Contents

1. Mathematical Methods and Tools for Modeling Complex Systems

New Methods in Potential Theory

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A theory of equigravitating bodies has been developed. They allow one to represent external force fields of the volume axially-symmetric figures through single integrals. The theory is developed in three directions. The first direction is related to the proof of existing equigravitating rods. Such rods can have both real and imaginary density distribution. However, the mass and the external potential of the rods remain real. The rod boundaries are marked with special points. (These are points of fractures on teh surface or else special points of analytical continuation of the external potential inside to the body.) At two special points there is a single equigravitating rod, otherwise the rods will be composite and or form equigravitating "skeletons". In case of isolated special points the external gravitating fields can be represented as a set of rods and mass points.

A second directionis based on the representation of the external gravitating field of volume bodies with the help of potentials of plane disks. All cases when such disks are located over the equigravitating rods have been described. The contrary is always valid: for a homogeneous disk or any non-uniform circle disk one can find an equigravitating rod and therefore an equigravitating volume body with an equatorial plane of symmetry. It is possible to build chains of equigravitating bodies of 'spheroid - disk - rod'.

A third direction is related to the development and expansion of the the application area of the method of cofocal transformations. This method is modified and applied both to continuous homogeneous ellipsoids (as made Maclourin, Ivory and Laplace), and to stratified non-uniform ones with stratification of the general type, as well as to homogeneous and non-uniform shells. Any elementary or thick ellipsoid shells (as well as continuous non-uniform stratified ellipsoids) connected by special confocal transformations have been found to be mutually gravitating.

Разработана теория эквигравитирующих тел, с помощью которых внешние силовые поля объемных осесимметричных фигур можно представлять через однократные интегралы. Теория развивается в трех направ-

лениях. Первое связано с доказательством существования эквигравитирующих стержней. Такие стержни могут иметь как реальное, так и мнимое распределение плотности, однако масса и внешний потенциал стержней остаются вещественными. Границы стержней отмечены особыми точками (это точки изломов на поверхности или особые точки аналитического продолжения внешнего потенциала внутрь тела). При двух особых точках эквигравитирующий стержень один, в противном случае стержни составные или образуют эквигра-витирующие "скелеты". При изолированных особых точках внешние гравитационные поля можно представить совокупностью стержней и точечных масс. Второе направление опирается на представление внешнего гравитационного поля объъмных тел с помощью потенциалов плоских дисков. Указаны все случаи, когда такие диски находятся по эквигравитирующим стержням. Обратное верно всегда: для однородного или любого неоднородного круглого диска можно найти эквигравитирующий стержень, а значит, и эквигравитирующее ему объъмное тело с эквато-риальной плоскостью симметрии. Удаѣтся построить цепочки эквигравитирующих тел типа "сфероид - диск - стержень". Третье направление связано с развитием и расширением области применения метода софокусных преобразований. Этот метод модифицируется и прилагается не только к сплошным однородным эллипсоидам (как это делали Маклорен, Айвори и Лаплас), но и к эллипсоидам слоисто-неоднородным со стратификацией самого общего вида, а также к однородным и неоднородным оболочкам. Любые элементарные или толстые эллипсоидальные оболочки (а также сплошные слоисто-неоднородные эллипсоиды), связанные специальными со-фокусными преобразованиями, оказываются эквигравитирующими друг другу.

Numerical Solution of Elliptic Problems with Non-Classical Interface Conditions

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A finite difference discretization of elliptic problems with discontinuous coefficients is investigated. The interface condition relates the jump of the normal derivatives and a second order elliptic operator in tangential variables. Error estimates of the method in Sobolev spaces are obtained. Numerical tests illustrate the features of the presented method.

Critical Dependencies in Three-Layered Josephson Junctions

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The dynamics of the Josephson phases in stacked long Josephson Junctions is described by Sakai-Bodin-Pedersen model. Partial critical dependencies of the kind current-magnetic field for three-layered Josephson Junctions are numerically investigated by using this model. Numerical procedure for finding the critical currents of the individual junctions for fixed parameters is proposed and realized. A correspondence between switching to nonzero voltage of the system and the loss of stability of some static solutions is found. For this reason the static problem is numerically investigated as well. In order to study the stability of possible static distributions a Sturm-Liouville problem is generated and solved. Critical currents for individual junctions are found for different values of the damping and coupling parameters at low magnetic field. We show that the individual critical currents depend on these parameters and that there is a domain in vicinity of zero magnetic field where the junctions switch to nonzero voltage simultaneously.

Non-Markovian Relaxation of Atomic Systems and Line Shape Calculations

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Non-Markovian relaxation equation for a system of two-level atoms in the limit of short-time memory is derived. The level populations and the shape of radiation lines are calculated. Influence of memory effects is observed and compared with Markovian approach calculations.

Nonstandard Finite-Difference Schemes for Reaction Diffusion Equation

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As is known, a system of reaction-diffusion PDE's provides a valuable mathematical models for a broad range of phenomena in the natural and engineering sciences. In many cases, the dependent variables represent physical variables that can not take negative values. Therefore, it is desirable to construct positivity preserving schemes.

In this talk we present a family of nonstandard finite-difference schemes preserving positivity and boundedness.

The proposed schemes can be considered as an extension of the well–known Mickens one.

About a Class of Finite Elements with Harmonic Basis Functions

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For approximation of high order vector-functions, a new class of finite elements with harmonic basis functions has been suggested. An algorithm of construction of the functions inscribed into a sphere, has been also developed. Examples of using the finite elements of this class are given.

About Nonlinear Effects and Photons Statistics on Conditions of Selective Reflection of Laser Radiation

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Some nonlinear properties of spectrums of selective reflection in inclined geometry have been investigated. Asymmetry of saturation of resonant reflection is considered. New nonlinear structures up on reflective resonances are described. Some applications of the found features of selective reflection for quantum optics problems and quantum information processing are discussed.

Application of Polynomial Approximation Method to Drop Evaporation

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The polynomial approximation method for measurement data of a dependent variable with errors in both dependent and independent variables introduced in our previous papers is proposed. Here we discuss and apply it to the physics of drop river water evaporation. We analyze the main steps of the method of data fitting within the error corridor in both dependent and independent variables. We compare various approximating curves with different polynomial degrees within the data intervals. The method is applied to the data obtained from optical measurements of sessile drop evaporation.

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Multi-Channel Atomic Scattering and Confinement-Induced Resonances in Waveguides

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We have developed a wave-packet propagation method [1, 2, 3, 4] for multi-channel scattering of atoms in a waveguide with harmonic confinement. This approach is employed to extensively analyze the transverse excitations and deexcitations as well as resonant scattering processes. We plan to discuss resent results obtained in the field of contemporary physics of ultracold atoms and molecules [5, 6]. It was found that ultracold atoms in the confined geometry of optical trap or atomic chip have specific properties. Moreover, modern nano-technologies permit to control theirs properties by varying the waiveguide width up to $a_\perp \sim$60 nm. We have found the strong dependence of the transmission coefficients for pair atomic collisions in a harmonic trap on the ratio $a_s/a_\perp$, where a_s is the atom-atom scattering length. By varying the trap (confinement) width $a_\perp$ it is possible to change the effective interatomic interaction and generate the confinement-induced resonances [1, 2, 3]. They were analyzed for the first time at non-zero energies as well as the excitation of the transverse atomic vibrations at such collisions [4]. Possible applications include: ultracold collisions in atomic traps, electron-impurity scattering in quantum wires and atomic interferometry.

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Software for Solution Faddeev — Yakubovsky Equation

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The multiple scattering approximation based on the modified Faddeev—Yakubovsky equations [1] for charged and neutral particles is applied to the calculation of the scattering amplitudes and cross sections of the different processes ion-atom, ion-molecular and atom-molecular collisions.

In three-body approximation the amplitude may be written in the form [2]:

$$f_{2-2} = f_c + \Psi_{2-2} v_1 (G_2 V_2 + G_3 V_3 + G_2 V_2 G_3 V_3 + G_3 V_3 G_2 V_2) \Psi_{2-2}$$

- for elastic scattering,

and

$$f_{2-3} = \Psi_{2-3} v_1 (G_2 V_2 + G_3 V_3 + G_2 V_2 G_3 V_3 + G_3 V_3 G_2 V_2 \Psi_{2-2}$$

- for break-up processes,

where

$f_c = \eta \exp(-i\eta \ln \sin^2 \theta/2 + 2iarg\Gamma(1+i\eta))/2(\mid k \mid \sin^2 \theta/2)$- Coulomb amplitude;

$$\cos(\theta) = (\vec{k}\wedge, \vec{k}');$$

$$\Psi_{2-2} = \varphi_{2-2}(x)\psi_c(y,p);$$

$$\psi_c(y,p) = e^{-\pi\eta/2}\Gamma(1+i\eta)\Phi(-\eta, 1, i \mid p \mid\mid \xi \mid);$$

$$\eta = n/2 \mid p \mid; \qquad \xi = \mid y \mid -(y,p);$$

$$\Psi_{2-3} = \varphi_{2-3}(x,k)\psi_c(y,p);$$

$$v_i = n_i/ \mid x_i \mid + v_i^s(x_i); n_i = \gamma Z_i Z_j / \sqrt{2\mu_{ij}};$$

$$\mu_{ij} = m_i m_j/(m_i + m_j);$$

$$V_i = V_i^1 + V_i^2; V_i^1 = v_i^s + n_i \chi_i(x_i, y_i, \nu)/ \mid x_i \mid;$$

$$V_i^2 = (1 - \chi_i(x_i, y_i, \nu)) n_i / \mid x_i \mid;$$

x_i, y_i, k_i, p_i, m_i, Z_i - coordinate, momenta and charge of i-particle; ψ_{2-2},ψ_{2-3} - wave functions of the bound and continuous states two particle subsystems; G_i, χ_i - Green and cutoff functions defined in [1]. The parameters ν, x_i, y_i chosen

such that χ tends to unity in the limit $x_i << y_i \to \infty$ and vanishes when $x_i \sim y_i \to \infty$, thus proving asymptotic decoupling of the scattering channels.

This expression agrees with the expression for neutral particles obtained in the multiple scattering approach [3], if to take into account that $V_i G_i = G_0 T_i$. The present model obviously takes into account the long range interactions and allows one to take the multiple scattering into account in an explicit fashion, as well as the resonances connected with it for an arbitrary number and location of the scattering centers.

In this approach the elastic, inelastic (rearrangement, charge-exchange) and ionization processes are considered simultaneously.

Using the eikonal approximation of Green function explicit expressions for the differential cross section in case three-body scattering are presented. Energy and angular distribution of electron and proton in scattering of the proton with hydrogen are calculated. The characteristic features in the ionization spectrum at forward angles (the continuum electron capture and binary encounter peak) and different mechanism of this processes are discussed.

Under conditions in which such features play a dominant role by determining the order of magnitude of the cross sections of the processes in which we are interested, the use multiple scattering approach allows us to obtain a simple and effective estimate of the cross section.

The calculations of the different processes in the scattering of ions with atoms, ions with diatomic molecules and electron with diatomic molecules $H^+ + H$, $H^+ + He$, $H_2^+ + He$ and $He^+ + He$ in three-body approximations are presented [3].

The results of these calculations are compared with the available experimental data and other calculations such as quasiclassical, (saddle point mechanism), classical, multiple-scattering treatment, Born and impulse approximation, semiclassical Faddeev-Watson approximation [3].

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Applying the WKB Method to the Bifurcation of an Everted Spherical Shell Made of Elastic Varga Material

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We apply the WKB method to the bifurcation analysis of everted a spherical shells composed of Varga material. incompressible cases are considered. The method is degenerate but we obtain explicit bifurcation criteria and compare with previous numerical approximations.

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Econometric Approaches to Modeling Reality: Advances and New Challenges

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Some new advances in econometrics, concerned with financial engineering and risk management are presented. Latest events on the world financial markets show impossibility of modern mathematical methods for analyzing, forecasting and crisis avertion. In this work some fresh paradigm in econometrics and applied statistics are considered.

We introduced dynamical correlation models in multivariate GARCH for modeling the behavour of nonlinear stochastic dependencies between equities and applicate them for reasonable financial problems such as portofolio, risk protection in conditions of high volatility.

Equation of State of Strongly Coupled Quark–Gluon Plasma – Path Integral Monte Carlo Simulations[1]

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A strongly coupled plasma of quark and gluon quasiparticles at temperatures from $1.1T_c$ to $3T_c$ is studied by path integral Monte Carlo simulations. This method extends previous classical nonrelativistic simulations based on a color Coulomb interaction to the quantum regime. We present exploratory PIMC simulations of a nonideal quark-gluon plasma. The main goal is to test this approach for ability to reproduce the equation of state known from lattice data [1]. To this end we use the simplest model of a QGP consisting of quarks, antiquarks and gluons interacting via a color Coulomb potential due to Gelman et al. [2] with several approximations for the temperature dependence of the quasiparticle masses. We report surprisingly good agreement with the lattice data for one of the parameter sets, which gives us confidence that the model correctly captures main properties of the nonideal QGP. Further, pair distribution functions and color correlation functions are computed indicating strong correlations and liquid-like behavior.

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Simulation of Magnetic Reconnection in 3D in Geometry

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The mathematical model of magnetic reconnection in the vicinity of critical points is discussed in the frame of 3D magnetohydrodynamics. We have considered the evolution of the magnetic field in the vicinity of the null point and null line in the driven magnetic reconnection regime. The model numerically solved with the help of Schnack method. The effective parallel code is developed for the realization of numerical algorithm. Some results of computational experiments characterizing the origin of difficult nonlinear structures have been done.

New Mathematical Approach and Computation Algorithm for Study of Quantum 3D Disordered Spin System in External Field

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A dielectric medium consisting of rigidly polarized molecules has been treated as a 3D disordered spin system. For investigation of statistical properties of this system on the scales of space-time periods of standing electromagnetic wave a microscopic approach has been developed. Using the Birgoff's ergodic hypothesis the initial 3D disordered spin problem is reduced to the two conditionally separate 1D problems along external electromagnetic field propagation. The first problem describes a quantum dynamics of disordered N-particles system with relaxation in medium, while the second one describes statistical

properties of disordered 1D steric spin-chains system. Basing on the constructions which are developed in both problems, the coefficient of polarizability related to collective orientational effects under the influence of external field was calculated. Using these investigations the Clausius-Mossotti (C-M) equation for stationary (effective) dielectric constant with taking into account the influence of standing electromagnetic field was generalized. As well the equation for permittivity function was generalized. It was shown that in weak standing electromagnetic field in the spin-glass system's is possibly catastrophe in the C-M equation which can substantially change behavior of permittivity function in the X-rays region on the macroscopic scale.

The developed approach allows creating a significant new effective parallel algorithm for computation of 3D spin-glass system on a scale of space-time's period of standing electromagnetic field.

Fitting of 3D Reaction Surface of Three-Atomic System in the Natural Collision Coordinates System

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As was shown recently [1], the problem of quantum reactive scattering in three-body system in *natural collision coordinates* (NCC) may be reduced to the inelastic single-arrangement problem. In other words in NCC system the initial multistep complex problem is possible to reduce to the problem of solution of first-order ordinary differential equation's system. The algorithm of numerical simulation in this case consists from two parts:

a) Computation of coefficients of equations describing a reactive scattering,

b) The numerical solution of aforementioned system of equations.

The realization of first part includes two important problems:

1. Fitting of the *ab-initio* calculations array of bi-molecular chemical reaction surface by a especial analytic form (in particular the programs package creation),
2. Using analytical form for a reaction potential, calculate the explicit form of coefficients in the scattering equation. To create program for calculation of coefficients in arbitrary points of grid, which are defined on the curve of *coordinate reaction* $\Im_{i,f}$.

Note that the 1) problem is solved by two steps. At first was investigated the reaction surface of collinear collision because near this surface is localized the part of the configuration space, important for exchange reaction in three-body system. In particular was shown, what the generalized Mors potential with the two coefficients which are functions from the coordinate changing along the curve "Coordinate Reaction"describes the peculiarities of surface of collinear collision very precisely. As shows numerical simulation on the example of $H+H_2$ reaction the both coefficients in mentioned case are being well described by Eckhart type potential function, which includes a set adjusting parameters.

On the second step were investigated properties of 3D reaction potential. As was shown with the help of numerical simulation (on the examples of H+H2 reaction and its isotopes), for other (nonzero) members of decomposition of 3D potential isn't suitable to use Eckhart function for the coefficients in generalized 2D Mors potential. In this case the coefficients depending on coordinate are being changed very fast, what is very bad for numerical simulation of dynamical problem. Nevertheless, this problem is being solved by a way of choice for coefficients of other class of analytical functions. As shown on the example of numerical simulation of hydrogen isotopes' reactions, 3D reaction surface may be represented in the form of decomposition with the help less than eight Legendre polynomial.

For computation of coefficients in the potential surface's decomposition is elaborated parallel code for numerical simulation.

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Numerical Solution of the Schroedinger Equation with a Degenerate Polynomial Potential of Even Power

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We have constructed a high-order finite difference scheme for the Schrodinger equation with the degenerate potential $U(x) = x^{2r}, r \in N$ which describes phase transitions in quantum systems. The eigenvalues are found for some values of r.

A Physical Approach to the Development of Computational Algorithms for Solving the Navier–Stokes Equations and Its Application in Jet Engine Analysis [1]

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Linearized finite-differenced Navier–Stokes equations result in a generalized saddle point system

$$\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

in which α and β represent the discrete velocities and discrete pressure, respectively. Here nonsymmetric A is a block diagonal matrix, where each block corresponds to a discrete convection-diffusion operator with appropriate boundary conditions. The rectangular martix B^T represents the discrete gradient operator while B represents its adjoint, the divergence operator.

It is clear that the system cannot be solved by standard methods of linear algebra. Solution algorithms for the generalized saddle point problems can be

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subdivided into two categories, which we will call segregated (decoupled) and coupled methods.

A new approach for reduction of computational cost of numerical algorithms for the Navier–Stokes equations in primitive variables formulation is proposed. The approach uses physical aspects of hydrodynamics for fast computation of "part" of pressure. For the given purpose, an auxiliary problem based on simplified Navier–Stokes equations and original pressure splitting is suggested. "Part" of pressure can be computed using mass conservation equations and high effective numerical methods proposed for the simplified Navier–Stokes equations. The paper represents detailed description of the approach and results of numerical experiments with benchmark and applied problems. Proposed approach leads to impressive reduction of the computational efforts at simulation of directed fluid flows [1, 2].

Results of the study will be used for interdisciplinary computations of elements of gas turbine engines. MSC.SimManager SimEnterprice technique makes it possible to obtain informational model of engineering data consisting of results of CFD simulation.

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Elimination of the Centre-of-Mass Motion in the Nuclear Shell-Model with Isospin

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An efficient procedure for large-scale calculations of the two-particle translational invariant coefficients of fractional parentage (TICFPs) for several j-shells with isospin is presented. The approach is based on a simple enumeration scheme for antisymmetric many-particle states and efficient algorithms for

calculation of the coefficients of fractional parentage for a single j-shell and several j-shells with isospin. The TICFPs may be obtained by diagonalizing the centre-of-mass Hamiltonian in the basis set of antisymmetric A-particle oscillator functions with singled out dependence on intrinsic coordinates of two last particles and choosing the subspace of its eigenvectors corresponding to the minimal eigenvalue equal to 3/2. An arbitrary number of oscillator quanta can be involved. We investigate the characteristics of the introduced TICFPs basis and the application of this procedure to the harmonic-oscillator shell-model approach.

Численное решение системы нелинейных дифференциальных уравнений, описывающей эволюцию полярона[1]

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В работе исследована численная схема для решения системы нелинейных дифференциальных уравнений, описывающей эволюцию полярона в однородной среде с модельными параметрами системы и для параметров, соответствующих H_2O. Выполнен анализ точности схемы вычислений. По результатам численных экспериментов сделан вывод, что если в системе уравнений с модельными параметрами в начальный момент времени полярон находился в конкретном состоянии (основном или возбужденном), то он сохраняется в этом состоянии независимо от наличия или отсутствия затухания в системе. Показано, что для модельного случая начальные распределения заряда, заданные суперпозициями, при наличии в системе затухания с течением времени эволюционируют в основное состояние, а при

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отсутствии в системе затухания эволюция в основное состояние не наблюдается. С параметрами, соответствующими H_2O, для тех значений времен, в которых был проведен численный эксперимент, эволюция в основное состояние не наблюдается, независимо от наличия или отсутствия затухания в системе.

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Investigation of Solutions of Boundary Problems for the Singular Perturbed Differential Equation of High Order[1]

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An algorithm is suggested for finding eigenvalues and eigenfunctions for one boundary problem for the equation of the high order (the sixth, the eighth, the tenth and the twelfth one) with small parameter ε at higher derivatives with a Coulomb potential. Investigations of the eigenvalues and eigenfunctions are carried out at various values of ε. The algorithm is realized with the use of a system of symbolical evaluations MAPLE.

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Моделирование тепловых процессов в однослойных и двухслойных материалах при прохождении тяжелых заряженных частиц высоких энергий[1]

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Разработана обобщенная модель термического пика, учитывающая движение иона внутри материала. Компьютерная программа SRIM-2007 [1] позволяет вычислять потери энергии тяжелых ионов при их прохождении через конденсированные среды. Проведенные расчеты (с использованием результатов программы SRIM-2007) показали, что время прохождения ионов урана с энергией 700 МэВ в никелевой мишени составляет $t_{\text{ион}} \approx 4 \times 10^{-12}$с. В предыдущих исследованиях [2] не учитывалось движение иона внутри материала и предлагался источник со временем действия $t_{\text{ион}} \approx 10^{-14}$с. Нами предлагается модель термического пика с новым источником, учитывающим движение иона внутри материала. Приведены некоторые результаты расчетов при облучении никеля ионами урана с энергией 700 МэВ и сравнительный анализ с предыдущими результатами [2], где не учитывалось движение иона внутри материала.

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Numerical Simulation of Heatmass Transfer Process in the Porous Material

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In papers [1-4] the inverse diffusion problems are solved in the isothermal approach for determination of a moisture transfer coefficient in porous materials with use of experimental data of moisture spatial distribution for different time moments.

In this contribution the model equations that describe transfer of heat, moisture and air in porous materials are formulated. A numerical study of the equations for moisture penetration to material, its drying and a comparative analysis of the obtained results with the results of [1-4] are carried out.

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Numerical Investigation of the Thermoelastic Effects in Materials Irradiated by Pulsed Ion Beams in Frames of a Thermal Spike Model[1]

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In works [1-2] formation and evolution of the thermoelastic waves arising in metals irradiated by pulsed ion beams in frames of a system of equations of the thermoelasticity are investigated.

We offer the modified thermal spike model considering the suggest thermoelastic effects in materials. A comparative analysis of results of numerical research in these equations with the results of the classical equations of thermoelasticity has been performed.

The results of the investigations have shown that the temperature of the sample and the thermoelastic waves in two approaches strongly differ, at that temperature twice. A dependence of the shape of thermoelastic waves on speed of switching on the source is explored.

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Numerical Energy Approach and QED Lines Moments Technique for Atoms and Nuclei in a Strong Laser Field

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New numerical models in the QED theory are developed for studying interaction of atoms with an intense and superintense laser field. Our approach is based on a description of system in the field by the k-photon emission and absorption lines. The lines are described by their QED moments of different orders, which are calculated within Gell-Mann and Low adiabatic formalism [1,2]. The corresponding energy approach uses the adiabatic Gell-Mann and Low formula for an energy shift dE with QED scattering matrice, which includes an interaction with the photon vacuum field and external electromagnetic (laser) field [1,3]. Thus it allows one to provide a uniform description of the different radiation processes as in absence of the laser field as directly in a strong laser field. In particular, we have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. and effect of the stochastic fluctuations in a field on the mujltiphoton resonances characteristics. For illustration there are gevin new data for the multi-photon resonance and ionization profile in Cs, Yb, Gd atoms. Besides, an efficiency of the QED energy approach is demonstrated by calculation of the two-photon ionization cross-sections for extended photon energy range (including above-threshold ionization) in Mg atom [3]. The analogous energy approach is for the first time developed for consistent description of the laser-nucleus interaction and corresponding multi-photon phenomena. The natural actual application of the presented approach is a formulaion of the consistent theory for the resonant process of nuclear excitation by electron capture NEEC (transition NEET) , in which a continuum electron is captured into a bound state of an ion with the simultaneous excitation of the nucleus. The preliminary estimates are obtained for the case of electric and magnetic multipole E2, M1 transitions in U, Yb , Gd etc. AC and DC strong field Stark effect for atoms is also studied within the energy approch and operator peturbation theory formalism. The zeroth order Hamiltonian, possessing only stationary states, is determined only by its spectrum without specifying its explicit form. We present here the calculation results of the Stark resonances energies and widths for a number of atoms (H, Li, Tm,U etc.) and for a whole number of low-lying and also Rydberg states [2]. We discovered and

analyzed the weak field effect of the giant broadening of widths for Letokhov-Ivanov re-orientation decay autoionization resonances in Tm etc. For the first time this effect is discovered in the U atom. We consider the nuclear dynamic (AC) Stark shift of low-lying nuclear states due to the off-resonant excitation by the laser field (laser intensity 10(25)-10(35) W/cm2). It is confirmed that the direct laser-nucleus interaction has to become of relevance together with other super-intense light-matter interaction processes such as pair creation.

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Electron-Beta-Nuclear Spectroscopy of Atoms and Molecules: New Numerical Models of Bound Beta-Decay and Decay of Isomeric States for Fully Ionized Atoms

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We discuss the cooperative electron-beta-nuclear processes in atoms and molecules, including the excitation, ionization, electronic rearrangement, induced by the nuclear reactions and beta-decay [1]. The relativistic many-body perturbation theory (PT) with the optimized Dirac-Kohn-Sham (DKS) zeroth approximation is used to calculate the beta-decay parameters for a number of allowed (superallowed) transitions (33P-33S, 241Pu-241Am etc) and study a chemical bond effect on beta-decay parameters [2]. A few factors are taken

into account: changing the integration limits in the Fermi function integral, energy corrections for different chemical substances, and the possibility of the bound beta-decay or other decay channels. We studied the electronic rearrangement induced by nuclear transmutation in the beta-decay . The half-life period 1/2 for beta-decay of tritium atom (ion) has been estimated while taking into account the bound beta-decay channel and some other accompanying effects. The estimated values of 1/2 for the tritium beta-decay and free triton decay are: (T1/2;a)=12.26 years (correction due to the electron-atomic effects (ΔT/T)a=0.82%) for the tritium atom and (T1/2;t) =12.36 years for the triton decay. These data are in physically reasonable agreement with experimental data. We firstly present the value 1/2 in a case of the beta-decay in the halogen-containing molecular tritium (3l): (T1/2;m)=12.28 years (3l); the correction due to the chemical bond effect is (dT1/2;am)=0.024 (i.e. 0.20%). The estimates for a ratio lb/lc of bound-state (lb) and continuum-state (lc) beta decay rates for the case of bare (207)Tl(81+) ions and isomeric states of fully ionized (144m)Tb etc are given. The similar effects are also studied for (187)Re. The effects considered are responsible for creation of elements in the space and astrophysical plasma. Besides, an approach proposed can be useful, providing perspective for the development of new nuclear models, search of the new cooperative effects on the boundary of atomic and nuclear physics, carrying out new methods for treating the spatial structure of molecular orbitals, diagnostics of the hydrogen-containing compounds by means of exchange of the hydrogen atoms by tritium, studying properties of energy releasing in the tritium (DT, TT) plasmas [1-4].

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Autoresonant Asymptotics in the Oscillating System with Weak Dissipation

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Autoresonance is a phase locking phenomenon occurring in nonlinear oscillatory system, which is forced by oscillating perturbation with slow varying frequency. The essence of the phenomenon is that the nonlinear oscillator selfadjusts to the varying external conditions so that it remains in resonance with the driver for a long time. This long time resonance leads to a strong increase in the response amplitude under weak driving perturbation. Many physical applications of the autoresonance are known in nonlinear physics. The main goal of the autoresonance theory is revealing of existence of such state.

In the lecture a system of two first-order differential equations arising in averaging nonlinear systems over fast one-frequency oscillations is considered. The dissipation term is a specific of the equations under consideration. An asymptotics at infinity for two-parameter growing solutions is constructed. This result gives a key to understanding the autoresonance in weak dissipative systems.

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Atomic Parity Non-Conservation in Atoms and Dynamical Enhancement of Weak Interaction: Numerical Modelling

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During the past decade, first of all the optical experiments to detect atomic parity on-conservation (PNC) have progressed to the point where PNC amplitudes can be measured with accuracy on the level of a few percents in certain heavy atoms [1,2]. Promising idea (Forston) is to apply the techniques of laser

cooling and ion trapping to measurement of the PNC in 6s 2S1/2-5d 2D3/2 transition of the singly ionized barium. To provide an adequate treating these experiments in terms of the standard model for a electro-weak interaction, comparison of the measured amplitudes with theoretically defined ones is required. In the quantum many-body systems with dense spectra of excited states weak perturbation can be significantly enhanced. We consider an enhancement of the PNC effects in heavy atoms and neutron-nucleus reactions. Using the PNC effects one can study quantum chaos in many-body systems, nuclear fission , distribution of neutrons in nuclei etc [1-3]. Nowdays the PNC in atomic systems has a potential to probe a new physics beyond the standard model. We systematically apply the formalism of the relativistic many-body perturbation theory [2] to precise studying PNC effect in heavy atoms (nuclei) with account for the relativistic, nuclear and radiation corrections. Earlier an efficiency of this approach has been demonstrated in the precise calculation of the hyperfine structure constants, E1, M1 transition probabilities for heavy atoms and heavy ions [3]. We present the preliminary calculation results for energy levels, hyperfine structure intervals, E1-,M1-transitions amplitudes in heavy atoms of 133Cs, 137Ba+, 207Pb, 119Sn. For comparison the analogous data (e.g.[1,2]) by Dzuba etal (Novosibirsk), Bouchiat etal (Paris), by Johnson etal (Indiana), by Johnson-Sapirstein-Blundell (Notre Dame) are presented. Comparison of calculated transition amplitudes with the measurement by Noeker et al gives the following data of weak nuclear charge Q(w) and the Weinberg angle.

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Numerical Modelling in a Theory of Electron Internal Conversion in Nuclides

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We consider spectra of the barium isotopes and turn attention on definition of the corresponding internal conversion electron coefficients. It is continued the discussion which began in [1,2]. The neutron- deficient nuclides of 125,127Ba are theoretically studied and the level structures for high-spin states are interpreted the framework of the RMF model. The electron internal conversion coefficients in the 125,127Ba nuclides are calculated on the basis of the relativistic Dirac-Fock method. A comparison is performed of the obtained theoretical data and data by Rossel et al [3], which are 1.1-10(3) and 8.5-10(4) for M2 and E3, respectively, the 24.0-keV transition can be considered mainly an M2 transition. The other aK values of the 79.4-, 114.3-, 128.7-, 134.3-, 220.4-, 243.0-, 253.3-, 269.6-, 285.6-, and 318.7-keV gamma transitions associated with the decay of 127La are deduced from the electron internal conversion measurements [4]. It is confirmed that the E1 transitions between parity doublets are characterized by a two to four orders of magnitude enhancement compared to those of more normal cases. A possibility of manifestation of stochastic elements (dynamic enhancement) and quantum chaos is discussed.

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Metric Analysis and Applications

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Interpolation and forecasting of functions are one of the main mathematics tasks. At present for solving many applied problems mainly with the help of computer technology it is necessary to develop a universal method of interpolation and forecasting of multivariable functions $y = f(\vec{x})$ including conditions of presence chaotic uncertainty in determined values of function for points $\vec{X_1}, \ldots, \vec{X_n} \in E^m$, with the help of which values of function in the other points of space E^m are reconstructed.

An application of a new method for interpolation and forecasting of single and multivariable functions is considered in this work, including its usage at presence of chaotic components. The new method called metric analysis is based on construction of weighting metric and metric uncertainty matrix which takes into account the degree of argument influence on variation of interpolated or forecasted function. The metric analysis in contrast to autoregressive model and SSA method allows one to forecast the dynamical processes deseribed with nonlinear equations.

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Mathematical Model and Toolkit for Social and Economic Monitoring in Regions

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The problem of monitoring the social and economic situation in regions has always been a currently central one for our country due to the vast territory and variety of life conditions in different areas. This urgency severely increases in crisis conditions. For acceptance of reasonable well-grounded managerial decisions monitoring should not be reduced to sociological research, but it should be founded on a deep mathematical base. Whereas the problem of description of economic subjects interaction is more or less clear, the social processes are much more difficult for analysis. In the presented discourse the attempt is made on the basis of leading political psychologists' latest research to formulate a model of social and economic processes in a region. The analysis of results of this model application allows one to reveal such characteristic modes which correspond to real processes in the society. Prototypes of information systems which can be used for monitoring in real conditions are offered. The problem of regional elections forecast is analyzed as an example for such system application.

Проблема социально-экономического мониторинга ситуации в регионах всегда была актуальна для нашей страны из-за большой теоритории и различных условий жизни в разных районах. В кризисных условиях эта актуальность еще более возрастает. Для принятия правильных управленьческих решений мониторинг не должен сводиться к социологическим исследованиям, но под ним должна быть серьезная математическая база.

И если задача описания взаимодействия экономических субъектов более или менее понятна, с социальными процессами дело обстоит сложнее. В сообщении на основании исследований ведущих политпсихологов делается попытка сформулировать модель социально-экономических процессов в регионе. Анализ решений этой модели позволяет выявить характерные режимы, которые связываются с реальными процессами в обществе. Предлагаются прототипы информационных систем, которые можно использовать для мониторинга в реальных условиях. В качестве примера анализируется задача о региональных выборах.

Hybrid Information System for Estimation of Risks in Financial Markets

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Nowadays there exists a large variety of forecasting methods based on neural networks technologies which allow to adequately simulate the nonlinear processes with noisy data in slowly varying markets. However, in the conditions of strong turbulence they are not capable to promptly response to swiftly changing environment, and, hence, to market conjuncture changes. It has grown in a very serious problem, as the decisions accepted on the basis of these technologies can be resulted in movement of hundreds billion dollars in the financial markets, and any incorrectly revealed tendency can lead to large losses. We will notice that this problem has recently arisen due to joining of new world players to the common economics, and due to, as a consequence, decrease in controllability of the international system. In the presented work the dynamic approach will be considered which properly operates in swiftly changing markets. It is based on a combination of neural networks technologies with algorithms of quantum mechanics calculations.

Сегодня существует множество методов прогнозирования, основанных на нейросетевых технологиях, которые хорошо позволяют моделировать нелинейные процессы с зашумленными данными на медленно меняющихся рынках. Однако, в условиях сильной турбулентности они не способны быстро реагировать на изменяющиеся условия, и, следовательно, на

конъюктурные изменения рынка. Эту выросло в очень серьезную проблему поскольку решения, принимаемые на основе этих систем, связаны с движением сотен миллиардов долларов, и любая неправильно выявленная тенденция ведет крупным потерям. Заметим, что эта проблема возникла совсем недавно, вследствие присоединения к мировой экономике новых мировых игроков и, как следствие, снижения управляемости международной системы. В данной работе будет рассмотрен метод(динамический подход), который работает на сильно изменяющихся рынках и основан на комбинировании нейросетевевых технологии с алгоритмами квантовой механики(квантовых вычислении.

Комплексный метод математического моделирования сложных инженерно-технических систем

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Значительную роль в промышленности и сельском хозяйстве играют сложные инженерно-технические системы, обеспечивающие централизованное снабжение потребителей тепловой энергией, топливом, водой и другими транспортируемыми продуктами. Все эти системы различаются назначением, масштабностью, принципами создания, физической сущностью протекаемых в них процессов. К ним следует отнести польдерные системы [1-2], магистральные нефте- и газопроводы [3] и многие другие промышленные объекты.

Предлагаемый комплексный метод математического моделирования инженерно-технических систем в данной работе рассматривается на примере польдерных систем, имеющих два уровня: систему проводящих открытых каналов с насосными станциями и систему осушаемых массивов с определенными уровнями грунтовых вод (УГВ), вертикальными потоками влаги от поверхности грунтовых вод, атмосферными осадками, поверхностными испарениями и транспирациями влаги корневой системой растений. Системы имеют трехмерную структуру, в которой пространственно - временные распределения УГВ и уровней воды в открытых каналах определяются горизонтальными переносами, а увлажнение корнеобитаемого слоя почвы - вертикальными, и заключается в теоретико-множественном описании объекта, декомпозиции исходной постановки на подзадачи, в разработке методов решения гидродинамических уравнений, интегрирование которых

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проводится вдоль контуров обхода графа инженерно-технических систем. Использование теории графов позволяет построить инвариантные математические модели.

Синтез системы разрешающих дифференциальных уравнений в частных производных осуществляется на ребрах направленного графа инженерно-технической системы (проводящие трубопроводы, каналы) с заданием граничных условий в вершинах графа (точки ветвления), при выполнении равенства входящих и выходящих потоков из точек ветвления проводящих трубопроводов (закон сохранения потока в узлах проводящей сети), что обеспечивает сквозной расчет параметров инженерно-технических систем.

Отметим, что каждому элементу базы ставится в соответствие вектор состояний, включающий характеристики элемента, параметры технологического процесса и событий, характеризующий нарушения технологических (функциональных) ограничений. Параметры векторов состояний образуют элементы нормативно-справочной, оперативной и расчетной информации базы данных.

При этом задаются номинальные значения управляющих параметров и их допуск, а также математические ожидания и дисперсии целевых функций.

Такой подход позволяет просчитывать различные варианты конструкций инженерно-технических систем, моделировать оптимальные условия работы и режимы эксплуатации инженерно-технических, а также проводить оптимизационные расчеты для получения совершенных конструкций этих систем независимо от конфигурации и числа элементов базы инженерно-технических систем.

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Research of a Sensitivity of an Integrated-Optical Sensor of Gaseous Substances at the Presence of a Statistic Additive Noise by the Method of Computer Modeling

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The dependence of the sensitivity of an integrated-optical waveguide sensor on the length of a waveguide sensor cell, efficiency of input of the laser radiation in a waveguide, absorption cross-section and a level of an additive statistic noise is studied. On data of the computer modeling it is established, that the integrated-optical sensor of the given type can find out the contents of gaseous ammonia in the air with the limiting theoretical concentration about 0.1 ppm for the magnitude of the a signal-to-noise relation about 20, length of a sensor cell approximately 4 cm and efficiency of input of a laser radiation in a waveguide not less than 40%.

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Computer Simulation of Acceleration of Ions and Electrons at Interaction of a Laser Pulse with Plasma [1]

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It is well known that the interaction of ultraintense laser pulses with plasmas is accompanied by the acceleration of charged particles, both ions and electrons. Results are presented two-dimensional particle-in-cell simulations of the acceleration of ions and electrons at interaction of a ultrastrong laser pulse with structured targets. These simulations show that the laser pulse drills a channel through the plasma slab, and electrons and ions expand in vacuum.

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Numerical Investigation of Passively Advected Vector Field in Anisotropic Turbulent Environment[2]

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The field theoretic renormalization group and operator product expansion is used for investigation of the influence of uniaxial small-scale anisotropy on the stability of the scaling regime, on the turbulent magnetic Prandtl number, and on the anomalous scaling of the single-time correlation functions of a passive vector quantity (weak magnetic field within kinematic magnetohydrodynamics) advected by the velocity field governed by the stochastic Navier—Stokes equation.

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The model is studied in one-loop approximation. The corresponding system of strongly nonlinear renormalization group differential equations for determination of Kolmogorov-like scaling regime which contain angle integrals is constructed and solved numerically. The turbulent magnetic Prandtl number as function of anisotropy parameters is found. The influence of small-scale anisotropy on the anomalous scaling of the correlation functions of a passive vector field is studied by the operator product expansion and it is shown that the critical dimensions of the corresponding composite operators depend also on the fixed point value of the reciprocal magnetic Prandtl number already in one-loop approximation unlike the isotropic case and the case with the so-called large-scale anisotropy. It demonstrates the fact that the anomalous dimensions of the structure functions, which are the same (universal) for the corresponding Kraichnan-like model, for the model with finite time correlations of the velocity field [1], and for the model with the advection by the velocity field driven by the stochastic Navier-Stokes equation in the isotropic case [2], can be distinguished by the assumption of the presence of the small-scale anisotropy in the systems even within one-loop approximation. The corresponding comparison of the anisotropic anomalous dimensions for the present model with that obtained within the corresponding model of passively advected scalar quantity is done.

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Numerical Analysis of Anomalous Scaling of Passive Scalar Advection by Anisotropic Navier–Stokes Turbulence[1]

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The influence of uniaxial small-scale anisotropy on the stability of the scaling regime, on the turbulent Prandtl number, and on the anomalous scaling of the single-time structure functions of a passive scalar quantity (concentration

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of an impurity, temperature, etc.) advected by the velocity field governed by the stochastic Navier-Stokes equation is investigated by the field theoretic renormalization group and operator product expansion within one-loop approximation of a perturbation theory. The corresponding system of strongly nonlinear renormalization group differential equations for determination of Kolmogorov-like scaling regime which contain angle integrals is solved numerically [1]. The turbulent Prandtl number as function of anisotropy parameters is found and compared to the corresponding one- and two-loop isotropic values [2]. The influence of small-scale anisotropy on the anomalous scaling of the structure functions of a passive scalar field is studied by the operator product expansion and it is shown that the critical dimensions of the corresponding composite operators depend also on the fixed point value of the reciprocal Prandtl number already in one-loop approximation unlike the isotropic case and the case with the so-called large-scale anisotropy. It demonstrates the fact that the anomalous dimensions of the structure functions, which are the same (universal) for the Kraichnan model, for the model with finite time correlations of the velocity field, and for the model with the advection by the velocity field driven by the stochastic Navier—Stokes equation in the isotropic case, can be distinguished by the assumption of the presence of the small-scale anisotropy in the systems even within one-loop approximation. The corresponding comparison of the anisotropic anomalous dimensions for the present model with that obtained within the models with a Gaussian statistics of the velocity field is done [3].

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Temperature Distribution in Nuclear Fuel Rod at High Burn Up

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Temperature distribution in the fuel rod of nuclear reactor is one of the most important factors that control the behavior of fission products in the pellets,

the diffusion and vaporization properties and so on [1]. This dependence has been intensively studied for prolonged lifetime of existing reactors. Yapici et al.[2] investigated the maximum temperatures in centerline of the fuel rod for different clad outer surface temperatures, melting points of the fuel materials, temporal heat generation, temperature distribution in the nuclear fuel rod and temporal variation of the neutronic data during rejuvenation periods. Pontedeiro et al. in [3] presented an improved lumped—differential formulation for one—dimensional transient heat conduction in a heat generating cylinder with temperature—dipendent thermo—physical properties typical of high burn-up nuclear fuel rods.

The fuel behavior is affected by the temperature distribution in the fuel that is related to change in the fuel microstructure with irradiation. One significant change in the fuel microstructure is the formation of a porous rim in the periphery of the high burn-up fuel. It was shown that the rim structure is formed through recrystallization and coarsened pore formation. The subdivided grains with high angle grain boundaries are the nuclei for recrystallization, and then the coarsened pores are formed by the sweeping out of small pores during grain growth on recrystallization.

We have studied the temperature distribution in nuclear fuel rod taking into account the fuel, the rim - layer, the gap, the film of the zirconium oxide and the cladding. Solving the nonstationary task of the temperature distribution in the nuclear fuel rod by the numerical simulation we have obtained that the evolution of the temperature in the rod to the stationary behavior goes the short time. This time is less then 45 secund for the maximum power in nuclear fuel rod. This fact allowed us to consider the solution of the stationary behavior of the nuclear reactor. We have solved this task using the analytical method and we have found the exact solution of the temperature distribution in the nuclear fuel rod. Exact solutions allows us to analyze the temperature distribution in details and to evaluate the influence of the rim - layer and the zirconium oxide on the temperature distribution in the nuclear fuel rod.

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Mathematical Modeling of Track Formation in High-Temperature Superconductors

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Nanodimensions ion track technologies are now of great importance for their enabling increase the critical current density in high-T_c superconductors. In spite of the manifest practical importance, no satisfactory theory of track formation for these materials exist so far. Although different mechanisms were suggested till now, the thermal spike model (TSM) was demonstrated to be the most matchable for this purpose [1]. Mathematical modeling of track formation in $YBa_2Cu_3O_{7-x}$ in the frame of TSM revealed some unexpected features of the process such as imposibility to formulate an appropriate Stephan problem, existence of the electronic quenching phenomenon which results in supersensitivity of track radii to small variations of the electron diffusivity value [2], and others.

It was shown in [3] that taking into account the superheating nonequilibrium processes allows one to stabilize the model and obtain a quantitative description of tracks in $YBa_2Cu_3O_{7-x}$ with both elliptical and circular cross sections. In the present paper, another even more crucial problem of TSM is considered. The fact is that electron thermal diffusivity, D_e, was considered previously as an adjustable parameter for varied types and energies of the impinging ions. Meanwhile, the self-consistency of the theory requires using a single function, possibly depending on electron temperature in the superconductor, $D_e(T_e)$, for the whole bulk of data. We show that such a function exists and takes quite reasonable physical values.

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Application of Nondifferentiable Optimization to Investigation of the Shape of Bodies

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An optimization method with space dilation in direction of the difference of two successive subgradients in transformation space for the calculation of the shape of bodies is presented. We discuss the method, its complexity and computer implementation.

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Numerical Study of Oscillating Solitons of the Parametrically Driven, Damped Nonlinear Schroedinger Equation [1]

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We investigated the parametrically driven damped nonlinear Schroedinger (NLS) equation

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = h\psi^* - i\gamma\psi, \tag{1}$$

that describes a large number of resonant phenomena in various physical media [1]. The time-periodic solitons of the NLS equation are determined, numerically,

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as solutions of the boundary-value problem on a two-dimensional domain. Stability and bifurcations of periodic solitons were classified by examining the Floquet multipliers of the corresponding linearised system [2]. Cases of weak, moderate and strong dissipation have been analyzed. Our results shed a new light on the form of the attractor chart [3] for the NLS equation. New stable temporally periodic two-soliton bound state has been found.

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Density Functional Theory Approach to Atomic Autoionization in an External Electric Field: New Numerical Relativistic Scheme

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In the last years extensive experimental and theoretical studies of photo-auto- and multiple ionization in strong laser fields have revealed a number of unexpected effects and features. Moreover, some phenomena should can be described as multi-photon ones and independent electron processes (see e.g. [1]). This was concluded on the basis of a detailed analysis of experimental data together with precise calculations of single photo-ionization rates [1]. Several experiments then revealed a pronounced YkneeY structure in the yield vs peak laser intensity, typically plotted with logarithmic axis because of the wide range of values covered. Further ingenious experiments that resolved the

joint momentum distributions of the outgoing electrons then showed that they often leave the atom with the same moments. This has triggered a number of theoretical studies of this process, including S-matrix calculations for the full cross sections [2], and investigations of simplified classical and quantum models. Among the models are so-called aligned-electron models, in which electrons move in a one-dimensional (1D) regularized Coulomb potential, or quasi three-dimensional (3D) ones with the centre of mass of the electrons confined to move along the field polarization axis. At the same time, an exact solution of the time-dependent Schro"dinger equation even for two electrons in a laser field remains a formidable task. It is well known that the autoionization phenomena in the heavy atomic systems should be considered exclusively within the relativistic formalism. The suitable basis is the time-dependent Dirac equation, which is remained by the very complicated problem to be solved. Surely, if one consider a dc electric field and its effect on the autoionization process in the atomic system, the standard atomic relativistic approaches can be used as the zeroth approximation. Besides, one must take into account a group of the known complicated correlation effects. Here we mean, for example, the relaxation processes due to Coulomb interaction between moving away electron (electrons in a case of the laser induces multiple ionization) and resulting in the electron distribution in the vacancy field have no time to be over prior to the transition. It is known that a consistent theory of the atomic autoionization is to take into account correctly a definite number of the correlation (polarization, relaxation) effects, including the energy dependence of the vacancy mass operator, the continuum pressure, spreading of the initial state over a set of configurations etc. It should be reminded that hitherto these effects are not described adequately in the modern theoretical scheme. As example, let us remind such widespread methods as the: Dirac-Fock, relativistic Hartree-Fock methods, random phase approximation (RPA) and RPA with exchange, different model and pseudo potential schemes, density-functional formalism and its relativistic generalization etc. In this paper we present a new relativistic density functional theory scheme to description of the atomic autoionization in an external dc electric and laser field within the S-matrix Gell-Mann and Low formalism and the relativistic perturbation theory [2]. New scheme has to be applied to studying the autoionization phenomena characteristics in the atomic and molecular (obviously heavy) systems, and quasi-molecules and solids. The novel elements consist in an implementation of the relativistic Dirac-Kohn-Sham density functional theoretical scheme to the S-matrix Gell-Mann and Low formalism according the method [2,3] and using the optimized electron wave functions (basises are generated within the QED scheme [3]) of the relativistic perturbation theory in order to describe the fundamental atomic characteristic of autoionization in an external field.

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Численное и аналитическое изучение параметрического возбуждения осцилляторов в зависимости от импеданса и частоты [1]

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Будем рассматривать двумерный и одномерный гармонический осциллятор. В статье Б. Я. Зельдовича показанно, что модуляция импеданса, а не циклической частоты, приводит к резонансу осциллятора. Целью работы была проверка этого утверждения непосредственно решением уравнений Гамильтона. Решение уравнений осуществляется двумя способами: численным и аналитическим. Рассмотрим лагранжиан следующего вида:

$$L(\boldsymbol{x}, \dot{\boldsymbol{x}}, t) = -\frac{1}{2}\boldsymbol{x}^T \hat{K} \boldsymbol{x} + \frac{1}{2}\dot{\boldsymbol{x}}^T \hat{M} \dot{\boldsymbol{x}} + \boldsymbol{x}^T \hat{\beta} \dot{\boldsymbol{x}}$$

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Где, $\hat{K}$ — матрица упругости, $\hat{M}$ — матрица масс, $\hat{\beta}$ — матрица поля магнитного типа. Определим циклическую частоту как $\omega(t) \stackrel{\text{def}}{=} \sqrt{\frac{K(t)}{m(t)}}$, и импеданс как $Z(t) \stackrel{\text{def}}{=} \sqrt{K(t)m(t)}$ Выражаем все параметры в уравнениях Гамильтона через импеданс и частоту. Пусть теперь частота терпит малые периодические возмущения, а импеданс остается постоянным, и наоборот. Решаем полученные системы численно. На основе полученных решений подтверждается вывод Зельдовича, что при модуляции частоты, но постоянном импедансе не происходит параметрического резонанса. В свою очередь, при модуляции импеданса даже при постоянной частоте происходит параметрический резонанс.

После этого, система для одномерного случая решается аналитически, пренебрегая членами второго порядка малости. Полученное решение хорошо согласуется с численным.

При численном решении было использовано открытое программное средство для численных расчетов SciLab. На языке SciLab была написана программа для решения систем ОДУ в одномерном и двухмерном случаях.

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Критерии устойчивости некоторых квазилинейных сингулярно возмущенных модельных задач и их приложения

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Для сингулярно возмущенной (с/в) квазилинейной задачи вида

$$\varepsilon\dot{x} = A(t,\varepsilon)x + \varepsilon f(x); \quad x(0,\varepsilon) = x^0; \quad x, f \in R^n, \tag{1}$$

к которой сводится математическая модель работы сердца Зимана [1, с.188]

$$\varepsilon\dot{x} = x - x^3 - y; \quad \dot{y} = x - x_0 \tag{2}$$

и задача о прохождении нервного импульса [1, с.190]

$$\varepsilon\dot{x} = -(x^3 + xy + z); \quad \dot{y} = -2(x + y); \quad \dot{z} = -y - 1,$$

с помощью методов работы [2] сформулированы конструктивные критерии устойчивости и возникновения в системе (2) бифуркации Хопфа и предельного цикла.

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Анализ квазилинейных неавтономных систем с нормальной матрицей

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Для квазилинейной неавтономной системы

$$\dot{x} = A(x,t)x, \quad x(0) = x^0, \quad x \in R^n \tag{1}$$

с нормальной матрицей $A(x,t)$ (которая может иметь кусочно-непрерывные элементы) в случае, если ее спектр $\{\lambda_j(x,t)\}_1^n$ удовлетворяет тождествам

$$a)\ Re\lambda_j(x,t) \equiv \sigma(x,t) \quad (\ j = \overline{1,n};\ |x| < \delta;\ t \geq 0\ );$$

или неравенствам

$$b)\ \sigma_1(x,t) \leq Re\lambda_j(x,t) \leq \sigma_2(x,t) \quad (\ j = \overline{1,n};\ |x| < \delta;\ t \geq 0\ ),$$

доказано, что модуль точного решения задачи (1) определяется дифференциальными соотношениями:

$$a)\ \frac{d|x|^2}{dt} = 2\sigma(x,t)|x|^2;$$

$$b)\ 2\sigma_1(x,t)|x|^2 \le \frac{d|x|^2}{dt} \le 2\sigma_2(x,t)|x|^2,$$

что позволяет (без использования аппарата функций Ляпунова) сформулировать критерии устойчивости решения или существования устойчивых предельных многообразий. Приведены нетривиальные примеры.

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Nonlinear Waves in a Liquid with Gas Bubbles

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Propagation of nonlinear waves in a liquid containing gas bubbles is considered. This problem is of interest as model to describe a various phenomena in the physics, chemistry and biology.

We assume that the gas phase is same radius bubbles and gas content is small. Processes of bubbles formation, destruction, agglutination and phase transitions are not taking into account. We neglect the relative motion of bubbles and fluid. It allows us to use the classical hydrodynamics equations for description of a mixture flow written with respect to average flow characteristics - velocity, density and pressure [1, 2].

The viscosity is considered on interphase boundary. We suppose, that gas in a bubble can warm up and cool down, but the liquid temperature is constant as its mass and heat capacity is much more than mass and heat capacity of a gas. We assume that distance between bubbles is much more then equilibrium

bubble radius. That allows us not to consider interaction between separate bubbles, and to use the dynamics and energy conservation equations for a single bubble at a deriving of the gas-liquid mixture state equation.

Perturbations with characteristic wave length much more than distances between bubbles are considered. We suppose, that deviations of bubble radius from equilibrium value are small, in comparison with radius.

With above mentioned assumptions the closed system of equations with respect to perturbations of pressure, bubble radius and a mixture velocity has been obtained. For the analysis of system technique of the multi scale method and the perturbation theory is used. With their help the nonlinear evolution equations for pressure waves describing in gas-liquid mixture are obtained. Some of the obtained equations are new. In the limiting cases of the isothermal regime results transform in already known. By means of the multi scale method influence of physical properties of gas-liquid mixture on evolution of pressure waves is investigated. The exact solutions of the nonlinear equations are obtained using the simplest equation method [3]. The dimensionless parameters values characterizing physical properties of a bubbly liquid at which there are exact solutions of traveling wave type are found. The periodic and solitary wave solutions are obtained and their dependence on dimensionless parameters is investigated.

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Nonlinear Wave Process in a Viscoelastic Tube

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Propagation of perturbations in a viscoelastic tube is investigated. The study of nonlinear wave processes in a viscoelastic tubes is of interest, as such tubes corresponds to some features of circulatory system vessels and

understanding of wave processes in them can promote prediction of development of some blood vessels diseases [1].

The quasi-one-dimensional model of a liquid flow in a tube is considered. It is supposed, that the axial component of a liquid flow velocity is much more than radial, and on boundary the condition of equality to zero of a velocity components is satisfied. It allows us to average the axial component of Navier-Stokes equation and the continuity equation on a vessel cross-section.

We assume, that the tube wall is homogeneous, isotropic, incompressible and consists from is viscoelastic material. The tube strain is characterized by a modification of its radius which depends on co-ordinate and time; wall strains are assumed small in comparison with tube radius, and characteristic lengths of waves much more than equilibrium radius. At the mentioned above assumptions it is possible to use the equation connecting pressure with a tube radius [2].

This equation together with the equations of a continuity and Navier-Stokes organises the closed system of equations for description of a quasi-one-dimensional liquid flow in an axial-symmetric viscoelastic tube.

For the analysis of this equations system technique of the multiscale method and the perturbation theory is used. With their help the system of the nonlinear evolution equations for description of pressure waves in a viscoelastic tube is derived. The suggested model allows us to analyze various cases of values of the physical parameters in mathematical model, and to obtain various types of the corresponding nonlinear evolution equations.

The simplest equation method is used for construction of exact solutions of the received nonlinear equations [3]. Periodic solutions and solitary wave solutions are obtained. Dependence of the exact solutions on dimensionless parameters is investigated.

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Computational Modelling One- and Multi-Photon Excitation and Dissociation Processes in Multi-Atomic Molecules and Functional Materials on the Basis of Dyes

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The paper is connected with computational studying the multi-photon excitation and dissociation processes in the free multi-atomic molecules and molecules in matrices. The first part of work is connected with experimental and computational theoretical studying processes running under relaxation of molecule from the high excited state, which is obtained during 1-quantum ($S0 \to Sn$) or two-quantum ($S0 \to S1 \to T1 \to Tn$) excitation [1,2]. The polymer layers with dyes (rezaurine, methylen blue, brilliant green etc) are studied and used as a working substance in dye-lasers, as photosensitive compound in processes of information processing etc. The kinetics of the decolouration is described by a system of the quantum kinetical equations. It has been shown that a relaxation of the molecule from the highly excited state includes as equilibrium as non equilibrium processes including the quantum transitions between intermediate purely electronic states. It has been found system could live in the intermediate electronic states during several vibrations, which are characteristic for this state. This effect results in possibility of realizing the dissociation process from the intermediate state, the electron transitions between highly-excited molecule and surrounding environment (matrice) etc. In second part of paper we present new numerical stochastic, quantum kinetics approach [3] to modelling multi-excitation and dissociation processes in the 12CF(3)Br, 13CF(3)Br molecules. In particular, it has been found a link between the integral characteristics of multi-photon processes with parameters of relaxation CF(3)Br in a medium of the buffer nitrogen gas. It has been defined the

output of multi-photon dissociation and absorbed energy for studied molecules. A process of excitation to continuum is described within a generalized kinetical equations model [3,4]. A key moment is connected with account of the stochastic diffusion mechanism in quasi-continuum. It is shown that in the pressure interval p<50-100Torr a dissociation output is mainly determined by influence of the rotational relaxation and the V-T relaxation is not significant. Above 200Torr the dissociation output is mainly determined by concurrence of two processes: the V-T relaxation and involving the molecules from the lowest levels. Stochastic model block is manifested in more correct description of the excitation dynamics in the quasi-continuum.

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Asymptotic Solutions of Boundary Problems for Singular Perturbated Infinite Order Differential Equations on Fractal Sets

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The asymptotic solutions of the boundary problems for the singular perturbated infinite order differential equations on the fractal sets are studied.

Transfer Matrix Method for Tunneling Transport[1]

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Effect of quantum tunneling governs the charge transport in a good deal of nano-electronics devices[1]. The semi-classical WKB approximation is widely used to calculate the stationary quantum transmission coefficient (QTC); however, it often lacks enough accuracy. In this paper we develop a transfer matrix method for calculating the quantum tunneling probability. A piecewise constant approximation[3] and a piecewise linear approximation[4] are considered and their drawbacks analyzed. To overcome them we have elaborated a hybrid method which combines piecewise linear and piecewise constant approximations depending on geometry of potential structure. As further development we constructed a new matrix approach which dispense with basic functions on the segments. It can be applied to any potential barrier. The technique has been tested on various potential barriers. It proves highly efficient for numerical simulation of stationary tunneling transport and can be applied to various nano-structures and nano-devices.

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Адиабатические моды плавно-нерегулярного открытого планарного волновода: нулевое приближение [1]

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Модель адиабатических мод позволяет проектировать плавно-нерегулярные профили толщин волноводных слоев с заданными характеристиками волноводных и вытекающих мод. Таким образом, адиабатическая модель дает возможность проектировать интегрально-оптические амплитудно-фазовые преобразователи, датчики (сенсоры, позволяющие получать, обрабатывать и предавать информацию о физическом строении, химическом составе, форме, положении и динамике исследуемой системы) и т.п.

Адиабатическая модель плавно-нерегулярных оптических многослойных волноводов в отсутствие нерегулярности совпадает с моделью регулярного волновода, выраженной в терминах продольных компонент полей волноводных мод. Данная модель использует формализм переходной матрицы. Этот же формализм можно применять для волноводных и постепенно вытекающих мод регулярного волновода. Мы реализовали данный подход для численного моделирования дисперсионных соотношений и амплитуд полей с помощью регуляризованного метода решения однородной системы линейных алгебраических уравнений.

High Probability State Transfer among Different Nodes of Spin 1/2 Chains with XY and XXZ Hamiltonians[2]

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We study the problem of the state transfer between different nodes of the spin 1/2 chain with both XY and XXZ Hamiltonians in the strong external magnetic field. The interest to this problem is stimulated by the development of quantum communication systems. Although the perfect state transfer (PST) is most popular in theoretical models, its realization in practice has two basic obstacles: (a) the nearest neighbour approximation of the Hamiltonian (rather then complete Hamiltonian) has been used for providing the perfect state

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transfer, and (b) different coupling constants may not be produced with absolute accuracy. Moreover, the perfect state transfer may be organized between the end nodes of the chain only, while the state transfers to the inner nodes are also important for the purpose of distribution of the excited state between several receivers.

For this reasons we suggest to concentrate on the high probability state transfer (HPST) (rather then PST) which has the following advantages: (a) it is not as sensitive to the values of coupling constants as perfect state transfer [1], and (b) it is possible to transfer the initial state not only between the end nodes of the spin chain, but also from the end to the inner nodes [2].

First, we study the HPST in the short alternating spin $1/2$ chain with the XY Hamiltonian in the strong external magnetic field [1]. We show that the exited state may be transfered between the end nodes of four-, six- and eight-node chains with probability 0.999, 0.997 and 0.989 respectively. We also demonstrated that the HPST into the inner nodes of such chains is impossible.

Then, we construct the spin $1/2$ chains with properly distributed week bonds allowing the HPSTs from the end node to either some of the inner nodes or to all of them [2]. Thus, we organize the HPSTs between all nodes of the four- and eight-node spin chains and between four symmetrical nodes of the six-node chain

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On Two-Field Solitons in 2 and 3 Dimensions

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We discuss existence and properties of two- and three-dimensional stationary solitons with non-trivial topology in gauge-invariant models describing interaction of scalar unit $O(N)$-invariant fields with vector $SU(n)$ fields.

Calculation of Asymptotic Expansions of Solutions of Quantum Well with Hydrogen-like Impurity

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Symbolic-numerical algorithms for calculation of asymptotic expansions of solutions of quantum well with hydrogen-like impurity [1] by using angular prolate spheroidal functions are elaborated. The efficiency of the algorithms is demonstrated by solving typical test examples and proving compatibility conditions of scattering problem in spherical and cylindrical coordinates.

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Method of Numerical Analysis for Determination of Type of Shock Structure in Media with Complex Dispersion [1]

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Method of numerical analysis for prediction of stationary shock structure type for low-dissipative media with complex dispersion is advised. This method is based on investigation of branches of stationary periodic solutions (solutions

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of ordinary differential equations) of non-dissipative version of the model under consideration. The method is firstly developed for generalized Korteweg–Burhgers equation

$$a_t + aa_x + a_{xxx} + a_{xxxxx} = \varepsilon a_{xx}$$

The method is proved by direct numerical solution of this partial differential equation. Correspondence between types of bifurcation diagrams of branches of periodic solutions and types of shocks obtained from numerical experiment is good.

Low-dissipative shock structures are described by averaged equations. Shock structure solutions of these equations contain internal non-dissipative resonance shock structures. Resonance means that for one side of shock we observe periodic wave zone and for other side we observe two-periodic wave zone. The ratio of periods is integer value $n = 1, 2, 3, ...$ For $n = 1$ for one side wave zone is replaced by uniform zone. This shock structure is observed for $\varepsilon = 0$ while other shocks are observed only for $\varepsilon > 0$. They become unstable if value of ε is decreased. Besides that non-stationary stochastic and time-periodic shock structures are found. Investigation of dependance of shock structure type of shock amplitude and dissipative parameter is fulfilled.

Let $\omega = \omega(k)$ is dispersion equation. Resonances are related with the fact that line $v = \omega/k$, here v is phase speed of solution, two times intersects dispersion curve for $k > 0$. So we may expect that similar effects will take place for other models with this property. The method is applied for magnetosonic waves of plasma equations (electron magnetics hydrodynamics). Similar solutions and similar correspondence between shock structure types and branch diagrams are found.

These results may be used for verification of numerical schemes and for determination of parameters of media by analysis of shock structure type observed in physical experiment.

Modeling the High Critical Temperature Superconducting Phase Transition in Cuprates within the Effective Two-Band Hubbard Model

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More than two decades after its discovery by Bednorz and Müller in 1986, the high critical temperature superconductivity in cuprates is still the great puzzle of the solid state physics.

Here we review the effective two-dimensional two-band Hubbard model proposed by Plakida et al. [1], as the reasonable simplest candidate to the consistent understanding of the unusual fundamental properties of the cuprates which have been evidenced by high precision investigations (occurrence of CuO_2 planes embedded in lamellar structures, existence of Fermi surface, the charge transfer nature of the cuprates, occurrence of families of cuprates characterized by either hole doping or electron doping, low density hopping conductivity, unconventional anomalous pairing, occurrence of the pseudogap in the normal state, kinetic energy minimization in the superconducting phase, spin-charge separation).

The model assumes a doped effective two-dimensional spin lattice in which the single fermion states are described by Hubbard operators that automatically obey the Pauli exclusion principle and its Hamiltonian is derived within a frame governed by the Weiss principle of the hierarchy of the effects following from the relative importance of the various interactions occurring in the system. The Hamiltonian is then investigated within the equation of motion method for 4×4 Green function (GF) sets.

Special emphasis is put on the progress obtained in the solution of the generalized mean field approximation (GMFA) GF problem [1]. The right formulation of the eigenvalue problem results in finite energy spectrum everywhere in the (δ, T) phase diagrams of these systems, with hybridization effects which are fully solved both for the normal and the superconductivity states. Rigorous consideration of the symmetry properties following from the crystallographic structure of the effective spin lattice, the invariance to spin reversal, as well as from the complicated algebra of the Hubbard operators result in consequences which accommodate several of the specific cuprate features within the GMFA-GF description of the effective two-band Hubbard model.

It becomes, however, apparent from this discussion that the solution of the full Dyson equation of the GF matrix is necessary to account for other properties of the cuprates.

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Bayesian Automatic Adaptive Quadrature

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Since a great many physical models get the observables as integrals that cannot be calculated analytically in terms of elementary functions, algorithms for their reliable floating point computation are highly needed, especially within numerical experiments investigating parameter dependent processes like doping dependent phase transitions ([1] at this Conference).

The computation of the integrals by automatic adaptive quadrature algorithms (AAQA) [2] was known for decades to result in bad and unpredictable failures [3].

Their elimination is only possible within a Bayesian approach which changes fundamentally the approach to the building of the binary tree of the subranges (BTS) over the integration domain as well as the generation and use of the information on the integrand function.

The concept of the *subrange status* (found in one of the four possible states – undefined, ill-conditioned, regular well-conditioned, improper well-conditioned – which are defined using both *global* and *local* conditioning criteria) allows adequate definition of the BTS. The recursive generation and the reordering in logarithmic time of the priority queue of minimal length associated to the BTS under *inheritance* of the information already acquired over the ancestor subranges results in the elimination of implicit assumptions on the local integrand conditioning as well as in sizeable decrease of the computation time.

Securing code robustness under adverse hardware and software environments is finally addressed.

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Asymptotic Solutions of Boundary Problems for Singular Perturbated Infinite Order Differential Equations with Fractal Quantum Potentials

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The boundary problems for the singular perturbated infinite order differential equations on the fractal sets are studied. Using the small parameter methods and the transfer matrix methods solutions for these problems are obtained.

Using this approach the solutions of the boundary value problem for the one-dimensional relativistic Schroedinger equation with the fractal quantum potentials are built. The convergence of these solutions to the solutions of the boundary value problem for the non-relativistic Schroedinger equation with the same potentials is shown. These results are compared with the solutions of the boundary value problem for the one-dimensional relativistic Schroedinger equation with the periodic quantum potentials.

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Variational-Iteration and Evolution Methods for Investigations of Few-Body Quantum Systems

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The effective variational-iteration and evolution methods, algorithms and programs for the numerical solutions of the boundary and evolutionary problems for the multi-dimensional Schrödinger type equation with homogeneous boundary conditions are developed in the framework of the Kantorovich and the

finite-element methods. The following problem-oriented complex program for numerical investigations of few-body quantum systems is created:

• KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach [1].

• ODPEVP: A program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm-Liouville problem [2].

• TIME6T: A program complex for the numerical solution of the Cauchy problem for the time-dependent Schrödinger equation [3].

The efficiency of the developed methods, algorithms and elaborated complex - program is confirmed by the eresults of the numerical analysis, the obtained theoretical error estimations of the solutions of the parametrical, spectral and evolution problems, and the modelling of some processes in few-body quantum systems such as excitation and de-excitation [4], photoionization and recombination of hydrogen-like atom in a uniform magnetic field [5] and ion channeling [6].

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Convergence of the Continuous Analogy of Newton's Method for Solving Nonlinear Equations

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In resent years much attention has been devoted to the development of new high-order iterative methods for solving nonlinear equations [1, 2]. Among them there are methods that were obtained by combining Newton's method with other one-step methods [7, 4]. On the other hand, so-called continuous analogy of Newton's method (CANM) or damped Newton's method with a parameter [5, 6] has often been used although its convergence order is less than that of the above mentioned methods. It is known that the suitable choice of this parameter allows us not only to extend the region of convergence, but also to control the convergence of the method in general. At present, there are some choices of this parameter that are often used in practice [5, 6].

In this talk, we will show that suitable choices of iteration parameter in CANM allow us even to speed up the convergence of the method.

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Stability and Bifurcations of Magnetic Flux Distributions in Josephson Junctions, Described by Double Sine-Gordon Equation

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Physical properties of magnetic flux in Josephson junctions are the base of the modern superconducting electronics. Tunnel superconductor-insulator-superconductor (SIS) Josephson junctions have sinusoidal current-phase relation, while with the decrease of the barrier transparency deviations from this relation take place. The sign of the higher harmonic is important for many applications, in particular in junctions like SNINS and SFIFS, where N is a normal metal and F is a weak metallic ferromagnet.

In this work static magnetic flux distributions in long Josephson junctions are investigated numerically taking into account the second harmonics in the Fourier-decomposition of the Josephson current. Stability analysis is based on numerical solution of a spectral Sturm-Liouville problem formulated for each distribution. The nullification of the minimal eigenvalue of this problem indicates a bifurcation point by change of one of the parameters.

The nonlinear boundary value problem corresponding to the model is solved using the continuous analog of Newton's method. Spline-collocation scheme for the linearized problems at each newtonian iteration is applied.

We have calculate some basic distributions along the junction and analyze their stability in dependence on the model parameters. A comparison with traditional SIS Josephson junction model is performed.

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Homogenization of Problems Arising in Low—-Frequency Electromagnetism[1]

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In conducting material, exposed to a low-frequency electromagnetic field, electric currents, the so-called eddy currents, are induced. The phenomenon is described by Maxwell's equations. In the case of heterogeneous material these equations are multiscale in their nature. We study the asymptotic behavior of eddy current model and compare the results with the numerical approximations obtained using the Heterogeneous multiscale method.

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Mathematical Modeling of Quantum Well Potentials via Generalized Darboux Transformations

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We apply the Darboux transformation operator technique to the generalized Schredinger equation with a position-dependent effective mass and with linearly energy-dependent potentials and show how to construct the quantum well potentials in nanoelectronic with a given spectrum. The method is illustrated by several examples.

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Modeling of Phase Transitions in Complex Fluid Dynamics

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A method of direct numerical simulation for some heterogeneous fluid dynamics with take of phase transitions will be presented. It is supposed that the fluids are compressible and inviscid (non-viscous). Heterogeneities of the fluids are considered as small drops or particles of one fluid within other fluid. Total number of the drops can be large enough and the drops may have phase transitions. Thus, simulations of the main fluid (or gas) with small transited drops dynamics are discussed. These are dynamics of multiphase flows really. Therefore it is possible to use general multiphase flow models in the case. But standard multiphase equations are not complete as a rule and various physical experiments are necessary for solving of the problem for concrete heterogeneous fluid dynamics. The situation is more difficult whenever phase transitions are possible.

Presented method is a combination of Harlow's particle-in-cell method and Belotserkovskii's large particles method (see, for example, [1]). The method is based on a discretization of conservation laws for masses, momentums, and energies in integral forms. The discretization is natural and numerical simulations are realized as direct computer experiments for the dynamics of main fluid together with transited drops without use multiphase flows approach. The method seems to be much more adequate to the mechanical and mathematical essence of the dynamics, because conservation laws are correct on the discrete level at least.

The method is designed to computer modeling of following physical processes. Let us consider graphite particles distributing uniformly in some fluid. More exactly there is medium with graphite particles and the medium can be considered under high pressure as "fluid"with corresponding state equation. Inducing conical shock waves in the heterogeneous medium, it is possible to observe dynamics and phase transitions of the graphite particles in computer experiments by the method, where the transitions are realized if the pressure or temperature is more (or less) than the critical pressure or temperature by relevant phase diagrams. Results of the computer experiments are in agreement

with results of physical experiments. The results are greatly depending on density of graphite particles and intensity of the shock waves.

The method seems to be perspective for numerical simulations of other absorption and diffusion processes in complex fluid and plasma dynamics (see, for example, [2]).

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Time Discretization Scheme for Maxwell's Equations with Silver—Müller Boundary Condition for Non-Perfect Conductor

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We study a time dependent eddy current equation for the magnetic field $\boldsymbol{H}$ accompanied with a non-linear degenerate boundary condition, which is a generalization of the classical Silver-Müller condition for a non-perfect conductor. More exactly, the relation between the normal components of electric – $\boldsymbol{E}$ and magnetic – $\boldsymbol{H}$ fields obeys the following power law

$$\boldsymbol{\nu} \times \boldsymbol{E} = \boldsymbol{\nu} \times \left(|\boldsymbol{H} \times \boldsymbol{\nu}|^{\alpha-1} \boldsymbol{H} \times \boldsymbol{\nu} \right)$$

for some $\alpha \in (0, 1]$. We design a non-linear time discrete approximation scheme using the well known Rothe's method.

Applying the theory of monotone operators we show the existence and uniqueness of a weak solution on each time step. This is done in a suitable function space under the minimal regularity assumptions on the boundary Γ and the initial data $\boldsymbol{H}_0$. The a priori estimates are helpful for proving the

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convergence of our method. The proof of convergence based on Minty-Browder's trick is regarded as the main theoretical result. Finally the error estimates describing the dependence of the error on the discretization parameter τ – the length of the time step, are derived.

The efficiency of the proposed method is supported by numerical experiments. Even though the problem is discretized in time, it still retains its nonlinear character. Therefore we apply the Newton method as a standard tool for solving nonlinear PDEs. We have studied the sensibility of our problem to the length of the time step τ, size of the mesh h and parameter of nonlinearity α.

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Оптимальное управление процессом электронагрева [1]

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Предметом исследования являются вопросы математического моделирования и построение оптимального управления тепловых и электрофизических процессов, описываемых взаимосвязанной системой уравнений

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Максвелла и теплопроводности. Рассматривается класс многомерных начально-краевых задач с учетом нелинейности заданных функций. Указанный класс задач является моделью многих современных технологий, где осуществляется распределенное или сосредоточенное воздействие на токопроводящие твердые поверхности (металлические, порошковые, композиционные, полупроводниковые). Цель работы заключается в разработке эффективных методов управления для нелинейных многомерных краевых задач теплопроводности.

В представленной работе используется система уравнений Максвелла, нелинейное уравнение теплопроводности, модель термонапряжений, теория возмущений операторов, методы функционального анализа, спектральная теория самосопряженных операторов, метод функции Грина, численные методы решений интегральных уравнений, теория интегральных преобразований, принцип максимума, а также методы поиска экстремума.

В теории индукционного нагрева можно выделить четыре больших класса задач оптимального управления.

Первый класс - это задача быстродействия, когда по условиям производительности оборудования требуется минимальное время нагрева при выполнении определенных ограничений на качество нагрева , а также при дополнительных фазовых ограничениях.

Второй класс задач - это так называемые задачи финитного управления с фиксированным временем нагрева, которое также решается с ограничением вида и рядом специфических фазовых ограничений, например, на скорость нагрева.

Третий класс задач - это задачи слежения. В таких задачах функционал максимизируется по фазовой переменной по фазовой переменной и по времени и среди всех значений выбирается минимальное.

Четвертый класс задач - это задачи простого синтеза. Здесь за решение задачи принимается любое допустимое управление, не обязательно оптимальное.

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An Adaptive Method and Fortran Programs for Smooth Approximation of Functions

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The approximation problem arises in many disciplines when the studied phenomenon is modeled by a continuous function measured only in a few discrete points. In this paper we present an improved adaptive method for smooth approximation of functions based on the variational approach of Talmi and Gilat [1] and on the principle of heuristic self-organization [2]. The essence of this method is that the approximating function minimizes an appropriate functional representing some measure for smoothness of the function. The problem is solved generally in L-dimensions. A package of FORTRAN programs for L = 1, 2, 3 is developed. Many tests with model functions are carried out. They show that this method manages well enough with the requirements of flexibility, sufficient accuracy both for the function itself and its derivatives and reasonable computer implementation. It was successfully applied in solving of real physical tasks also [3, 4].

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Modeling of Thermal Surface Roughening by Processing of Data Obtained from Crystal Morphology

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Surface roughening [1] at constant temperature and low supersaturation was observed on highly purified single crystals (adamantane and camphene), grown in sealed ampoules. After spontaneous transformation, their equilibrium shapes were drop-like with entirely nonsingular surfaces (adamantine at 18 K below melting point Tm = 546 K [2], camphene at 23 K below Tm = 323 K [3]). Both crystals showed thermal reversibility of shapes and sizes. The obtained temperature dependent morphological data were statistically processed and fitted to theoretical models, such as mean field, XY, etc. A simple approach defines the roughening transition by vanishing of step free energy, i.e. by measuring the temperature of facet disappearance. The aim is verification of the type of transition (continuous or second order), strict determination of the roughening temperature Tr, quantitative proof of the molecular roughness above Tr, etc.

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Generation of n-Loop Topologies in Models of Developed Turbulence[1]

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By using pure graph theory the problem of generation of all n-loop topologies ($n \geq 1$, $n \in \mathbb{N}$) for potentially divergent Feynman diagrams which contribute to the corresponding two-point one-irreducible Green functions in field theoretic models of problems of fully developed turbulence is solved. The completeness and uniqueness of the sets of the n-loop topologies is proved and effective algorithms for their constructions are found.

The general theory is used for generation of the corresponding n-loop Feynman diagrams in the theory of fully developed turbulence based on the stochastic Navier-Stokes equation where two types of propagators and one interaction vertex exist. The corresponding general algorithm is found and all Feynman diagrams are constructed for $n = 1, 2, 3, 4$, and 5.

Hamiltonian Formulation of Ideal Ferrohydrodynamics

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An interesting class of intelligent materials are magnetic fluids, or ferrofluids, which without magnetic field are homogeneous colloidal suspensions of ferromagnetic nanoparticles coated with surface-active dispersive medium (typical diameters of particles range from 5 to 10 nm) in a carrier liquids. Ferrohydrodynamics describes evolution of a magnetic fluid, carrying a magnetic field. The continuous models of ferrohydrodynamics have been studied in recent years from different points of view. The concept of frozen magnetization in nonconducting magnetic fluid was used in deducing ferrohydrodynamics equations

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[1]. An important consideration when constructing new fluid models is the existence of a Hamiltonian structure [2]. In the report the Hamiltonian formulation of a nonconducting ideal magnetic fluid model with frozen magnetization is presented. We have received the noncanonical Poisson bracket and have shown that this bracket produces the system of equations containing in [1] with the appropriate Hamiltonian.

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Multioperator's Method for Constructing the Bilinear Forms Closed System for Pair Vectors and Corresponding to Them Linear Relatively Operators Models[1]

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Lets for pair vectors (arithmetical vectors, functions or vector-functions) $(\mathbf{u}, \mathbf{y})$, belonging to some Euclidean space, and the set of operators $\{A_i, i = 0, 1, 2,\dots\}$ can be constructed pair subspaces $U \subseteq E$, $Y \subseteq E$, linear spans of respectively linear independent vectors

$\{A_n\mathbf{u}, n = 0, 1, 2,\dots N\}$ and $\{A_k\mathbf{y}, k = 0, 1, 2,\dots K\}$.

If $U \cap Y \neq \emptyset$, then two matrix equations are correct

$$\det(\mathbf{G}_Y - \mathbf{P}^*\mathbf{G}_U^{-1}\mathbf{P}) = 0,\ \det(\mathbf{G}_U - \mathbf{P}\mathbf{G}_Y^{-1}\mathbf{P}^*) = 0,\ (*)$$

where $\mathbf{G}_U$, $\mathbf{G}_Y$ are bilinear forms $< A_i\mathbf{u}, A_j\mathbf{u}>$ and $< A_i\mathbf{y}, A_j\mathbf{y}>$ Gram's matrices, respectively bases $A_i\mathbf{u}$ and $A_j\mathbf{y}$, $\mathbf{P}$ is matrix of bilinear forms $< A_i\mathbf{u}, A_j\mathbf{y}>$. The system of different bilinear forms is closed by (*). Matrix equations (*) are conditions of linear relatively operators A_i correlations between vectors $\mathbf{u}$, $\mathbf{y}$ in kind of equations (models)

$a_0A_0\mathbf{u} + a_1A_1\mathbf{u} + \dots + a_NA_N\mathbf{u} = b_0A_0\mathbf{y} + b_1A_1\mathbf{y} + \dots + b_KA_K$. (**)

Coefficients in (**) are connected by equations

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$(a_0, a_1, \ldots a_N) = (b_0, b_1, \ldots b_K)\mathbf{P}^*\mathbf{G}_U^{-1}$, $(b_0, b_1, \ldots b_K) = (a_0, a_1, \ldots a_N)\mathbf{P}\mathbf{G}_Y^{-1}$

and are solutions of linear equation's systems

$$(b_0, b_1, \ldots b_K)(\mathbf{G}_Y - \mathbf{P}^*\mathbf{G}_U^{-1}\mathbf{P}) = \mathbf{0},\ (a_0, a_1, \ldots a_N)(\mathbf{G}_U - \mathbf{P}\mathbf{G}_Y^{-1}\mathbf{P}^*) = \mathbf{0}.$$

This method can be used for model constructing and classification of processes and system.

Моделирование токовых обмоток в электрофизических установках

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В работе рассматриваются вопросы моделирования токовых обмоток сложной конфигурации с различным сечением кабеля. Разработан удобный инструментарий для задания подобных обмоток. Обсуждаются проблемы, возникающие при вычислении магнитного поля от токовых элементов с использованием закона Био-Савара. Предлагаются численные методы, учитывающие сингулярность используемых интегральных уравнений.

Pioneering Space Research in the USSR and Mathematical Modelling of Large Problem of Radiation Transfer [1]

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This review is to recall to scientists of the older generation about some historical pages of our memory and about many famous researchers, teachers and colleagues. As to the younger researchers and foreign colleagues, it will be useful for them to get to know about pioneer advancements of the Soviet

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scientists in the field of information and mathematical supply for cosmonautic problems on the eve of the space era. Main attention is paid down to the scientific experiments conducted on the piloted space vehicles and the research collectives who created the information and mathematical tools for the first space projects. The role of Mstislav Vsevolodovich Keldysh, the Major Theoretician of cosmonautics, is in particular emphasized, who determined in the most degree the basic directions of development of space research and remote sensing of the Earth and planets that are shortly called as REMOTE SENSING.

Two Greatest epoch-making scientific projects - atomic and cosmic - have favoured the enermous progression of Soviet science, which could competitive with World science in 20-th century. The solving of large problems on computer was demanded to realize of the engineering and constructing projects in the first time. The bases of the new technology were laid, which would be called as "mathematical modelling"or "computer sciences".

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Sheet Current Model for Inductances Extraction of Superconductor Microstructures[1]

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Sheet current model for microelectronic superconductor structures, based on Maxwell and London equations, is presented. For this model, numerical method for current density calculation and inductances extraction is evaluated.

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The resulting equations are solved using finite element method and matrix of self and mutual inductances is calculated as well as current distribution in conductors. Then, current distribution can be used for calculation of boundary conditions for Josephson junctions equations. The program and results of calculations are presented.

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Developing Monotone Difference Schemes for Hyperbolic Type Equations[1]

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For the simplest one-dimensional linear transport equation $u_t + \lambda u_x = 0, \quad \lambda = const > 0$ there are a lot of difference schemes which can be written in the next form $u_m^{n+1} = \sum\limits_{\mu,\nu} \alpha_\mu^\nu(\tau,h) u_{m+\mu}^{n+\nu}$, $\mu = 0, \pm 1, ..., \quad \nu = 1, 0, -1, ...$, on the arbitrary grid templates (including multi-layer and implicit) and we can write the approximation conditions for these schemes:

- 1^{st} order: $\sum\limits_{\mu,\nu} \alpha_\mu^\nu(\tau,h) = 1$, $\sum\limits_{\mu,\nu} (\mu - \nu\sigma)\alpha_\mu^\nu(\tau,h) = -\sigma$, $\sigma = \lambda\tau/h$
- and higher: $\sum\limits_{\mu,\nu} (\mu - \nu\sigma)^k \alpha_\mu^\nu = -(-\sigma)^k, \ k = 2, 3, ...$

There are a few monotonicity criteria for these difference schemes:

[1] This work is supported by the grant of Russian Foundation for Basic Research

- monotone by Friedrichs schemes: $\alpha_{\mu}^{\nu}(\tau, h) \geqslant 0$ (1)
- monotone by Godunov linear schemes, in which for any grid point:

$u_{m+1}^{n+1} - u_{m}^{n+1} \geqslant 0$, if $u_{m+1}^{n} - u_{m}^{n} \geqslant 0$ (and vice versa) (2)

- monotone by Harten schemes

$$TV(u^{n+1}) = \sum_{m} |u_{m+1}^{n+1} - u_{m}^{n+1}| \leqslant \sum_{m} |u_{m+1}^{n} - u_{m}^{n}| = TV(u^{n}) \qquad (3)$$

- monotone by Van Leer schemes

$$\begin{cases} \min\left\{u_{m}^{n}, u_{m-1}^{n}\right\} \leqslant u_{m}^{n+1} \leqslant \max\left\{u_{m}^{n}, u_{m-1}^{n}\right\} & \text{if } \lambda > 0 \\ \min\left\{u_{m}^{n}, u_{m+1}^{n}\right\} \leqslant u_{m}^{n+1} \leqslant \max\left\{u_{m}^{n}, u_{m+1}^{n}\right\} & \text{if } \lambda < 0 \end{cases} \qquad (4)$$

We made extension of monotonicity criteria (2)-(4) for the difference schemes on the multi-layer grid templates for linear and nonlinear hyperbolic equation systems.

Развал бризера для эффективного уравнения с дисперсией. Асимптотика на границе корректности

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Рассматриваются эффективные уравнения, возникающие при осреднении уравнений, которые описывают волновые процессы в периодических слоистых средах [1-2].

Решается задача Коши с разрывными начальными данными:
$u(x, 0) = 0$ при $x < 0$, $u(x, 0) = 1$, при $x \geq 0$. Для уравнения

$$U_{tt} = U_{xx} + U_{ttxx}$$

было доказано [3-4] существование решения типа "бризер":

$$U(x, t) = \frac{1}{2} + \frac{\mathrm{sgn}(x)}{2} cos(t) + \mathrm{O}(\sqrt{x^2 t}), \qquad t \to \infty,\ |x| < ct^{-1/2}.$$

Результаты численных экспериментов указывали также на существование решения типа бризер для уравнения

$$U_{tt} = U_{xx} + ibU_{ttx} + U_{ttxx}, \quad |b| < 2.$$

При достаточно больших t проявилась разница в поведении решения рассматриваемой задачи (при $b = 0$ и вещественной части решения при $b \neq 0$). При $b \neq 0$ амплитуда осцилляций уменьшается, в то время как зона осцилляций расширяется. В работе [4] построены асимптотики при больших t для решения рассматриваемой задачи в случае $b = 1$, подтверждающие доставерность процессов деформации бризера, выявленных при численном моделировании. Предварительно строится интегральное представление решения. На границе корректности (при $b = 2$) меняется вид подинтегральной функции. Проведено дополнительное исследование. Доказано, что в предельном случае зона существования бризера сужается до $O(t^{-1})$ против $O(t^{-1/2})$ для $b = 0$. Построены асимптотики при больших t, указывающие, что в пределе (при $b = 2$) зона осцилляций занимает всю вещественную ось. Результаты численных экспериментов, подтверждают существование экзотических асимптотик, предсказанных теоретически.

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Об одном аспекте метода матричной линеаризации систем нелинейных дифференциальных уравнений в частных производных

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Метод матричной линеаризации систем нелинейных дифференциальных уравнений в частных производных [1] в идейном плане достаточно прост. Однако в итоге мы получаем, вообще говоря, связанную систему

линейных дифференциальных уравнений. Построение аналитических решений такой системы само по себе является нетривиальной задачей. В настоящем сообщении рассматривается одна возможность построения этих решений для определчнного класса начальных условий. А именно рассматриваются полиномиальные начальные условия. В этом случае вполне возможно применение довольно простого способа построения самих решений с помощью экспоненты от дифференциально-матричного оператора. Эта методика основана на работе [2].

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Неэллипсоидальные конфигурации вращающихся намагниченных ньютоновских политроп с малым индексом

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В докладе показана эффективность составленного и реализованного сим-вольно-численного алгоритма для решения уравнения равновесных вращающихся ньютоновских политроп с малым индексом n. Найден аналитический вид нового класса неэллипсоидальных конфигураций ньютоновских политроп - предельные клиновидные фигуры, имеющие форму кругового клина. Вычислены значения главных кривизн поверхности конфигурации вблизи экватора. Найдено семейство предельных точек $e_L(n)$. Для

параметра асимметрии X получено кубическое уравнение и на его основе определено семейство критических точек (точек бифуркации). Доказано существование первой предельной критической точки со значением $n_m = 0.1161$.

In this report we was shown and The realized symbol-numerical algorithm for the decision the equations of equilibrium rotating Newtonian polytropics with the small index n. The analytical kind of a new class is found nonellipsoidal configurations of Newtonian polytropics - limiting wedge-shaped the figures having the form of a circular wedge. Are calculated Values of the main things curvatures surfaces of a configuration near to equator. We found of family of limiting points $e_L(n)$. For asymmetry parameter X the cubic equation and on its basis is received the family of critical points (bifurcations points) is defined. Existence of the first limiting critical point is proved with Value $n_m = 0.1161$.

Кольцеобразные пузыри в распределении плотности быстровращающихся ньютоновских политроп с индексом $n > 1.25$

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В работе доказано существование у ньютоновских быстровращающихся политроп с индексом $n \geq 1.254$ областей, в которых плотность близка нулю. Эти области (пузыри) имеют кольцеобразную структуру. Проведена проверка выполнения граничных условий на поверхности пузыря. Подробно исследуется зависимость конфигурации пузырей от параметров сплюснутости e и быстроты вращения конфигурации ε. В случае уравнения состояния нерелятивистского вырожденного нейтронного газа ($n = 1.5$) получены ограничения на период вращения T конфигурации в области существования пузыря при произвольном значении ее массы m $11.579 \cdot 10^{-3}$сек$\leq T \cdot \frac{m}{m_\odot} \leq 11.917 \cdot 10^{-3}$сек.

In work existence at Newtonian polytropics rapidly rotating with an index $n \geq 1.254$ areas in which the density is close to zero is proved. These areas (bubbles) have ring-shaped structure. There was performed the check up of performance of the boundary conditions on a bubble surface. Explicitly association of a configuration of bubbles on parameters of flatness e and speed of rotation ε of a configuration is investigated. In the case of the equation of

the condition nonrelativistic degenerate neutron gas (n=1.5) restrictions on period of rotation T of a configuration in the region of bubble existence are received at arbitrary value the configuration's mass m $11.579 \cdot 10^{-3}$s$\leq T \cdot \frac{m}{m_\odot} \leq 11.917 \cdot 10^{-3}$s.

A Model of Steady Glass Fiber Drawing Process as a Non-Linear Eigenvalue Problem

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New numerical method for modeling the steady drawing process of a glass fiber is presented. The method is based on the one-dimensional version of the equations of motion coupled by the heat transfer equation. The drawing zone is separated into two parts: melted (liquid) and solidified zones. These zones are then smoothly matched in an unknown section whose coordinate is treated as spectral parameter. The corresponding non-linear eigenvalue problem is solved by means of the continuous analog of Newton method combined by spline-collocation scheme. The effects of Stanton and radiative numbers as well as the effect of air-drag are investigated.

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Generalized Sequence and Its Application to Calculation of the Density of Resonance States

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The parallel method of calculation the generalized sequence [1] is developed by using of area decomposition method. Properties of sequence are investigated for the symmetric tridiagonal matrices. With the application of property of Sturm theorem [2] to the generalized sequence we calculate the density of resonance states [3].

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2. Methods and Software for Experimental Data Processing

Track Fitting by Parabolic Model of Kalman Filter

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We consider a problem of track fitting using the measurements of track hits in the ZOX-plane of the STS detector. The parabolic model of Kalman filter is applied for estimation of the track parameters.

Robust Method of Dielectric Tensor Evaluation from Spectrophotometric Data[1]

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The main mathematical formalism employed here is based on the Berreman matrix method and the Kramers-Kronig relations. The matrix method, which is applicable to a multilayer optical system of arbitrary anisotropy, describes the light propagation with the help of equation which couples known incident, and unknown reflected and transmitted waves. The problem of finding optical dielectric tensor for each layer of the optical system knowing only measured intensities of reflected and transmitted light is quite complicated, but is very important and actual for design of new optical devices like photovoltaic cells, LEDs, and informational displays.

The perturbed measured intensities and are known only for the part of the spectral range therefore the problem of the permittivity tensor evaluation is the ill-posed problem. Fortunately, the physically realized dielectric tensor has the analytical structure that is equivalent to the Kramers-Kronig relations. Therefore we propose an algorithm in which the imagine part of the permittivity tensor is presented as sum of Gaussians-like peaks and the real part is calculated in according to the Kramers-Kronig relation. Thus, the solution of the inverse

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problem can be obtained as a parametric representation in a special class of analytical functions. This is the essence of the used regularizing procedure. Further evaluation (restoring) of the unknown permittivity tensor is done by a nonlinear fitting using some variation of Nelder-Mead algorithm.

Study of Electron Energy Losses in the CBM TRD

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We analyze the distributions of energy losses for electrons in the transition radiation detector (TRD) of the CBM experiment [1]. The energy deposits in one-layer TRD prototype (test-beam in GSI (Darmstadt, February 2006) and Monte Carlo simulations for the n-layered TRD realized in frames of the CBM ROOT [2] for momenta in the range of 1 GeV/c to 13 GeV/c were used in this study. The ionization losses of charged particles in a medium is a well-known process [3], but the behavior of the energy losses on transition radiation (TR) has a more complicated character. In order to understand the details of the TR simulation in the TRD, we performed the procedure for approximation of the electron energy losses in one layer of the TRD. This procedure permits one to extract the transition radiation part from real measurements and to bring the Monte Carlo simulation [4] into the agreement with real measurements.

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Electron/Pion Identification with the TRD Applying a Multilayer Perceptron

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A problem of pion-electron identification based on their energy losses in the transition radiation detector (TRD) of the CBM experiment [1] is considered. For particles identification an artificial neural network (ANN) was used [3, 4], a multilayer perceptron realized in JETNET and ROOT packages. It is demonstrated that, in order to get correct and comparable results, it is important to define the network structure correctly [4]. Recommendations for such a selection are given. In order to achieve an acceptable level of pions suppression, the energy losses need to be transformed to more "effective'' variables. The dependency of ANN output threshold for a fixed portion of electron loss on the particle momentum is presented.

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Electron/Pion Identification with the Transition Radiation Detector in the CBM Experiment

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The CBM (Compressed Baryonic Matter) Collaboration [1, 2] builds a dedicated heavy-ion experiment to investigate the properties of highly compressed baryon matter as it is produced in high energy nucleus-nucleus collisions at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany. The measurement of charmonium (J/ψ meson) is one of the key goals of the CBM experiment. For detecting J/ψ meson in its dielectron decay channel the main task is the electron/pion separation. To solve the mentioned problem, a multilayered transition radiation detector (TRD) is used. TRD must provide an effective electron identification and a sufficient pions suppression. The required pions suppression is a factor of about 100-200 [2].

The problem of electron/pion identification using n-layered TRD consists in the following: having a set of energy losses in n layers of the TRD, one has to decide to which particle, electron or pion, this set is relative. Taking into account that each of the particles under consideration possesses its own distinctive form for the energy loss distribution, it is necessary to solve a typical pattern recognition problem, namely, to determine which of the energy loss distributions the analyzed sampling is related to.

In order to solve the mentioned above problem, we have elaborated algorithms and implemented various approaches based on i) artificial neural network (ANN) of a feed-forward type [3, 4], ii) statistical criteria traditional for such type problems: a mean value method and a likelihood functions ratio method [6], iii) nonparametric goodness-of-fit ω_n^k criterion [5], iiii) a combined approach, i.e. combination of the mean value method and ω_n^k-test [6]. The work discusses the characteristic properties of the energy losses by electrons and pions in the TRD layers and special features of applying ANN and statistical methods to the considered problem. A comparative analysis is performed on the power of the statistical criteria and ANN.

In the work we use both the real measurements of energy losses of electrons and pions with the momentum $p = 1.5$ GeV/c in the single-layer TRD prototype (test-beam in GSI, February 2006) and the Monte Carlo simulations for the n-layered TRD realized in frames of the CBM ROOT [7].

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Online Event Selection in Heavy Ion Experiments

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ALICE and CBM are heavy ion experiments at CERN (Switzerland) and FAIR/GSI (Germany) with track multiplicities up to several thousands of tracks per event. Therefore, the online event reconstruction and selection at input rates up to 10 MHz is one of the most challenging tasks of the experiments. Because of a high track density, the cellular automaton based track finder includes the Kalman filter based track fitter. Motivated by the idea of using the SIMD unit of modern processors, the Kalman filter based track fitting algorithm has been investigated in order to increase the speed of the track finding stage of the event reconstruction. The speed of the algorithm has been increased in 120000 times, running on a Cell Blade computer. The fully SIMDized cellular automaton track finder with the included SIMD Kalman filter based fitting

routines shows 1000 times increase of the reconstruction speed with respect to the initial scalar version, running on the same Pentium 4 based computer.

The Kalman filter based track fit has shown to be a well suitable benchmark for parallelizing the algorithms of data reconstruction in high-energy physics. A real-time performance of the multi-threaded SIMD Kalman filter based fitting routine of 0.1 microsecond per track has been reached on the Intel Core i7 CPU. The algorithm has been also ported to the NVIDIA CUDA framework. It has been shown a throughput of $21.7*10^6$ tracks per sec on the NVIDIA GTX 280 graphics card. In addition, a many-core architecture code named Larrabee can be considered an interesting platform to further scale the Kalman filter in the threading and vectorization dimensions. Less architecture-dependent programming frameworks, such as OpenCL and Intel Ct, may also better support future changes in architecture.

The Basic Element Method in Polynomial Approximation and Smoothing Problems

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To increase the solution efficiency in the polynomial approximation and smoothing problems, a base element method (BEM) is suggested. The essence of the method consists in decomposition of the algebraic polynomial via quadratic and cubic elements, obtained with the aid of cross-ratio functions. The main properties of BEM comprise: threefold reduction of the order of derivatives in function decomposition, uniform approximation along the entire length, expansion of the approximation interval, direct relationship of model and data, the use of continuous parameters for adjustment of computation accuracy and stability. The use of BEM opens new possibilities for increasing the efficiency of LSM procedures, when resolving polynomial regression problems.

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Methods to Reveal Hidden Signal Structure and Their Applications

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The goal of the paper is to describe methods used to reveal the hidden structure of signals that have no distinct structure by their processing.

The approaches used in the methods proposed are connected with increase of data resolution and search for signal instability and spectrum variation domains in various modes. Algorithms are based on the maximum entropy method, calculation of signal entropy and wavelet-conversion.

In the maximum entropy method, the hidden structure of spectra manifests itself owing to the band width decrease procedure [1]. A change in the mode of the process is characterized by high signal entropy values that reflect the chaotic pattern and instability of transition moments. A change in the mode of the process is also marked by variations in spectra.

The IR spectrum structures revealed have provided new data on the isomorphic replacements and structural characteristics of silicates. A high-resolution estimate of the NGR spectrum of amorphous diadochite has shown that diadochite corresponds to destinezite. Similar estimates of the blurred NGR spectra of hydrated and radiation-irradiated biotites were used to trace structural transformation dynamics in detail.

Processing of seismograms with wavelet-algorithms has revealed the moments of arrival of various types of seismic waves , and determination of the coordinates of the sources of seismic events with their help. The algorithms can be used to increase the resolution of geophysical data [2].

Wavelet and entropy algorithms were employed to reveal the bifurcation points of river runoff and solar and seismic activity.

The characteristic feature of the methods is the minimum use of a priori information. The methods proposed are more general-purpose, simple and economical than instrumental measurement improvement methods.

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Geophysical Applications of a Statistical Model

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In the paper, the results of the use of a statistical model for solving some tectonic problems are reported.

Based on data of the statistical study of the Fennoscandian Shield, the evolution of magmatism was reconstructed [1,2]. The thickness of lava flow was found to vary with time in accordance with Fibbonaci series of numbers [1]. To interpret this relationship, a model of stepwise formation of magma effluent channels was proposed.

The fracturing of the Valaam sill was studied [3]. The polar distributions of the directions of fractures of a dip jointing were constructed for different sectors and analysed. Multiple fracturing grows to a maximum in the direction 340 and agrees with the radial strike of the Pasha-Ladoga horst-graben system forms the tectonic framework of the region.

The magnitude distribution of the events from the NEIC Catalogue has revealed at least five components that correspond to different types of earthquakes. Quakes that have a magnitude over 4.5 occur more commonly in the mantle than in the Earth's crust. For major and very minor earthquakes, there are depths at which seismic foci are most likely to form. The analysis of the monthly distribution of seismic events has supported our assumption that crustal earthquakes occur more often in October-November and in April-May, when the tangential acceleration of the Earth's movement along the orbit attains maximum values. The bifurcation points of the process were determined from the time dependence of seismicity.

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Feature Extraction for Data Input to Neuro-Classifiers

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Artificial neural networks (ANN) are widely used now, in particular, in problems of experimental data classifying and recognition. However, despite of known ANN advantages, their practical applications are faced with many difficulties caused, as a rule, by restrictions of inter-neuronal connections due to insufficient sizes of training samples and a great dimension of each data vector in such samples. Therefore the problem of the essential compression of data to be input to ANN-classifier without loosing significant information is of great importance.

In the given paper this problem is considered on the example of the quite substantial task of the genetic protein structure analysis, which is important for genetic biology researches in radiobiology and, especially, in agricultural applications for breeding cereals and other crops. Such analysis is usually carried out by studying electrophoretic spectra (EPS) of gliadin (alcohol soluble protein) of the inspected grain cultivar [1]. EPS digitization produces a densitogram with 4 thousands counts which intensity changes inherits the genetic structure of a protein as its unique marker. The multicriterion problem of the cultivar identification by their spectra lead to the idea of its solution by an artificial neural network trained on an expert data base. The peculiarity of obtaining each EPS as a set of 17 strips on polyacrylamide gel substrate requires elaborating special preprocessing software for densitogram smoothing, pedestal eliminating, as well as compensating such digitization defects as signal noise, variability of spectrum borders and illumination, their non-linear starches due

to electrophoresis nonstationarity. These procedures are realized by wavelet filtering and Hemming neural network application [2].

On the next stage of extracting most informative features several alternative approaches have been studied: (1) the densitogram is coarsen from 3900 points into 200 segments with averaged density as input fields for ANNs [3]; (2) such a well-known way of feature extraction as the principal component analysis (PCA) was also applied in its neural network implementations, which allows to avoid cumbersome calculations of covariance matrices and their eigenvectors; (3) the next approach is to recognize all well-pronounced peaks, fit them by some of bell-shaped function, like a Gaussian, in order to evaluate their parameters: amplitude, width and position to be input to ANN; (4) then heuristics of experts shown that not only the width and intensity of peaks on densitograms was be taken into account, but the order of their alternating is also very decisive, therefore it was proposed to split each densitogram into a number of zones, in order to calculate the rank of a peak occurred in every zone; (5-6) input data compression by both discrete Fourier (DFT) and wavelet (DWT) transformations.

All these methods have been used for feature extraction from samples formed by experts for 30 different sorts. Each sample contains more than 100 EPS cultivars for every sort. Then extracted features were used to train ANN of three-layer perceptron type in order to test the efficiency of correctly recognized cultivars. Substantial efforts were applied to optimize ANN parameters. The comparative study of the recognition efficiency with the methods listed above shows their high sensitivity to the number of sorts to be classified. Three first methods show fast drop of efficiency lower 95% after 3-5 sorts, the 4th method kept efficiency 97% till 7 sorts and only DFT and DWT approaches could keep 95-97% up to 20 sorts. A further development of feature extraction methods and a study of possibility to develop a hierarchy of classifying ANNs are intended.

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About Finding k-Jet Zeros with Using Annealing

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In report discuss method of determinate zeros of k-jets with using annealing. In this method may be find zeros of k-jets of the 1-st. rang. Discussed accuracy of this methods and its advantage and its problems.

Training Neural Networks with PSO and Other Population-Based Algorithms

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Artificial Neural Networks are excellent classification tools widely applied in computational physics. Gradient descent based methods for neural network training, such as back propagation of error, are usually used. However, due to its hill climbing nature, back propagation may not always be the best choice for neural network training. An overview of alternative population-based training algorithms is provided, paying special attention to particle swarm optimization algorithm. Example applications are also discussed.

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Method of the Main Components for Description of Internal Dynamics of Weakly Bound Clusters

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The dynamics of weakly bound atomic and molecular complexes is sophisticated and it cannot be described by well known method of normal modes. New approaches to present their internal dynamics are relevant for understanding of fundamental processes in molecular physics and chemical reactions. Method of the main components has been suggested for effective description of internal dynamics of nonrigid van-der-Waals atomic clusters [1]. The main idea of the method is to decompose the motion in n-dimensional phase space (or subspace) into m (m=1,2ЖЌn) orthogonal components such that the linear superposition of m modes approximates the dynamical properties in the most accurate matter. The method helps to reduce dimension of the phase space effectively and gives the key for understanding of internal dynamics of complex nonlinear systems. In the present work method of the main components is applied to study dynamics of such molecular systems as small water clusters with number N (N=2-6) of water molecules at different quasi-states of the clusters. For interaction between water molecules the rigid TIP5P [2] potential function is used, and phase trajectories are calculated by classical molecular dynamics method. A law of energy distribution among the modes is determined. It is shown that the internal temperature of the system is connected with the numbers of effective modes (main components).

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Fast Ring Recognition Algorithm for the RICH Detector of the CBM Experiment at FAIR

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The Compressed Baryonic Matter (CBM) experiment at the future FAIR facility at Darmstadt will measure dileptons emitted from the hot and dense phase in heavy-ion collisions. In case of an electron measurement, a high purity of identified electrons is required in order to suppress the background. Electron identification in CBM will be performed by a Ring Imaging Cherenkov (RICH) detector and Transition Radiation Detectors (TRD).

In this contribution we will present algorithms and software which have been developed for electron identification in RICH detector. Efficient and fast ring recognition in the RICH detector is based on the Hough Transform method which has been accelerated considerably compared to a standard implementation. Ring quality selection is done using an Artificial Neural Network. Due to optical distortions ellipse fitting and radius correction routines are used for improved ring radius resolution.

These reconstruction methods allow for a high purity and efficiency of reconstructed electron rings. The developed algorithms is very robust to a high ring density environment. They were tested on large statistics of simulated events and are included into the CBM software framework for common use.

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Fast Global Tracking for the CBM Experiment at FAIR

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The Compressed Baryonic Matter (CBM) experiment at the future FAIR accelerator at Darmstadt is being designed for a comprehensive measurement of hadron and lepton production in heavy-ion collisions from 8-45 AGeV beam energy, producing events with large track multiplicity and high hit density. The CBM setup consists of several detectors including as tracking detectors the silicon tracking system (STS), the muon detector (MUCH) or alternatively a set of Transition Radiation Detectors (TRD). Finally, hits from the Time of Flight (TOF) detector are attached to global tracks.

In this contribution, the status of the global track reconstruction software including track finding in MUCH and TRD and track-to-hit merging in TOF is presented. The track reconstruction procedure includes track finding, track fitting, track propagation and finally track selection. The track propagation algorithm takes into account an inhomogeneous magnetic field and includes accurate calculation of multiple scattering and energy losses in the detector material. Track parameters and covariance matrices are estimated using the Kalman filter (KF) method and a modified KF where weights are assigned to hits and simulated annealing is used. Three different track finder algorithms based on track following with track seeds from STS and KF track fitting have been developed either use track branches, nearest neighbor or weight methods. The track reconstruction efficiency for central Au+Au collisions at 25 AGeV beam energy using events from the UrQMD model is at the level of 93-95%.

Since CBM has to process terabytes of input data produced at high collision rate, it is extemly important to develop a fast track reconstruction algorithm. The speed up of the reconstruction algorithms has been studied. The significant memory and combinatorics optimization have been done. SIMD, a powerful feature of modern CPUs, allows to vectorize part of the code, resulting in further speed up. Including these improvements in our global track reconstruction it could be accelerated by approximately 10 times compared to the original version.

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GEANT4 Code Application for Radiation Environment Prognostication at the NICA Complex

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The operation of a high-energy ion facility provokes secondary radiation along an accelerator ring and especially at the local sites of maximum beam losses (outlet devices, targets, and beam dumps). An essential condition for the commissioning of a relativistic heavy ion accelerator is appropriate radiation shielding for every radiation element of the complex. The shielding design is connected with two crucial problems: the estimation of the source term and the prognostication of the neutron fluence and equivalent dose distributions around the shielding.

As regards the first problem, the experimental data on the double differential cross section and secondary neutron production in thick targets for a primary uranium beam with the energy of several GeV/n are practically lacking. Few Monte Carlo multipurpose codes able to simulate the uranium ion interaction

with, and transport into, the matter are now available. A comparison of FLUKA, GEAT4, and SHIELD simulations with unique experimental data on neutron production in a 1GeV/n ^{238}U beam interaction with a thick Fe target was performed to find the most suitable code. As a result, the GEANT4 code was chosen to carry out a simulation of the NICA (Nuclotron-Based Ion Facility at JINR) complex radiation shielding. Forming the secondary radiation field inside and behind the ordinary concrete shielding was analyzed as well. Some regularities of the secondary neutron field generation in a 4.5 GeV/n uranium beam interaction with thick targets are discussed.

As concerns the second problem, it was found that the crucial point determining the NICA shielding design is that the yearly equivalent dose at the border of the Laboratory site must not exceed 1 mSv. The radiation situation at long distances from NICA will be formed by neutrons which escaped from the shielding of the NICA radiation sources and were then multiscattered in the air and ground ("skyshine"neutrons). The GEANT4 calculations of the "skyshine"neutron radial distributions around all the elements of the NICA complex were carried out, and guidelines for the shielding construction were worked out for different operation modes of the complex.

PACS: Keywords: Monte Carlo code; Shielding data; Relativistic heavy ions; Secondary radiation field; Thick target, Neutron yield; Attenuation curve; Neutron fluence and equivalent dose.

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The Application of Linearization Technique for Finding Drift Characteristics of Wire Detectors[1]

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The iteration algorithm for particular case of problem of finding drift characteristics for wire detectors is presented. It is based on using linearization technique, proposed many years ago in our institute. Its specificity is in the possibility to take into account practically arbitrary number of tracks.

Reference Points Based Approximation and Asymptotic Normality[2]

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A three-part polynomial scheme is presented as a basic building block for piecewise smoothing of noisy data. The approximation model of the scheme leverages a reference points based representation of polynomials. The quasy-smooth transition between the three components is ensured by an appropriate localization of the reference points. The parameter of the central part is computed by a recursive formula that yields an asymptotically normal estimate.

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Математическое моделирование хронотомографических процессов реконструкции 2-D объектов.[1]

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Представлен метод реконструкции плотности распределения по проекциям, используя специально разработанную функцию реконструкции.

Продемонстрирована эффективность данной функции для реконструкции функции распределения по проекционным данным хронометрических измерений. Также продемонстрирован результат моделирования случайного разброса проекций по координатам на плоскости изображения, с последующей коррекцией, непосредственно перед реконструкцией. Обсуждается применения данного метода для восстановления изображений в сканирующей зондовой микроскопии.

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Two Methods for Ellipse Fitting in the CBM Experiment

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Since the elliptic model of Cherenkov radiation rings in the RICH detector of the CBM experiment [1] was recently accepted supplementally to the previous circular one [2], the ellipse fitting algorithm based on the Kepler equation of ellipse with the following MINUIT minimization [3] has been elaborated and used now as the default method. To avoid time-consuming MINUIT application we propose a new direct ellipse fitting algorithm based on the Taubin method [4, 5].

In this contribution we describe the second algorithm and fulfil the comparative study of both algorithms using obvious notations: - Minuit and Taubin Fitters correspondingly. It is important to stress that the Taubin method is non-iterative and, therefore is much faster than the Minuit Fitter, besides it is statistically more accurate [4, 5]. After detailed testing on the great statistics of simulated data corresponding software implementing the Taubibin-based algorithm is also included in the CBM Framework [6].

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About Improving Accuracy of Graphic Pattern Recognition by Increasing of Range of Image Representation

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The standard eight bit image range in noise environment is too small to effective image processing and pattern recognized of form graphic object. To improve it in report is to attempt to wide dynamic range of image to sixteenth bits. The result is present in report and discussed.

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3. Computer-Algebra Software, Symbolic-Numeric Methods and Algorithms

The Addition and Multiplication Properties of Orthogonal Polynomials[1]

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A sequence of orthogonal polynomials $\{Q_n(x)\}$ can be uniquely specified in a few ways: via a measure on some domain, three-term recurrence relation, generating functions or integral representation. We will discuss their usage for deriving of addition formula of the type $Q_n(x+y) = \sum_{k=0}^{n} C_{n,n-k}(x)Q_k(y)$ and multiplication formula $Q_n(xy) = \sum_{k=0}^{n} D_{n,n-k}(x)Q_k(y)$. Adequate computer-algebra software will lead along the consideration.

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An Average Growth Rate of the Random Fibonacci-Padovan Sequences

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An integer recurrent sequence $u(n) = u(n-1-r) + u(n-2-r)$, $n \geq 3$, where r is a random value equal to 0 or 1 with the probabilities and respectively, is called a random Fibonacci-Padovan sequence.

In the present report we show that the average growth rate of such sequences, $\lim(u(n)^{(1/n)})$ is equal to the greatest positive root of some special cubic equation.

Multi-Level LP-Structures in Rewriting Systems

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The lattice-based algebraic systems containing the semantics of a set of rules of the conditional equational theory (or a term rewriting system) are introduced. The following basic questions are considered for the given model: completeness, equivalent transformations, structure of closure, logical reduction. The obtained results can be applied to analysis and automatic optimization of the corresponding set of rules.

Complexity of Bounding Polynomial Roots

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We discuss the efficiency of methods for bounding real roots of polynomials. We study the optimality and establish results on the complexity.

Common LISP Based REDUCE

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A common Lisp–based computer algebra system REDUCE under CMUCL/GCL interpreters is presented. The concurrent using of the modules written in Common Lisp and Snandard Lisp and CMUCL/GCL specific questions in compilation and optimization are discussed.

An Implementation of the Heaviside Algorithm

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The so-called Heaviside algorithm is intended for solving initial value problems for linear ordinary differential equations with constant coefficients. It is based on the operational calculus approach. We use it in frames of Mikusinski's Operational Calculus.

An implementation of the Heaviside algorithm using a computer algebra system is considered with special attention to the features determining its efficiency.

Some aspects of the extension and application of the Heaviside algorithm are discussed as well.

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Functional Equations for Feynman Diagrams

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New types of relationships between Feynman integrals are presented. It is shown that Feynman integrals satisfy functional equations connecting integrals with different values of scalar invariants and masses. A method is proposed for obtaining such relations. The derivation of functional equations for one-loop propagator- and vertex - type integrals is given. It is shown that a propagator - type integral can be written as a sum of two integrals with modified scalar invariants and one propagator massless. The vertex - type integral can be written as a sum over vertex integrals with all but one propagator massless and one external momenta squared equal to zero.

The proposed method is also applied to one-loop box integrals needed in calculations of radiative corrections to heavy-quark production and Bhabha scattering. We present relationships between these integrals with different arguments and box integrals with all propagators being massless. It turns out that functional equations are rather useful for finding imaginary parts and performing analytic continuations of Feynman integrals.

The presentation is based on recent publications [1, 2].

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Virtual Modeling to String Theory

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We analyze methods of virtual modeling of closed and open strings in different backgrounds and apply selected of the methods to visual representation of string interaction. It is impossible to visualize string propagation in 10 or 26 dimensional spaces. But it is possible to give a visual representation of projections on 2D or 3D subspaces. Methods of the projections in various spaces

are presented and discussed. In conclusions we consider theoretical foundations of extensions of virtual modeling methods and their possible applications.

A short tutorial on virtual modeling and simple examples of visualization will be done.

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О выборе алгоритма умножения для полиномов и полиномиальных матриц

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Исследуются алгоритмы умножения для плотных и для разреженных полиномов и полиномиальных матриц в разных числовых областях. Приводятся выражения для сложности операций умножения полиномов и полиномиальных матриц как математического ожидания числа аддитивных и мультипликативных операций. Приводится табуляция полученных выражений сложности для набора параметров, представляющих практический интерес. Представлены результаты экспериментов с реальными программами, вычисляющими произведения полиномов и полиномиальных матриц исследуемыми алгоритмами. Обсуждается сравнение экспериментальных результатов с теоретическими и возможность построения процедуры автоматизирующей выбор лучшего алгоритма в зависимости от диапазона параметров.

DIRAC: Computer-Algebra Tool for Studying the Structure and Dynamics of Highly-Charge Heavy Ions

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During the last five years, the Dirac package has been found to be an efficient tool for studying the properties and dynamical behaviour of few–electron heavy ions [1]. Owing to its user–friendly interface, this package became accessible not only to experts in relativistic atomic theory, but also to many scientists who have to deal with atoms and ions only occasionally. Here, we present an extension of the Dirac program for calculating the properties of the radiative bound–bound and bound–free in heavy atomic systems. In particular, the new Maple and Mathematica procedures support the symbolic as well as numerical computations of a whole variety of transition properties including total cross sections, angular distributions and polarization properties of x–ray radiation, and others.

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On Decomposition of Nonlinear Differential Systems into Involutive Subsystems

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In this talk we consider some constructive aspects of algebraic completion of polynomially-nonlinear systems of partial differential equations (PDEs) to involution. To optimize the computational costs of prolongations and projections to be done in the course of completion one can use separation of independent variables for the equations in the system based on theory of involutive divisions. To preserve the solution space by performing completion one has to make sure that the initials and separants of equations in the system do not vanish on its solutions. This condition is fulfilled by performing the triangular decomposition

of the nonlinear differential system into algebraically simple subsystems. We discuss this method and show how algebraic Groebner bases can be used to avoid unnecessary splittings. Finally, we show how to combine the splitting method with the involutive completion technique to decompose of a nonlinear PDE system into a finite set of involutive and algebraically simple subsystems with disjoint set of solutions.

SLIPM— a MAPLE Code for the Numerical Solving of Sturm—Liouville Partial Problem Basing on the Continuous Analog of Newton's Method

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A MAPLE program for solving the Sturm-Liouville partial problem based on the continuous analog of Newton's method (CANM) is presented. The program code is the development of the original FORTRAN programs SLIP1, SLIPH4 [1-2]. We propose two new algorithms to calculate initial values of the iterative parameter in the driver program. It may be the additional possibility to optimize the numbers of iterations in the convergence domain. The program has a user-friendly graphic visual interface. The program has been tested on series of examples [3]. The algorithms and their implementations in the program are described and discussed.

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Computational Tools for Representation Theory of Affine Lie Algebras

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We describe computational algorithms for construction of representations of affine Lie algebras and computation of branching coefficients of representations of affine Lie algebra to representations of affine sub-algebra. Also we introduce the implementation of these algorithms as Maple package and present examples studied with these computational tools.

Interlacing Solutions of Linear Difference Equations[1]

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The search for solutions in the form of the interlacing of finite sums of hypergeometric sequences plays an important role in the Hendriks-Singer algorithm ([1]) for constructing all Liouvillian solutions of a linear homogeneous difference equation $L(y) = 0$ with polynomial coefficients. We show that Hendriks - Singer's procedure for finding the interlacing solutions can be simplified. We also show that

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[2]Work is partially supported by the RFBR, grant no. 07-01-00482-a.

– the space of solutions of $L(y) = 0$, spanned by the solutions of the form of the the interlacing of m ($1 \leq m \leq \mathrm{ord}L$) hypergeometric sequences, posses a cyclic permutation property, and

– if $L(y) = 0$ has Liouvillian solutions, then it has, in particular, solutions of a quite simple form (so-called m-fractional solutions).

In addition we describe adjustments of the implementation described in [2] of the Hendriks-Singer algorithm to utilize the presented results.

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Вычисление характеристических полиномов матриц: последовательные и параллельные алгоритмы

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Исследуются алгоритмы вычисления характеристических полиномов матриц. Получены теоретические выражения, характеризующие сложность алгоритмов, позволяющие сравнивать их между собой и выбирать лучший алгоритм в зависимости от конкретной задачи. Получен новый алгоритм, имеющий асимптотически лучшую оценку сложности в кольцевых операциях.

Разработаны программы для вычисления характеристических полиномов матриц. Выделены области параметров входных данных и указаны лучшие алгоритмы в этих областях. Результаты экспериментов для целочисленных и полиномиальных матриц показали, что асимптотически лучшее время имеют новый алгоритм и алгоритм Данилевского с применением Китайской теоремы об остатках. При малых порядках матрицы меньшее время вычисления имеет лучший из прямых алгоритмов – алгоритм Сейфуллина.

Разработаны параллельные алгоритмы вычисления характеристических полиномов матриц на основе алгоритма Данилевского и нового алгоритма с применением Китайской теоремы об остатках. Граф каждого

параллельного алгоритма имеет вид бинарного дерева за счет применения дихотомического деления множества модулей. Получены параллельные программы для вычисления характеристических полиномов матриц. Результаты экспериментов для целочисленных матриц показали, что ускорение вычислений находится в пределах от 50% до 90%.

An Algorithm for Symbolic Solving Systems of Partial Differential Equations

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An algorithm for symbolic solving systems of partial differential equations by means of multivariate Laplace-Carson transform. There is considered a system of n equations with m as the greatest order of partial derivatives and right hand parts of a special type. Initial conditions are input. As a result of Laplace-Carson transform of the system according to initial condition we obtain an algebraic system of equations. A method to obtain compatibility conditions is discussed.

The algorithm of solving the system consists of three main steps:

I. Laplace-Carson transform of the system.

II. Solving of the algebraic system.

III. Establishing of compatibility conditions.

IV. Inverse Laplace-Carson transform of the solutions as the solution of the data system.

To provide the symbolic character of all computations we carry out the following:

1) Represent all given functions as sums (or series) of exponents with polynomial coefficients.

2) Factorize D (as full as possible).

3) Represent the solution of algebraic system as sums (or series) of algebraic fractions with exponential coefficients.

Computer Realization of Regularized Method for a Wavefront Set Recovering on the Base of Hartmann Test with the Help of Analytical Calculations in Axiom CAS[1]

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On the first (auxiliary) stage of computer experiment with the help of analytical calculations in Axiom from the given Fourier coefficients of the wavefront set Zernike expansion we construct the Hartmann test data on the given mesh in the unit disk using pseudorandom numbers generator.

On the second (principal) stage of computer experiment with the help of analytical calculations in Axiom CAS we construct the matrix of stabilization functional for regularized algorithm for a wavefront set recovering on the base of Hartmann test. We also give a computer realization of this algorithm.

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On Integrability of a Planar ODE System

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We consider an autonomous system of ordinary differential equations, which is solved with respect to derivatives. To study local integrability of the system near a degenerate stationary point, we use an approach based on Power Geometry method and on the computation of the resonant normal form. For a planar 5-parametric example of such system, we found the complete set of necessary and sufficient conditions on parameters of the system for which the system is locally integrable near a degenerate stationary point.

Автоматизация средствами компьютерной алгебры качественного анализа заданной системы алгебраических дифференциальных уравнений с параметрами: алгоритмы классификации фазовых портретов в пространстве параметров и качественная устойчивость генерации фазовых портретов

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Решения систем ОДУ с дробно-полиномиальными правыми частями на конечном или бесконечном интервале времени могут достигать бесконечных значений за бесконечное или конечное время. При этом, возможно, в

некоторых точках производные искомых функций по времени принимают бесконечные значения.

Корректное определение бесконечных значений переменных достигается вложением исходного пространства в компакт $R^n \to T^{2n}$.

Интегрируемые функции на компакте имеют ограниченную вариацию, интегрирование ведется по параметру, отличающемуся от времени (натуральному, например). С компактностью связана устойчивость численного интегрирования.

Преобразование исходной системы уравнений и начальных условий к новым переменным выполняется автоматически в пакете Maple12. Построен механизм автоматического перебора качественно отличных фазовых портретов, который сопоставляет каждому портрету соответствующий набор параметров и позволяет составить альбом графических иллюстраций. Механизм основан на анализе характеристических уравнений для особых точек системы. Предлагаемый метод использовался при численном интегрировании уравнений Эйнштейна, отличающихся чрезвычайно широким диапазоном значений интегрируемых функций и в неограниченной области [1]. Некоторые решения при этом обнаруживают особенности (локализация во времени и в пространстве) сходные с рассмотренными в [2].

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Об экспериментах с алгоритмом Фужера F4

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Алгоритмы J.-C. Faugere, известные как алгоритмы F4 (1999) и F5 (2002), открыли эру матричных алгоритмов вычисления стандартных базисов полиномиальных идеалов. Программы, написанные их автором, являются лучшими программными реализациями, которые используются сегодня для вычисления базисов Гребнера. В настоящем докладе обсуждаются результаты экспериментов, которые проводились с программными реализациями алгоритма F4 в среде Java, а также перспективы создания параллельной программы для алгоритмов F4 и F5.

Symbolic & Numeric Schemes for Analysis of Deterministic and Stochastic Systems with Aftereffect[1]

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A phenomenon of different delays is an essential element of objects functioning. Therefore deterministic and stochastic differential equations (DEs, SDEs) with divergent arguments and integro-differential equations (IDEs) have been attracting added interest both from theoretical and practical viewpoints. Such equations are encountered in those areas, where properties of an object depend on a hereditary effect, and serve as models for different processes, viz., an automatic control for technical devices and engineering procedures, development of economic and social systems, autonomous vessel course stabilization, struggle for existence in biology, population dynamics, etc.

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There are deterministic and stochastic, linear and nonlinear ordinary DEs with single and multiple constant and variable delays, neutral DEs, systems excited by continuous and discrete fluctuations, SIDE with additive and multiplicative noises, deterministic partial DEs (PDEs) with single constant delay, tasks of estimation of stochastic sensitivity for linear dynamic systems with delay under consideration.

Our schemes for study of such systems are based on extensions of phase spaces [1] and implemented due to Mathematica code programs. These schemes allow to transform equations with divergent arguments into equations without delays and to use standard Mathematica tools such as function NDSolve.

These techniques were applied to study a number of linear and nonlinear models. Among them there are deterministic DEs of Lottka-Volterra, Van der Pol-Duffing, Minorsky, auto-oscillation in a long current line and B-cell response dynamics; SDEs of a nonlinear system with multiple delays and pantograph; PDEs of Burgers and burning with delay; linear SDEs of car motion effected by front-to-rear delay and a rough road and random dynamics of pollutions discharged into a cascade of natural water bodies; a modified Black-Schools SDE for option price effected by an additive jump-like Poisson excitation and a constant lag etc.

Moreover we present the iterative method of successive differentiation for calculation of a Green matrix-function for linear deterministic and SIDEs, few approximate procedures of linear SIDEs transformation into SDEs and corresponding examples.

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Reduction-Level Parallel Computations of Gröbner and Janet Bases[1]

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In previous papers [1, 2] we presented algorithm for parallel calculation of Gröbner and Janet bases that works in terms of parallel normal forms computations. The realization was quite promising but faced problem of "starvation" (e.g. in some moments of time only few processors was fully loaded). In this talk an approach to raise scalability and avoid "starvation" will be presented. Experimental results of parallel computations on eight core SMP machine will be shown.

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Symmetries, Gauge Invariance and Quantization in Discrete Models[1]

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Different aspects of discrete symmetry analysis in application to deterministic and non-deterministic lattice models are considered. One of the main tools for our study are programs written in C.

In the case of deterministic dynamical systems, such as cellular automata, non-trivial connections between the lattice symmetries and dynamics are revealed. In particular, we show that formation of moving soliton-like structures — analogs of "spaceships" in cellular automata or "generalized coherent states" in quantum physics — is typical and caused by the existence of non-trivial symmetry group.

In the case of mesoscopic lattice models we consider algorithms for computing microcanonical partition functions and searching phase transitions. These algorithms involve the use of symmetry groups of the models.

We consider also gauge invariance in discrete dynamical systems and its connection with quantization. We propose an approach to introduce quantum structures in discrete systems, based on finite gauge groups. In this approach quantization can be interpreted as introduction of gauge connection of a special kind. We illustrate our approach to quantization by a simple model and suggest its generalization.

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On Computation of the Bifurcation Points for the Logistic Map

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The logistic map is a discrete-time analogue of the continuous logistic Verhulst's equation and has the form of a one-parameter nonlinear recurrence relation

$$x_{n+1} = \mu x_n(1 - x_n), \quad \mu > 0\,. \tag{1}$$

Detecting the bifurcation values of parameter μ is a hard computational problem [2]. It is described by the following system of polynomial equations

$$\begin{cases} x_2 = \mu x_1(1 - x_1\,,) \\ x_3 = \mu x_2(1 - x_2)\,, \\ \dots \\ x_n = \mu x_{n-1}(1 - x_{n-1})\,, \\ x_1 = \mu x_n(1 - x_n)\,, \\ \mu^n \prod\limits_{k=1}^{n} (1 - 2x_k) = 1\,. \end{cases} \tag{2}$$

From the system (2) one can compute a polynomial in μ by doing elimination of the variables $\{x_1, \dots, x_n\}$. This can be achieved by computing a Gröbner basis for a degree compatible term order and then by constructing a univariate polynomial in μ that belongs to the ideal generated by the system (2). The last construction is done by the linear algebra methods applied to the ideal as

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a vector space generated by the power products in $\{x_1, \ldots, x_n, \mu\}$. In doing so, computation of roots of the univariate polynomial obtained is a much more simple problem to detect the values of μ directly from the multivariate system (2).

We discuss the algorithmic aspects of this approach the specialized computer algebra system *GINV* [1] to compute the bifurcation polynomial in μ for $n = 9$. Among the real roots of this polynomial we found the bifurcation point $\mu = 3.687196\ldots$.

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Distributed and Recursive Representation of Polynomials in Computing Boolean Gröbner Bases by the Pommaret Division Algorithm[1]

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Recently Boolean Gröbner bases were successively applied, as a universal algorithmic tool, to solving various scientific problems in cryptography, model checking and SAT (Satisfiability). In the present talk we apply the involutive

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algorithm based on Pommaret division to computation of Boolean Gröbner bases for the lexicographical monomial ordering. In doing so, we consider two distinct representations of Boolean polynomials: distributive and recursive. We implemented these representations in two distinct C++ packages called BPB-I and BPB-II (BPB abbreviates Boolean Pommaret Basis) where the former package implements the distributive representation and the latter one implements the recursive one. We present the results of our computer experiments with BPB-I and BPB-II based on some standard benchmarks.

Analysis of ODE systems by algorithms of Power Geometry in CAS Maxima[1]

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We consider algorithms of Power Geometry to calculate asymphtotic expansions of solutions of ODE systems. Author develops the collection of functions of the computer algebra system Maxima to apply these algorithms. We tested these functions by computation of known asymphtotic expansions of solutions of the autonomous Henon-Heiles ODE system. We consider the usage of these functions to calculate asymphtotic expansions of solutions of the non autonomous N. Kowalewski ODE system.

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Limit Cycles in a Mathematical Model of Three Interacting Species

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The paper presents a mathematical model for describing the dynamics of populations of three interacting species, predator and its two preys in the form of the system of differential equations

$$\begin{cases} \dot{x} = x \cdot (a - b_2 \cdot z), \\ \dot{y} = y \cdot (c - d_2 \cdot z), \\ \dot{z} = z \cdot (-e + h_1 \cdot x + g_1 \cdot y), \end{cases} \in G^+ \qquad \begin{cases} \dot{x} = x \cdot (a - b_1 \cdot z), \\ \dot{y} = y \cdot (c - d_1 \cdot z), \\ \dot{z} = z \cdot (-e + h_2 \cdot x + g_2 \cdot y), \end{cases} \in G^-$$

where the right-hand side has a discontinuity on the surface S. A package of symbolic-numerical software in Maple invironment is developed for integrating the system and presenting its solutions graphically, trajectories for certain parameter values are made up. It is shown that in such a model the presence of predator is enough (even with the lack of competition) to stabilize the populations of preys without causing either of them to completely extinct.

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Pattern Matching Summation in MAPLE [1]

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We consider an implementation of the pattern matching summation approach in MAPLE. In spite of existing of modern summation algorithms, this approach is still of some practical value, since it allows finding a result significantly faster in the case when the approach is applicable. The implementation is done as a package `PatternMatchingSummation`. We describe the package structure, its internal representation of patterns, its features to extend the set of patterns, its pattern matching mechanism, and present examples of using the package.

We consider pecularities of using summation formulae from handbooks as patterns. To receive right results it is often required to make additional study of formula's definition area.

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Applications of Computational Algebra to Studying Polynomial Systems of Differential Equations

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We discuss applications of methods of computational algebra to studying some problems of qualitative theory of differential equations, namely, the center and isochronicity problems, and the problem of estimating the number of small-amplitude limit cycles bifurcating from an equilibrium point (the cyclicity problem). An essential step in resolving the first two problems is finding the irreducible decomposition of polynomial variety generated by some polynomials (the so-called focus and isochronicity quantities). We discuss an approach to perform such decomposition using modular arithmetic.

The third problem (the problem of cyclicity) is reduced to computing a basis of the ideal generated by the focus quantities. We show how to compute a basis in the case, when the ideal in question is a radical ideal, and in some cases, when the ideal is not a radical.

We also characterize the set of all time–reversible systems within a particular family of polynomial differential equations and give an efficient computational algorithm for finding this set. An interconnection of time-reversibility, the center problem and invariants of the rotation group is discussed as well.

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Новые гомографические решения в ньютоновой задаче многих тел[1]

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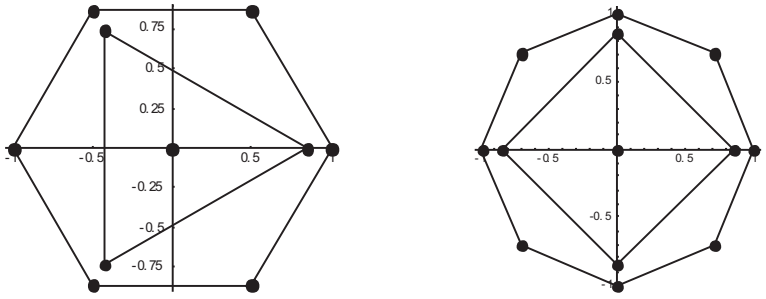
В работах [1-3] найдены новые точные частные решения ньютоновой проблемы (n>3) тел, геометрически изображаемые правильными многоугольниками одной и той же размерности, вращающимися с одинаковой угловой скоростью вокруг общего центра, являющиеся центральными конфигурациями в терминологии Лагранжа и Винтнера [4].

Нами исследована проблема существования концентрических центральных конфигураций, геометрически изображаемых правильными многоугольниками разной размерности n и 2n, вложенными друг в друга. Для n=3 это будет конфигурация, состоящая из равностороннего треугольника, вложенного в правильный шестиугольник, а для n=4 - квадрат, вложенный в октагон. Необходимые и достаточные условия существование таких центральных конфигурации в проблеме многих тел получены с использованием методов компьютерной алгебры. Рассмотрен вопрос о применении КАМ-теории в исследовании устойчивости этих центральных конфигураций [5,6].



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Evolution Equations for Roots and Coefficients of Polynomials and Related Generalized Dynamics

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Invariant theory as a study of properties of polynomials under translational transformations is developed. Class of polynomials with congruent set of eigenvalues is introduced. Evolution equations for eigenvalues and coefficients remaining the polynomial within proper class are formulated. The connection with equations for hyper-elliptic Weierstrass and hyper-elliptic Jacobian functions is found. Algorithm of calculation of eigenvalues of the polynomials based on the evolution process is elaborated. The generalized dynamics with n-order characteristic polynomials is built.

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Многослойные кольцевые структуры [1]

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Исследование проблемы существования и устойчивости конфигураций материальных точек, взаимно гравитирующих по закону Ньютона [1], совместно с точным решением задачи „об осе-симметричном взаимодействии n-тел“ [2] и с методами конструирования кольцевых структур [3] позволяет создавать алгоритмы построения многослойных кольцевых структур. Используя методы численного интегрирования дифференциальных уравнений, авторы определили и исследовали некоторые устойчивые и неустойчивые модельные структуры.

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The Number of Fixed Length Cycles in an Undirected Graph Explicit Formula in Case of Small Lengths

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Modifications of Ross and Harary algorithm to formularize the number c_k of cycles of length k in an undirected graph in terms of its adjacency matrix are developed. We consider general undirected graphs as well as bipartite graphs. Computer algebra implementations of the algorithms enable us to construct formulae at least for $k \leqslant 12$ in general case and for $k \leqslant 14$ in case of bipartite graph.

We show that, for any fixed value of $k \geqslant 8$ and space complexity quadratic in order n of a graph, the time complexity of computing c_k is $O(n^{[k/2]} \log n)$. In case of bipartite graph, for $k = 8, 10, 14$ better estimations are obtained: $O(n^3 \log^2 n)$, $O(n^4 \log^2 n)$, $O(n^6 \log^2 n)$.

Original Ross and Harary algorithm [1] was designed to formularize the matrix R_k of self-intersecting open walks of length k. Using matrix R_{k-1}, the number of cycles of length k is computed [2]. However the formula constructed specifically for c_k, has less terms and an order of magnitude more efficient than the formula for R_{k-1}. In case of bipartite graph, further formula reduction is possible.

k	4	5	6	7	8	9	10
Number of terms for R_{k-1}	3	9	32	101	348	1225	4555
Number of terms for c_k (arbitrary graph)	3	3	10	12	35	58	160
Number of terms for c_k (bipartite graph)	3		7		20		59

Formulae obtained for c_k in general case extend previously known expressions for $c_3, \ldots, c_6$ [3, 4, 5]. The time complexity of computing latter values and c_7 is $O(r(n))$ where $r(n)$ is complexity of $n{\times}n$-matrices multiplication [5]. Another previously known formularization of c_k in terms of graph's adjacency matrix [6] results in complexity $O(2^n r(n))$ for any fixed value of k. Being simplified it leads to complexity $O(n^k \log n)$ which is inferior to our estimations.

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4. Modeling in Biophysics, Bioinformatics, and Physical Chemistry

Analysis of Numerical Investigations Regarding the Supercritical Fluid Expansion in the RESS Process

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In this work, we detail the CFD simulations of the RESS (rapid expansion of supercritical solution) process which is employed to get microparticulates of selected materials with controllable morphology and narrow size distributions using supercritical fluid (especially the carbon dioxide). The numerical computation of supercritical fluid flow is extremely challenging because of the complexity of the involved physical processes and the different space and time scales involved. This project aims to analyze advanced mathematical modeling of the supercritical fluid expansion in the RESS process in order to optimize operating parameters from a comparison of published works in the field. Particularly, the research goals are to examine numerically influences of temperature, pressure, composition, flow rate and reactor dimensions on the fluid hydrodynamic to undertake study of transport and growth of the recrystallized particles.

Network Libraries of Computable Models as the Reactive Distributed Systems

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For computable models and numerical methods on the basis of the reactive distributed systems with a graphic interface the concept and the architecture of network object-oriented information libraries are discussed. Calculation of modelling situations is driven by the events and workflow constructed by the user using components saved in library and their data.

The library is intended for saving, easy access and the calculation of wide range set of models solved by iterations, including complex models on the basis of systems of equations of private and ordinary derivatives.

The example of calculation of complex system of mass transfer model and population dynamic model by means of working system Niva is shown.

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The Spectroscopic Studies and Structural Behavior of Binary Liquid Mixtures of Alkoxyethanol with Amides Using DFT

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The spectroscopic and molecular simulations studies of liquids and their mixtures have great relevance in understanding the molecular interactions among the components. When the binary mixture is used as solvent media, specific solvent - co-solvent interaction can intervene to modify the structural properties and molecular arrangement of pure liquids. The effect of simultaneous presence of ether (-O-) and hydroxyl (-OH) group on thermodynamic properties and corresponding behaviour of alkoxyalkanols in the mixtures is of great importance from both practical and fundamental point of view to understand the interactions. The amides are very good aprotic prolific medium for organic and inorganic compounds due to high polarity and possessing donor-acceptor -CO-NH-peptide bond an important tool in interpretation of complex

molecules of biological interest. The excess molar volumes, VmE and the IR 1 and 1H NMR spectra have been measured and interpreted for binary mixtures of 2-methoxyethanol, or 2-propoxyethanol, or 2-isopropoxyethanol, with N,N-dimethyl formamide, N,N-dimelhyl acetamide , 2-pyrrolidinone, N-methyl-2-pyrrolidinone. The excess molar volumes are negative over the whole mole fraction range. The shifts in the C=O and O-H stretch have been used to interpret the excess molar volumes. The DFT calculation at B3LYP/6-31G* and B3LYP/6-311++G** levels has been carried out to identify the structures of H-bonded dimmers and to predict the frequency shifts in O-H and C=O str. vibrational modes.

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Toward Protein-DNA Stereochemical Recognition Codes: Identification and Classification of Homeodomain-DNA Complexes Based on Their Interfaces

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In our previous work, using the original interface-based structural alignment procedure, we analyzed in detail the interfaces of five homeodomain-DNA

complexes and inferred both invariable and variable protein-DNA contacts that can serve as possible stereochemical rules for formation of such interfaces. Here we find that application of some of those rules selects the homeodomain-DNA complexes from the entire set of protein-DNA complexes. Other rules can serve to classify the family of homeodomains into subfamilies basing on properties of their interfaces with DNA.

Toward Classification of Promoter DNAs According to Their Electrostatic Potentials

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We have reported calculation of electrostatic potentials of long (up to 1000 nucleotide pairs) DNA fragments, such as complete promoter regions of E. coli (hundreds of DNA sequences), using the original adaptation of multigrid Poisson-Boltzmann equation solver for distributed computation (Grid) media. Here we propose several techniques for converting the obtained 3D distributions of electrostatic potentials into characteristics according to which the promoters may be efficiently classified according to their electrostatic potentials.

The Structural Changes of Magnetic Nanoparticles Clusters in Magnetic Fluids Provoked by Thermodiffusion

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The structuralization of magnetic particles in magnetic fluids due to the thermodiffusion induced by laser light illumination was experimentally observed in two types of magnetic fluid based on mineral oil and kerosene. In case of magnetic fluid based on mineral oil the positive thermodiffusion (S $>$ 0) has been observed, while the indication of negative thermodiffusion (S $<$0) has been observed in magnetic fluid based on kerosene. Both phenomena have been studied by means of the forced Rayleigh Scattering (FRS). Numerical simulations confirmed aggregation observed after laser illumination in case of negative thermodiffusion and allowed the authors to estimate the value of the negative Soret constant ($S \approx -10^{-2}K^{-1}$) [1].

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Numerical Modeling of Magnetic Drug Targeting

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A special focused magnet, designed for the use in the magnetic targeted drug delivery system, has been constructed. The mapping of the field distribution has also been calculated by means of numerical computing. Numerical modeling of the adhesion condition for a magnetic fluid drop in the magnetic field with obtained design showed that the constructed focused magnet generates a sufficient magnetic force for the capture of a magnetic drop on the vessel wall and can be used 2.5 - 3 cm deeper in the organism, comparing with the prism permanent magnet which could allow the non-invasiveness of the magnetic drug targeting procedure.[1]

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Phase Front Evolution in Desiccated Colloidal Droplets[1]

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Drying of drops of colloidal suspension is important in different applications including medical tests [1].

Several models were proposed to explain the complex dynamics of the drop shape [2, 3, 4]. The models are based on simplified descriptions of the drop geometry. Moreover, the author supposes that gel has no effect on both evaporation and hydrodynamics and volume fraction of the colloidal particles in sol is constant.

In our model, gel stops any hydrodynamical flow and volume fraction of the colloidal particles varies in time.

The model is described with the several equations. We accept that the air–liquid interface is a spherical cap [2, 3, 4].

From mass conservation

$$\frac{d\Phi}{dt}\left(r_f^2 h_f + \frac{H^3}{6} + \frac{H}{2}r_f^2\right) + r_f\frac{dr_f}{dt}(2\Phi h_f + \Phi H - 2\Phi_g h_f) + \\ + \frac{\Phi}{2}\frac{dH}{dt}(H^2 + r_f^2) + \Phi r_f^2\frac{dh_f}{dt} = 0,$$

where $h_f(t)$ is the height of the sol–gel phase boundary, $r_f(t)$ is the position of the sol–gel phase boundary, $H(t)$ is the height of the drop apex, $\Phi(t)$ and Φ_g are the volume fraction of the colloidal particles in solution and in deposit, respectively.

$$r_f H\frac{dr_f}{dt} + \frac{1}{2}\frac{dH}{dt}(H^2 + r_f^2) + r_f^2\frac{dh_f}{dt} = -\frac{2}{\rho}\int\limits_0^{r_f} J(r,t)r\,dr,$$

where $J(r,t)$ is the evaporation rate.

We suppose that the dynamics of the drop height is

$\frac{d}{dt}(h_f + H) = V_0\left(1 - \frac{\Phi}{\Phi_g}\right)$, where V_0 is a constant connected with evaporation rate.

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Simulation of Electron Emission from a Surface of Nanostructures[1]

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A problem of numerical simulation of electronic emission from a surface of nanostructures is considered. The surfaces of a silicon micro-cathode and a carbon nanotube are taken as test structures. The both structures have active nanometer elements that can stimulate the electron emission. Electron heating near the emitting surface is taken into account using a quasi-hydrodynamic approach. A real electric field distribution around the nanostructures is calculated. The tunneling of electrons through the emitting surface is considered both by means of formula Fauler-Nordheim and by means of a direct numerical calculation in Shottki model.

To solve the numerical problem, an original scheme with an irregular triangle grid is used with a finite-volume approximation of the quasi-hydrodynamic equations on the grid. Semi-explicit time and space numerical schemes are used for analyzing the model. A parallel algorithm for providing of calculations on multiprocessor computer systems has been created.

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The emission characteristics of the nanostructures have been studied numerically. A comparison of thresholds of emission for two ways of calculation of the tunneling factor has been performed. The results may be used as a basis for both analysis and synthesis of semiconductor devices in vacuum micro- and nanoelectronics.

Modeling of Human's Three-Vertebra System and Optimization of Fixation Constructions

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The mathematical description [1] of dynamic processes by differential II' th sort equations Lagrange, made on the basis of the settlement scheme of a human's 3-vertebra complex presented as system of discrete concentrated weights, connected elastic elements and possessing in the certain geometrical parameters are in a basis of mathematical model of calculation of loadings on the human's vertebra.

The system of the differential equations of II order is reduced to system of I sort 14 ordinary nonlinear differential equations of the order which is realized by conducting half-integer time layers j+1/2 at construction the difference scheme providing increase of the order of accuracy of the numerical decision of the differential equations and countable stability of algorithms of the numerical decision of systems with greater number of the differential equations.

Feature of the numerical decision of system with greater number of the ordinary differential equations of the first order with quasi-linear in the factors, consisting of two vector equations is that the given system of the equations is solved concerning trajectories of movements of material points derivative of generalized coordinates which are tangents of corners of inclinations of tangents lead to points of these trajectories.

In work calculations of optimum parameters of rigidity Cct1 and Cct2 stabilizing partial rigidus designs for 3-vertebra a complex of the person [2,3] are resulted. By optimization of parameters requirements of preservation of

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physiologically normal loadings of elements of a complex at least a square of a difference of loading on vertebra in a complex with a pathology and without it are chosen. In conditions of astable position of the backbone connected with destruction intervertebral of a disk or a vertebra body, an optimum variant of its stabilization is application of fixing designs of elastic type. It allows to keep distribution эпюр loadings on vertebra bodieswithin the limits of the values close to natural. Let's note, that to each element of base the vector of the conditions including the characteristics of an element, parameters of technological process and the events, describing infringements of technological (functional) restrictions is put in conformity. Parameters of vectors of conditions form elements of the normative-help, operative and settlement information of a database.

Thus rating values of operating parameters and their admission, and also population means and dispersions of criterion functions are set.

Such approach allows to count various variants of fixing designs of plates, to model optimum conditions of their work, and also to spend optimization calculations for reception of the perfect designs of these systems, irrespective of a configuration and number of elements of base spine systems.

О математической модели трехпозвонкового комплекса человека и оптимизации параметров фиксирующих конструкций

В основу математической модели расчета нагрузок на позвонки человека положено математическое описание динамических процессов дифференциальными уравнениями Лагранжа II-го рода, составленных на основе расчетной схемы трехпозвонкового комплекса человека, представленного как система дискретных сосредоточенных масс, связанных упругодемпфирующими элементами и обладающих определенными геометрическими параметрами [1].

Система дифференциальных уравнений II порядка сводится к системе 14-ти обыкновенных нелинейных дифференциальных уравнений I порядка, которая реализуется путем ведения полуцелых временных слоев $j+1/2$ при построении разностных схем, обеспечивающих повышение порядка точности численного решения дифференциальных уравнений и счетную устойчивость алгоритмов численного решения систем с большим числом дифференциальных уравнений.

Особенностью численного решения системы с большим числом обыкновенных дифференциальных уравнений первого порядка с квазилиней-

ными коэффициентами, состоящей из двух векторных уравнений является то, что данная система уравнений решается относительно производных от обобщенных координат траекторий движений материальных точек, которые являются тангенсами углов наклонов касательных проведенным к точкам этих траекторий.

В работе приведены расчеты оптимальных параметров жесткости Cct_1 и Cct_2 стабилизирующей полуригидной конструкции для трехпозвонкового комплекса человека [2,3]. При оптимизации параметров выбраны требования сохранения физиологически нормальных нагрузок на элементы комплекса как минимум квадрата разности нагрузки на позвонок в комплексе с патологией и без нее. В условиях нестабильного положения позвоночника, связанного с разрушением межпозвонкового диска или тела позвонка, оптимальным вариантом его стабилизации является применение фиксирующих конструкций упругого типа. Это позволяет сохранить распределение эпюр нагрузок на тела позвонков в пределах значений, близких к природным.

Заметим, что каждому позвонку ставится в соответствие вектор состояний, включающий характеристики элемента, параметры динамического процесса и событий, характеризующий нарушения технологических (функциональных) ограничений. Параметры векторов состояний образуют элементы нормативно-справочной, оперативной и расчетной информации базы данных.

При этом задаются номинальные значения управляющих параметров и их допуск, а также математические ожидания и дисперсии целевых функций.

Такой подход позволяет просчитывать различные варианты фиксирующих конструкций пластин, моделировать оптимальные условия их работы, а также проводить оптимизационные расчеты для получения совершенных конструкций этих систем, независимо от конфигурации и числа элементов базы позвоночных систем.

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Simulation of Physical and Chemical Phenomena and Processes in the Course of Evolution of Unicellular Organisms

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Based on the developed simulation technique of the functioning of animate systems the probabilities of the existence of genetically steady biological kinds of live objects are calculated. The possible reasons for probability discontinuous behaviour of speciation of unicells with the various genome sizes, adapted for different environmental conditions (temperature and aggression) are shown. Evidence for larger expediency of symbiotic presence of mitochondrions in eukaryote cells in comparison with other energy sources, for example, polyphosphates is produced. The genetic reason of evolutionary success of syngenesis over agamic reproduction is revealed. A.Weismann dogma about larger evolutionary stability of gametal cells genome, than somatic is confirmed. The calculations are carried out under the assumption of evolutionary conservatism of genetic stability systems of modern cells: reparations and apoptosis.

Identification of Internal Points of Macromolecular System for Statement of Parameters of Poisson—Boltzmann Equation[1]

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Solvent environment plays a crucial role on the structure and function of biological macromolecules, such as DNA, RNA and proteins. Exact determination of direct interactions between the macromolecules and the solvent molecules still remains a very hard mathematical and computational problem.

The existence of cavities should be taken into account by solving different problems connected to the molecular properties. In the presented work some special triangulation [1] which includes inside possible cavities points of the

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system of overlapping spheres is considered. It can be used for making decision if the grid point lies inside the area bounded by the molecular surface. It provides more realistic dielectric constant values for the Poisson-Boltzmann equation (PBE) describing the electrostatic potential of interaction in the protein-liquid systems [2].

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Conformational Properties of Hydrocarbon Chains of Natural Lipids: Unperturbed State and Liquid-Crystalline State (Computer Simulation Study)[1]

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Monte Carlo computer simulations of hydrocarbon chain molecules containing cis double bonds in the main chain were carried out. Variations of C-C torsion angles of the molecules were considered to be continuous. An importance sampling procedure was used for the efficient generation of chain conformations in the unperturbed state [1, 2]. This approach has already been employed for the study of various properties of hydrocarbon oligomers [3, 4]. The molecule-fixed coordinate system with the axes along principal axes of inertia of each molecule conformation was used. The intramolecular C-C and C-H bond ordering properties, the bond orientation distribution functions with respect to the principal axis of inertia, and their temperature dependencies in the range between 278 and 403 K were studied for oligomers with 14–22 carbons and 1–6 cis double bonds [5, 6].

Temperature factors of the end-to-end chain distances and the shape of C–C and C–H bond orientation distribution functions in polyunsaturated chains

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with methylene-interrupted cis double bonds were shown to be considerably lower than those in saturated chains [7]. The characteristics of the unperturbed chains were compared with those obtained by molecular dynamics simulations for the acyl lipid chains in hydrated homogeneous bilayers consisting of unsaturated lipids, in the liquid-crystalline phase, and with the available experimental data. The order parameter characteristics of lipid hydrocarbon chains in the liquid region of the bilayers are found to be qualitatively similar to those of single unperturbed hydrocarbon chains.

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Method of Adaptive Artificial Viscosity

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A new method of adaptive artificial viscosity (AAV) of solution to multidimensional equations of gas dynamics for the Euler variables in the Cartesian co-ordinates system is considered. The calculations of 2D test gas dynamics problems by a new adaptive artificial viscosity net method, are described in detailed in [1]. The equations are considered for an ideal gas. Test problems are taken from [2]-[4]. The results of the comparison of AAV2D with other methods are published in [2]-[4].

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Polaron in Molecular Chain with Dispersion

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At present time it is supposed that solitons are one of the mechanisms of charge transfer in biopolymers. Using computer simulations we researched the polaron states of 1D discrete model "quantum charged particle + classical molecular chain"and dependence on value of dispersion in classical chain. It was shown that both total system energy and polaron radius are increasing with dispersion growth. Calculated results are in good agreement with analytical estimations obtained from virial relations.

Effect of Let and Track Structure on Cell-Cycle Delay and Statistical Distribution of Chromosome Aberrations

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Investigations of the genetic effects of particle exposure are of particular interest in relevance for application of particle beams in therapy and prediction of radiation risk in space. The key issue in understanding biophysical effects of radiation is the difference in energy deposition following irradiation with photons and heavy charged particles (Ritter 2000, Nasonova 2001, Nasonova 2004, Tenhumberg 2007, Peng 2009). Following microdosimetric concepts, distribution of imparted energy can be estimated from the knowledge of range and stopping powers of penetrating charged particles in an irradiated object. For particles, the energy is inhomogeneously deposited along the trajectory of an ion penetrating the matter with a local dose distribution within a particle track following the 1/r2 dependence. In contrast, in the case of X-rays, the energy deposition is spatially uniform.

Due to the high local energy deposition within the particle track, a traversal of a single ion through a cell nucleus can result in multiple chromatin breaks. This lesion "clustering"determines non-Poisson distribution of aberrations among cells. Additionally, contributions to damge coming from independent individual tracks give rise to a compound distribution well approximated by a mixed statistics (Virsik and Harder, 1981, Gudowska-Nowak 2005, 2007).

We have analyzed chromosome aberration data obtained for human lymphocytes exposed to X-rays and C (LET = 175 keV/μm and 29keV/μm) and Fe-ions

(LET = 155 keV/μm). For cytogenetic analysis lymphocytes were collected in metaphase at 48,60,72 and 84 post-irradiation. For the time-course analysis a modified mathematical approach proposed by Scholz (1998) has been used. To account for the different kinetics of high and low-LET induced damage, the total amount of aberrations induced within the entire population has been determined. For each subgroup of aberrant cells the flux through mitosis was analyzed revealing correlation between delay in mitosis and number of aberrations carried by a cell. This observation is of particular importance for the proper estimation the biological efficiency of C ions and health risks associated with radiation exposure.

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Computational Approaches to 2D and 3D Modeling of the Macro-Architecture of Native Chromosomes in Sperm Genome of Drosophila Melanogaster

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As the first justified concept over 125 years of the history of the basic scientific ideas on large-scale arrangement of eukaryotic interphase chromatin in cell nucleus, 2D and 3D spatial macro-architecture of haploid chromosomes in Drosophila sperm nucleus was sequentially reconstructed using the detected non-random distribution of γ-ray- and neutron-induced inversion and translocation breakpoints along the euchromatic chromosome maps with their clastering around heterochromatin [1,2]. For modeling and visualization of the spatial chromosome structures, some approaches to using a software program complex for 2D and 3D modeling [3,4,5] have been elaborated. As a first step, a 2D model was constructed as a B-spline comprising of 40 standard chromosome sections. Among them, the sections with inversion (translocation) breakpoints were moved closer to the heterochromatin and two chromosome regions with the gene-markers which often interact each other over distance $L = \sqrt{N}$ (N - the number of inversion and translocation breakpoints detected) at $L_{min} = 4nm$. In this model, each section occupies 9 degrees of a circular expansion relative to the centre with the gene-markers. Then, numerous refinements of the model have been introduced so the chromosome sections in the 3D model do not cross each other within the volume of cell nucleus. Therewith, the chromosome sections without breakpoints were constructed as a "giant"relaxed loops on the periphery of this nucleic volume. At the final step, a knotty primitives are arranged at regular intervals along the line of the spline obtained. Finally,

coloration and labeling of chromosome sections as well as a choice of model illumination were carried out sequentially. As a result, the reconstructed spatial configurations of haploid chromosomes in Drosophila sperm nucleus are defined as highly specific and universal for all large chromosomes megarosette-loop structures having the unitary heterochromatic compartment. These structures are radically distinct from the linear-polar Rabl's configuration of interphase chromosomes in animal and plant somatic cells bearing witness to high specificity of molecular-biological mechanisms of self-organization of the germ cell haploid genome during post-meiotic stages of its differentiation from earlier spermatids to mature sperms.

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Physical Principles in Economics

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It seems like, there is a little in common between physics and economics... However number of physics and economical processes and phenomenons have same mathematical formulations. This report is dedicated to certain analogies in such a different problems. Following topics are discussed in the report:
i. Statistical equilibrium and problems planning production;
ii. Functions of supply and demand and principle le Chatelier.

Фрактальная модель динамики цен на нефть в период 2008 год - начало 2009

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В докладе проведен фрактальный анализ динамики цен на нефть в 2008 и 2009 годах, в течение которых имели место сильные взлеты и падения цен на нефть, на основе ранее разработанной авторами статьи математической модели. Выявлены два наиболее характерных участка кривой динамики нефтяных цен и для них определены значения коэффициентов линейного тренда и фрактальной размерности. Сделан прогноз цены на нефть на конец 2009 года.

In this report the fractal analysis of dynamics of oil prices in 2008 and 2009 during which one strong flights and falls in prices on petroleum took place, on a ground before the paper of mathematical model designed by authors is made. Two plots of curve dynamics of the petroleum prices and for them a defined value of factors of rectilinear trend and fractal dimension are revealed. The oil price prognosis on the extremity of 2009 is made.

Software Complex for Computing Maps of Molecular Surface of Helical Proteins and Nucleic Acids[1]

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A software program complex for investigation of the surface of biopolymer molecule proteins and nucleic acids is worked out. It includes three program codes: SURFACE-2008, PROT-Z and DNA/RNA-Z. These codes are based on the known program SURFACE [1, 2] designed earlier for the surface cartography of globular proteins in frames of MS DOS. New codes are realized in the DELPHI language in the framework of OC Windows, they have similar graphical interfaces for setting the control parameters and for presenting the computational results.

The code SURFACE-2008 is a modification of SURFACE for OC Windows together with both changing the coloring of atoms of amino acids and nucleotide bases in the Aitov-Hummer projections and including the compact saving of protein maps in the JPG-format.

New algorithms, not used earlier in the SURFACE code, are included into PROT-Z and DNA/RNA-Z codes. The PROT-Z code is intended for construction of maps of helical protein molecules, and the DNA/RNA-Z code – for helical DNA and RNA molecules. An original scheme of the cylindrical

[1]This work is supported by RFBR grant 07-07-234.

projection for the fragments of helical molecule on a plane is implemented in both codes. In this scheme, an axis Z of helical fragment of the molecule is directed along the vertical axis of the cylinder projection. The atoms are represented as spheres with the given van-der-Waals radii. Definite problems inherent, both to specificity of cylindrical projection and peculiarity of double-chained helical structures of DNA and RNA, were overcome.

The most important features of the software complex are as follows. The scale of the map along the vertical axis of the cylinder can be chosen which allows one to avoid misrepresentation of atom images. As a result, the main axis can be pointed accurately, in unit of Å. The molecular relief of the surface is also calculated. Colors of atoms can be chosen by variety of types, such as polarity or some other chemical properties. The selected part of the map can be enlarged in scale. Distances between pairs of any atoms can be determined from the map. An algorithm of simultaneous visualization of atoms of the front and back subspaces against the main cylinder axis is realized. It also takes into account a possibility of atom's shading in the radial projection on the cylinder surface. A possibility is provided to interrupt the running program and continue its work later starting from the interrupted point.

The software complex involves the codes PROT-Zcompact and DNA/RNA-Zcompact which represent the modified Linux versions of codes PROT-Z and DNA/RNA-Z and are destined for organization of massive calculations of the map parameters in the distributed computing media. These parameters are used in full versions of corresponding programs for graphical presentation and further analysis of maps.

There are also additional service programs for the selecting definite chains and their segments of DNA or RNA from atomic coordinates of PDB-files (Protein Data Bank).

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On Massive Calculations of Maps of Molecular Surface of Helical Proteins and Nucleic Acids[1]

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An approach has been developed for organizing massive calculations of the maps of a molecular surface of helical proteins and nucleic acids in the distributed computing media. Two new program codes PROT-Zcompact and DNA/RNA-Zcompact which represent modified Linux versions of codes PROT-Z and DNA/RNA-Z [1] were elaborated for calculations of the surface maps of the helical protein molecules and the helical DNA/RNA molecules. In order to organize massive computing of a large set of molecules, the graphical interface and the input of control parameters in a dialog mode are eliminated from the PROT-Z and DNA/RNA-Z codes. To input the control parameters and to run codes PROT-Zcompact and DNA/RNA-Zcompact, a special script-program is used. For graphical presentation and further analysis of the maps obtained in such a way, corresponding full versions of codes PROT-Z and DNA/RNA-Z are used.

[1]This work is supported by RFBR grant 07-07-234.

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5. New Generation Computing Tools, Distributed Scientific Computing

ParCA2: Arcitecture and Experiments

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An architecture of the parallel computer algebra system ParCA is presented. The results of last experiments with the cluster of the Joint Supercomputer Center of the Russian Academy of Sciences is discussed.

Символьное обращение плохо обусловленных матриц в Grid-среде сервисов доступа к системе компьютерной алгебры Maxima[1]

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В докладе приводится пример использования Грид-среды, сформированной из сервисов удаленного доступа к системам компьютерной алгебры Maxima, установленных на настольных компьютерах, для обращения плохо обусловленных матриц в режиме символьных вычислений без потери точности.

Описываются два распределенных сценария вычислений: сочетании LU-разложения и параллельном вычислении столбцов обратной матрицы; блочной декомпозиции с использованием дополнения Шура.

Приводятся результаты численных экспериментов по "точному"обращению матриц Гильберта (с экспоненциальной зависимостью числа обусловленности от размера матрицы) относительно большой размерности (до

[1]Работа поддержана грантом РФФИ №08-07-00430-а

400), подтвердивших эффективность предложенного подхода. Показано, что использованный при реализации вычислительного сценария "неявно-адаптивный"алгоритм балансировки вычислительной нагрузки позволяет достаточно эффективно использовать временно неиспользуемые вычислительные мощности многоядерных процессоров настольных компьютеров.

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Beam Dynamic Calculation by NVIDIA® CUDA Technology

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The optimization of the central region structure of the cyclotron requires a tedious iterative procedure using a substantial amount of the particle tracking in the machine. The problem becomes even more complicated when the beam space charge effects should be taken into account. The solution of the problem

was attempted via upgrade of the recently developed computer code CBDA [1] based on the beam dynamics calculation by the NVIDIA CUDA parallel computing architecture.

The main part of calculation was performed without application of the CPU, and only a video card with GPU of about 100-200 processors was used. An application of the video card with the GPU instead of multi-processor computer is very cost effective solution in this case.

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Enabling Science through Emerging HPC Technologies

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For the last two decades most software applications have enjoyed regular performance gains, with little or no software modification, as each successive generation of microprocessors delivered faster CPUs. However, system builders have now hit physical limits which have slowed the rate of increase of CPU performance and the computing industry is moving inexorably towards multiple cores on a single chip. Nevertheless, general purpose many-core processors may not deliver the capability required by leading-edge research applications. High performance may be more cost-effectively achieved in future generation systems by heterogeneous accelerator technologies such as General Purpose Graphical Processing Units (GPGPUs), STI's Cell processors and Field Programmable Gate Arrays (FPGAs). Innovative algorithms, software and tools are needed so

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that HPC application scientists can effectively exploit these emerging technologies.

By presenting some recently published work on the use of GPUs in scientific computation [1, 2, 3], this talk will examine some of the challenges and opportunities presented by emerging HPC technologies. Recent results on using GPUs to compute large numbers of two-dimensional radial integrals required in the package 2DRMP [4, 5] will also be presented.

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Software Package for Modeling Problems of Mechanics of Continua Using Modern Multiprocessor Systems

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A software package for solving problems of mechanics of continua is presented. This package contains instruments which allow user to solve the specified

problem from the very beginning (designing solution region's geometry, setting boundary conditions) to the end (viewing end result using provided visualization instrument). These instruments are oriented on using parallel computing algorithms and modern multiprocessor systems. The package includes 4 components: geometry editor to design solution's region and set boundary conditions, mesh generator to create suitable grid or mesh, visualizer which displays result and allows one to present it in different forms and a component called 'shell' which connects 3 other components in one interface and controls the data flow between a client computer and a multiprocessor system. User directly interacts only with a shell component, so he does not need to know how package components work with each other and with the multiprocessor system. User has to pass through 4 steps to solve a problem: designing solution's region and setting boundary conditions in editor, generating mesh using provided mesh generator, starting problem solving on a remote multiprocessor system, viewing results in visualizer. All these steps could be done using the shell component of the package.

C$: A High-Level Programming System for High-Performance Graphics Processors[1]

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Graphics processing units (GPU) have been used recently for solving computationally-intensive problems. A number of programming tools exist for modern GPUs. However, those tools require specific knowledge of target GPU architecture as well as low-level programming to achieve high performance. In fact, low-level optimizations can account for as much as an order-of-magnitude increase in GPU performance in certain problems.

To address those issues, we propose C$, a higher-level approach to GPU programming. Programmers are provided with a high-level C#-like language for application development. The sequential part of the program is executed on

[1]This work is supported by AMD/ATI fellowship award and Intel Stipend for young researchers

CPU in .NET environment, while the execution of parallel part is offloaded to GPU. Runtime system performs data transfer management as well as program optimizations for specific GPUs. Evaluation of the system on a number of problems shows performance comparable with that of highly-optimized hand-tuned code, while demonstrating clear advantages in terms of code complexity and portability.

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6. Models and Algorithms of Quantum Computation and Quantum Information

Special Stochastic Representation of Quantum Mechanics and Solitons

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The special stochastic representation of Quantum Mechanics is suggested. The basis of this representation is a linear combination of soliton solutions to some nonlinear field equations, the particles being identified with the soliton configurations. The wave function of the particle proves to be the vector in the random Hilbert space. The many-particles wave function is constructed via the many-solitons configurations. It is shown that in the point-like limit, when the proper size of the soliton configuration vanishes, the main principles of Quantum Mechanics are restored. In particular, the expectation values of physical observables are obtained as Hermitian forms generated by self-configated operators and the spin-statistics correspondence stems from the extended character of particles-solitons.

From Hudson's Theorem to Generalized Uncertainty Relations

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Coherent Gaussian states play an important role in quantum mechanics in general, and in particular, quantum optics and quantum information with continuous variables. A particular property of these "quasi classical" states is the positivity of the Wigner function. Moreover, the Gaussian states are the only pure quantum states with positive Wigner function. This is the content of fundamental Hudson's theorem. By the argument of continuity one could expect that the mixed states with a positive Wigner function, which are close to

pure states, are necessarily "close" to the Gaussian form. Small Hilbert-Schmidt distance would imply a small value of the trace overlap between the quantum state and the corresponding Gaussian state determined by the same covariance matrix as the quantum state in question. We have derived the tight lower bound on the trace overlap for one-mode mixed states have shown that it is saturated by mixtures of the number states. Our bound recovers a lower bound on the purity of states, given the purity of the corresponding Gaussian states. In the limit of pure states it recovers the fact that only the Gaussian pure states saturate the Heisenberg uncertainty relation. For the mixed states, the purity bound extends the Heisenberg uncertainty relation to the "purity bounded" uncertainty relation. In the same way our bound on the overlap further extends the Heisenberg uncertainty relation. The calculations are simplified by the fact that the derived bound is saturated by mixtures of the number states. The identification of the region where these mixtures have a positive Wigner function takes us closer to an extension of the Hudson's theorem to mixed states.

A Computer-Algebraic Approach to the Simulation of Multi-Qubit Systems

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Quantum computations and quantum information theory have attracted much interest during recent years owing to its great promise to solve problems that are *intractable* otherwise. Despite of the recent advancements in this field, however, there remain a large number of difficulties to be resolved both, in theory and experiment. For instance, one of the major difficulties in dealing with complex systems concern their decoherence and how the entanglement is lost or transfered between the individual subsystems, if they are coupled to some environment. To overcome this and other problems, computer-algebraic simulations may provide a helpful route in studying multi-qubit systems and how the quantum coherence can be protected against various noise mechanisms.

Therefore, in order to better understand the entanglement and decoherence in $N-$qubit quantum systems, we recently developed the Feynman program [1], a computer-algebraic approach within the framework of Maple, which

facilitates the symbolic and numerical manipulation of quantum registers and quantum transformations. Originally, this program concerned the definition of data structures and useful operations as well as the implementation of (quantum) measures and bounds for the entanglement of multi-qubit systems. With two recent additions to the program [2], moreover, we now also support various noise models (so-called quantum operations), the duality between quantum states and quantum operations (known as Jamiołkowski isomorphism) as well as a simple access to quantum measurements. — In this talk, I shall discuss and display by means of several simple but intuitive examples how the program can be applied interactively, both for education and research in the field of quantum information.

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Teleportation and Local Reality

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In framework of an algebraic approach, we consider teleportation procedure. It turn out that using the quantum measurement nonlocality hypothesis is unnecessary for describing this procedure. We study the question of what material object are information carriers for quantum teleportation.

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Entanglement Measure for Pure Multiparticle States and Its Numerical Calculation[1]

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We describe an entanglement measure for pure multiparticle states (the minimum of Shannon's entropy of orthogonal measurements). This measure is additive, monotone under LOCC, and coincides with the reduced von Neumann entropy on bipartite states.

A method for numerical calculation of this measure by genetic algorithms is also presented. Moreover, the minimization of entropy technique is extended to fermionic multiparticle states.

Multi-Qubit Teleportation Algorithm and Teleportation Manager

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Two new variants of the teleportation protocol over three-qubit states are suggested. Namely, we assume that three persons $(A, B.M)$ are involved in the scheme. M is a manager who wants to make a teleporting of a qubit $|D\rangle = \alpha|0\rangle + \beta|1\rangle$ (with unknown α, β) to A or B using one quantum channel (one entangled state). Moreover, we want that M would choose the recipient (A or B) only at the final stage of the algorithm. It is a first version of our protocol. A second version is related to another possibility given by our scheme. Namely, it allows M to control the result of the teleportation of a qubit from A to B by creation of proper entangled state of A and B. This state is used for the conventional two-qubit teleportation of a qubit from A to B (note that A and B do not know the type of this entangled state and, consequently, cannot predict the result of the teleportation, the manager predetermines the result).

A version of quantum secret sharing based on the generalization of the suggested teleportation scheme on many-qubit case is described. A problem of creation of a classical secret key in the framework of our approach is also discussed.

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Vertically Coupled Double Quantum Dots in High Magnetic Fields[1]

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We have investigated the electronic structure of vertically coupled double quantum dots in a magnetic field within local density functional theory. The dots are identical and two-dimensional. Many-body effects are taken approximately into account by using a local intra-layer exchange energy.

The system of Kohn-Sham equations has been solved numerically. In the case of identical quantum dots the Schroedinger equation has been solved for one quantum dot. For tunnel splitting $\Delta = 0$ meV we have magic numbers M = 5, 7, 10, 13. The nature of these magic numbers is deal with occupation of antisymmetric state. So for M = 5 the angular moments of electrons are m_s= 1 and 2 and m_a = 2, i.e. two electrons are occupied symmetric state and one electron is occupied antisymmetric state.

Comparison of results ($\Delta = 0.2$ meV) with exact results [1] has shown that the divergence is about 5 percents. As Δ increases, new magic number states occur (M = 6, 9, 12, 15) as in the case of a single dot containing three electrons. In this case all electrons are occupied symmetric state.

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Parametric Resonance in the System of Two Spins in the Driven Regime

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We study the dynamics of a system of two interacting spins [1]. The problem is of considerable interest, for example, in studies of NMR in liquids. Under the action of a constant magnetic field along with a rotating radio-frequency field, the system performs resonant transitions between its energy levels. In this work we show that if the amplitude of the radio-frequency field is harmonically modulated with the proper frequency (depending on the average value of the amplitude) then the parametric resonance takes place, the regularity of the transition dynamics breaking down and the entropy of the probability distribution of visiting the states increasing essentially as compared with the case of the monochromatic pulse.

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Entangled States in Two-Particle Quantum Systems and Violation of the Bell-Type Incoherence Inequalities for Correlation Tensor Components

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The general structure and properties of nonfactorizable ("entangled") two-particle states have been considered. In particular, spin correlations in systems of two particles with spin 1/2 have been studied in detail, and it is shown that for nonfactorizable two-particle spin states the Bell-type incoherence inequalities for the correlation tensor components (which were established previously in [1] for incoherent "classical"mixtures of factorizable states of two spin-1/2

particles) may be essentially violated – i.e. in some cases the modulus of sum of two diagonal components of the correlation tensor may exceed unity.

As concrete examples, in particular, the spin correlations in the $(p, {}^3He)$ system formed in the reaction $\pi^+ + {}^4He \to p + {}^3He$ [2], in the muon and τ lepton pairs produced in the processes $e^+e^- \to \mu^+\mu^-$, $e^+e^- \to \tau^+\tau^-$ [3] and in the lepton pairs generated in the two-photon annihilation processes $\gamma\gamma \to e^+e^-\,(\mu^+\mu^-, \tau^+\tau^-)$ have been analyzed . It is demonstrated that, in all these cases, the final two-particle spin state represents a characteristic example of "entangled"state and, in doing so, one of the incoherence inequalities is *necessarily* violated . Thus, spin correlations of final particles in all the above processes have the strongly pronounced quantum character.

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Diagonalization of the XXZ Hamiltonian in the Problem of Quantum State Transfer in One-Dimensional Cyclic Systems [1]

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The exact diagonalization of the different Hamiltonians of one-dimensional spin systems is possible only in the approximation of nearest-neighbor interactions. However the XXZ-Hamiltonian for the problem of a qubit transfer in a ring consisting of 2N spins can be diagonalized in general case. The point is that only the single excitation of the XXZ-Hamiltonian is responsible for one

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qubit transfer from the first ring node to the (N+1)-th node in the considered problem.

In order to diagonalize the block of the XXZ-Hamiltonian which describes the evolution of the system in the single excitation space we use the methods developed for diagonalization of cyclic matrices [1,2]. As a result, we obtain the total spectrum of this block. Every eigenvalue is represented as the sum of contributions of interactions of nearest neighbors, next nearest neighbors, and so on. The full set of eigenvectors is also obtained.

Using the obtained spectrum we have found the quantum state fidelity[3] for quantum state transfer in rings with 60 spins. We also study the concurrence of the entangled state of spins 1 and N+1 at different assumptions on spin-spin interactions.

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Inhomogeneous One-Dimensional Spin Modes for Solving Problems of Quantum Information Theory [1]

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It is well known that the spin system (s=1/2) described by the XY-Hamiltonian in the uniform transverse magnetic field is very useful for solving a lot of problems of quantum information theory [1]. However, the possibilities of this model are restricted. In particular it is impossible to solve the qubit addressing problem in homogeneous systems. The perfect state transfer between the ends

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of homogeneous spin chains can be performed only if a number of nodes is not more than 3.

We consider inhomogeneous open spin chains with different coupling constants using the approximation of nearest neighbor interactions. We also assume that the magnetic field varies along the chain. The XY-Hamiltonian of such inhomogeneous open chains can be diagonalized in some cases. Thus we diagonalized the XY-Hamiltonians of open alternating chains [2,3] and, more general, open chains with coupling constants periodically changing along the chain [4].

As a result, we organized a transfer of quantum states in sufficiently long chains and calculated the quantum entanglement in inhomogeneous systems.

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О квантовых "демонах Максвелла"

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В работе поставлен вопрос о допустимости "квантовых демонов Максвелла глубоко изученный в классической физике, но также имеющий интерес с точки зрения квантовой логики. В работе делается вывод, что квантовые закономерности, в отличие от классической физики, по-видимому, допускают существование "квантовых демонов Максвелла"и уменьшение энтропии системы спинов, по крайней мере, с теоретической или логической сторон основных квантовых постулатов.

In this work the attention to the question on an admissibility of "quantum Maxwell demons deeply studied in the classical physics, but also having interest from the point of view of quantum logic is brought. In work the conclusion

becomes that quantum laws, in difference from the classical physics, apparently suppose existence of "quantum Maxwell Demons"and reduction of entropy of spin system, at least from the theoretical or logic parties of the basic quantum postulates.

Quantum Computing with Squeezed Polarization States of Light in Doped Materials

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In our work we investigate the problem of electromagnetic field propagation in atomic systems at regime of resonant atomic-field interaction. A special interest to these systems is connected with quantum coherent effects and optical interference that take place during absorption and re-emission of light in multi-level atomic systems. In the work we develop nonlinear approach to coherent resonant atom-field interaction [1] that yields new possibilities for drive amplitude/phase characteristics and quantum fluctuations of light by changing the control field parameters. We focus our attention on the case when the optical losses in the atomic system are almost zero at the presence of giant negative nonlinearity. These conditions provide high efficient cross-interaction of probe electromagnetic fields and a practical possibility to generate nonclassical light in the system. In particular we offer M-type nonlinear model of optical field interaction with atomic system for realization of polarization squeezing. The problem of formation of the entangled atom-optical states in Bose-Einstein condensate of quintic-level atoms in regime of induced cross-interactions between two-mode probe fields is under investigation too. We propose necessary conditions and concrete schemes to generate polarization-squeezed light in terms of Stokes parameters.

In other limit we investigate processes of nonlinear cross-interaction of single-photon pulses in optical materials on the base of optical matrices doped by clusters of rare-earth atoms. Such an interaction leads to formation of time-bin entangled photon states in these systems. Here we present the concept of quantum processor which manipulates phase shifts of one-photon light pulses in doped material and special measurement procedure [2]. These principles can be used to develop systems of distributed quantum information processing, and also for design of laboratory experimental set-up of quantum processor.

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On the Integrity Basis for Polynomial Invariants of Mixed Two Q-bit Systems[1]

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The ring $\mathcal{R}_{SU(2)\otimes SU(2)}$ of $SU(2)\otimes SU(2)$ invariant polynomials in elements of the density matrix of the entangled q-bit pairs is studied. The special integrity basis for $\mathcal{R}_{SU(2)\otimes SU(2)}$ is described and constraints on its elements due to the Hermicity and semi-definiteness of the density matrix are given explicitly in the form of inequalities. This basis has the property that only a minimal number of primary invariants of degree 2, 3 and one lowest degree 4 secondary invariant that appear in the Hironaka decomposition of $\mathcal{R}_{SU(2)\otimes SU(2)}$ are subject to the polynomial inequalities.

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Chaos in the Phase Qubits

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In recent years there were proposed and studied, both theoretically and experimentally, several types of the superconducting quantum bits (qubits). One of them, the so-called phase qubit, which is not considered a viable proposal any more, was based on a Josephson junction in the high temperature superconductors. The quantum phase of this dynamical system with the twice degenerate ground state can exhibit the nonlinear behavior under an external high frequency bias. We studied this mathematical model by numerical simulations and found conditions for the onset of chaos.

Implementation of Some Algorithms for Quantum Computation with Mathematica

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A *Mathematica* package [1] for simulation of quantum circuits is presented. The package provides a user-friendly graphical interface for generating quantum circuits and computing the circuit unitary matrices. Arbitrary circuit is represented internally as a symbolic table whose elements correspond to different

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one- and multi-qubit gates. Its unitary matrix is computed by means of the *Mathematica* build-in linear algebra facilities. The package is quite universal and can be used for designing and testing different quantum algorithms, several examples are considered as demonstrations. In particular we demonstrate an implementation of Grover's search algorithm in unstructured data base.

For a circuit constructed from the Toffoli and Hadamard gates, which form a universal set of quantum gates, there is a special routine to generate a system of multivariate Boolean polynomials [2]. This system is such that its number of common roots in the finite field F_2 defines the matrix elements of the circuit matrix [3]. In its extended form this option of our program allows to implement Shor's integer factoring algorithm in terms of the Hadamard and (generalized) Toffoli gates [4].

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Dirac-like Quasiparticles in Graphene

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The graphite films with a single atomic layer of carbon (graphene) have the low-energy "relativistic-like"quasiparticle excitations which in the continuum approximation are described by two-dimensional massless Dirac equation. Historically, the field theoretical study of graphene started before [1, 2] its actual discovery [3]. The Dirac-like character of carriers in graphene leads to several unique electronic properties including magneto-oscillations of electrical conductivity, unusual quantum Hall effect, and a universal value of optical conductivity.

We study the gap opening in graphene which is an analogue of the Ychiral symmetryY breaking that occurs in quantum field theory. We suggest that physics underlying the recently observed removal of sublattice and spin degeneracies in graphene in a strong magnetic field describes a quantum phase transition connected with the generation of an excitonic gap.

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Quantum Communication Speed Improvement with the Use of Realistic Parallel Detectors Considering the Privacy Amplification Algorithms[1]

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Single photon detection quality is the main property of any quantum cryptography setup. It defines main parameters: error probability and bit rate. The higher the detection probability higher the detector noise counts probability. For the telecom fiber the most suitable detectors are InGaAs-InP avalanche photodiodes [1-3]. These photodiodes has the so called aftrepulsing probability - the probability to have the noise count just after the previous detector count what restricts maximum frequency. To reduce this effect we propose to connect several detectors in parallel. This method increases the dark count probability but due to the repetition rate increase an overall efficiency increases.

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Quantum Gates through Multiple Optical Interactions[1]

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We present results of quasi-phase multiple interactions designed in one-dimensional multilayered media consisting of layers with different $\chi^{(2)}$ nonlinearities that interchanged by linear dispersive layers. The key to this approach is the idea of manipulating overall group delay mismatches between the various fields in each layer by appropriate choosing of the dispersive parameters. This physical mechanism is used to make multiple optical parametric interactions in higher orders of perturbation theory in a factorized form through elementary interactions in application to elaboration of quantum optical gates. We concentrate on the composite system that is the multilayered structure consisting in nonlinear blocks separated with dispersive segments. Each block is a structure of periodically poled crystals i.e. consists of a sequence of alternately interchanged layers with $\chi^{(2)} > 0$ and $\chi^{(2)} < 0$. We observe behavior of such $\chi^{(2)}$ multilayered structure in the case of both strong nonlinearity and perfect quasi-phase-matching that play extremely important role in the creation of quantum gates. We also investigate how the properties of multilayered structure affect the Bell measurement and investigate the efficiency of CNOT gate.

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Modeling and Visualization of Quantum Bifurcations [1]

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The new method for numerical simulation of quantum distributions in phase-space for open quantum systems, particularly, the Wigner functions are presented. For this goal the reduced density operator of a quantum system is represented via an ensemble of quantum states for random time intervals instead of an ensemble of stochastic quantum states as in the standard approach. This method also leads to novel analytical approximate results for the Wigner functions and for the systems that may be localized around semiclassical phase trajectories. As an application, the model of coupled two oscillators driven by a monochromatic force in the presence of dissipation and decoherence is analyzed for the operational regime in which the system displays instability or chaotic behavior. The system of interest is characterized by the Hopf bifurcation which connects a steady state dynamics of oscillatory modes to a self-pulsing temporal dynamics. Relatively far from the Hopf bifurcation that is realized for more intensive driving forces, the system exhibits the critical phenomenon of period-doubling. The both two regimes are analyzed analytically as well as numerically on the framework of the Wigner functions of the oscillatory modes.

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Scaling Invariance for Dissipative Chaos[1]

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It is known that dissipative chaos might satisfy to scaling invariance in a classical limit [1]. We discuss this statement from the point of view of quantum-to-classical transition for a model of anharmonic driven dissipative oscillator with time-modulated parameters [2]. On the other side, we apply the scaling ideology for study the ranges of chaos in quantum and semiclassical dynamics. Chaotic dynamics is analyzed numerically within framework of both the Poincaré section in classical description and the Poincaré section of a single stochastic trajectory in quantum description. We concentrate on analysis of nontrivial operational regimes for which the system displays chaotic behavior in quantum treatment, while the dynamics is not chaotic in classical description.

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Entanglement Control in a Two-Dimensional Quantum Dot in a Magnetic Field[1]

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A two-dimensional anisotropic oscillator is considered as an effective confinement potential for non-interacting electrons in a perpendicular magnetic field. The exact solutions for this model are used to illuminate shell phenomena in an isolated quantum dot. With the aid of these solutions we analyse the entanglement between the electron states as a function of time for the lowest shells depending on the strength of magnetic field.

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Poster section

Upper Hybrid Wave Driven Electron Acceleration in a Plasma

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An intense short pulse laser propagating through plasma in the presence of a magnetic field excites a large amplitude upper hybrid wave in its wake. The upper hybrid wave has phase velocity equal to the group velocity of the laser and transverse spot size comparable to the spot size of the laser. It effectively accelerates energetic electrons to relativistic energies via cherenkov and cyclotron resonance interactions. The magnetic field localizes the electrons in the region of large amplitude while the upper hybrid wave accelerates them in along the magnetic field. The electrons that originate off axis typically at normalized position X=1.0, Z=0.0 with normalized momentum P_z=0.1, P_x=0.0, attain the maximum energy $\approx$ 12.5 MeV, for the normalized wave amplitude A_0=2.0, B_0=0.2 normalized transverse and longitudinal wavenumber K_x=0.74, K_z=1.05.

Percolation Theory and Criticality in Two-Dimensional Growth Models

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We give a review on our recent findings on evidences of conformal invariance in the level sets of random growth surfaces. We also present a new type of criticality found for multifractal-like surfaces and show that there exists a SLE theory describing the level sets of the surface.

Математическое моделирование некорректной обратной задачи магнитостатики

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В данной работе решается задача поиска конструкции магнитной системы для создания магнитного поля с требуемыми характеристиками в заданной области. На основе анализа математической модели магнитной системы предлагается подход к решению одной нелинейной задачи магнитостатики, которая описывается уравнением Фредгольма:

$$H(z) = \int_S J(s)G(z,s)ds, \quad z \in U, \quad s \in S,$$

где $J(s)$ – функция распределения плотности тока в системе, $G(z,s)$ – функция Грина, аналитический вид которой зависит от геометрии источников тока и от точки z, принадлежащей области определения поля H. Необходимо определить распределение плотности тока $J(s)$, а также расстановку источников тока для создания поля H. Известно, что такие задачи относятся к классу некорректных обратных задач. В работе предлагается метод решения этих задач с помощью регуляризованных итерационных процессов по А.Н.Тихонову. На примере конкретной магнитной системы проводится численное исследование влияния различных факторов на характер создаваемого магнитного поля.

In this paper the problem of searching for the design of the magnetic system for creation a magnetic field with the required characteristics in the given area is solved. On the basis of analysis of the mathematical model of the magnetic system rather a general approach is proposed to the solving of the inverse problem, which is written by the Fredgolm equation:

$$H(z) = \int_S J(s)G(z,s)ds, \quad z \in U, \quad s \in S,$$

where $J(s)$ – is distributed density function of current in the system, $G(z,s)$ – is a Green function, the analytical form of the function depending on the

current source geometry and on z point, falling into the definition area of field H.

It was necessary to define the current density distribution function $J(s)$ and the existing winding geometry for creation of a required magnetic field.

It is known that such problems are incorrect ones. In the paper a method of solving those by means of regularized iterative processes is proposed. On the base of a particular magnetic system we perform a numerical study of influence of different factors on the character of the magnetic field being designed.

Модернизация магнита СП-40 спектрометра НИС с целью увеличения объема однородного поля

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Проектирование и конструирование магнитных систем электрофизических установок требует предварительного математического моделирования. Математическое моделирование необходимо и в процессе наладки и в последующей эксплуатации установки. Хотя расчеты полей магнитных систем проведены нами на основе решения ряда прямых задач магнитостатики, мы их относим к классу обратных задач магнитостатики, так как осуществляем фактически поиск оптимальной конструкции токовых элементов и железного ярма для наперед заданного распределения магнитного поля. В данной работе представлены результаты численного моделирования распределения магнитного поля некоторых модификаций спектрометрического магнита СП-40, используемого в экспериментальной установке NIS ЛВЭ ОИЯИ. Численным путем выбрана конфигурация магнита СП-40, для которой ширина области однородности магнитного поля увеличилась с 0,5 м до 1,0 м, т.е. в два раза.

The design and construction of magnetic systems of electrophysical installations require a preliminary mathematical modeling. The mathematical modelling is necessary in the process of adjustment and subsequent operation of an installation. Calculations of fields of magnetic systems, although performed on the basis of solving the direct magnetostatic problems, are related to the class

of inverse magnetostatic problems, since they actually include the search for an optimal design of current elements and an iron yoke for a given magnetic field distribution. In this work, a method of the numerical solution of the magnetostatic problem for domains with boundaries containing cusps is proposed. Using this numerical method, magnetic systems of rectangular configuration were modeled with a high accuracy. In particular, the calculations of some modifications of the magnetic system SP-40 used in NIS LHE JINR experimental installations are presented. By the numerical modeling a configuration of magnet SP-40 is constructed, and the uniformity of its magnetic field is increased on 100% as compared with the really existing configuration of the magnet.

Modeling of the New Optimal Laser Photoionization Schemes for Separating and Sensing Isotopes and Nuclear Reactions Products

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Laser photo-ionization (LPI) method is one of the most perspective methods for separating isotopes, isomers, nuclear reactions products etc [1]. The proposed optimal LPI scheme is based on laser excitation of atoms into Rydberg states and further auto- or collisional ionization. To carry out computer modelling optimal LPI scheme parameters we used the operator perturbation theory,the Focker-Plank stochastic equation method and density matrices formalism [1,2]. We studied laser separating and sensing Na, U, Cs (Cf) isotopes. In experiments by Letokhov et al. (Russia) and Moor (USA) two dye-lasers are used for Na separation. The 1-st laser provided a saturation of the resonant Na transition: 3s $^2S_{1/2}$-3p $^2P_{1/2}$. The wavelength of 2-nd laser is tuned in region of 4210-4490A. The excitation cross section for Na isotope at first step of the scheme is $\sigma = 10^{-12} cm^2$; the ionization σ from excited 3p state 10^{-17}cm^2, from ground state 10^{-19}cm^2. The relations of these σ are $\sim 10^5$, 10^7. This provides the known non-efficiency of the standard LPI. Using above indicated mechanisms is more effective from energetic point of view. Our estimate shows that the stochastic ionization σ =4.8 10^{-14} cm^2. The LPI scheme for U includes the steps: i). Excitation of the 235U isotopes from the ground $5f^36d7s^2$ -$^5L_6^0$ state and low lying metastable $5f^36d7s^2$ -$^5K_5^0$ state with energy 620.32 cm^{-1}; ii). Transition to Rydberg state and then autoionization (laser field) or collision ionization. A scheme for sensing the nuclear reaction products is considered on example of

the fusion ^{252}Cf isotope on the unsymmetrical coils (Cs etc). LPI sensing the Cs isotopes is based on resonant excitation of Cs ($6s^2S_{1/2}$ - $7p^2P_{3/2}$, 4555A and $6s^2S_{1/2}$- $7p^2P_{1/2}$, 4593A) and further autoionization (+electric field). Sensing reaction products results in detecting Cs atoms as spontaneous nuclear fusion coils.

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Mathematical Aspects of Modeling of Required Operation Modes of Multi Purpose Isochronous Cyclotrons[1]

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The mathematical and computer modeling of required operation modes of multipurpose isochronous cyclotrons is presented. The considered procedure is based on the calculation of currents in trim coils of correction of the basic magnetic field ($I_i, i = 1, 2, \ldots, n$) at a certain level of current in the main coil (I_{mc}). A series of numerical and physical experiments on calculation of the basic operation mode of the multipurpose isochronous cyclotron AIC144 (proton, kinetic energy E_k =60 MeV, rotation frequency F_0 =26.25 MHz),

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confirmed both the necessity of including the evaluation of solution stability into the calculation, and the possibility of producing the beams of protons in the range of acceleration radii without essential phase losses in the range of isochronization radii of the required magnetic field.

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Quantum Computation of Populations Dynamics of the Resonant Levels for Atomic Ensembles in a Laser Pulse: Optical bi-stability Effect

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Present paper has for an object (i) to carry out numerical quantum computation of a temporal dynamics of populations' differences at the resonant levels of atoms and nuclei in a large-density medium in a non-rectangular form laser pulse and (ii) to determine possibilities that features of the effect of internal optical bi-stability at the adiabatically slow modification of effective field intensity appear in the sought dynamics. It is known that the dipole-dipole interaction of atoms in dense resonant mediums causes the internal optical bi-stability at the adiabatically slow modification of radiation intensity. The experimental discovery of bistable co-operative luminescence in some crystals showed that an ensemble of resonant atoms with high density can manifest the effect of optical bi-stability in the field of strong laser emission. The Z-shaped effect is actually caused by the first-type phase transfer. On basis of the modified Bloch equations, we simulate numerically a temporal dynamics of populations differences at the resonant levels of atoms in the field of pulse with the non-rectangular cosh form. Furthermore, we compare our outcomes with the similar results, where there are considered the interaction between the ensemble of high-density atoms and the rectangularly- and sinusoidally-shaped pulses. The modified Bloch equations describe the interaction of resonance radiation with the ensemble of two-level atoms taking into account the dipole-dipole

interaction of atoms [1,2]. A fundamental aspect lies in the advanced possibility that features of the effect of internal optical bi-stability at the adiabatically slow modification of effective filed intensity for pulse of the cosh form, in contrast to the pulses of rectangular form, appear in the temporal dynamics of populations differences at the resonant levels of atoms.

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Formulation of Scattering Problem for the Fourth Order Differential Equation with Small Parameter at Higher Derivative [1]

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An algorithm is suggested solution of a scattering problem on a spherical rectangular potential well for the equation of the fourth order with small parameter ε at a higher derivative. At $\varepsilon \to 0$ a comparative analysis of solutions of the fourth order equation with Schroedinger equation solutions is carried out. The algorithm is realized with the use of a system of symbolical evaluations MAPLE.

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Numerical Models in a Theory of the Hadronic Atoms and Superheavy Atomic Ions: Spectra, Energy Shifts and Widths

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Paper is devoted to the numerical calculation of the spectra, radiative corrections, energy widths and shifts for some hadronic atoms and heavy ions with account of the definite nucleus structure modelling. One of the main purposes is establishment a quantitative link between quality of the nucleus structure modelling and accuracy of calculating energy and spectral properties of systems. We apply our numerical code [1,2] to calculating spectra of the hadronic (pion, kaon) atoms. A new, highly exact, ab initio approach [2] to relativistic calculation of the spectra for superheavy ions with an account of relativistic, correlation, nuclear, radiative effects on the basis of gauge-invariant QED perturbation theory is used. Zeroth approximation is generated by the effective ab initio model functional, constructed on the basis of the comprehensive gauge invariance procedure [2]). The potential includes the core ab initio potential, the electric and polarization potentials of a nucleus (the Fermi model, the gaussian form of charge distribution in the nucleus and the uniformly charged sphere are considered). For low orbits there are important effects due to the strong hadron-nuclear interaction (pion atom). The energy shift is connected with length of the hadron-nuclear scattering (scattering amplitude under zeroth energy). For superheavy ions the correlation corrections of high orders are accounted within the Green functions method. The magnetic inter-electron interaction is accounted in the lowest order, the Lamb shift polarization part- in the Uhling-Serber approximation, self-energy part - within

the Green functions method. We carried out calculations: 1).energy levels, hfs parameters for some heavy Li-like ions for different models of charge distribution in a nucleus; 2). Shifts and widths of transitions (2p-1s,3d-2p, 4f-3d) in some pionic and kaonic atoms (18O, 24Mg etc.) and also K-4He [3].

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Generalized Multiconfiguration Model of Decay of the Multipole Giant Resonances

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It is known that an account of complex configurations has significant meaning for adequate explanation of the widths, structure and decay properties of the multipole giant resonances (MGR). Here we present generalized multiconfiguration model to describe a decay of high-excited states, which is based on the mutual using the shell models (with limited basis) and microscopic model of pre-equilibrium decay with statistical account for complex configurations 2p2h, 3p3h etc in some analogy with the Zhivopistsev-Slivnov model. All possible configurations are divided on two groups: i). group of complicated configurations 'n1', which must be considered within shell model with account for residual interaction; ii). statistical group 'n2' of complex configurations with large state density p(n,E). To take into account a collectivity of separated complex configurations for input state a diagonalization of residual interaction on the increased basis (ph, ph+ phonon, ph+2 phonon) is used. All complex configurations are considered within the pre-equilibrium decay model by Feschbach-Zhivopistsev et al [2] with additional account of Yn1Ɣ group configurations. Giant resonance is treated on the basis of the multi-particle shell model Initial wave functions of MGR for nuclei with closed or almost closed shells are found from diagonalization of residual interaction on the effective 1p1h basis. Process of arising a collective state of MGR and an emission process of nucleons are

described by the corresponding diagram with V(mu) effective Hamiltonian of interaction, resulted in capture of muon by nucleus with transformation of proton to neutron and emission by antineutrino. Isobaric anagoges of isospin & spin-isospin resonances of finite nucleus are excited. Proposed model of decay of the multipole giant resonances is tested on analysis of reaction (mu-n) on the nucleus 40Ca. Wave functions of initial input state are calculated in the model of shells with oscillator-like wave functions. Our theoretical results are compared with experimental data and other calculation results [2].

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Numerical Modelling of the Chaotic Ionization of the Rydberg Atoms in an Electromagnetic Field

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In last years a phenomenon of chaotic ionization and photoionization of atomic systems in low-frequency electromagnetic fields attracts a great interest [1,2]. Above many reasons very essential moment is connected with a possibility of realizing quantum chaos phenomenon in a system. Earlier it was shown that an ionization process for highly excited H atom states by a strong low frequency electromagnetic field is realized through a mechanism of diffusion on atomic states which are strongly perturbed by a field. An important feature of process is in a stochastic character of electron vibrations. In order to describe a stochastic dynamics of hydrogen atom, several models were developed. The most simplified model uses diffusion like equation [2]. More sophisticated numerical calculations are presented in refs. [2]. Experimental observation of chaotic effect was carried out for the H atom from the state with ground quantum number n=60 in a field of frequency w=9,9 GGz. In series of papers by Casati

et al [3] a dynamical chaos effect for hydrogen atom in a field was at first correctly described by the non-linear classic mechanics methods. If a hydrogen atom in a field problem is studied in many details, the analogous problem for multi-electron highly excited atoms is far from their adequate solution. In this aspect an especial interest attracts studying the highly excited dynamic Stark resonant states for alkali elements atoms in a electromagnetic field. This problem is also stimulated by experimental discoveries of the near threshold resonances in the photo ionization cross sections for hydrogen and alkali atoms in a electric field [4]. Here we study a phenomenon of chaotic ionization of non-hydrogenic Rydberg atoms on example of alkali atoms. All results are obtained by using quasi-stationary, quasi-energy states method and the model potential one [5].

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Computational Technology for Modelling and Optimization of Magnet Systems for Electrical Motors Based on COMPOTE/MP Capabilities

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A computational technology is proposed for analysis and optimization of magnet systems for motors. The technology uses a combination of complementary 2D and 3D magnetostatic models. The original computer code COMPOTE/MP is capable of simulation of field maps for various stator/rotor positions using preset coil currents. The field maps are then used to predict magnetic fluxes, ponderomotive forces, emf, moments and other parameters, as well as their integral values and expected variations at steady-state operation. This technology makes it possible to modelize magnet systems with awkward-shaped coils and/or media interfaces, permanent magnets and non-linear steels with known B-H curves. The pre- and post processing tools give f possibility to develop parametrized models for a range of magnet systems. Calculated field and temperature maps are available in files formatted so as to suit as inputs for popular programs for stress and thermal analyses. A special component of the COMPOTE/MP code provides transfer of distributed EM loads onto a finite-element mesh as a set of equivalent nodal loads. This enables solving coupled problems typical in motor design.

The presented technology has been used in the design and manufacture of high-capacity ac electronic motors with permanent magnets for all-wheel drive Belaz heavy trucks, shipbuilding, oil-transfer pumps, and 3000 rpm electric drives.

Расчет магнитных потерь в электрических двигателях, содержащих постоянные магниты, на основе численного моделирования распределения магнитного поля с использованием комплекса программ COMPOTE/MP

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На практике условия предельно допустимого нагрева определяют один из важнейших параметров электрической машины удельные электромагнитные нагрузки, к которым обычно относят индукцию, линейную токовую нагрузку и плотность тока.

Предельно допустимый нагрев определяется величиной и распределением мощности потерь в объеме электрической машины. Потери также определяют величину коэффициента полезного действия и экономичность машины в целом. Одними из основных являются магнитные потери в стали магнитопровода, которые возникают при переменном перемагничивании; они слагаются из потерь на гистерезис и потерь на вихревые токи. Эти потери являются основным источником тепловыделений (мощности потерь) в стали электродвигателя и используются для последующего проведения теплового и вентиляционного расчётов с целью анализа температурного состояния и теплоотвода в машине.

Поскольку практический интерес представляют общие магнитные потери, в качестве основного метода их расчета применялся подход с использованием величин удельных потерь в стали в переменном синусоидальном магнитном поле. Использовались известные значения этих величин

$P^{'}_{1.0/50}, P^{'}_{1.5/50}$ для амплитудных значений индукции B_0= 1.0Тл, 1.5Тл и частоты f_0= 50 Гц, приведенные для известных марок сталей и толщины их листа согласно ГОСТ 21427.2-83. При расчете мощности потерь вводился также коэффициент увеличения потерь, учитывающей влияние механической обработки листов стали. Пересчет удельных потерь для отличных от приведенных выше значений индукций и частоты проводился по формуле

$$P = P^{'}_{B_0/f_0} \cdot (f/f_0)^{\beta} \cdot (B_m/B_0)^{\alpha}, \qquad [1]$$

где $\alpha \cong 2, \beta \cong 1.5$ и зависят от марки используемой стали. Такой подход в технической литературе носит название метода расчета потерь в стали по заводским данным [1, 2] и базируется на анализе и обобщении экспериментальных данных испытаний электрических машин.

При характерных для анализируемых конструкций толщинах листа приведенная выше формула применима для сравнительно узкого диапазона частот и по этой причине позволяет определять так называемые основные потери в стали от основной гармонической составляющей индукции.

Расчет и определение потерь, обусловленных высшими гармониками статора и ротора (которые носят название добавочных) требует учёта реакции вихревых токов. При высоких частотах, когда имеют место, главным образом, потери на вихревые токи, их действие может быть учтено согласно [1] умножением величины потерь по формуле (1) на коэффициент $k_m \leq 1$, равный $k_m = 3/kd(\sinh kd - \sin kd)/(\cosh kd - \cos kd)$, где $kd = \sqrt{\mu\omega/2\rho}$, d-приведенная толщина листа; μ- магнитная проницаемость стали; ρ- ее удельное сопротивление; $\omega = 2\pi f$.

Поскольку в установившемся режиме работы машины имеют место периодические процессы изменения электромагнитных величин, для расчета потерь величина поля в каждой точке в пределах объема электрической машины представляется в виде ряда временных гармоник. Для их расчета используются пространственные распределения компонент вектора магнитной индукции в объеме ротора и статора, отвечающие различным временным точкам периодического процесса, обусловленного вращением ротора и изменением тока в пазах машины. Полные потери определяются как сумма потерь от каждой гармоники в отдельности.

Расчеты проводятся для рабочего режима с учётом реальной формы кривой тока и условий коммутации тока в пазах машины.

В расчетах учитывается анизотропия магнитных свойств стали статора.

Кратко приведены данные расчётов конкретного двигателя. В результате численного моделирования находятся пространственные распределения удельной мощности тепловых потерь и определяются значения полной

мощности тепловыделений в различных конструктивных элементах электрической машины.

В частности, получено, что основная часть тепловыделений в стали (порядка 80-90%) обусловлена первой гармоникой поля при его разложении в ряд Фурье на интервале, определяемом двойным полюсным делением ротора. Тепловыделения в роторе фактически являются поверхностными и ≈90% полной мощности потерь локализованы в приповерхностном слое с радиальной толщиной Δr=12-13мм вблизи воздушного зазора. При этом величина и распределение поверхностной плотности тепловыделений в роторе в азимутальном направлении определяется величиной и распределением квадрата средней индукции поля по зубцам статора. Наличие такой зависимости приводит к сильной неоднородности распределения тепловыделений в роторе (вдоль его окружности) в рабочем режиме из-за поперечной реакции якоря.

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Численное моделирование поля магнитных систем электрофизического оборудования с учётом их взаимного влияния

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Численное моделирование поля магнитных систем, входящих в состав электрофизического оборудования различного назначения, часто приводит к необходимости учета их взаимного влияния друг на друга. Решение такой задачи электромагнитной совместимости часто затруднено тем, что:

- каждая система адекватно описывается своей детальной конечно-элементной сеткой; построение общей сетки, включающей в качестве подобластей две или более "локальные"сетки весьма трудоёмко;

- размерность общей сетки настолько велика, что задача не может быть решена за приемлемое время или в принципе;
- влияние одной системы на другую описывается не в терминах сеточных подходов, а задано, например, в виде формул, включая квадратуры, или набора выходных данных в виде распределений величин в пространстве, полученных с помощью других программ.

Примерами таких ситуаций могут служить, например,

- учет влияния полей рассеяния Международного термоядерного реактора - токамака ИТЭР на его же систему инжекции нейтральных частиц;
- учет влияния полей магнитной системы установки ИТЭР на испытательные модули бланкета ИТЭР, которые расположены в экваториальных патрубках вакуумной камеры установки;
- уччт взаимного влияния магнитной системы циклотрона и магнитного канала вывода заряженных частиц.

Предложен алгоритм решения данной задачи, который базируется на отдельном учете наличия магнитного поля, порожденного "внешними"по отношению к анализируемой магнитной системе источниками, и на решении нелинейной пространственной задачи магнитостатики с использованием "традиционной"конечно-элементной постановки.

Предложенный подход был реализован в виде модернизированного комплекса программ COMPOTE/MP (COMPOTE/MULTY PURPORSES). Он позволяет рассчитывать как влияние отдельных частей магнитной системы друг на друга, так и общий случай взаимного влияния нелинейных систем.

Numerical Simulations of Electro-Magnetic Transients in ITER Cryopumps with Use of Typhoon Code

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The reference design of the International Thermonuclear Experimental Reactor exhaust pumping system is based on eight cryopumps, connected to the torus via four ducts, each of them containing a pump in a direct line of sight and a branched pump. The torus cryopumps will be installed in the lower port cells of ITER.

The cryopump is made for the most part of non-magnetic stainless steel, and eddy currents induced in the cryopump and adjacent structures electrically connected to the cryopupmp during transients will cause additional mechanic and thermal loads on the conducting components.

The cryopump assembly can be separated into four main sub-components: the pump housing assembly, the 80K system, the 4.5K system, the pump valve assembly.

The events when eddy currents are induced in the cryopump structure include: centered plasma disruptions, vertical plasma displacement events, toroidal and poloidal field coils fast discharge.

The objective of this work was to estimate electromagnetic (EM) loads on the ITER Torus Cryopump for most dangerous loading conditions from EM loads point of view.

The TYPHOON code was used for this analysis. The TYPHOON code is designed for an advanced 3D simulation of transient electromagnetic processes using a conducting shell approach. The code is dedicated to 3D simulation of quasi-stationary eddy currents using a shell approximation in an integral-differential formulation to model conducting multi-connected shells, spaced arbitrary, in terms of a electric vector potential (the T-Ω method).

Preliminary simulations made in 2001 with the use of a simplified cryopump model [5] demonstrated low EM loads on the cryopump if the cryopump is electrically insulated from Vacuum Vessel (VV). The problem was divided into two low-dimension sub-tasks solvable successively:

1. simulation of eddy currents in VV components (ignoring the cryopump influence on VV eddy currents) due to the plasma current variations;
2. simulation of eddy currents in the cryopump due to the VV eddy currents and the plasma current variations.

According to the reference design, the cryopump has 2 electric contacts with the conducting structures of the VV cryoport: 1) the pump plug has electrical contact with the cryoport flange all around; 2) the cryoport bellow is welded to the pump housing front flange. To allow for the electric contact, the cryopump and surrounding structures should be modelled together. Due to electric contact between the cryopump and VV components, a cross-flow of eddy currents may occur, that results in increasing EM loads on cryopump as compared with the previous results in [5].

Due to geometry complexity and a variety of conducting details of the cryo-systems, it was decided to consider them as detailed as possible. This resulted in a model requiring all computation resources available on a standard PC. The highly detailed calculation model developed for the cryopump allows accurate modeling of the cryopump subcomponents to be carried out without losing the calculation accuracy. The whole calculation model describes a 40-degrees sector of the ITER machine. The sector includes: double walled VV with ports and ribs, divertor inboard and outboard rails, blanket triangular support, upper and equatorial port plugs, cryopump, plasma, CS, PF and TF coils. Necessary portions of the existing FE mesh can be re-built if the design be modified or another operation scenario be taken.

For each considered plasma event the total EM loads: forces, moments and AC losses have been calculated for the cryopump components. Using special numerical procedures and software [6], the obtained EM loads can be transformed into nodal loads in the format suitable for further structural or thermal-hydraulic analysis with the use of finite elements codes (for example, ANSYS or VINCENTA [7]).

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Quasi-3D Numerical Simulation of TF Coil Thermal-Hydraulic Parameters During the Fast Energy Discharge

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Results of thermohydraulic simulations are presented. The simulations have been made to study parameters of cooling channels and the quench line for helium extraction under the toroidal field coil fast energy discharge in the ITER

magnet system. a full-scale quasi-3D calculation model has been developed. The model allows a thermohydraulic analysis of a TF coil together with its hydraulic scheme and the helium at the fast discharge or the loss of superconductivity. The simulations have been performed with the original code VENECIA.

The calculation model includes:

- all 14 layers of a TF coil winding pack;
- interturn heat transfer and helium counterflows in adjacent layers of the winding pack;
- 4 relief valves installed at the inlet and outlet of 18 TF winding packs to control helium mass flow rates;
- all 74 cooling channels of TF coils grouped into two parallel branch;
- 2 valves used to control mass flow rates at the inlet of both branches of the cooling channels;
- individual description of time and space variations of heat losses associated with eddy currents and neutron heating for each cable;
- heat loading of the return/supply cryolines;
- local sub-model of a centrifugal pump for forced circulation;
- local sub-model of a liquid helium bath modelled as a volume with the liquid and vapour fractions in thermodynamic equilibrium, the LHe level is controlled by a J-T valve and a cold compressor;
- heat exchanger inside the LHe bath;
- TF winding cooling interface tubes connected with the tank for extracted helium.

The thermohydraulic simulations of the TF fast discharge have revealed that:

1. It takes 15 min to extract helium from the TF case and about 200 s to exhaust the winding.
2. Due to small diameter of the quench tubes and fast warming of the helium inside, the maximum pressure in the TF case exceeds 2.0 MPa. The same reasons lead to a 1.8 MPa pressure spike in the TF winding quench circuit at 10 s of the fast discharge.
3. He pressure and temperature inside the cold quench tank of reach, respectively, 1 MPa and 42 K at 200 s and keep rising due to equalizing of temperatures between the helium and the tank wall.

Modelling, Optimization and Synthesis of Magnet Systems for Isochronous Cyclotrons with COMPOTE/MP Code

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An efficient computational technology is proposed for electromagnetic analysis, optimization and synthesis of magnet systems for isochronous cyclotrons at all stages of their design and adjustment. Magnet systems are modelled with the use of precision 3D magnetostatic models. The original computer code COMPOTE/MP provides modelling of field maps with allowance for a magnet system geometry and coil currents. Simulated field maps are used to determine influence functions of coils and structure components. Thus, a variational problem of magnet system synthesis can be defined as to provide a known field distribution. Computational models are generated with regard to fabrication/maintenance/procurement/cost saving requirements. The code provides accommodation for nonlinear magnetic properties of different materials used in the manufacture of a modelled magnet system. Models use realistic B-H curves measured over a typical operating field range.

Simulated results are presented in output files in formats suitable for further computations with the use of different codes, particularly, for the stress analysis. A special component of the COMPOTE/MP code transforms distributed EM loads in their nodal equivalents associated with a given finite-element mesh. Also, expected strains of the magnet system may be taken into account in field map simulations in order to correct the field configuration.

A desired isochronous field is obtained by iterative solving a self-consistent problem on the basis of precise 3D field simulations and particle dynamics analysis. The inputs for COMPOTE/MP field map simulations are data from a trajectory analysis. Resulting 3D field maps are formatted so as to serve as inputs for trajectory analysis computations. Such algorithm makes it possible to form a closed iterative adjustment of the required field distribution.

A comparison between simulated and measured data demonstrates that the proposed technique provides formation of a desired isochronous field accurate to 0.1%.

Finally, the magnet system may be optimized using both measured and simulated data.

This method has been effectively applied to design and manufacture of a number of isochronous cyclotrons at JINR and the Efremov Institute.

VENECIA: New Code for Simulation of Thermohydraulics in Complex Superconducting Systems

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In 1998 the computer code VINCENTA was introduced for full scale thermohydraulic simulations of transients in ITER superconducting magnets and their cryogenic systems. The code was intensively used for detailed modelling of the ITER coils as well as multiparameter analysis and design/operation optimisation.

The code was originally strictly ITER-oriented but constantly growing computational complexity and demand for new applications initiated its radical modification. The advanced code named VENECIA is based on the database approach and has extended range of use and new functionalities. VENECIA enables detailed modelling of thermohydraulic transients for both siperconducting and warm magnet systems, in a whole and in their components, using realistic geometry and operational conditions. An efficient algorithm makes it

possible to analyse behaviour of a range of compressible coolants (He4, HeII, N, H_2O) under a variety of conditions. Different coolants can be used in a single calculation model simultaneously. A global computational model is generated using a set of basic local sub-models linked together that provides simple and generalised modelization of a magnet system. Such modelling allows due regard for properties of different materials, non-linear effects or specific geometry. Also the code gives predictions of space and time variations for various heat loads.

As compared to VINCENTA, VENECIA is more flexible and universal code modeling applicable for a wide range of devices including thermonuclear facilities, accelerators and transport systems, MRI-magnets, superconducting motors, generators and storage rings, experimental and diagnostic devices for scientific research, superconducting cables and joints.

As an example, a calculation model is described which was used for the thermohydraulic analysis of the toroidal field magnet system in the ITER machine.

Supercritical Systems of Nonlinear Evolution Equations: Crtitical Behaviour and Blowup

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Numerical adaptive algorithms for investigation of threshold configurations of supercritical evolutionary equations was developed. Decay of regular static spherically symmetric solutions in the $SU(2)$ Yang-Mills-dilaton (YMd) system of equations under the independent excitation of their unstable eigenmodes has been studied self-consistently in the nonlinear regime [1, 2]. The considered regular YMd solutions form a discrete family and can be parametrised by the number $N = 1, 2, 3, 4...$ of their unstable eigenmodes in linear approximation. We have obtained strong numerical evidences in favour of the following statements: i) all static YMd solutions are distinct local threshold configurations, separating blowup and scattering solutions; ii) the main unstable eigenmodes are only those responsible for the blowup/scattering alternative; iii) excitation of higher unstable eigenmodes always leads to finite-time blowup; iv) the decay

of the lowest $N = 1$ static YMd solution via excitation of its unique unstable mode is an exceptional case because the resulting waves propagate as a whole without energy dispersion revealing features peculiar to solitons. Parallel computing with use of the message passing interface (MPI) was done on cluster CICC JINR and SIMFAP parallel cluster at IFIN-HH Bucharest [3, 4].[1]

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Invertible Dynamical Systems and Quanputing

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General method of construction of the linearly extended reversible dynamical systems formulated. Applications of the method for finite and infinite dimensional dynamical systems shown.

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