian Supercomputer Center SB RAS and using computational resources of Novosibirsk State University.

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## On $N$ -soliton Interactions of Manakov Model with Gain/Loss Terms

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We analyze the dynamical behavior of the  $N$ -soliton train in the adiabatic approximation of the perturbed Manakov model:

$$i\frac{\partial \vec{u}}{\partial t} + \frac{1}{2}\frac{\partial^2 \vec{u}}{\partial x^2} + (|u_1|^2 + |u_2|^2)\vec{u} = i\vec{R}[\vec{u}], \quad (1)$$

where  $i\vec{R}[\vec{u}]$  are the perturbative terms:

$$iR[u] = i(\gamma u + \beta|u|^2u + \eta|u|^4u) + V(x)u, \quad V(x) = A \cos(\Omega x + \Omega_0), \quad (2)$$

describing linear and nonlinear gain/loss and a periodic external potential  $V(x)$ .

We show that the evolution of the  $N$ -soliton train is described by a perturbed complex Toda chain (PCTC). This PCTC is compatible with our earlier results on the subject derived by other methods, see [1,2,3].

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## Integrable Nonlocal Multi-Component Equations with $\mathcal{PT}$ and $\mathcal{CPT}$ Symmetries

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We will present extensions of  $N$ -wave and derivative NLS types of equations with  $\mathcal{PT}$  and  $\mathcal{CPT}$ -symmetries [1]. The types of (nonlocal) reductions leading to integrable equations invariant with respect to  $\mathcal{C}$  – (charge conjugation),  $\mathcal{P}$  – (spatial reflection) and  $\mathcal{T}$ - (time reversal) symmetries are described. The corresponding constraints on the fundamental analytic solutions and the scattering data are derived.

Based on examples of 3-wave (related to the algebra  $sl(3, \mathbb{C})$ ) and 4-wave (related to the algebra  $so(5, \mathbb{C})$ ) systems, the properties of different types of 1- and 2-soliton solutions are discussed. It is shown that the  $\mathcal{PT}$  symmetric 3-wave equations may have regular multi-soliton solutions for some specific choices of their parameters [1].

Furthermore, we will present multi-component generalizations of derivative nonlinear Schrödinger (DNLS) type of related to **A.III** symmetric spaces and having with  $\mathcal{CPT}$ -symmetry [2]. This includes equations of Kaup-Newell (KN) and Gerdjikov-Ivanov (GI) types.

Based on a joint work with Vladimir Gerdjikov and Rossen Ivanov.

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## About Nonlinear Guaranteed Estimation

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Problem of guaranteed estimation with no statistical description of disturbances plays an important role in control theory. In this talk, we consider a nonlinear system  $\dot{x} = f(t, x) + B(t)v(t)$  with an observation process  $y(t) = g(t, x) + w(t)$ , where functions  $v(\cdot)$ ,  $w(\cdot)$  are uncertain disturbances. Suppose that the initial state  $x_0$  and the disturbances are restricted by a priori constraint

$$F(x_0) + \int_0^T \left\{ f_0(t, w(t)) + |v(t)|_{Q(t)}^2 + |v_0(t, x(t))|_{Q(t)}^2 \right\} dt \leq 1, \quad (1)$$

where  $|v|_Q^2 = v'Qv$ , and the function  $v_0(t, x) = \langle br / \rangle Q^{-1}B'V_x/2$  may be found from the linear partial Lyapunov equation

$$V_t = -f'(t, x)V_x + f_0(t, y(t) - g(t, x)), \quad V(0, x) = F(x). \quad (2)$$

Here  $Q(t)$  is a symmetric and positive definite matrix; the symbol  $'$  means the transposition. The functions  $F(\cdot)$  and  $f_0(\cdot, \cdot)$  are continuous and non-negative. Denote by  $J(v(\cdot))$  the left side of constraint (1), where  $w(t) = y(t) - g(t, x(t))$ . It is easy to see that  $\min_{v(\cdot)} J(v(\cdot)) = V(T, x)$  under boundary condition  $x(T) = x$ . Thus, the set  $\mathbf{V}(T, y) = \{x : V(T, x) \leq 1\}$  consists of all states  $x(T) = x$ , for which there exist the initial state and the disturbances such that constraint (1) holds and observation equations is fulfilled. The set  $\mathbf{V}(T, y)$  is said to be multiple estimate at the instant  $T$ . We focus on two main problems. First, we can consider the constraint (1) without the summand  $|v_0(t, x(t))|_{Q(t)}^2$ . This leads to nonlinear Bellman equation like (2) with function  $W(t, x)$  and to the another multiple estimate, i.e. the set  $\mathcal{V}(T, y) = \{x : W(T, x) \leq 1\}$ . We compare one set with another and discuss the approximation of these sets. The approximation is our second task. At the beginning we do this for linear systems, where the sets may be calculated explicitly. After that the finite-difference approximation of the initial nonlinear system is considered and corresponding multiple estimates are built. We prove the convergence of approximating sets to the initial ones in Hausdorff metric. The text is illustrated by examples. Applications to flight problems are considered as well.

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## Design and Testing Based Experimental Data of a MEMS-INS/GPS Navigator with ANFIS Data Fusion Algorithm

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The paper presents the design and experimental testing results of a MEMS-INS/GPS navigator with a data fusion algorithm based on an adaptive neuro fuzzy inference system (ANFIS). The work has been performed during a research project related to the development of INS/GPS integrated navigators based on smart data fusion algorithms. In the paper, the structural design of the MEMS-INS/GPS integrated system mechanism and the training procedure of the fuzzy inference system are firstly exposed. Further, the evaluation with experimental data of the integrated navigator based ANFIS algorithm is presented. The integrated navigator proposed scheme works in two different phases: the training phase and the prediction phase. In the training phase, the GPS data are available and the scheme uses training data packages with ten inputs (the IMU outputs (three accelerometers and three gyros), the components of the INS attitude solution (attitude angles - roll, pitch and yaw), the outage time of GPS signal from the navigator clock) and six outputs (the differences between the components of global position and North-East-Down (NED) speed components from INS and GPS navigation solutions). The experimental model of the MEMS-INS/GPS navigator incorporates three miniaturized inertial sensors (LPY510AL – Biaxial gyro, LPR510AL – Biaxial gyro, MMA 7361L – Three-axial accelerometer), a GPS module (u-blox NEO-6M) and a dsPIC 33EP5-12MU810 microcontroller. The inertial sensors data were acquired with 100 samples/s, while the GPS receiver provided data once per second. To test the proposed integrated navigator, the hardware structure has been boarded on a testing car. In a first step, the experimentally acquired data were used to tune the ANFIS algorithm, while, at the next steps, an evaluation of the obtained integrated navigator has been performed. Three different scenarios were used: open sky detection (access to GPS signal all the time), GPS signal interruption, INS detection only.

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## Computing the Reachable Set Boundary for an Abstract Control Problem

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An abstract control system defined by a differentiable mapping  $F$  of a Banach space  $X$  into a Banach space  $Y$  is considered. A reachable set of the system is an image  $G = F(U)$  of a given set  $U = \{u \in X : \varphi(u) \leq 1\}$ ,  $\varphi(u)$  is a continuous functional on  $X$ . The set  $U$  is treated here as a constraint on the control  $u$ . Assuming that some regularity conditions are fulfilled, we prove that any control  $u \in U$  such that  $F(u) \in \partial G$  is a local solution to an auxiliary optimization problem. The necessary (necessary and sufficient in some cases) conditions of optimality for this problem give a characterization of the boundary points of  $G$  and provide the basis for the development of numerical procedures. As an example we apply this approach to a nonlinear affine-control system with joint integral constraints on the control and the state. We describe a numerical algorithm based on the Pontryagin maximum principle for computing the reachable set boundary and provide results of numerical simulations.

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## On Some Approaches for a Free Surface Fluid Flows Modeling

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Study of fluid flows in the presence of a 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 should possess by 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 flows) and CABARE method possessing the properties mentioned above. The test calculations and comparison with some theoretical, experimental data and calculations of other authors will be demonstrated.

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## Ultrafast Laser Excitation of CO/Pd (111) Probed by Sum Frequency Generation: Pump Laser Energy Effect on the Induced CO photo-desorption

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The desorption of CO from Pd (111) induced by femtosecond laser pulses is probed by IR + vis sum frequency generation (SFG). A large redshift of the main band, a broadening, and a strong decrease in intensity are observed; these originate from coupling of C-O stretch to low frequency modes (the frustrated rotation). Simulation based on two temperature model of electron and phonon heat baths within the substrate, show that CO desorption from the Pd(111) is an electron-mediated process, this corresponds well with the results obtained by two pulse correlation. SFG spectra show a development of a second band at high frequency at negative delay, which disappears at positive delay, due to an interference phenomenon between disturbed and undisturbed states of the SFG pulse. The CO desorption is becoming important with increasing the pump energy. We compared CO photo-desorption from Pd(111) to others metals, indeed the most probable hypothesis that makes the difference between metals is the position of CO 2p\* adsorbate resonance, into which substrate electrons may be excited. Other factors may play a role as the distance and the strength of CO-Metal.

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## Study of Histidine in Myoglobin with a Novel 3D Visualization Method

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Distal as well as proximal histidine play an important role in the oxygen delivery of myoglobin, thus they were both subjects of extensive research. Here we study them by a novel 3D-visualization method based on the construction of a series of orthonormal coordinate frames along the side chains, while mapping the atoms positions onto a unit sphere for better visualization. The results are consistent with the actual biological structure, which suggests the method can reliably depict the spatial orientation of side-chain covalent bonds in a protein. Our results provide a new perspective to further understanding the structure and function of histidine in myoglobin and could eventually be advanced into a protein-structure prediction tool.

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## Some Interval and Trend Statistics with Non-Gaussian Initial Data Distribution

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The research of Student statistics,  $\chi^2$  and Hald-Abbe trend statistics, Fisher statistics with non-Gaussian distribution of the initial data is carried out. An estimation of the significance levels shift and confidence probabilities values of these statistics depending on the kurtosis of the initial data a priori distribution is determined. Adopted in researches a priori statistical model of the data generation

is selected as a decomposition model of non-Gaussian probability density of initial data a priori distribution in Gram-Charlier series. The main question is to determine the form of  $\chi^2$  statistic for a priori distribution, due to Student and Fisher statistics are based on a  $\chi^2$  statistic. As follows from the carried out analysis, even very small kurtosis differences from its value for the normal distribution essentially shift the  $\chi^2$  distribution quantiles, that is important for determining the interval dispersion estimates at a given significance level. Student and Fisher  $\chi^2$ -related statistics are obtained by corresponding nonlinear transformations. A detailed analysis of the results shows, that the interval estimates and tests in which Student's statistics are used (mean value estimation, equality of means in the samples, etc.) do not suffer significant changes. For Fischer statistics, opposite, the quantiles shift is statistically significant, especially at a significant difference in degrees of freedom. Therefore, tests based on Fisher statistics and its modifications ( $v$ -distribution,  $z$ -distribution) for non-Gaussian samples may be accompanied by loss of significance levels more than 5%. First of all, this concerns the dispersions equality estimates and the equality of means at a given dispersion. We carried out the analysis of time series non-Gaussian distributions influences on the following trend statistics: cumulative sums, Hald-Abbe statistics and Fisher's criterion. The results of threshold levels calculations for Hald-Abbe trend statistics showed a high degree of stability of the investigated statistic to the distribution kurtosis in range of confidence probabilities (0.9...0.95) and the number of freedom degrees (number of series samples) more than 20. The difference of the accepted a priori statistical model of data generation from Gauss model leads to a substantial shift of the significance levels of interval estimates statistics and trend statistics.

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## Footprint of Point Mutations in Domain Decomposition of Large Proteins

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Even isolated single-point mutations in key structural/functional domains of biomolecules can significantly change their conformation and essentially modulate

their biological activity. In computational studies of such objects, it is of primary importance to identify measurable macroscopic parameters, which substantiate these transformations and allow for their prediction in absence of experimental data. We explore the sensitivity of the earlier developed SMCC method for identification of stable over time semi-rigid domains in large biomolecules to single-point mutations in the investigated biomolecules on the example of an important signaling molecule - human interferon-gamma (hIFN $\gamma$ ) and two artificially mutated forms with point mutations introduced in those regions, which are responsible for the binding to its extracellular receptor and for its biological activity.

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## Coarse Graining in MD Structure Studies: Cluster Formation from Peptides in Water Solution

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Their broad-spectrum antimicrobial activity against bacteria, viruses and fungi makes antimicrobial peptides (AMPs) a promising candidate for alternative therapies by multi-drug resistant bacterial strains. We aim at understanding the stages and dynamics of AMPs action on the target membrane. To this end, we performed coarse-grain molecular dynamics (CG-MD) simulations of a sample peptide (indolicidin, IL) solutions under different conditions (temperature and concentration). We observe a self-assembly process with a saturation threshold. Thus, a detailed knowledge of AMPs behavior prior to the interaction with the target membrane is a prerequisite for understanding AMPs mode of action and for designing of synthetic peptides with predefined properties as novel antivirals and antibacterials.

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## Random Forests Models of Particulate Matter PM10: A Case Study

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Air pollution and high concentrations of fine particulate matter (PM) are extremely harmful to human health, ecosystems and the climate in many countries around the world. To solve this type of air quality problems, a huge number of studies has been devoted. It is important to note that pollution sources have a local character for each urban region and depend on a large number of factors such as meteorological, manufacturing, domestic, transport and other. In the field of mathematical modeling and processing of accumulated measured data for PM with aerodynamic size up to 10 microns (PM10), along with classical statistical methods, powerful, flexible data mining techniques and approaches such as neural networks, fuzzy logic, regression trees, multivariate adaptive regression splines, random forest (RF), and more are adapted. This study explores the possibilities of the random forest method for modeling the concentrations of PM10 in Blagoevgrad, Bulgaria. Average daily data over 9 years (2009-2018) and a large number of input variables as predictors are used - meteorological and temporal. The constructed models show high-performance both in fitting and forecasting the measured data. The forecasting process is performed by a multi-step procedure with 3-day horizon ahead using data not included in the construction of the model. A specific objective of the investigation is thus to test the stability of the RF models in forecasting future pollution levels.

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## Waves over a Variable Bottom - Hamiltonian Approach

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We derive model equations for water waves propagating over uneven bottom using the Hamiltonian formulation of the water-wave problem. The assumptions are for a homogeneous incompressible, inviscid, irrotational fluid medium bounded by a free surface. The Hamiltonian of the system is expressed in terms of the so-called Dirichlet–Neumann operators. Specific scaling of the variables is selected which leads to approximations of Boussinesq and Korteweg–de Vries types, taking into account the effect of the slowly varying bottom. The arising KdV equation with variable coefficients is studied numerically.

Joint work with A. Compelli and M. Todorov

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## Tails and Probabilities for Extreme Outliers

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The task of estimation of the tails of probability distributions having small samples seems to be still opened and almost unsolvable. The paper tries to make a step in filling this gap. In 2017 Jordanova et al. introduce six new characteristics of the heaviness of the tails of theoretical distributions. They rely on the probability to observe extreme outliers. The main their advantage is that they always exist. This work presents some new properties of these characteristics. Using them six distribution sensitive estimators of the extremal index are defined. A brief simulation study compares their quality with the quality of Hill, t-Hill, Pickands and Deckers–Einmahl–de Haan estimators.

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## Numerical Reconstruction of the Right-Hand Side with Separable Variables of the Parabolic Equation

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In this paper we consider an inverse problem with two redefinition conditions for the multidimensional parabolic equation of identification of the right-hand side, defined as a product of functions that depend on spatial variables and time. For numerical solution of the given inverse initial-boundary value problem a conjugate gradient method is used in combination with the method of finite differences with a purely implicit time approximation. Herein, in each time layer a computational algorithm is based on a special decomposition, where a transition to a new time layer is provided by solving two standard elliptic problems. The results of computational experiment for model problems with quasi-real solutions are discussed, including the results of problems with overdetermination conditions specified with random errors.

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## Statistical Data Analysis to Identification of Operating Modes of Electronic Units

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In the research the clustering of measurement results of thermophysical properties by modes of an electronic unit behavior is discussed. An electronic unit (EU) is a rectangular aluminum frame, on which printed circuit boards with electronic components are installed. The dissipated by the electronic components heat is removed from the EU through the flat bottom surface of the frame. A laboratory test bench is used for investigations of thermal operation modes of the EUs. The test bench is a vacuum chamber with a heat removing base which provides temperature maintenance in the range from  $-30^{\circ}\text{C}$  to  $+60^{\circ}\text{C}$  within  $\pm 1^{\circ}\text{C}$ . For measurements the EUs are installed on the heat removing base in the vacuum chamber. Temperatures are measured by sensors located at various points of the EUs. The laboratory test bench provides the EUs operation both in the atmosphere and in a vacuum at a pressure of no higher than  $1.3\text{E-}3\text{Pa}$  ( $1.\text{E-}4\text{mmHg}$ ). The operating mode of the EUs

is determined by the set of powers which are given to a certain group of electronic components and by ambient conditions (atmosphere or vacuum). The following data and measurement results are available to analysis: the temperature of the heat removing base, the ambient temperature, the temperatures read from sensors in the EUs. The normalized “pseudo-temperatures” corresponding to the processed temperatures from the sensors are used to clustering. The “pseudo-temperatures” are obtained in the following way. First, the influence of the temperature of ambient and of the heat removing base on measured temperatures is determined by linear regression. Then, this influence is subtracted from the temperature of the sensors, and the result is normalized by standard deviation. To k-means clustering we use the results of more than 200 measurements. This data corresponds to nine operating modes of the EUs in the atmosphere and in a vacuum. A stable clustering of the operating modes of the electronic units has been obtained.

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## The Nonlinear Processes in Active Geophysical Monitoring

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The modern concept of earthquake source development is as a process of development of a system of cracks. Broadening of the spectra of the initial sounding seismic oscillations also results from vibroseismic sounding of fractured dilatancy media typical for earthquake preparation zones. The applicability of the parameters of wave field nonlinearity in the form of possible prognostic characteristics of the earthquake source development process is justified. One of the methods used to monitor the developing geodynamic processes in seismically active zones is based on regular sounding of the medium by powerful seismic vibrators, with subsequent analysis of the time dynamics of the seismic field parameters. Such monitoring is accompanied by some nonlinear processes taking place at the stages of radiation and propagation of seismic oscillations. One of them is due to the peculiarities of constructions of different vibrators and the processes of its interaction with the underlying surface. Others develop in the medium of seismic wave propagation. Such processes enrich the seismic wave field with additional lower and higher frequency components. In this paper it is shown that allowance for these processes increases noise immunity of vibrational correlograms (analogs of explosive seismograms), as well as their time resolution, contributing to an increase in the accuracy of measurements of the arrival types of the main wave types. The results of an

analysis and formulated conclusions presented in this paper are based on numerical calculations and experiments.

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## Holomorphically Projective Mappings of Special Kahler Manifolds

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Let us treat non-trivial holomorphically projective mappings of Kahler manifolds with limitations on the Ricci tensor. The limitations on the Ricci tensor take form of the differential equations in covariant derivatives. The class of Kahler manifolds that permits reciprocal holomorphically projective mappings can be characterized by its mobility degree  $K_n$  in relation to holomorphically projective mappings. The special Kahler manifolds are classified by the mobility class that they exhibit by necessity. The obtained results contribute to the well-known aspects theory of holomorphically projective mappings of Kahler manifolds.

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## Coupling Model of Coating Synthesis on Plane Substrate

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The synthesis of materials and coatings from the mixtures of the components capable to exothermic reactions with the formation of phases with special properties is interested for various applications. To describe the synthesis process and understand fundamental physical regularities controlling the composition and properties formation in technological situations one can use the classical theory of combustion



synthesis. However we should pay attention to the stress-strain state of specimen especially when the chemical reactions proceed in solid phase. To obtain dense product some researchers have use a special mechanical loading, quasi static or dynamic compaction, and etc. Even without external mechanical loading the stresses and strains stipulated by the high temperature gradients and properties change during chemical reactions could be the cause for special conversion regimes, including slow and quick ones. This problem needs a special investigation applicable to different technological situations. In this report, the problem on reaction front propagation is discussed for the coating synthesis on plane substrate. This situation is typical for example for intermetallic coating synthesis initiated by laser or electron beams. In this report, the asymptotic solution of type of traveling wave is constructed in the approximation of small strains for the conditions of reaction propagation along thin layer placed on the substrate for the heating of which the additional heat is necessary.

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## Optimizing Parallelization by the Cluster Platform Avitohol of the CFD Method of a Trimaran

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Computing of fluid dynamics is gaining popularity over the last years and requirements such as accuracy and speed are getting bigger. One of the biggest problems for the industry is how a Computational Fluid Dynamics (CFD) simulation could be parallelized and optimized in order to achieve better performance when solving complex engineering problems. Achieving the best possible performance depends not only on hardware architecture, but also on application software and its parallelization capabilities. A subject of this investigation is a trimaran model of a service boat – one of the complicated cases in ship hydrodynamics. Pressure based Navier-Stokes differential equations have been used to describe the trimaran model. OpenFOAM (version 2.3.0) software which is deployed on the hybrid supercomputer system Avitohol, is used in our tests to investigate the solution and parallelization of the model. This supercomputer consists of 150 HP Cluster Platform SL250S GEN8 servers with 2 Intel Xeon E 2650 v2 CPUs and 2 Intel Xeon Phi 7120P coprocessors. We apply pure MPI and a hybrid model of MPI + OpenMP to investigate the

parallelization of the model under consideration. The numerical results demonstrate a good convergence with the theoretical study as well as that the hybrid parallel model is proper for the acceleration of the OpenFOAM solver comparing it with pure MPI ways. From the other hand the simulation results lead to find solutions for complex problems faster than real-time experiments contributions.

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## Mathematical Model for Eddy Current Testing of Electrically Conducting Materials with Cylindrical Flaws

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Consider an air-core coil carrying alternating current located above a conducting metal plate with finite thickness  $d$ . The plate has a flaw with reduced electrical conductivity in the form of a circular cylinder located above the plate. The axis of the coil coincides with the axis of the flaw. Such a configuration can be used to model corrosion in metal plates in case thickness of the corroded part increases. The system of the Maxwell equations is solved by the method of truncated eigenfunction expansions. The electromagnetic field is assumed to be zero at a sufficiently large radial distance from the coil. The method of separation of variables is used to construct the solution in each region (air above and below the plate and conducting regions with and without the flaw). The problem is solved first for the case of a single-turn coil. The solution for the coil of finite dimensions is obtained using superposition principle. The interface conditions give a nonlinear equation containing Bessel functions. Complex roots (or eigenvalues) of this equation are computed numerically using contour integral technique. The change in impedance of the coil is obtained by means of a semi-analytical method. Computations are performed for different values of the parameters of the problem.

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## Infinite Quantum Graphs

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The notion of quantum graph refers to a graph considered as a one-dimensional simplicial complex and equipped with a differential operator (“Hamiltonian”). From the mathematical point of view, quantum graphs are interesting because they are a good model to study properties of quantum systems depending on geometry and topology of the configuration space. They exhibit a mixed dimensionality being locally one-dimensional but globally multi-dimensional of many different types. We will review the basic spectral properties of infinite quantum graphs (graphs having infinitely many vertices and edges). In particular, we will discuss recently discovered fruitful connections between quantum graphs and discrete Laplacians on graphs.

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## Computational Experiment to Solve the Stefan Problem with Nonlinear Coefficients

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The components of the first wall and the divertor of the experimental fusion reactor ITER are expected to experience serious thermal load during the discharge. The most intense of these pulsed thermal loads lead to melting of even such a refractory material as tungsten, which will cover the divertor plates. The melting of the surface layer can result in increase in material transport along the surface and formation of drops of material, which are dangerous to the hot plasma. The simulation of pulsed heat load by electron beam is significantly different from that by plasma flow. The limitation of heating of material in the former case is caused by the cooling of the surface by intense evaporation, as against the vapor shielding in the latter case. The results of computer simulation of tungsten evaporation

will be presented. Mathematical model of the evaporation of tungsten based on the numerical implementation of the equations of gas dynamics together with the Stefan problem.

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## Influence of Glycosilation on Human Interferon Gamma – a Molecular Dynamics Study

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Interferon gamma (IFN $\gamma$ ) is an important cytokine, which plays a key role in the formation and modulation of immune response. Human IFN $\gamma$  (hIFN $\gamma$ ) is a homodimer, organized primarily in an  $\alpha$ -helical globule, but it contains also a long positively charged unstructured C-termini. Under physiologic conditions the cytokine is independently and differentially glycosilated at ASN<sup>25</sup> and/or ASN<sup>97</sup>. Glycosilation promotes the folding and dimerization of the protein and extends its circulatory half-life by protecting hIFN $\gamma$  C-termini from proteolytic degradation, but does not affect receptor binding affinity. We developed model structures of monoglycosilated at either ASN<sup>25</sup> or ASN<sup>97</sup> or diglycosilated full-length native and N-terminally tagged hIFN $\gamma$  dimers. The structure and dynamics of the models were studied using molecular dynamics simulations. We report how the carbohydrate chains interact with the receptor-binding sites in the cytokine, with its flexible highly positively charged C-termini and the added N-terminal tag peptides.

**Acknowledgements.** The simulations were performed on the supercomputer Avitohol@BAS and on the HPC Cluster at the Faculty of Physics by St. Kl. Ohridski University of Sofia. This research was supported under the programme for young scientists' career development at the Bulgarian Academy of Sciences (DFNP-17-146/01.08.2017).

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## Mathematical Model of heat Transfer in an Electric Machine

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During the operation of an electric machine, the heat is generated by an electric current flow in the stator winding and rotor winding or just stator winding. This heat is transmitted to other parts of the electric machine and discharged outside naturally and through forced cooling. From a geometric point of view, in the simplest case, an electric machine is viewed in the form of complex two or three-layer cylinder with a perfect or non-perfect thermal contact between the layers. The paper's objective is to build the mathematical model of temperature field of an electric machine, which, from a mathematical point of view, can be represented in the form of a multilayered area with different physical characteristics of the layers and with the operating internal and external sources of heat. Moreover, the temperature field of an electric machine depends on the axial coordinate. In this work a mathematical model of the temperature field of a radial section of a three-layer cylinder is constructed in one of the layers of which the internal sources of heat act, and to the other two, which have different heat-physical properties, heat is transmitted by thermal conductivity. The mathematical model for determining the temperature distributions in a multilayer cylinder has the form of conjugate boundary value problem with impedance type boundary conditions. The constructed mathematical model describes the temperature field of electric machine that consist of two-layer rotor where the heat sources are absent and stator made of composite material aluminium-iron. Stated geometrically, aluminium stator with electric current flowing through it and where Joule heat emission is taking place has a look of 2-leafed rose. An algorithm for solving this problem has been proposed.

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## A Method of Approximate Reachable Set Construction on the Plane for a Linear Control System with Uncertainty

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The problems of construction of reachable sets of control systems or their estimates are in demand in control theory, since allow to estimate the capabilities of such systems on a finite time interval. At present, analytical methods for external ellipsoidal estimates construction of reachability sets are widely used for bilinear control systems with uncertainty. Such methods are implemented in the form of step-by-step algorithms, the use of which allows for a relatively short time to obtain ellipsoidal estimates in n-dimensional Euclidean space. But in a number of cases, due to the complex form of the reachable set, an ellipsoidal estimate is not enough to investigate the capabilities of the system. In this case, there is a need for approximate methods of a reachable set construction that are resource-intensive, require a sufficiently long computation time, but allow more accurate estimation of the reachable set. The presented research is devoted to the development of an algorithm for the approximate construction of the reachable set of an bilinear control system with uncertainty. This algorithm is based on operations with polygons and is intended for solving problem in the plane. In this algorithm the uncertainty in the matrix of the system is considered as the control of the second player, which makes it possible to apply methods similar to approaches from the theory of differential games to its solution. The difference is that the second player acts in conjunction with the first thereby expanding the capabilities of the control system. Such approach, with a change in the properties of the system components to diametrically opposite ones, falls within the concept of radical re-implementation.

**Acknowledgement.** This research was supported by Russian Foundation for Basic Research (Project 18-01-00544).

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## Using Cloud Computing for Reachable Sets Calculation for Control Systems

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At present, there is a wide range of mathematical problems for the solution of which a lot of computing resources are required. In a number of cases, in order to accelerate calculations, researchers use parallel computing technology to develop solution algorithms and implement them in the form of programs. One of such resource-intensive tasks that have a good parallelization potential is the problem of approximate calculation of reachable set of control system. It is known, that the best tool for maximizing the potential of parallel computations is the supercomputer. Unfortunately, not all researchers involved in solving resource-intensive problems have access to supercomputer. In this regard, there was a need for alternative tools that are available to a wide range of users and at the same time have significantly greater computing power than a personal computer. These tools include cloud computing. The presented work is devoted to the study of the effectiveness of using cloud computing in a corporate cloud on the example of calculating reachable sets of control systems. In the framework of the study, a multiplatform program in C language was developed. This program is based on the algorithm of approximate calculation of reachable sets and uses the OpenMP parallel computing technology. Using this program, a number of numerical experiments were performed. The results of these experiments allowed us to evaluate the effectiveness of cloud computing with respect to the problem of reachable sets calculation.

**Acknowledgement.** This work was supported by the UrB RAS program (project No. 18-1-1-6).

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## Estimates of the Reachable Set of the Lotka-Volterra System under Uncertainty

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The present paper is devoted to the construction of ellipsoidal estimates for reachable sets of the nonlinear Lotka-Volterra system with uncertainty in the initial data. This model is a classical model of the populations dynamics of type “prey-predator.” This mathematical model is successfully used in biology, demography, physics, economics, and so on. The problem is studied under uncertainty conditions on initial set. Initial set is assumed to be unknown but bounded with given bounds and any additional statistical information on the number of “predators” and “preys” is not available. In this paper we use ellipsoidal methods for approximation of the reachable set, that is, the set in the phase space to which a phase point may be driven from the set of the initial states in a given time. These methods allow to effectively construct an estimate of the reachable set without using resource-intensive calculations. The aim of this paper is to study the properties of the reachable set of the Lotka-Volterra model. Within the framework of the investigation, the algorithm for ellipsoidal estimation is constructed. A numerical simulation is performed.

**Acknowledgement.** The research was supported by Russian Science Foundation (RSF) (project No.16-11-10146).

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## A Customer Segmentation Approach in Commercial Banks

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The results of various recent analyzes of retail banking trends show that proper classification of borrowers is fundamental for the development of successful business. The increasing competition in both banking system and non-bank institutions requires the use of modern market strategies and individual approaches to customers. One of the main priorities in the banking sector is to improve customer segmentation and take it into account in the design and distribution of new products. A common tool to improve competitiveness is the designing of a special range of products and



services targeting loyal customers or offering them special discounts for existing products. This represents the so-called “Loyalty program,” which includes the issuance of various types of cards for such customers. Three clusters (segments) of loyal borrowers: “platinum,” “gold” and “silver,” are identified in the present work, using K-means Clustering. A database of 100 borrowers from a commercial bank branch that took secured consumer loans is analyzed. The clients are defined as loyal based on their credit history (they have less than 3 missed payments for the last year). Three variables are used for their segmentation. Initially, the original segmentation variables are taken as input data for the analysis, and further study on standardized segmentation variables is carried out. The potential segmentation strategies are formulated depending on the leading segmentation variable. A comparative analysis of the results of both methods examined (with original and standardized segmentation variables) and of a two-step clustering (obtained in a previous study from one of the authors) is made within each of the strategies. It is specified which type of cluster analysis suits best to each of the strategies.

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## Dynamic Systems, Similar to the Time Scale

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A similarity sign is the coincidence of regularities of the dynamic systems states changing at the different time scales. The necessary and sufficient similarity conditions of general (Cauchy problem) and particular solutions of ordinary linear differential equations that describe transient processes in linear stationary dynamic systems are proved. The similarity criteria of linear stationary dynamic systems are proposed. Non-stationary linear dynamic systems with varying parameters, for which the self-similarity property is defined, are considered. A non-stationary linear dynamical system is called self-similar, after completion of transient processes in which, caused by a change of its parameters, the dependencies of the state coordinates changing are the same and differ only by the time scale. The self-similar nonstationary linear dynamic systems of the first and second orders are investigated. The self-similarity conditions of the processes of nonlinear dynamic

systems states changing at small deviations from their steady-state modes are obtained. The applied problems of similar and self-similar dynamic systems investigation, particularly, the systems of aircraft gas turbine engines and subordinate regulation systems of electric drives are solved. The aircraft gas turbine engine is represented as a state space model, the companion matrix of the characteristic polynomial in which is a  $\lambda$ -matrix. On the basis of the eigenvalues and eigenvectors problem solution for this matrix, the self-similarity conditions of the transient processes of engine turbine revolutions changing were obtained. We proved that in a wide range of flight modes changing the transient processes of engine turbine revolutions changing have the same regularities. Comparison of simulation results and experimental data of turbine revolutions changing for aircraft gas turbine engine with several turbines is carried out. The proposed approach allows to perform synthesis of the control actions in complex systems that provide a similarity of dynamic properties in different modes.

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## **Induced Voltage, Magnetization Waveforms and the Spectral Response at the Grain Boundaries of YBCO Superconductors and the Critical State Model**

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Critical state model for granular superconductors is applied to study the nonlinear ac response of Y-Ba-Cu-O superconductors at the grain boundaries. The measured induced voltage waveforms are studied and explained at different temperatures and the corresponding calculated waveforms are shown to match the data. The intergranular hysteretic magnetization losses and the first 10 spectral components of the ac harmonic response are also measured and calculated at different temperatures.

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### 3D Mathematical Model for Evaluation of the Mass-Inertial Characteristics of the Upper Limb: Analytical Results

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We present a new 3D mathematical model of the for evaluation of the mass-inertial characteristics of the upper limb of the Bulgarian men and women. The model is based on the experimental data of the representative anthropological investigation of 5290 individuals (2435 males and 2855 females) of the Bulgarian population at the age between 30-40 years [1] as well as on our own anthropometric measurements of 50 Bulgarian men and 50 women of the same age. Using the model suggested, after deriving the corresponding analytical expressions needed, we calculate analytically and estimate numerically the mass-inertial characteristics of the segments: the mass, center of mass, the volume, and the principal moments of inertia. We present a comparison between the results obtained within this model with our previous results reported in [2], as well as with other data for Caucasian reported in literature. The investigation presented provides data for a set of parameters of the Bulgarian men and women for which no direct measurements are available. The model proposed is oriented to application in medicine (orthopedics and traumatology), rehabilitation robotics, computer simulations, sports and areas such as simulation of the human behavior in space, ergonomics, criminology and other areas.

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## Using of Fuzzy Mathematical Models in Automated Systems for Recognition of High Molecular Substances

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The aim of the study is to provide fuzzy mathematical models suitable for use in automatic systems for recognition of high molecular substances at their gel electrophoresis under denaturing conditions. For this purpose we described the fuzzy scale based on motion activity of known high molecular substances taking into account the shape of their traces. We used the method for construction of fuzzy dependencies of the traces models, which was proposed previously by us. To automate the process we constructed computer algorithm which leads to increasing of the accuracy and validity of the findings while the detection of new proteins.

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## Verification of Applicability in Space Domain of the Inverse Filtering with Evolution Control for Reconstruction of Images Obtained by Radar Scanning

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The aim of the study is verification of applicability in space domain of the inverse filtering of the evolution control under noise presence. For this purpose we determine its resolution by testing the ability to resolve several closely placed objects. We used experimental data of radar scanning of metal strips with a horn antenna. To automate the process we use original software.

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## Estimation of Parameter-Dependent Plates Vibrations on the Basis of the Asymptotic Method

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We consider the modified method of parameter continuation (MMPC) as an asymptotic technique for estimating the frequencies and shapes of both parametric oscillations and nonlinear vibrations of plates with parameter-dependent boundary conditions. Unlike known methods, which are usually used for such estimations, MMPC estimations depend from the initial plate shape. It describes real vibration shape of plate with different conditions on its edges. The comparison with numerical calculations confirms the advantages of proposed method and its accuracy.

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## Parametric Control of the Processes of Making Recommendations in Economic Policy

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The goal of the research is to propose methods for solving the actual problem of economic growth and suppressing the volatility of macroeconomic indicators (inflation, employment) at the country, the regional economic union, and the world economy levels based on the developed global multi-country macroeconomic model in the class of dynamical stochastic general equilibrium models (DSGE models) and parametric control theory. Methodology for developing of the model, calibration and estimation of parameters; assessing the conditions of transferability of the results of computational experiments to the investigated subject area; macroeconomic

analysis, and solving problem of economic growth and suppressing the volatility of macroeconomic indicators in the retro and forecasting intervals is based on system analysis, parametric control theory and approaches within the DSGE modeling. The novelty lies in the construction of the model, which differs from the known ones by expanded the composition of the regions (Kazakhstan, Russia, Belarus, Armenia, Kyrgyzstan, the United States, the European Union, China and the Rest of the World), expanded composition of agents (patient and impatient households, producers of oil, traded non-oil and non-traded products, second-tier banks, central banks and governments), complicated of agents' behaviors (by introducing different financial frictions, uncondition economic policies, intermediate commodities, and i.e.); two-step estimation; model testing (by using the evaluation of stability indicators, retroprognosis, estimating the closeness of the first and second order moments observed and calculated data, analyzing impulse responses, local sensitivity analysis, comparison of the marginal likelihoods); results of macroeconomic analysis and solution of parametric control problems. As results theoretical recommendations in the field of economic policy on economic growth and suppression of volatility of economic indicators at the levels of individual countries, the Eurasian Economic Union and the world economy were developed.

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## Evolution of a Performance-Efficient Air Pollution Model

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Air pollution modeling in a large scale area is extremely tough numerical task, even with the most powerful up-to-date parallel computing systems on hand. The Danish Eulerian Model (DEM) is a powerful and sophisticated large scale air pollution model, with a long development history. Over the years it was used successfully in different long-term environmental studies for the European region. By processing a huge amount of data (most of it - for the quickly changing meteorological conditions), the model is able to calculate the variable concentrations of a number of pollutants and other closely related chemical species over a long time period. Moreover, various accumulative quantities (AOT40, AOT60, etc.) are calculated on yearly basis. Thus huge data sets appear and are to be processed along with the complicated calculations. With the rising power of the modern supercomputers and the novel developments in the up-to-date parallel implementation of the model (UNI-DEM), great improvement has been achieved in the speed of

calculations. As far as the transfer and I/O processing of the huge data sets is concerned, this lately became a strong bottleneck for the overall performance of the code. One way to deal efficiently with this problem will be discussed here. The effect of the improvements will be shown by experiments on some of the most powerful parallel supercomputers in Europe. For some applications it is highly desirable to simplify as much as possible the model, keeping the reliability of its output results. A careful sensitivity analysis is needed in order to decide how to do such simplifications. On the other hand, it is important to analyze the influence of variations of the initial conditions, the boundary conditions, the rates of some chemical reactions, etc. on the model results in order to make right assumptions about the simplifications which are to be done. Analysis of that kind can give valuable information about the performance of reliable and reasonable simplifications. It can also identify parameters and mechanisms, the accuracy of which should be improved, because the model results are quite sensitive to their variations.

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## **Interspike Interval Distribution for a Continuous-Time Random Walk Model of Neurons in the Diffusion Limit**

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One of the milestones in theoretical neurobiology was the introduction of the perfect integrate and-fire (PIF) neuron model by Gerstein and Mandelbrot [1]. In this model the voltage across the neuron membrane obeys a simple random walk kinetics. In the present work, we generalize this model, using the concept of continuous-time random walk [2], for the PIF model presented in Ref. [1]. CTRW models are fundamentally different from the regular random walk models (e.g., in Ref. [1]) as the probability density of the walk in the long-time limit behaves in a non-Gaussian way, which is a serious extension of the Gaussian case, due to which, e.g., the CTRW becomes a foundation of anomalous transport and diffusion. As experiments from many different areas reveal that anomalous diffusion is ubiquitous in nature, signaling that it may be generic for complex heterogeneous systems [3], we propose, based on the CTRW approach, a diffusion-like equation with distributed-order time fractional derivatives for the kinetic description of spike generation in the stochastic firing process of a PIF neuron model. The effect of a temporally correlated random activity of synaptic inputs, which arises from other neurons forming local and distant networks, is modeled as a waiting time

distribution with an asymptotic power law behavior in the underlying mesoscopic CTRW model. Using a first-passage-time formulation in an external uniform force field, we find exact expressions for the Laplace transforms of the output interspike interval (ISI) density and of the survival probability. More precisely we analyze the properties of the ISI distribution in the case of the double-order time-fractional diffusion equation, which is characteristic for the general situation. Similarities and differences between the behaviors of the ISI densities at decelerating and accelerating subdivisions are also discussed.

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## Studying Performance of Distributed Batch Asynchronous Advantage Actor-Critic Algorithm

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We introduce a parallelized distributed architecture for deep reinforcement learning's Batch Asynchronous Advantage Actor-Critic (BA3C) algorithm, producing current state-of-the-art results over multiple gaming tasks. We have developed a robust method of synchronous distributed training on large CPU clusters, that successfully trains neural networks to excel at a wide range of Atari 2600 games. Our implementation shows very promising scaling capabilities and surpasses current leading algorithms, in the Atari domain, in terms of training efficiency.

Presented results focus on optimizing algorithm to work on multiple machines, and performance tuning of asynchronous reinforcement learning algorithms on large computer clusters with the idea of bringing the training time down from hours to minutes. In this context, different hardware configurations within the cluster, e.g. number of nodes, cores per CPU, threads per node, as well as batch size are considered. The goal of the work is to come up with a solution that optimizes a



robust single-machine learning algorithm to scale efficiently on multiple CPU-based workers.

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## Mining Smartphone Generated Data for “User Action Recognition” – Preliminary Assessment

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Recently, smartphones became a very interesting source of data, due to the fact that they can include as many as different 14 sensors. Therefore, it has been recognized that generated streams of data can be used in a number of different contexts. Among them one can find, for instance, crowd sensing mechanisms (allowing study of user mobility patterns) or eHealth applications (helping users to reach individualized fitness goals).

In this context, observe that collected data can be used not only to find out what users are doing, but also to verify activities they declare. For instance, to establish if the user did actually use bicycle to “travel from point A to point B” (rather than going by car). As a matter of fact, the latter is precisely the case of an application, which has been developed to “incentivise” workers to use bicycles (in particular, to travel to work). The specific question that is being addressed is: how to “teach” smartphone to correctly recognize user activities (especially, mode of transportation). To answer this question, machine learning mechanisms have been applied to raw sensor data, obtained from actual cell phones. Furthermore, it is important to balance sensor power consumption and computational requirements, with correctness of prediction and response time.

In the presentation, we will compare results of application of recurrent neural networks, being one of the most powerful and popular means to process time series

data, with more traditional approaches (decision trees, SVNs, etc.). Finally, we present approaches that leverage domain knowledge in order to make classifiers more reliable and requiring less processing power (and less energy).

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## Applying Semantic Technologies within a Port Internet of Things Ecosystem – Case Study

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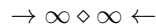
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Internet of Things (IoT) deployments proliferate globally. One of the areas where they find use are large multimodal logistics centers. For example, ports of today become filled with sensors and actuators. In this context, in the port of Valencia, intelligent lights system has been installed. Here road lamps, within terminals, are to react to presence of vehicles to turn light on and off and thus reduce electricity consumption (and light pollution). However, as it turned out, utility of this system is limited due to the fact that it is working only with port owned machinery, as it is not capable of interacting with trucks that pick/deliver containers. Interestingly, this problem can be combined with (and extended by) issues involved in management of access to the port (logistics center, in general). Here, not only trucks of companies that have contracts signed with the port have to be allowed in (and then interact with intelligent lamps), but also trucks that have been subcontracted by holders of original contracts should be treated as the “original ones.”

To address these issues, it has been proposed to apply semantic technologies. The aim of the presentation will be to discuss the approach and show how it has been implemented and tested.



## The Non-Isothermal Mathematical Model of Particle Beam Action on the Target with Coating

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The treatment of a metal surface by particle beam is accompanied by a variety of physical and chemical phenomena. It is known that the particle impact on the target surface leads to the appearance of stresses. Usually the processes of impurity introduction and stress redistribution are interdependent in theoretical works. But these processes influence each other. The implanted impurities can meet internal surface separating several areas with different structure or orientation. Also it may be the border separating coating or thin layer from target material. That is why the propagation velocity of mechanical waves in transition across the border is changed. As a result, the concentration wave velocity is changed too. The paper is aimed at investigating the initial stage of particle beam action on the target surface with coating. The model allows considering the processes occurring after interaction of particle flux with target – stress generation. Assume that: ions have sufficient energy for generation mechanical perturbations; strain and stress are elastic; strain, velocity and acceleration are small. Then the mass balance equation, the heat equation and the equation of motion are used for describing the interaction of diffusion wave, heat wave and stress (strain) wave under particle beam action. The coupled problem is solved using an implicit difference scheme. The developed numerical algorithm provides the stability and convergence.

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## An Application of Survival Model in Insurance

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In actuarial science, biology and demography, a life table (also called a mortality table or actuarial table) is of particular importance. This table shows the probability for a person at certain age to die before his or her next birthday (“probability of death”). In other words, it represents the survivorship of people from a certain population. An important benefit from life tables is that they could be used to make predictions on demographics of different populations. The life table observes the mortality experience of a single generation, consisting of 100 000 births (for example), from birth until no lives remain in the group. In order to price insurance products, and ensure the solvency of insurance companies through adequate reserves, actuaries must develop projections of future insured events (such as death, sickness, and disability). For that purpose, actuaries develop mathematical models of the rates and timing of the events. They do this by studying the incidence of these events in the recent past, and sometimes developing expectations of how these past events will change over time and deriving expected rates of such events in the future, usually based on the age or other relevant characteristics of the population. An actuary’s job is to form a comparison between people at risk of death and people who actually died to come up with a probability of death for a person at each age number. In the process of analysing the population decline, an important role has the force of mortality, i.e. the number of deaths in a particular population, scaled to the size of that population, per unit of time (most often one year). In many applications, it is very important to obtain survival models. In this paper we consider a life table for males: United States, 2010, and construct a quadratic survival model. Next we proof its adequacy and present a force mortality interpretation and an application in insurance.

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## Fourier Approximation for Modeling Limit of Insurance Liability

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The liability limitation clause is a required element of any insurance policy. Determining such a limit requires an interruption (one or more) in the distribution of the claim process used for estimating the financial balance. These distributions are found in the literature as truncated distributions. This in turn leads to the question how to proceed with such mixed continuous/discrete distributions if one needs comprehensive analysis, including derivatives, mass functions, accurate simulations random variables with such distributions etc. In the present work the process of claiming as a stochastic process is defined by the important properties of the Poisson process. The question about defining models of the claim process, which arise in practice when imposing a limitation on liability for the individual payment of claims by the insurer is considered. There are different approaches for approximating the distribution functions for solving these issues. The focus in this paper is placed on an algorithmic method for approximation of functions of distribution with a trigonometric Fourier series, giving analytical form of these functions and allowing simulations to be made in the area of interruption of the obtained particular distribution.

Results for one of the basic distribution in the insurance practice – Gamma distribution are presented. The results are compared with normal approximation. Any approximation leads to errors. For estimating and forecasting some of the most often used errors in the analysis are considered two methods – minimax estimation and the least square method. Considered regression models to predict the error, depending on the distribution parameters, provides an opportunity for comparative analysis when using generators of random variables. The achieved algorithmic method could be applied for estimating and forecasting the process of claiming and classical risk models.

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## A 4-Variate Gompertz Type Diffusion Model: Computational Aspects and Applications

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This work focuses on modeling the growth dynamics for measurements of tree variables in a forest stand. Stochastic differential equation (SDE) models allow us a better understanding of biological processes driving the dynamics of natural phenomena. In this study, we propose a system of the Gompertz type 4-variate fixed effect parameters SDEs to quantify the dynamics of tree size components distribution against the age in a forest stand with a sigmoid form trend for the mean value of tree size components. The new derived 4-variate probability density function and its marginal univariate, bivariate, trivariate and conditional univariate distributions are applied for the modeling of stand attributes such as the mean diameter, height, crown base height, crown width, volume and slenderness ratio. All parameters were estimated by the maximum likelihood procedure using real-life data set. The results are implemented in the symbolic algebra system MAPLE.

**Key Words:** 4-variate stochastic differential equation; univariate lognormal distribution; conditional distribution; Gompertz

**Acknowledgements.** This work was supported by the European Union Investment in Lithuania project 09.3.3-LMT-K-712.

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## Noise-Induced Excitability in the Hodgkin-Huxley Neuron Model

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We study the probabilistic behavior of the Hodgkin-Huxley neuron model in presence of the random forcing of the parameter of the injected (external) current.

Excitable regimes (spiking and bursting) in this model are frequently associated with the parametric zone of self-oscillations. We show how the phenomenon of the noise-induced excitement can occur in the zone of stable equilibria (quiescence regime). A parametric analysis of the stochastic excitability in the Hodgkin-Huxley model is carried out. Statistics of interspike intervals and probabilistic distributions of mixed-mode oscillations are studied.

**Acknowledgements.** The work was supported by Russian Science Foundation (N 16-11-10098).

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## Analysis of Stochastic Cycles Induced by Periodic Forcing

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We consider nonlinear dynamical systems forced simultaneously both periodically and stochastically. The periodic modulation generates oscillatory regimes in the form of cycles. Additional stochastic forcing results in the dispersion of random trajectories around these cycles. To analyze this dispersion quantitatively, we develop a mathematical approach based on the probabilistic asymptotics. For weak noise, the asymptotics of random trajectories dispersion is found in a form of the periodic function. This function is a solution of the boundary value problem for some deterministic linear differential equation. The elaborated mathematical method is applied to the analysis of the stochastic oscillations in one-dimensional model.

**Acknowledgements.** The work was supported by Russian Science Foundation (No 16-11-10098).

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## Modeling of Fan Waves Taking into Account the Resistance to Separation of Domino-Slabs in a Fan-Shaped System

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Recent laboratory studies showed that the propagation of shear rupture in hard rocks at stress conditions corresponding to seismogenic depths is associated with consecutive creation of inclined small slabs in the fracture tip. Due to rotation caused by shear displacement of the fracture interfaces, such slabs form a fan-shaped structure representing the fracture head. The fan-head is characterized by very low shear resistance and can propagate as a wave of extreme dynamics through intact rock mass at shear stresses below the frictional strength. In our research, we analyze the laboratory physical model of the system of rotating bonded slabs on inclined plane, which was created to imitate the process of fan formation and propagation. Mathematical model of the dynamics of this system as a mechanical system with a finite number of degrees of freedom is realized by means of the Merson method for numerical solution of ordinary differential equations. We consider two different approaches describing the resistance to separation of slabs in a fan-structure. In the first of them, the value of limiting couple force is assumed to be given. In the second one, a nonlinear tension diagram for the bonds between the slabs with a characteristic tooth simulating the initial strength of the bonds is determined. Comparison of the computational results by these two approaches shows a good qualitative and quantitative correspondence. The influence of viscous friction on the process of motion of a fan is analyzed. Dependencies of the velocity of motion on the geometrical parameters of a fan-system are obtained, too.

**Acknowledgements.** This work was supported by the Centre for Offshore Foundation Systems (The University of Western Australia).

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## Linear Instability of the Peregrine Breather: Numerical and Analytical Investigations

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We study the linear stability of the Peregrine breather both numerically and with analytical arguments based on its derivation as the singular limit of a single-mode spatially periodic breather as the spatial period becomes infinite. By constructing solutions of the linearization of the nonlinear Schrödinger equation in terms of quadratic products of components of the eigenfunctions of the Zakharov-Shabat system, we show that the Peregrine breather is linearly unstable. A numerical study employing a highly accurate Chebychev pseudo-spectral integrator confirms exponential growth of random initial perturbations of the Peregrine breather.

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## Methods of Padé-Type Multidimensional Approximations Application for Solving Boundary Value Problems

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As well as the Padé approximations itself, multidimensional approximations of such type can be used both to expand the domain of convergence and to accelerate the rate of convergence of series. We consider the modified method of parameter continuation (MMPC) as an asymptotic technique for solving boundary value problems in noncanonic domain. MMPC implies the use of multidimensional Padé-type approximants. In this paper we consider the application of several types of multidimensional Padé-type approximants depending on the problem specificity

which is being solved. The comparison with numerical calculations confirms the advantages of proposed methods and their accuracy.

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## Resonant Response in Bounded Nonlinear Wave Systems

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Resonant phenomena in bounded domains can pose distinct challenges both from physical and mathematical standpoints. It is well known that resonant behavior can arise in bounded domains under weak forcing, leading to significant amplifications in the response. Canonical examples include acoustic resonance in open and closed tubes and other geometries. Exactly how this resonant behavior manifests itself depends crucially on the underlying features of the system, i.e., is it continuous, is it shocked, etc.

In order to gain a better understanding of this process and the underlying mathematical features which drive the outcomes, we will present and discuss a simple class of nonlinear PDE model systems, then we explain how the features of this problem such as the form of nonlinearity, boundary conditions, and the nature of spectrum play a fundamental role in the qualitative nature of the response. These are then studied in more detail both from an analytical and numerical perspective. Of particular interest will be the description and characterization of the transition between various response regimes.

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## The Semi-Lagrangian Approximations of Transfer Operators in Time-Dependent Equations

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The approximation of transfer operators in time-dependent equations obviously depends on demands of stability or the fulfillment of conservation laws. For example, the approximation of the continuity equation for the mass conservation law in the compressible Navier-Stokes system would be monotone and also ensures the fulfillment of this conservation law at a discrete level. Another important conservation law is the conservation of kinetic energy. In our talk, at first we will present the semi-Lagrangian approximations of the transfer operator for different conservation laws using the one-dimensional parabolic equation as an example. Then we will demonstrate their application to the Navier-Stokes equations both for incompressible liquid and for compressible gas. We will provide these approximations with some numerical examples. Note that semi-Lagrangian approximations can give better properties of the discrete schemes in comparison with the traditional difference schemes or the finite element ones with up-wind means. So, the semi-Lagrangian approximations can help to avoid the Courant-Friedrichs-Levy condition due to adaptive stencils for discrete equations. Another advance consists in the elimination of first-order derivatives from the finite element formulation that improves the properties of discrete analogues. For example, the semi-Lagrangian approximation in combination with the finite difference or finite element method results in grid problems with inversion of symmetric matrices at each time layer unlike the traditional discrete approximations with non-symmetric matrices.

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**Elastic High-Performance Computing Platform for  
Real-Time Data Analysis  
(Xeon Phi, Kubernetes, Docker, Apache Kafka)**

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Using the power of high performance computing together with the flexibility of loosely coupled event-driven software architectures provides a lot of benefits especially, when it comes to processing real-time data. This paper outlines the architecture of a general-purpose platform leveraging event-driven micro-services architecture in combination with Event Sourcing and powerful High-Performance Computing core. The platform is aimed to software applications that process and analyze huge amount of data in a real-time or near-real-time fashion from variety of sources, having as requirement downtime-less upgrade and scaling capabilities. The first-class citizens of this platform are applications in the domains of IoT, trading, meteorology and traffic control. The reference implementation of this platform used as foundation for this research consists of two main components, the hardware based on Intel Xeon Phi Knights Corner family and Kubernetes as main container orchestration solution leveraging both Xeon processors and co-processors for maximum performance. On the application level the platform uses Apache Kafka as Event Sourcing mechanism that allows to treat the applications as state machines, providing capability to perform “step back in time” or “multi-window event processing.” We present the architecture of the platform and initial experiments that demonstrate the feasibility of our approach. Related to project “Development and Investigation of quasi-Monte Carlo Algorithms for Extreme Parallel Computer Systems” <http://www.grid.bas.bg/ENDFNI-I028/index.html>.

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## Numerical Modeling of Multiphysics Blood Filtration Problem in Liver Lobule

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Earlier in the paper A. Bonfiglio et al. was carried out numerical simulation of blood circulation in the liver lobule. In this paper multiphysics model for blood filtration in the liver lobule is considered. Multiphysics model consist of double porosity model for blood flow process in lobule, linear elasticity model for lobule deformation process, also anisotropy effects are taken into account. A numerical algorithm is based on the finite element approximation in space and using time explicit-implicit approximation.

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## Junction Trees Construction: Application to Bayesian Networks

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The junction tree shows the important relationship between graph theory and efficient probabilistic inference through a very important and interesting mathematical property of junction trees, the running intersection property. This paper examines an alternative method for constructing junction trees that is essential for the efficient computations of probabilistic enquiries posed on Bayesian networks. It presents a new method for converting a sequence of subsets in a Bayesian network into a proper set of cliques satisfying the running intersection property. We propose an algorithm in two versions (one of which is original) that allows a sequence of cliques possessing the running intersection property to be built. The obtained set of cliques and separators coincide with the junction tree obtained by the moralization and triangulation process, but it has the advantage of adapting to any computational task by adding links to the graph.

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## Bayesian Network Model for Temperature Forecasting in Dubai

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In this paper, we deal with the problem of weather forecasting using Bayesian networks. The study focuses on the data representing Dubai weather conditions. The variables used in this study are as follows: maximum and minimum temperature, mean temperature, mean relative humidity, rainfall, and wind speed. The National Centre of Meteorology and Seismology (NCMS) gathered the weather data from Dubai Airport Station located at latitude:  $25^{\circ}15'$  and longitude:  $55^{\circ}20'$  starting from January 2004 to December 2014. The values available represent month averages. We used these data to learn the Bayesian network structure and parameters. Inference in the Bayesian network helped in forecasting the maximum and minimum temperature of the succeeding months through dynamic Bayesian networks. The model showed 72% and 90% overall precision in forecasting minimum and maximum temperature, respectively.

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## Parallel Implementation of the Algorithm Describing the Behavior of Liquid Crystals under the Action of Electric Field

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Mathematical model for description of the dynamic processes in liquid crystals under weak mechanical, temperature and electric perturbations was proposed. This model is based on the representation of a liquid-crystal medium as a fine-dispersed continuum. At each point of this continuum, the domains of a liquid crystal can move in accordance with laws of the dynamics of viscous or inviscid liquid and can rotate relative to a liquid, encountering resistance to rotation. In this work a numerical algorithm for analysis of the influence of electric field on a liquid crystal and its parallel implementation are represented. We consider a layer of a liquid-crystal medium under the action of periodic electric field, created by appearance of charges on the plates of a capacitor. In the exterior part of a layer, the potential of

electric field satisfies the Laplace equation. Its solution is constructed by the method of straight lines. Inside a layer, the equation taking into account the anisotropy of a medium is solved by means of iterative method using a recurrence relation. In the presence of electric field, the molecules of a crystal experience the action of bulk forces and couple stresses, which can be used as right-hand sides of the basic equations of mathematical model. The algorithm is implemented using the CUDA technology for computer systems with graphics accelerators. Main stages of the algorithm are executed sequentially, the parallelization of computations is performed inside each of the stages. Parallel program contains modules realizing the method of straight lines with the use of a three-point sweep, the Fourier transform and the SLAE solution method by means of the LU-decomposition and the iterative method of solving the equation for potential. Some numerical results are represented.

**Acknowledgements.** This work was supported by the Russian Foundation for Basic Research (project no. 18-31-00100).

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## **Multiscale Model Reduction of the Flow Problem in Fractured Porous Media Using Mixed Generalized Multiscale Finite Element Method**

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Mathematical modeling of a flow in fractured porous media is important problem in subsurface simulations. Therefore, the development of mathematical models and efficient computational algorithms for numerical modeling of such processes is an actual problem. The mathematical model should take into account the entire complex of complicated, multiscale processes occurring in fractured porous media. The fracture network requires a special approach in the construction of a mathematical model and computational algorithms. In this paper, we construct a coupled mixed dimensional model for simulation of the flow process in the fractured porous media. Mathematically the problem is described by a coupled system of

equations consisting a  $d$ -dimensional equation for flow in porous matrix and a  $(d-1)$ -dimensional equation for fracture networks with a specific exchange term for coupling them. In order to reduce size of the system and efficient solution of the presented problem, we construct coarse grid approximation using Mixed Generalized Multiscale Finite Element method. We will present results of the numerical simulations using our proposed multiscale method to illustrate its performance.

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## On Statistical Invariants, Groups and Broken Symmetries for Algebraic Confidence Covers

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Hartigan's "typical value theorem" (1969) [3] is the basis for random subsampling, a resampling plan which uses group theory to construct confidence intervals for the center of a symmetric distribution on a real line. Atkins and Sherman [1] derived a group-theoretic condition on a set of subsamples of a random sample from a continuous random variable symmetric about 0 to be sufficient to provide typical values for 0.

Nowadays, in the "Big Data" era, subsampling from a complex data can be viewed as a natural solution to the computational issues induced by the immoderate size of databases. Since ignoring the survey scheme can impede estimation by introducing a non-negligible bias, it might be helpful to derive statistics under symmetry (or other group action) constrain. While a plethora of analyzes has already been conducted to provide unbiased and efficient estimation of average quantiles, to our knowledge, such is not the case for phenomena involving invariance under the action of a finite reflection group, e.g., the hyperoctahedral groups of  $B_n$  type. We have addressed this issue in Francis, Stehlík and Wynn [2]. Beside that, surprisingly, generating functions for such structures (e.g.,  $B_n$ ) follow asymptotics of Hájek-Šidák CLT (1967). Structures (e.g.,  $B_n$ ) can naturally introduce invariances, under which statistician can build up covering nets in higher dimensions. Such knowledge provide us omnibus covering nets, which cannot be obtained by inverting of severely directed nonparametric multivariate rank tests (see recent paper Jurečková and Kalina [4]). New possibilities for building proper subsampling and algebraic confidence covers are given.



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## Deviation Analysis using Applicable Methodologies for Impact Assessment on the Ambient Air Component from Industrial Sites

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In completing an Environmental Impact Assessment report for impact assessment on the ambient air component, three methodologies are applicable for drawing up an inventory on an annual basis of the estimated values of the pollutant quantities, emitted from the assessed site. They are the following: 1) AP-42, Compilation of Air Pollutant Emission Factors (EPA – U.S.Environmental Protection Agency ) 2) EMEP/EEA air pollutant emission inventory guidebook (EEA – European Environmental Agency) 3) Updated unified methodology for inventory of harmful substance emissions in the air, approved by the Bulgarian Ministry of Environment and Water. The paper presents an impact assessment on the ambient air component for a particular site using any of the applicable methodologies. The study focuses on establishing the deviations of the estimated emission values of the emitted pollutants by the various methodologies compared to the actual values of the pollutants specific to the site after putting it into operation. The purpose of the research is to determine the methodology that provides a sufficient degree of certainty for the site’s predicted results before putting it into operation and to ensure the ambient air quality in the investment area.

**Keywords:** ambient air, pollutant, environmental impact assessment, forecasting

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## Two-Color Self-Focusing of Optical Beams

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The effect of self-focusing is responsible for the collapse of high-power gaussian beams in free space. Nonlinear Schrodinger Equation (NLSE) is the mathematical model that correctly describes this dynamics. Collapse is a fundamental phenomenon and is well-studied. It has an important application in the area of filamentation, collapse leads to ionization of the air and creation of plasma channel. Collapse of a single beam is linked to the power of the ground state Townes soliton profile of 2-D NLSE. In the recent work [1], the extension of Townes soliton for two-color beams were obtained. In this talk, I will describe new types of spatial collapse events of two-color beams being both at resonance and non-resonance as well as the effect of dispersion on temporal dynamics.

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## Statistical Analysis of the Implementation of Resource-Saving Technologies for Rapeseed Production in Southeastern Kazakhstan

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Rapeseed production has grown in Republic of Kazakhstan nowadays because of the variety of existing possibilities for the rapeseed using. New resource-saving

technologies for rapeseed growing are implemented in Kazakhstan. For these new technologies it is needed to know which are the factors that influence the production of rapeseed and how each factor influence the yield and the quality of this culture. The careful study of these factors is necessary for better understudying the process of the growing aimed increasing the yields and quality of the rapeseed in Southeastern Kazakhstan. The principles of rational use of the natural resources of the rapeseed agro-ecosystem at the southeastern part of Kazakhstan are described. Resource-saving technologies for rapeseed growing save significant part of energy costs per unit of rapeseed production and give good opportunities to strengthen the stability of its agro-environmental systems. They also provide important conditions for the natural recovery of agro-ecological factors and soil fertility. It is needed to combine the three basic scientific principles for sustained development of agro-economics: creating an optimal soil structure, preserving and improving soil fertility; stabilizing ecophysical health status as a whole; optimizing the environmental conditions for rapeseed growing and increasing yields. A statistical analysis of data connected with atmospheric characteristics and technological parameters of rapeseed production in Southeastern Kazakhstan is provided and commented in the paper.

**Key words:** Rapeseed, resource-saving technology, statistical analysis

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## IST Numerical Methods for Solving Nonlinear Evolution Equations

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In this talk a survey and a method of derivation of certain class of numerical schemes and an implementation of these schemes will be presented. These schemes are constructed by methods related to the Inverse Scattering Transform (IST) and can be used as numerical schemes for their associated nonlinear evolution equations. They maintain many of the important properties of their original partial differential equations such as infinite numbers of conservation laws and solvability by IST. Numerical experiments have shown that these schemes compare very favorably with other known numerical methods.

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## Homogenization for Nonlocal KPP Reaction-Diffusion Equations in Periodic Media

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We examine the front propagation and homogenization properties of a Fisher-KPP type reaction-diffusion equation with generic periodic reaction term and nonlocal diffusion which generalizes the fractional Laplacian. Following a certain hyperbolic scaling of the space and time variables, we use techniques of viscosity theory to determine a locally uniform limit for the Hopf-Cole transform of the solutions. Working backwards, we also derive the asymptotic behavior of the original solution.

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## Mathematical Modeling of HIV Dynamics with Virus-to-Cell and Cell-to-Cell Transmissions

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We propose and analyze a within-host model for the dynamics of HIV to investigate the effect of virus-to-cell and cell-to-cell transmissions. We will incorporate mitosis of the healthy target cells which is described by a logistic term and two routes of infection, via binding of a virus to a receptor on the surface of a target cell to start genetic reactions (virus-to-cell infection), and the direct transmission from infected cells to uninfected cells through the concept of virological synapse in vivo (cell-to-cell infection). Then we will further analyze models of drug therapy with multiple delays accounting for a period of the chemical reaction in the virus-to-cell infection, an intracellular incubation period in the cell-to-cell infection, and a period of the immune lag incurred by antigenic activation and selection.

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## Gravitational Waves: Ripples in Spacetime's Geometry

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A key prediction of Einstein's theory of general relativity, namely the existence of gravitational waves (GW), has recently been tested. More specifically, on September 14, 2015, the Laser Interferometer Gravitational-wave Observatory recorded GW, emitted a billion light-years away by a coalescing binary of two stellar-mass black holes (the detection was announced in February 2016). GW correspond to ripples in spacetime itself, they are not waves of any substance or medium. Like electromagnetic waves, GW move at the speed of light and carry energy. The study of the universe using GW is not just a simple extension of the optical and electromagnetic possibilities, it is the exploitation of an entirely new spectrum that could unveil parts and aspects of the universe inaccessible so far. The enormous technological effort to build ultra-sensitive detectors has been followed by an intense quest for developing computer methods to solve Einstein's equations. Having invested so much to detect GW, it is crucial that we be able to interpret the waveforms detected. In this talk, I present a brief historical overview and some of the challenges of the GW science.

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## Solving a Singularly Perturbed Elliptic Problem by a Cascadic Multigrid Algorithm on the Shishkin Mesh

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A two-dimensional linear elliptic equation with parabolic and regular boundary layers is considered in the unit square. It is solved by using an upwind difference scheme on the Shishkin mesh which converges uniformly with respect to a small perturbation parameter. The scheme is resolved based on an iterative method. It is known that the application of multigrid methods leads to essential reduction of arithmetical operations amount [1] and the references therein. Earlier in [2] we investigated the cascadic two-grid method with the application of Richardson extrapolation to increase accuracy of the difference scheme uniform with respect to a perturbation parameter, using an interpolation formula uniform with respect to a

perturbation parameter. We obtained that the usage of the auxiliary mesh with the number of nodes in two times less than the initial mesh leads to increase accuracy of the difference scheme by an order uniform with respect to a perturbation parameter. In this paper multigrid algorithm of the same structure is studied. We also used an interpolation formula uniform with respect to a perturbation parameter. We construct an extrapolation of initial guess using numerical solutions on two coarse meshes to reduce the arithmetical operations amount. The application of the Richardson extrapolation method based on numerical solutions on the last three meshes leads to increase accuracy of the difference scheme by two orders uniform with respect to a perturbation parameter. Different iterative methods are compared. The results of some numerical experiments are discussed.

**Acknowledgement.** Research has been supported by the program of fundamental scientific researches of the SB RAS No I.1.3., project No 0314-2016-0009.

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## Loan Portfolio Payment Flows Management Considering Macroeconomic Parameters Forecast

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Markov model of the loan portfolio dynamics considering the process of new customers attraction as a control action from the bank management is described. Unlike the models, that do not take into account the attraction of new customers, the proposed model describes not only the structure, but also the volume of the loan portfolio, which allows to model and predict changes in quantitative lending indicators in dynamics when changing bank management decisions on the organization of selection procedure. When choosing the optimal management strategy such

indicators as portfolio income and risk are used. In accordance with the adopted approach in the financial analysis, portfolio income will be described based on the analysis of payment flows using its net present value (NPV). The risk of the loan portfolio will be calculated as a share of problem loans. The model also takes into account dependence of the incoming applications flow quality from external economic factors. The problem of choosing the optimal management strategy of the bank by two criteria (NPV and a share of problem loans) based on the Markov model of the loan portfolio structure dynamics considering the forecast of macroeconomic parameters is formulated.

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## Efficient Quasi-Monte Carlo Methods for Multiple Integrals in Option Pricing

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Nowadays quasi-Monte Carlo methods have become a popular computational device for problems in finance. We consider European style options. In the special case when the payoff function is the exponential function, with an appropriate choice of the constants involve in the formula for the value of the European option, we obtain a multidimensional integral of the exponential function over the unit hypercube. We compare several quasi-Monte Carlo methods based on lattice rules for different multidimensional integrals up to 30 dimensions. It is well known as long as the integrand is sufficiently regular lattice rules outperform not only the plain Monte Carlo method, but also other types of low discrepancy sequences. The performance of a lattice rule depends heavily on the choice of the generator vectors. We considered the simplest lattice rules, called “rank 1” rules, and use a lattice generated by multiples of a single generator vector. The advantages and disadvantages of the different quasi-Monte Carlo methods under consideration have been discussed. The methods have never been compared before on European options and that motivates the study.

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## Statistical Analysis of Air Quality Measurements Data from Automatic Mobile Station for City of Ruse, Bulgaria

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In the frame of SANDI project (Support Actions to create New RDI partnerships in trans-border area in order to bring together Business and Research for accessing European Funds - SANDI, (2011-2013) [http://www.comoti.ro/en/participarea\\_la\\_proiecte\\_europene\\_2\\_12.htm](http://www.comoti.ro/en/participarea_la_proiecte_europene_2_12.htm) between COMOTI and Ruse University measurements of air quality characteristics were provided. Mobile automatic station of COMOTI institute was placed in front of Ruse University and 14 different atmospheric characteristics were measured on 26 and 27.06.2012. The data were measured continuously at 3 minutes and after this, mediation was performed for each hour in order to compare it with the legislative limits.

This paper deals with the descriptive statistics of these data. Also, the mobile station data measured were compared with the official data from the two stations in the city of Ruse, Bulgaria. Correlation and regression analysis of the measured data were made and commented in the paper.

**Keywords:** Air quality measurements, Atmospheric characteristics analysis

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## Stable Mode of Dendritic Growth with Allowance for the Convective Heat Transport near the Solid/Liquid Phase Transition Interface

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Convection plays an essential role in the growth of dendrites. Convection may influence the transport of heat and substances as well as mechanical deformation of dendritic crystals. In this paper, the effect of convective heat transport that substantially changes the dendrite tip diameter and its tip velocity is demonstrated. In addition, the Gibbs-Thomson condition connecting the phase transition temperature has been taken into account with allowance for the kinetic contribution arising from the effect of attachment kinetics at the phase transition boundary. In this paper the growth of an anisotropic dendrite under conditions of convective heat transfer at the solid-liquid interface was analyzed theoretically. An analytical solution is obtained for the temperature distribution in the liquid phase for the parabolic and paraboloidal forms of the needle-like dendrite. The stability analysis is carried out and the integral of microscopic solvability is defined. The selective ratio for the stable growth rate of the dendritic tip and its diameter is derived.

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## Two-Dimensional Interaction of Internal Solitary Waves

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Study of Internal wave in stratified fluid is important, for example, associated with transport and mixing process in the ocean. In particular stable solitary wave with large amplitude and long wavelength is studied intensively in order to clarify the dynamics of its generation and propagation. In theoretical studies, some weakly nonlinear equations which can be systematically derived from fundamental equations have been proposed. These equations, including Korteweg-de Vries (KdV) equation, have the solitary wave solution which interact without deformation. But most

pioneer studies were limited to one-dimensional modeling. Concerning the two-dimensional interaction in which line solitons interact with different angle of propagation direction, different kind of interaction can be seen. Depending on the interaction angle the new soliton is generated and steady propagates (soliton resonance). This phenomena was firstly discussed by Miles (1970) for surface water wave and has studied by many researchers. Recently mathematical studies about integrable Kadomtsev-Petviashvili (KP) equation, which is two-dimensional extension of KdV equation, advanced its understanding. In this talk this resonant phenomena is numerically studied by two-dimensional model equations which has one-dimensional line soliton solution. It is clarified that the “nonlinear resonant” phenomena can be seen not only the integrable systems but also the non-integrable model equation.

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## **Statistical Study of the Influence of the Atmospheric Characteristics upon the Particle Mater (PM10) Air Pollutant in the City of Ruse, Bulgaria**

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Air pollution by particle matter with a diameter between 2.5 and 10 $\mu\text{m}$  (PM10) is going up recently in Ruse region, Bulgaria [1, 2]. Also recently it becomes clear that the mean values of the temperature in Ruse region are slightly goes up for the last 40 years and they are bigger than the mean temperature for Bulgaria. This could be interpreted as a proof for climate change and warming in Ruse region. The presence of PM10 maybe affects and changes somehow the main atmospheric characteristics - temperature, atmospheric pressure and humidity.

The sources of dust on the territory of Ruse region, Bulgaria are industry, transport and domestic heating by solid fuel. PM10 levels for Ruse mark a significant increase during the autumn-winter period compared to the levels during the spring-summer period [1, 2, 3]. The biggest peak of PM10 levels for the autumn-winter period is usually observed in January months. It is in January that the number of days in which there is exceedance of the limit values of the PM10 levels is maximum observed. It becomes clear, that there is a relationship between PM10 contamination levels and ambient air characteristics.

In our work [3] we examined in more details the influence of the temperature on the PM10 contamination during January months. The lower the temperatures are, the higher the PM10 levels are. Also in January months the day and night temperatures are the lowest and usually they do not pass 0°C for many days of the

month. To understand better this relationship we provide a statistical analysis of ambient air PM10 contamination during winter periods [3]. Correlations between the measured PM10 values and the respective temperatures measured for January months for different years were presented in [3].

This paper is one continuation of [3] and is devoted to examine the PM10 pollution in Ruse region during winter and its relationship with some atmospheric characteristics (atmospheric pressure and humidity). It presents a statistical analysis of the level of PM10 air pollution in Ruse using data from the monitoring stations in the city. The measurements cover the period since 2011 up to now. Descriptive statistics of PM10 and atmospheric characteristics – pressure and relative humidity as well as linear regression modeling are presented and commented in the paper.

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## Mathematical Modeling of the Fluid Flow and Geomechanics in the Fractured Porous Media using Generalized Multiscale Finite Element Method

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In the reservoir simulation, mathematical modeling of the fluid flow and geomechanics in the fractured porous media plays an important role. A coupled poroelastic

models can help for better understanding of the processes in the fractured reservoirs. In this work, we consider a discrete fracture model (DFM) for coupled flow and mechanics problems. Mathematical model describes by the coupled system of equation for displacement and pressure. The fundamental point is that the system of equations is coupled: the equation for the motion includes the force, which is proportional to the pressure gradient, and the pressure equations include the term, which describes the compressibility of a medium. Fracture networks have complex geometries, exist in the multiple scales and typically have very small thickness compared to typical reservoir sizes. Due to high permeability, fractures have a significant impact on the flow processes. In this work, we consider a discrete fracture model for coupled flow and mechanics problems. We construct coarse grid approximation using Generalized Multiscale Finite Element method (GMsFEM). In this method, we solve local spectral problems for construction of the multiscale basis functions for pressure and displacements. We present numerical results for two-dimensional model problem.

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## Simulation of Thermal Interaction of Multiple Wells Open Loop Geothermal System

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A heat distribution model of an open geothermal system with multiple wells is considered. This system consists of two wells: a number of production wells with hot water, which is used and became cooler, and an injection well, which returns the cold water into the productive layer (aquifer). This cold water is filtered in the productive layer (porous soil) towards the inflow of hot water of the production wells. A productive well network is considered for delivering hot water. In the paper the productive wells interaction is considered from the point of view the temperature in the wells optimization.

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## Numerical Modeling of Seismic Wave Propagation under the Action of Electromagnetic Pulse Source

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Oil and gas producers are interested in effective methods of search and localization of hydrocarbon saturated formations. The classical geophysical methods may not be so effective due to the complex mosaic structure of oil deposits. It is proposed to improve the accuracy of seismic exploration by means of the electromagnetic pulse source “Yenisey” in combination with a highly dense system of points for receiving of the seismic signal. High density of seismic points increases considerably the prognosis of the formation properties. And the use of single sources reduces the effect of a spatial filter on the seismic signal. Unlike the explosive works and vibratory methods, the electromagnetic pulse source “Yenisey” gives well-defined parameters of the impact pulse on the medium excitation. Parallel numerical algorithm for the modeling of acoustic wave propagation in layered medium under the action of pulse source “Yenisey” is developed. The material properties in each layer are different depending on the type of the medium, i.e. hard rocks, soils. The results of numerical modeling allow to analyze the reflected waves of seismic signal when passing a thin layer of the medium. The parallelization of computations is performed by the CUDA (Compute Unified Device Architecture) technology for supercomputers with graphics processing units.

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## Algorithm of Time Step Selection for Numerical Solution of Boundary Value Problem for Parabolic Equations

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We propose an algorithm allowing automatic time step evaluation when solving the boundary value problem for parabolic equations. The solution is obtained using guaranteed stable implicit schemes, and the step choice is performed with the use of the solution obtained by an explicit scheme. Formulas for explicit calculation of the time step are derived using the estimation of the approximation error at new time step. Calculation results obtained for model problem demonstrate reliability of the proposed algorithm for time step choice.

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## GARCH Models for Particle Matter Air Pollutants in the City of Ruse, Bulgaria

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The main air pollutant in Ruse is particle matter PM10, as can be seen from our previous work [1]. The average annual rates at the two measuring stations in the city are near the norm, but over the daily norm are 25% and 15% of the observations respectively. The maximum reported values exceeds 3.52 and 4.35 times respectively the daily norm of 50 (mg/m<sup>3</sup>). Almost all values above the norm, in particular 81% and 91% respectively are measured in the winter months. The two time series exhibit clearly expressed time-varying volatility. In [1] and [2] we obtained ARIMA models for the levels of PM10 measured at the two stations. Natural logarithm transformation was used to ensure the stationarity of the time

series. The goal of this paper is to analyze and forecast volatility of the two original data time series using GARCH models.

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## Estimation of Parameter-Dependent Plates Vibrations on the Basis of the Asymptotic Method

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We consider the modified method of parameter continuation (MMPC) as an asymptotic technique for estimating the frequencies and shapes of both parametric oscillations and nonlinear vibrations of plates with parameter-dependent boundary conditions. Unlike known methods, which are usually used for such estimations, MMPC estimations depend from the initial plate shape. It describes real vibration shape of plate with different conditions on its edges. The comparison with numerical calculations confirms the advantages of proposed method and its accuracy.

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## Mathematical Simulation of the Acoustic Wave Propagation through Absorbing Layers on the Ground

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Among modern geocological problems an important problem is that estimation the geocological risks for the environment from the impact of powerful acoustic waves generated by technogenic and natural explosions of increased danger including powerful quarry and polygonal explosions, technogenic roads noises, earthquakes, etc. Of greatest interest is to study of seismic and acoustic effects from mass explosions, since they determine the integrity of industrial and residential objects. Along with the meteofactors increasing the environmental risks from explosions there are factors that lead to weakening of acoustic vibrations from explosions. These include the presence of a snow cover, forest massifs, and relief along the propagation path of acoustic waves. Particular statements of the problems of acoustic oscillations propagation associated with the estimation of the influence of individual factors on the characteristics of propagation were considered earlier. The problem of acoustic oscillations propagation under such conditions is a multi-factor one. In the present paper, authors estimated weakening characteristics taking into account influence of absorbing layers (vegetable and snowy) to the surface propagation of acoustic waves from infralowfrequency vibrational sources. In the "air - absorbing layer - ground" model the problem of interaction of acoustic waves falling at a given angle on a ground covered absorbing layer with seismic waves arising in the ground is studied. The question of the influence of the absorbing layer on amplitudes of seismic waves excited in the ground is investigated. A system of differential equations of the gas dynamics, wave and elastic equations with boundary conditions is constructed. It describes the propagation of incident and reflected acoustic waves in the air, and refracted and reflected waves in the absorbing layer and ground. The amplitudes and pressures of reflection and refraction of acoustic and seismic waves are calculated and analyzed depending on the different characteristics of the absorbing layer.

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## Symplectic Numerical Method for Boussinesq Equation

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In this talk we study the fourth order Boussinesq equation with a single nonlinearity. We rewrite this equation in the Hamiltonian form and construct a finite difference scheme, which preserves the symplectic structure of the initial problem. To illustrate the new scheme we present many computational results. We compare the performance of the symplectic scheme with the existing conservative finite difference schemes.

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## Method for Solving an Inverse Problem of Heat Transfer Based on the Integral Equation

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The paper is devoted to the problem of linear heat transfer in a homogeneous object when the temperature measurements are carried out only in a boundary domain and it is required to calculate the temperature at the internal control points. This problem is represented as one-dimension inverse problem for parabolic PDE when the nonzero conditions are given on one boundary domain of the rod. In this problem, it is required to calculate the unknown boundary function on another end and then to find the temperature values at the internal points.

In this contribution, the authors reduce the inverse problem to an integral equation via the Laplace transforms. The resulting equation characterizes the direct dependence of the unknown boundary function on the initial data. The algorithm for numerically solving the integral equations based on the regularizing technique is also developed. The proposed approach ensures the stability of numerical solution and eliminates the elements of operational calculus from the computational procedure. The reliability of the approach were verified by comparing the numerical results with the test functions.

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## Deformation and Fracture Based on Wave Dynamics

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Fracture of solids is discussed based on a recent field theory of deformation. Using a physically-based formalism analogous to electrodynamics, this field theory describes all stages of deformation comprehensively. A set of field equations similar to Maxwell equations have been derived, and their wave solutions have been obtained. Elastic deformation is characterized by the oscillatory behavior of the displacement field that propagates as sinusoidal waves (the deformation wave). The irreversibility of plastic deformation is characterized by the decaying behavior of the deformation wave where the energy dissipative dynamics is represented by a non-conservative field force acting on a quantity called the deformation charge. It has been observed that in an early stage of plastic regime the deformation charge drifts at a velocity proportional to the particle velocity. The dynamics of fracture is characterized by a solitary-like wave, which represents stress concentration leading to the final fracture. It has been observed that the drift velocity of the deformation charge decreases with development of deformation and that at the final fracture the deformation charge becomes completely stationary. While the field theory explains deformation and fracture self-consistently, the connection to the conventional dislocation theory has not been fully understood. Recent analysis indicates that the dynamics of deformation charge in the transition from the late plastic deformation to final fracture regimes is well explained by known behaviors of dislocations under the influence of external load. The energy dissipative force on the deformation charge is explained as the frictional force that dislocations undergo when they move. The decrease in the drift velocity of deformation charge is explained by known time dependence of dislocation velocity. All these observations indicate it possible to develop a new fracture mechanics theory consistent with the present field theory and dislocation theory.

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## Nonstationary Boussinesq Viscous Medium Flow for a Solid

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The translational movement in a viscous medium a homogeneous solid with a sufficiently smooth surface is considered. The center of mass moves along the curve connecting the origin of the coordinate system with a given point of space. Such motion is provided by a control force applied to the center of mass along the tangent to the curve of the trajectory. The problem is to determine the control force, under the action of which the mass center of the body at a given time reaches a predetermined point in space with minimum expenditure of energy to overcome the viscous resistance. To calculate the drag the Boussinesq approach is used. The problem does not involve any geometric restrictions on the control force. In such a situation, impulse components may appear in the composition of the optimal control force. Therefore, an attempt to solve this problem using known classical variational procedures is not correct. The original problem is reduced to an auxiliary problem that does not contain constraints on the phase coordinates and products of generalized functions.

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## Numerical Simulation of Formation of Hydrated Electron States

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Formation of hydrated electron states in water is investigated within the polaron model which is described by a system of nonlinear partial differential equations. The time-dependence of the absorption band width of the hydrated electron has been accounted in this framework in order to improve an agreement between numerical and experimental data. New results of numerical simulation are presented as well as description of numerical scheme and parallel implementation.

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## Parallel Implementation of the SANS Analysis of the PTNS-Based Vesicles Structure

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The parallel Asynchronous Differential Evolution (ADE) method [1, 2] with adaptive correlation matrix (ACM) [3] is implemented for the analysis of the drug-delivering phospholipid transport nanosystem (PTNS). ADE is appropriate to solve multidimensional global minimization problems appearing in the complex biological systems analysis and allows effective parallel computer implementation [1]. A vesicular structure of the indomethacin when incorporated into phospholipid nanoparticles is investigated. The experimental spectra have been measured at the

small-angle spectrometer YuMO (FNLP JINR, Dubna). The small angle neutron scattering (SANS) data from the polydispersed populations of the unilamellar PTNS-based vesicles in heavy water have been investigated. The analysis is based on the separated form-factors (SFF) method [4, 5, 6]. Several models for the vesicular structure is discussed and analyzed using SFF modeling. The average radius and polydispersity of vesicles as well as parameters of internal structure of bilayer, have been determined by fitting to SANS spectra. The numerical results are discussed in comparison to the results of the analysis of the small angle synchrotron X-ray spectra from the PTNS system elaborated in the Orechovich Institute of Biomedical Chemistry (Moscow) [7]. Respective minimization problem is solved by means of the ADE-ACM algorithm [1, 3]. The efficiency of our MPI-based parallel computer code for the SFF-ADE procedure is also demonstrated.

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## An Algorithm for Computing Reachable Sets of Control Systems under Isoperimetric Constraints

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We consider a reachability problem for a nonlinear affine-control system with integral constraints, also known as isoperimetric constraints. The constraints supposed to be quadratic in control variables. Under controllability assumptions it is proved that any admissible control that steers the control system to the boundary of its reachable set is a local solution to some auxiliary optimal control problem with vector-valued cost functional and terminal constraints on a trajectory. This leads to the Pontriagyn maximum principle for boundary trajectories. We propose here a numerical algorithm for computing the reachable set boundary based on the maximum principle and provide some numerical examples.

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