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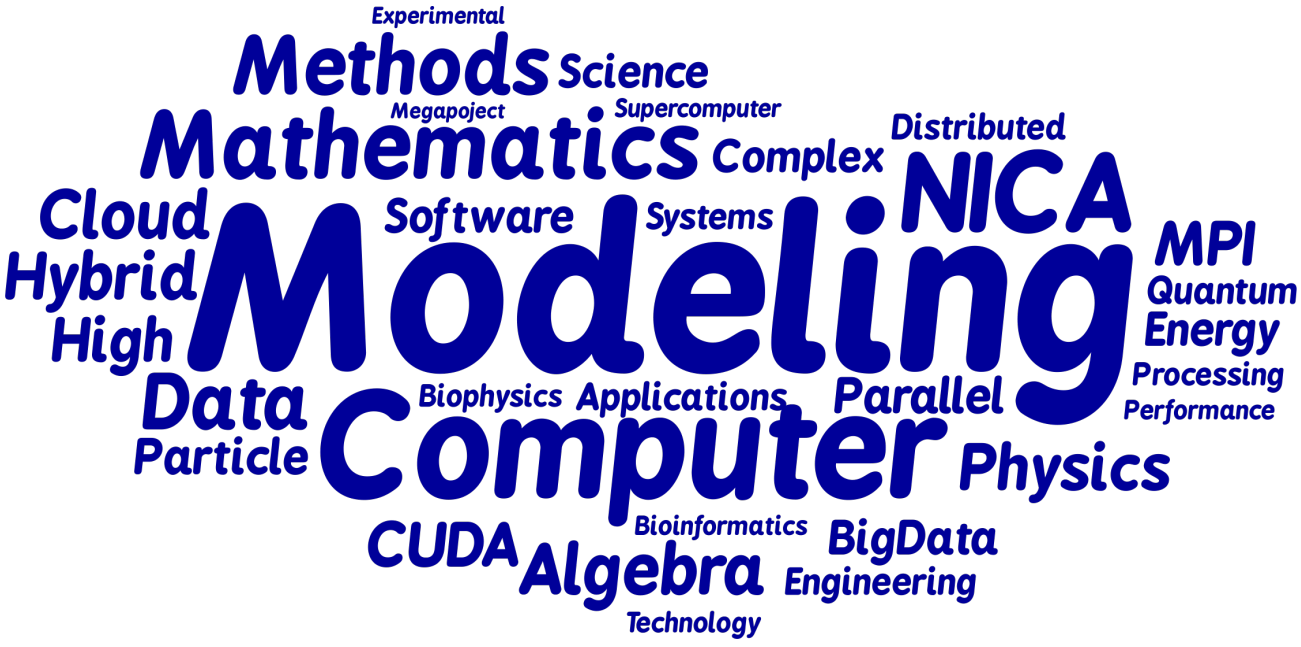
MMCP'2017

Book of abstracts

3–7 July, 2017
Dubna, Russia



Joint Institute for Nuclear Research
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MATHEMATICAL MODELING AND COMPUTATIONAL PHYSICS

Book of abstracts of the International Conference

Dubna, July 3–7, 2017

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ И ВЫЧИСЛИТЕЛЬНАЯ ФИЗИКА

Тезисы докладов международной конференции

Дубна, 3–7 июля, 2017

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The book contains the abstracts of the reports submitted to the International Conference "Mathematical Modeling and Computational Physics" (MMCP'2017).

Full texts of the reports approved by the MMCP'2017 Advisory Committee will be published separately.

Математическое моделирование и вычислительная физика (MMCP'2017): Тезисы докладов международной конференции (Дубна, 3–7 июля 2017 г.). — Дубна: ОИЯИ, 2017. — 158 с.
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В сборник включены аннотации докладов, представленных на международную конференцию «Математическое моделирование и вычислительная физика» (MMCP'2017).

Полные тексты докладов, отобранные программным комитетом, будут опубликованы отдельно.

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The Conference follows the rich traditions of the previous conferences on mathematical modeling, numerical methods and computational physics which started in Dubna, Russia, in 1964, e.g., “Computational Modeling and Computing in Physics” (1996), “Modern Trends in Computational Physics” (1998), V International Congress on Mathematical Modeling (2002), “Mathematical Modeling and Computational Physics” 2006 (in Slovakia), 2009 (in Dubna), 2011 (in Slovakia), 2013 (in Dubna) and 2015 (in Slovakia).

The book is organized in three main parts: plenary lectures, contributed communications, and posters. The contributed communications are split into several sections covering respectively distributed and parallel computing in science and technology, mathematical methods and application software for modeling complex systems, bioinformatics and computational biophysics, mathematical methods and software for experimental data processing, computer algebra, and quantum computing with applications.

Конференция продолжает богатые традиции предыдущих конференций по математическому моделированию, численным методам и вычислительной физике, которые проводились в Дубне еще с 1964 года; например, «Численное моделирование и вычислительная физика» (1996), «Современные тенденции вычислительной физики» (1998), V Международный конгресс по математическому моделированию (2002), «Математическое моделирование и вычислительная физика» 2006 (Словакия), 2009 (Дубна), 2011 (Словакия), 2013 (Дубна) и 2015 (Словакия).

Сборник содержит аннотации пленарных лекций, секционных и постерных докладов. Предоставленные доклады охватывают широкий спектр задач в области математического моделирования сложных физических и технических систем, биоинформатики и вычислительной биофизики, распределенных и параллельных вычислений, обработки экспериментальных данных, компьютерной алгебры и квантовых вычислений.

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Plenary session

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Bioinformatics and computational biophysics

Computer algebra and quantum computing with applications

Poster session

PLENARY SESSION

SOLUTION OF MAGNETOGASDYNAMICS PROBLEMS WITH THE HELP OF HIGH PERFORMANCE COMPUTER SYSTEMS

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New approach to an obtaining of the equations of magnetic gas dynamics is offered. This approach is based on complex-valued locally Maxwellian distribution function. By means of the approach the equations of ideal magnetic gas dynamics are received. The analog of quasidynamic system of the equations is also constructed, describing magnetic and gasdynamic processes taking into account dissipation of an impulse and energy. The elaborated kinetic models and numerical algorithms of their analysis were tested on the example of well-known tasks. The offered algorithms easily adapt to architecture of modern high-performance computer systems.

FRACTIONAL STOCHASTIC FIELD THEORY

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Models describing evolution of physical, chemical, biological, social and financial processes are often formulated as differential equations with the understanding that they are large-scale equations for averages of quantities describing intrinsically random processes. Explicit account of randomness may lead to significant changes in the asymptotic behaviour (anomalous scaling) in such models especially in low spatial dimensions, which in many cases may be captured with the use of the renormalization group. Anomalous scaling and memory effects may also be introduced with the use of fractional derivatives and fractional noise. Construction of renormalized stochastic field theory with fractional derivatives and fractional noise in the underlying stochastic differential equations and master equations and the interplay between fluctuation-induced and built-in anomalous scaling behaviour is reviewed and discussed.

HIGHER-ORDER PARTIAL DIFFERENTIAL EQUATIONS FOR DESCRIPTION OF THE FERMI-PASTA-ULAM AND THE KONTOROVA-FRENKEL MODELS

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We consider the following dynamical system:

$$m\frac{d^2 y_i}{dt} = F_{i+1,i} - F_{i,i-1} - f_0 \sin\left(\frac{2\pi y_i}{a}\right), \quad (i = 1,\ldots,N), \tag{1}$$

where y_i measures the displacement of the *i*-th mass from equilibrium in time *t*, the force $F_{i+1,i}$ describes the nonlinear interaction between atpms dislocations in the crystal lattice in case of dislocations

$$F_{i+1,i} = \gamma(y_{i+1} - y_i) + \alpha(y_{i+1} - y_i)^2 + \beta(y_{i+1} - y_i)^3, \quad (2)$$

and f_0, a, γ, α, β are constant parameters of system (1).

The system of equations (1) is the generalization of some well-known dynamical systems. At $\alpha = 0$ and $\beta = 0$ the system of equations (1) is the mathematical model introduced by Frenkel and Kontorova for the description of dislocations in the rigid body [1]. In this model it was suggested that the influence of atoms in the crystal is taken into account by term $f_0 \sin\frac{2\pi y_i}{a}$ but the atoms in case of dislocations interact by means of linear low. Assuming that $N \to \infty$ and $h \to 0$ where *h* is the distance between atoms, we can get the Sine-Gordon equation.

In case of $f = 0$ and $\beta = 0$ system of equations (1) is the well-known Fermi-Pasta-Ulam model [2] which was studied many times. It is known that the Fermi-Pasta-Ulam model is transformed at $N \to \infty$ and $h \to 0$ to the Korteweg-de Vries equation [3].

The main result of work [3] was the introduction of solitons as solutions of the Koryeweg-de Vries equation. It was shown in 1967 that the Cauchy problem for this equation can be solved by the Inverse Scattering transform [4].

Assuming $f_0 = 0$, $\alpha \neq 0$ and $\beta \neq 0$ at $N \to \infty$ and $h \to 0$ one can find the modified Korteweg-de Vries equation for the description of nonlinear waves.

In papers [5,6] the author took into account high order terms in the Taylor series for the description of nonlinear waves in the Fermi-Pasta-Ulam and the Kontorova-Frenkel models assuming that $\alpha \neq 0$ and $\beta \neq 0$ and did not obtain nonlinear integrable differential equations in mass chain. Here we assume that the interaction between dislocations in crystal is described by means of nonlinear low at $\alpha \neq 0$ and $\beta \neq 0$ and consider the other equations. The aim of this talk is to present the nonlinear partial differential equations corresponding to dynamical system (1) and to discuss the properties of these equations.

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PETROV-GALERKIN FINITE ELEMENT METHOD FOR FRACTIONAL ADVECTION-DISPERSION EQUATIONS

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First, we shall make a short introduction the concepts of fractional calculus and differential equations of fractional order that include both, steady-state and time dependent problems. This type of problems arise in mathematical modeling of asymmetric super-diffusion processes in highly heterogeneous media.

Further, we shall present variational formulations of Petrov-Galerkin type for one-dimensional fractional boundary value problems with either a Riemann-Liouville or Caputo derivative of order $\alpha \in (3/2, 2)$ in the leading term and involving both convection and reaction terms. The well-posedness of the formulations and sharp regularity pickup of the weak solutions are established.

A novel finite element method is developed, which employs continuous piecewise linear finite elements and "shifted" fractional powers for the trial and test space, respectively. The new approach has a number of distinct features as it allows deriving optimal error estimates in both L^2- and H^1- norms and produces well conditioned linear systems, since the leading term of the stiffness matrix is diagonal matrix for uniform meshes. Further, in the Riemann-Liouville case, an enriched FEM is proposed to improve the convergence. Extensive numerical results are presented to verify the theoretical analysis and robustness of the numerical scheme.

ON THE LOAD BALANCING PROBLEM

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We present new results on the Load Balancing Problem that concerns and assignment of given jobs to a set of machines each of which can process a subset of jobs. Each job requires one unit of processing time and must be assigned to some machine that can process it. The jobs have to be assigned in such a manner that minimizes the total completion time. We exploit graph theory models and the divide-and-conquer nature of the semi-matching problem. We derive three algorithms for the optimal semi-matching problem. The first one runs in time $O\left(\sqrt{n} \cdot m \cdot \log n\right)$ on a graph with n vertices and m edges. The second one is randomized and computes an optimal semi-matching with high probability in time $O\left(n^{\omega} \cdot \log^{1+o(1)} n\right)$, where ω is the exponent of the best known matrix multiplication algorithm. Since $\omega < 2.38,$ this algorithm breaks through $O\left(n^{2.5}\right)$ barrier for dense graphs. In the case of

planar graphs, the third one computes an optimal semi-matching in deterministic time $O\left(n \cdot log^4 n\right)$. The character of designed algorithms allows parallelisation and distributed computing.

DISENTANGLING COMPLEXITY IN BAYESIAN AUTOMATIC ADAPTIVE QUADRATURE

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The present report discusses a Bayesian automatic adaptive quadrature (BAAQ) solution for numerical integration which is simultaneously robust, reliable, and efficient, hence able to yield guaranteed output in numerical experiments involving sudden unexpected modifications of the behavior of the integrand function.

An essential ingredient of the solution is the multiscale approach [1]. Within it, for integration ranges of macroscopic length, which are of primary practical interest, an early decision path for the integrand profile (IP) scrutiny is defined which enables fast solution of four basic problems: (i) identification of simple integrals; (ii) check of the need to relax the user requested accuracy parameters; (iii) end of computation diagnostic for simple integrals; (iv) hints on manifestly ill-conditioning IP features.

For integrals which are neither trivial, nor manifestly ill-conditioned, the Clenshaw-Curtis quadrature is activated within the approach discussed in [2]. This enables further identification of unresolved ill-conditioning features. We are thus left either with a hopefully well-conditioned integral, for which the standard automatic adaptive quadrature [3] is expected to yield reliable output, or with a manifestly ill-conditioned problem for which an improved version of the full BAAQ machinery [4] is activated.

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A NEW ORBITAL FREE SIMULATION METHOD BASED ON THE DENSITY FUNCTIONAL THEORY

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We propose a practical way to simulate multi-atomic systems without using of wave functions (orbitals). Our approach is based on the theoretical concept of the last years (FTT 2012, Sarry AM, Sarry MF; JETP 2013, Bobrov VB, Trigger SA) claiming that the universal functional of kinetic energy does not exist. We construct kinetic functionals for each type of atoms and then use them for complex systems. On examples of clusters containing Al, Si, C, and O we have shown that our method can describe structures and energies of multi-atomic systems not worse than the Kohn-Sham method but faster.

AN ATTEMPT TO BUILD A SMART REAL-TIME SYSTEM FOR HEAVY ELEMENT RESEARCH: APPROACHES, MATHEMATICAL OBJECTS, ALGORITHMS, EQUATIONS

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The Dubna Gas-Filled Recoil Separator is the most advanced facility currently in use in the field of research of Superheavy Nuclei (SHN) [1]. During last year's, IUPAC established the priority of the DGFRS experiments in the discovery of new Z=114-118 elements. Definitely, the DGFRS detection system and method of "active correlations" have played a significant role in these discoveries [2-4]. Author defines abstract mathematical objects, like correlation graph and incoming event matrixes of a different nature in order to construct a simple procedure of detecting rare events, yet more exhaustive compared to the present one, using real-time detection mode. In this case one can use any of $n \cdot (n+1)/2$ correlation graph edges to "trigger" beam irradiation pauses and thus provide "background free" conditions to search for ultra-rare alpha decays. Here n is the number of correlation graph nodes. Schematics of these algorithms are considered. Elapsed time value is used as matrix element for each event type. In the case of DSSSD detector-based system those matrices have dimension (X, Y), where X, Y are the numbers of horizontal and vertical strips, respectively. Proposals for test experiments with heavy-ion-induced reactions that can be used to check these approaches are considered. Some attention is paid to the forthcoming launch of a new FLNR ultra intense heavy ion DC-280 cyclotron for heavy element research. A role of a new protection and parameter monitoring system is discussed in a brief. Method to use more flexible correlation time intervals, using e.g. either V.B. Zlokazov's BSC (Background Signal Combinations) or K.H. Schmidt's LDSC (Linked Decay Signal Combinations) approach [5-7], except for fixed time intervals, is reported. In the last case, condition for the beam stop can be considered in the form of equation: $Pcorr(t,\nu) < \varepsilon$, where PCORR is random probability value for a given correlation chain (i) measured in a real-time mode at the moment t, ν is mean rate parameter for a given DSSSD pixel, and ε is a preset small positive value.

Of course, in this case one should additionally define one extra matrix related to event rate for each pixel of DSSSD. Some attention is paid to an analytical expression for SHE recoil registered with the DGFRS detection system.

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MULTISCALE MULTILEVEL APPROACH TO SOLUTION OF NANOTECHNOLOGY PROBLEMS

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The multiscale multilevel approach for solution of nanotechnology problems by supercomputer systems is presented. The approach is based on combining the continuum mechanics models and the Newton's dynamics for individual particles. This combination includes three scale levels such as macroscopic, mesoscopic and microscopic levels. For gas-metal technical systems we use the following models. The quasihydrodynamic equations system is used as a mathematical model at the macrolevel. The system of Newton's equations is used as a mathematical model at the meso- and microlevels. Numerical implementation of the approach is based on the method of splitting into physical processes. The quasihydrodynamic equations are solved by finite volume method on grids of different types. The Newton's equations of motion are solved by the Verlet integration in each cell of grid independently or in groups of connected cells. Within the framework of this general methodology the four classes of algorithms and methods of their parallelization are offered. Parallelization technology is based on the principles of geometric parallelism and efficient partitioning the computational domain. Special dynamic algorithm is used for load balancing the solvers. The testing of developed approach was made by the example of the nitrogen outflow from balloon with high pressure to vacuum chamber through the micronozzle and microchannel. Obtained results confirm the high efficiency of the developed methodology.

COMPUTATIONAL METHODS IN RELATIVISTIC ATOMIC PHYSICS

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Owing to recent advances in accelerator and storage ring techniques, more possibilities arise to study formation of quasi-molecules in slow heavy-ion collisions. Today, these (quasi) molecules are believed to be a versatile tool for investigating a number of fundamental problems in modern physics. In particular, analysis of molecular spectra can provide unique knowledge on the relativistic, many-body and quantum electrodynamics (QED) effects in the non-perturbative domain of high nuclear charges and super strong electromagnetic fields. Moreover, the electron-positron pair production that occurs under such extreme conditions might be utilized to explore the properties and behaviour of physical vacuum and, even, to search for new particles.

Theoretical description of super-heavy quasi-molecules is a complicated task which requires solution of the two-center Dirac equation. During the recent years, we have developed several methods for dealing with such a two-center problem. The methods utilize finite basis sets constructed from B-splines and provide an efficient access to a complete (quasi-) molecular spectrum, including not only bound states but also positive- as well as negative-continuum solutions. In my contribution, I will review these novel computational approaches and will show their application for the analysis of the structure and dynamics of quasi-molecules.

CONTEMPORARY PROBLEMS OF NUMERICAL MODELING OF UNIQUE STRUCTURES, BUILDINGS AND COMPLEXES

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The following contemporary problems of mathematical modelling of unique structures, buildings and complexes are under consideration: modeling of interaction of buildings and structures with a foundation with allowance for real properties, stage-by-stage construction and actual operation history; structural analysis with allowance for physical, geometrical and other nonlinearities; structural analysis with allowance for structural and technological specificity of buildings and facilities; numerical modeling of wind flows and loads, experimental validations of wind load analysis; seismic analysis; progressive collapse analysis of buildings and facilities with allowance for real dynamic highly nonlinear effects of elastoviscoplasticity and large displacements; development and refinement of methods and algorithms for solution of large-scale computational problems; development of calibratable predictive mathematical and computer models as part of structural health monitoring systems at the stages of erection and operation of buildings and facilities; application of algorithms of aerodynamics for modelling of snow sedimentations, explosion loads and distribution of hazardous emissions; numerical modeling of three-dimensional nonstationary roblems of fire resistance; solution of coupled problems of aerohydroelasticity. Development of proprietary

software and verification of software in the Russian Academy of Architecture and Building Sciences are considered as well.

MATEMATICAL MODELING OF RESONANT PROCESSES IN CONFINED GEOMETRY OF ATOMIC AND ATOM-ION TRAPS

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Mathematical modelling of resonant processes in confined geometry of optical and electromagnetic traps is an actual problem of physics of cold atoms and ions. The conventional theory for free-space resonant scattering is not valid for confined scattering and new approaches, including effects of the confinement, are needed. In our works we have developed a computational methods [1-4] for resonant collisions in tight atomic waveguides and have found several novel effects in its application: the confinement-induced resonances (CIRs) in multimode regimes including effects of transverse excitations and deexcitations [2], the so-called dual CIR yielding a complete suppression of quantum scattering [1], and resonant molecule formation with a transferred energy to center-of-mass excitation while forming molecules [5]. The last effect was recently confirmed in the Heidelberg experiment [6]. Our calculations have also been used for planning and interpretation of the Innsbruck experiment on investigation of CIRs in ultracold Cs gas [7].

Our talk is devoted to computational aspects of the developed theoretical models, based on the nondirect product DVR [4,8,9], for the time-dependent and stationary Schrödinger equations with a few spatial variables. We also plan to discuss resent results obtained with the developed approaches for the confined dipole-dipole [10] and atom-ion scattering [11]. Particularly, we investigate very complicate problem of influence of the ion micromotion in Paul traps [12] on the resonances.

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ONLINE EVENT RECONSTRUCTION IN THE CBM EXPERIMENT AT FAIR

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One of the main purposes of the physics program of the future heavy-ion experiment CBM (FAIR, Germany) is to understand the properties of strongly interacting matter at very high baryonic densities and to study the possibility of a phase transition to a deconfined and chirally restored phase of quark matter. The experiment will operate at high interaction rates up to 10 MHz, that requires a full event reconstruction in real time.

In order to make an efficient event selection online a clean sample of particles has to be provided by the reconstruction package called First Level Event Selection (FLES). The FLES package operates in two stages. First, particles registered in the CBM detector system are reconstructed. Then short-lived particles decayed before or inside the setup are searched based on their charged and neutral daughter particles. Since the FLES package is developed to run on many-core computer architectures, the reconstruction of particles is done in parallel that provides a possibility for a global competition between particle candidates. Such a global event reconstruction significantly improves suppression of a combinatorial background and provides for further physics analysis a very clean sample of particles produced at different stages of heavy-ion collision.

The event reconstruction procedure and the results of its application to simulated collisions in the CBM detector setup are presented and discussed in details.

SHAPE APPROXIMATION BASED ON HIGHER-DEGREE POLYNOMIALS

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The planar shape (contour) of an object is a fundamental source of information in a pattern recognition problem. Obtaining the relevant information set rests on difficult procedures and is a key problem in pattern recognition [1]. A method is proposed for the segmentation of contours with a complex geometrical form. It is based on a parametric piecewise approximation of 12th order spanned by a polynomial model defined by basic elements [2]. Higher-order polynomial approximation [3,4] allows to optimize the number of segments on the contour and to obtain analytically the dependence of the curvature for more exact calculation of informative signs that are invariant to geometrical transformations. The algorithm based on this method as well as specific examples are described in detail.

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GENERALIZED TECHNIQUES IN NUMERICAL INTEGRATION

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Integration by parts is one of the most popular techniques in the analysis of integrals and it has frequently been used to create divergent series or asymptotic expansions of integral representations. The product of the technique is usually a divergent series formed from evaluating boundary terms; however, sometimes the remaining integral is also evaluated. Striking examples are the Euler series arising from integrating the Euler integral by parts and examples arising in molecular structure calculations.

In this contribution, we explore a generalized and formalized integration by parts to create equivalent representations to some challenging integrals and we introduce a numerical algorithm, called the staircase algorithm, which is shown to be robust and leads to an unprecedented accuracy.

As a demonstrative archetype, we examine the infinite-range Fresnel integrals, the Twisted Tail, Airy functions and Bessel integrals.

DYNAMICAL AND THERMODYNAMIC ELECTRONIC PROPERTIES OF DNA

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Dynamical properties of electron motion in molecular chains are considered. The charge motion is described in terms of quantum mechanics, whereas vibrational degrees-of-freedom are treated both classically and quantum mechanically.

The dynamics of charge migration was modeled to calculate temperature dependencies of its thermodynamic equilibrium values such as energy and electronic heat capacity in homogeneous adenine fragments. The peak on the graph of electronic heat capacity is observed at the polaron decay temperature.

A typical charge transfer/transport pattern can physically be viewed as a polaron and/or soliton. A closed analytical expression for charge carrier velocity dependence on electric field has been derived and analyzed in detail.

Special attention is given to: dynamical behavior of electrons in rigid chains, band structure of regular polynucleotide chains, dynamics of polaron states formation in Holstein

chain, polaron motion in an electric field, the role of dispersion, Bloch oscillations and breather states.

The work was supported by RSF project 16-11-10163.

KINETIC, MONTE-CARLO AND MULTIPARTICLE MODELS OF THE PROCESSES IN PHOTOSYNTHETIC MEMBRANE

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Processes in photosynthetic membrane proceed at wide time scales from 10-12s-1 (charge separation in photosynthetic reaction centers of Photosystems I and II) till dozen of milliseconds (interactions with Calvin-Benson cycle of CO2 fixation).

The paper presents the results of the work on kinetic and computer modeling performed at the Dept. of Biophysics, Biological faculty MSU. Kinetic models of the primary photosynthetic processes in thylakoid membrane are based on systems of ordinary differential equations, describing the processes in multi-enzyme complexes of Photosystem I, Photosystem II and Cytochrome b6f complex, coupled to transmembrane proton and other ions transport and generation of transmembrane electrochemical potential. These models describe simultaneous kinetic changes of different variables, including concentrations of electron carriers at different redox states, electrical and electrochemical potential values; fluorescence induction and adequately simulates a set of fluorescence induction curves experimentally recorded at different light intensities under continuous illumination and after a short laser flash.

Monte-Carlo models simulate the consequence of individual elementary stages of electron-transport processes in ensembles of several millions electron transport chains, which number is comparable with the number of photosynthetic reaction centers in a real algae cell. Models of this type could be simply modified according to the data of electron transport chain organization at different growth conditions.

The multiparticle computer models describe processes proceeding in the simulated membrane “scene”, which includes stroma, lumen and in transmembrane compartments constructed according to structural data. We simulate interactions of ensembles of molecules in solution and in the heterogeneous interior of a cell. In the models protein molecules move according to the laws of Brownian dynamics, mutually orient themselves in the electrical field and form complexes on the 3D scene. After the interacting molecules approach each other and produce the preliminary complex, we switch off molecular dynamic procedure to simulate intermolecular conformation activity leading to the formation of the final complex, in which the redox reaction occurs. The method allows to visualize the processes of molecule interactions and to evaluate the rate constants for protein complex formation reactions in the solution and in the interior of the photosynthetic membrane. 3D multiparticle computer models for simulation of complex formation kinetics for plastocyanin with photosystem 1 and cytochrome bf complex, ferredoxin with photosystem 1 and ferredoxin:NADP+-reductase are considered. Effects of ionic strength are featured for wild type and mutant proteins. The computer multiparticle models demonstrate non-monotonic dependences of complex formation rates on the ionic strength as the result of long-range electrostatic interactions. The models of interactions Cytf-Pc and Pc-PSI in lumen of thylakoid, taking into account the influence of the charge of the membrane, are developed. Directed electron transport Cytf–PSI via Pc is simulated according to experimental data. The models reveal the role of complex

geometry of the interacting proteins and spatial organization of photosynthetic membrane.

Kinetic and multiparticle computer models allow to evaluate the parameters of photosynthetic processes which cannot be determined experimentally and reveal physical mechanism of regulation of photosynthetic electron transport and coupled processes of energy transformation.

The work was supported by grants of the RFBR (grants N 14-04-00302, 14-04-00326, 17-04-00676).

PRECISE FREQUENCY-PATTERN ANALYSIS REVEALS THE FUNCTIONAL STRUCTURE OF COMPLEX SYSTEMS

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A method for the analysis of complex oscillating electrical systems was proposed [1], based on the multichannel measurements of magnetic field through the hundreds of seconds. Using whole registration time, the Fourier transform of the data is performed, leading to detailed spectra with many frequency components. Further analysis results in total decomposition of the system into functionally invariant entities, each of them having invariant field pattern. The method of functional tomography is described, making it possible to distribute in space the energy of magnetic field sources. Method was verified on the physical phantoms with highly satisfactory results. This approach was applied in different studies of the human brain [2], heart and hand, providing the three-dimensional arrays of sources distribution in the space of measurement. Generally corresponding to anatomy of the systems under study, those 3D arrays reveal their functional structure. Recently the method was successfully applied to localization of magnetic nanoparticles without pre-magnetization or displacement of the sample [3].

This work was partially supported by the Russian Foundation for Basic Research (grants 16-0700937, 16-07-01000, 17-07-00677, 17-07-00686), by the Program I.33P for Fundamental Research of the Russian Academy of Sciences, and by the CRDF Global (USA) (grants CRDF RB1-2027 and RUB-7095-MO-13).

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MACHINE LEARNING AND COMPLEX NETWORKS FOR PRECISION AND SYSTEMS BIOMEDICINE

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The talk will present our research at the Biomedical Cybernetics Group that I established about three years ago in Dresden. We adopt a transdisciplinary approach integrating information theory, machine learning and network science to investigate the physics of adaptive processes that characterize complex interacting systems at different scales, from molecules to ecosystems, with a particular attention to biology and medicine. Our theoretical effort is to translate advanced mathematical paradigms typically adopted in theoretical physics (such as topology, network and manifold theory) to characterize many-body interactions in complex systems and quantitative biomedicine. We apply the theoretical frameworks we invent in the mission to develop computational tools for systems and network analysis. In particular, in biomedicine we deal with: prediction of wiring in biological networks, combinatorial and multiscale biomarkers design, precision biomedicine, drug repositioning and combinatorial drug therapy. In general, we devise theoretical models of structural organization in complex networks and we leverage this knowledge to create novel and more efficient algorithms and to perform advanced analyses and predictions of patterns in complex systems. This talk will focus on two main theories. Firstly, Minimum Curvilinearity, which is a theory for topological estimation of nonlinear relations in high-dimensional data [1] (or in complex networks [2]) and its relevance for machine learning applications in biomedicine. The new topic on the impact of Minimum Curvilinearity for network embedding in the hyperbolic space will be also treated [3]. Secondly, we will discuss the Local Community Paradigm (LCP) [4,5], which is a theory proposed to model local-topology-dependent link-growth in complex networks and therefore it is useful to devise topological methods for link prediction in monopartite and bipartite [5] networks. In particular, we will discuss the impact of this new method for pioneering topological methods for network-based drug-target interaction prediction and repositioning [6].

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QUANTUM DYNAMICS OF A HOLE MIGRATION THROUGH DNA

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A model predicting the behavior of a hole acting on the DNA strand was investigated. The hole-DNA interaction on the basis of a quantum-classical, non-linear DNA single strand model was described. The fact that a DNA molecule is formed by a furanose ring as its sugar, phosphate group and bases was taken into consideration. Based on the model, results were obtained for the probability of a hole location on the DNA base sequences as well as on the sugar-phosphate groups mated with them.

The above considered model results in the following conclusions: the hole migration is a quantum phenomenon. The tunnel effect, owing to which the hole migrates through the chain bypassing the bases with a high ionization potential, influences the process of its migration considerably. The period of the hole migration lies in the range of time scales on which various processes in biomolecules and their solutions occur; the sugar-phosphate backbone possesses conducting properties affecting the hole migration process through the DNA strand considerably.

MONTE CARLO SIMULATION OF EARLY BIOLOGICAL DAMAGE INDUCED BY IONIZING RADIATION AT THE DNA SCALE: OVERVIEW OF THE GEANT4-DNA PROJECT

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INTRODUCTION

Modeling accurately biological damage induced by ionizing radiation at the scale of the DNA molecule remains a major challenge of today's radiobiology research [1]. In order to provide the community with an easily accessible mechanistic simulation platform, the general purpose and open source "Geant4" Monte Carlo simulation toolkit [2] is being extended in the framework of the "Geant4-DNA" project [3] with a set of functionalities allowing the detailed simulation of particle-matter interactions in biological medium. These functionalities include physical, physico-chemical and chemical processes that can be combined with nanometer size geometries of biological targets in order to predict early DNA damage. We will present an overview of the Geant4-DNA project and discuss on-going developments.

THE GEANT4-DNA EXTENSION OF GEANT4

The main developments undertaken by the Geant4-DNA collaboration [3-5] cover three main areas:

- Physics processes: several sets of physics processes are available in order to describe the dominant discrete physical interactions of electrons, protons, hydrogen atoms, alpha particles and their charged states in liquid water, the main component of biological medium. These can be combined with existing Geant4 processes for the description of other processes, such as

photon interactions.

- Physico-chemistry and chemistry processes: such processes can simulate water radiolysis from physical interactions, that is the creation, the diffusion and mutual reactions of molecular species in liquid water, up to 1 microsecond after irradiation.

- Detailed geometries of biological targets: benefiting from Geant4 geometry modeling capabilities, it is now possible to simulate accurate geometries of biological targets, such as the DNA molecule.

OUTCOME

All features described above are fully accessible [6] through the Geant4 simulation toolkit and can be run using a freely downloadable Linux (TM) CentOS (TM) virtual machine [7]. We hope that this platform and its future developments will be useful for the further mechanistic understanding of ionizing radiation effects in biological targets, especially when high spatial resolution (nanometer) and low energy (few electonsVolts) simulations are required.

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MULTISCALE SIMULATIONS OF TARGETS FOR PHARMACOLOGICAL RELEVANCE

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Molecular dynamics simulations of proteins may differ by the granularity of the underlying force fields (from quantum to coarse grain). At times, it is very useful to combine different descriptions in a hybrid description. Here I will present recent hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) – and MM/coarse grain (CG) based investigations of targets for pharmaceutical intervention. The predictive power and limitations of these multi-scale methods will be illustrated. The talk will close with a brief survey of multi-scale simulations within the recently formed consortium of the Human Brain Project, one of the two flagships grant funded by the EU.

The HPC-Leap, BioExel, Human Brain Project EU grants, along with the German agencies DFG and BMBF agencies are acknowledged for funding part of this research.

DYNAMICS OF QUANTUM CORRELATIONS IN BIPARTITE GAUSSIAN OPEN QUANTUM SYSTEMS

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In the framework of the theory of open systems based on completely positive quantum dynamical semigroups, we make a comparison of the behaviour of continuous variable quantum correlations (quantum entanglement, entropic quantum discord, geometric quantum discord, quantum steering) for a system consisting of: 1) two non-coupled; 2) two coupled bosonic modes embedded in a common environment of the form of a thermal bath or of a squeezed thermal bath. We solve the Markovian master equation for the time evolution of the considered system and describe the quantum correlations in terms of the covariance matrix for Gaussian input states. Depending on the values of the parameters characterizing the initial state of the system (squeezing parameter, average photon numbers), the coefficients describing the interaction of the system with the reservoir (temperature, dissipation constant), and on the intensity of the interaction between the two modes, one may notice phenomena like generation of quantum correlations, their suppression (sudden death), periodic revivals and suppressions, or an asymptotic decay in time of quantum correlations.

PARTIAL ANALYTICAL INTEGRATION OF STIFF NONLINEAR COSSERAT PARTIAL DIFFERENTIAL EQUATIONS AND ITS APPLICATION TO SIMULATION OF SLENDER STRUCTURES

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We apply modern computer algebra methods and software for the Lie symmetry analysis to the governing Cosserat system of twelve nonlinear partial differential equations (PDEs) describing dynamics of nearly one-dimensional flexible structures (rods, fibers, cables, etc.) and construct the general analytical solution to the kinematic part (six equations) of the system. The obtained solution depends on two arbitrary analytical vector functions, and we show that its knowledge helps to resolve stiffness of the governing Cosserat system. Based on this result we develope algorithms based on combinations of numerical (exponential integration) and analytical (solver of differential equations built-in Maple) treatments of the dynamical part of the governing PDE system. Our approach allows for larger step sizes compared to pure numerical solvers and at the same time combines efficiency and accuracy without sanctifying one for another. Based on this observation, we create a hybrid semi-analytical solver for highly viscous two-way coupled fluid-rod problems which allows for the interactive high-fidelity simulations of flagellated microswimmers, as a result of a

substantial reduction of the numerical stiffness. Besides, we present in the talk experimental comparison of our method with the so-called α-method, the best one among pure numerical methods developed for integrating Cosserat equations, and demonstrate superiority of our method.

NEW POSSIBILITIES AND APPLICATIONS OF THE METHOD OF COLLOCATIONS AND THE LEAST RESIDUALS

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In the numerical method of collocations and the least residuals (CLR), the boundary differential problem using the collocation method is projected into a finite-dimensional linear functional space. To find the solution of the obtained approximate problem, an overdetermined system of linear algebraic equations (SLAE) is written out and it is required that on its solution the minimum of the discrepancy functional of all its equations is attained. From this requirement and the presence of a piecewise analytic solution of the approximate problem, a number of merits of the method follows. In particular, the algorithms of the CLR method are relatively simple to apply in non-canonical regions and on irregular grids. It is relatively simple to build variants of the method of increased accuracy, including those for sufficiently ill-conditioned problems and with singularities in the solution of the initial differential problem. Its algorithms are easily parallelized. In the CLR method, modern algorithms of computational mathematics are effectively used: multigrid complexes, Krylov subspaces, preconditioners, irregular grids. The presented report will give a brief overview of the latest results obtained in the CLR method and demonstrate its indicated properties.

MODELING QUANTUM BEHAVIOR IN THE FRAMEWORK OF PERMUTATION GROUPS

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The trajectory of a quantum system is a sequence of unitary evolutions of vectors in a Hilbert space, interspersed with observations – projections of the vectors in some subspaces, that are specified by measuring devices. The result of quantum observation is random and its statistics is described by a probability measure defined on subspaces of the Hilbert space. Gleason's theorem gives a general construction of all possible probability measures on subspaces of a Hilbert space. In fact, this construction reproduces the Born rule for quantum probabilities. Quantum-mechanical description can be made constructive, if we replace the general group of unitary transformations of the Hilbert space by unitary representations of finite groups. It is known that any linear representation of a finite group can be realized as a subrepresentation of some permutation representation. Thus, quantum mechanical problems

can be formulated in terms of groups of permutations. Such a constructive approach allows us to clarify the meaning of a number of physical concepts. Combining methods of computational group theory with Monte Carlo simulation we study models based on the natural and standard representations of symmetric groups.

QUANTUM CORRELATIONS IN BIPARTITE SYSTEMS

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Quantum correlations are different from all other correlations in many-particle systems. They depend on measurements. Quantum correlations are responsible for the advantages of quantum devices over their classical counterparts and ensure efficient work of all quantum devices, including quantum computers. Entanglement is a measure of quantum correlations for pure states. According to the current understanding, total correlations, classical and quantum, can be described by the mutual quantum information [1,2]. In order to separate quantum and classical correlations, one should perform a total system of projective measurements over one of the subsystems of a bipartite system [1,2]. As a result of those measurements, at least a part of quantum correlations disappears. Performing minimization of the quantum conditional entropy over all possible total sets of projective measurements, one can annihilate all quantum correlations and separate the contributions of classical and quantum correlations to the mutual quantum information. The contribution of quantum correlations to the mutual quantum information is called quantum discord [1].

The calculation of quantum discord is a very difficult problem because it requires complex optimization. The problem can be solved in general bipartite systems only with numerical methods. We consider here some cases where quantum discord can be found analytically [3,4].

First we consider quantum correlations in a bipartite heteronuclear $(N-1)\times 1$ system in an external magnetic field. The system consists of a spin ring with an arbitrary number $N-1$ of spins on the ring and one spin in its center [3]. The spins on the ring are connected by the secular dipole-dipole interaction (DDI) and interact with the central spin through the Heisenberg zz-interaction. We show that quantum discord can be obtained analytically in the high-temperature approximation. The model allows us to find contributions of different parts of the spin-spin interactions to quantum correlations [3].

We investigate also [4] quantum correlations in a two-spin system with the DDI in NMR multiple-pulse spin locking experiments [5]. We demonstrate that quantum correlations are absent in the multiple-pulse spin-locking with $\pi/2$-radio-frequency pulses even at long times. At the same time, entanglement emerges after several periods of the pulse sequence with $\pi/4$-radio-frequency pulses. We demonstrate the dependence of entanglement on the number of periods of the multiple-pulse sequence. Quantum discord is obtained for the multiple-spin-locking experiment at different temperatures [6].

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USAGE POWER GEOMETRY AND NORMAL FORM METHODS IN SIMULATION OF DEGENERATED NONLINEAR ODES STUDY

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The report describes power transformations of degenerate autonomic polynomial systems of ordinary differential equations which reduce such systems to a set of non-degenerate systems. The original problem is separated in a number of partial nilpotent tasks.

There is an example of building exact first integrals of motion of a degenerate planar system in a closed form as functions of system parameters.

Joint work with Profs. Alexander Bruno and Valery Romanovski.

MODELING OF PHYSICAL PROCESSES AND COMPUTATIONAL METHODS

FUNCTIONAL INTEGRAL APPROACH TO SYSTEM OF STOCHASTIC DIFFERENTIAL EQUATIONS

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Various physical, chemical, and biological systems with fluctuations or noise are described by stochastic differential equations (SDEs). Constructing a SDEs for the modeled system such that the stochastic part is related to the structure of the system is considered in [1,2].

Evaluation of probability density function (PDF) and other quantities describing a solution of system of SDEs is considered in this work. To solve this problem, we use the Onsager-Machlup functional [3] to represent a PDF through a functional integral. In the general case, we cannot find a PDF on a small time interval Δt corresponding to an arbitrary SDE. However, we can find an expression for a PDF on a small time interval Δt which is true up to summands of orders higher than one with respect to Δt. Using this expression we can write a PDF in the form of functional integral. Case of system of SDEs is more complicated than case of SDEs. Therefore, we consider the Onsager-Machlup functional technique only for the flat space when the diffusion matrix for system of SDEs defines a Riemannian space with vanishing curvature.

A method for the approximate evaluation of the arising functional integrals is considered. Following this method, we distinguish among all trajectories the classical trajectory for which the action takes the extreme value. The classical trajectory is found as the solution of the multidimensional Euler-Lagrange equation. Further, to compute the integral, we use the decomposition of action with respect to the classical trajectory.

For SDE that is for one-dimensional case this method is considered in [4].

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FULLY DIFFERENTIAL CROSS SECTIONS FOR SINGLE IONIZING 1-MEV P+HE COLLISIONS AT SMALL MOMENTUM TRANSFER

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We present ultra high resolution data on single ionization of helium under impact of 1-MeV protons in comparison with theoretical calculations. Good agreement between theory and experiment [1] is obtained. Three initial trial helium wave functions are employed: a weakly correlated Roothaan-Hartree-Fock function, a simple Silverman-Platas-Matsen function of the configuration interaction family, and a strongly correlated function [2]. Multidimensional singular integrals which defining differential cross sections are calculated using special transform for each above trial function.

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APPLICATION OF HARMONIC OSCILLATOR BASIS WITH DIFFERENT SIZE PARAMETERS FOR CALCULATION OF GROUND STATE ENERGY OF COULOMB THREE-BODY SYSTEMS

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The new harmonic oscillator (HO) expansion method [1] is applied to calculate non-relativistic ground state energy of a number of Coulomb three-particle systems with two identical particles for up to 28 excitation HO quanta. The novelty of the method is the introduction of different size parameters in the Jacobi coordinates instead of only one unique oscillator length parameter in the traditional approach. It has been found that variational

calculations of the ground state energies of these systems using the proposed basis with different size parameters converge much faster than in the traditional treatment with only one oscillator length. Particularly, for systems with molecular character the second nonlinear variational parameter is vital for reasonable convergence. The results obtained in basis with different sizes are compared with the ones calculated in traditional basis with the same oscillator length for each Jacobi coordinate and with those given in the literature [2].

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QUASICROSSINGS OF THE ENERGY TERMS IN THE TWO-COULOMB-CENTRE PROBLEM

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The first three corrections to the bound state energy, separation constants, and wavefunctions of hydrogen-like ion in the field of remote $(R \gg 1)$ point charge are calculated by means of the modified perturbation theory. The consistent scheme for obtaining WKB expansions for solutions of the quasiangular equation in quantum mechanical two-Coulomb-centre problem $Z_1 e Z_2$ is developed. In the framework of this scheme, the quasiclassical angular Coulomb spheroidal wavefunctions for large distances between the fixed positive charges (nuclei) are constructed for the below-barrier motion of the negative particle (electron). The quasiclassical expression for the exchange interaction ΔE of potential curves at the points of their quasicrossing is found. It can be used further for the calculation of cross sections of charge exchange processes between hydrogen or hydrogen-like atoms and bare nuclei.

MODELING TURBULENCE VIA NUMERICAL FUNCTIONAL INTEGRATION

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We investigate the possibility of modeling turbulence via numerical functional integration. By transforming the incompressible stochastic Navier-Stokes equation into a functional integral we are able to calculate equal-time spatial correlation of system variables using standard methods of multidimensional integration. In contrast to direct numerical simulation, our method allows for simple parallelization of the problem as the value of the integral at any point is independent of other points. Thus the entire problem does not have to fit into available memory of any one computer but can be distributed even onto several supercomputers and the cloud.

We present the mathematical background of our method and its numerical implementation. The implementation is composed of a fast serial program for evaluating the integral over a given volume and a Python wrapper that divides the problem into subvolumes and distributes the work among available processes. We use various existing programs/libraries written mostly in C/C++ for integrating subvolumes. We show preliminary results obtained with our method and discuss its pros, cons and future developments.

FINITE-DIFFERENCE SPLITTING SCHEME FOR THREE-DIMENSIONAL SCHROEDINGER EQUATION, DESCRIBING TUNNELING FROM ANHARMONIC ATOMIC TRAPS

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We present an efficient computational scheme to integrate the time-dependent three-dimensional Schroedinger equation. The time-evolution operator is calculated with a second order split-operator technique and spatial derivatives are approximated with a sixth-order finite-difference method.

The efficiency of our implicit scheme is demonstrated in comparison with a high-order direct method [1] for an exactly solvable problem of a harmonic oscillator.

Our method was successfully applied to a tunneling problem of two interacting atoms confined in a one-dimensional optical trap by “walls” of an anharmonic potential [2]. By computing a time-evolution of a population of the trap states we extract tunneling rates of the atoms [2].

By using the above examples, we demonstrate a linear dependence of a computational time of the method on a number of spatial grid points and a fast convergence with respect to a step of integration over time and spatial variables. The computational method can be extended to more complicated problems in higher dimensions.

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OPTIMAL APPROXIMATION OF BIQUARTIC POLYNOMIALS BY BICUBIC SPLINES

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Recently an unexpected approximation property between polynomials of degree three and four was revealed within a framework of two-part approximation models in 2-norm, Chebyshev norm and Holladay semi-norm.

Namely, it was proved that if a two-component cubic Hermite spline's first derivative at the shared knot is computed from the first derivative of a quartic polynomial, then the spline is a clamped spline of class C^2 and also the best approximant to the polynomial.

Although it was known that a 2×2 component uniform bicubic Hermite spline is a clamped spline of class C^2 if the derivatives at the shared knots are given by the first derivative of a biquaartic polynomial, however the optimality of such approximation remained an open question.

The paper's goal is to resolve this problem. Unlike the spline curves, in the case of spline surfaces it is insufficient to suppose that the grid should be uniform and the spline's derivatives computed from a biquartic polynomial. We show that the biquartic polynomial coefficients have to satisfy some additional constraints to achieve optimal approximation by bicubic splines.

MECHANISM OF CONTROLLING THE PROCESS OF THE CONVERGENCE OF THE NEWTON ITERATION METHOD

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A mechanism for controlling the convergence of the continuous analog of the Newton method (NAMN) with the use, as a control parameter, of the step variation coefficient of the difference scheme for the numerical solution of the differential equation of the NAMN. Using the example of a developed algorithm for a modified NAMN, it was shown that it is possible to control the characteristics of the convergence of NAMN using the step change coefficient of the difference scheme for the numerical solution of the differential equation of the NAMN

as a control parameter. The development and implementation of mechanisms for controlling the iterative processes of solving the equations will make it possible to significantly reduce the time required to calculate the required value, which will significantly improve the efficiency of the algorithms for solving nonlinear equations.

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SPECTRAL MULTI EXPONENTIAL APPROXIMATION AS A ROBUST TOOL FOR ANALYSIS OF COMPLEX SYSTEMS

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The behavior of various systems in living and nonliving matter may be characterized mathematically by a linear combination of exponential functions. Many types of scientific experiments are often conducted in such a way that changes in some characteristic variable in response to some perturbation are recorded. These measurements yield data referred to as a signal. Assuming the signal by its nature is a linear combination of exponential functions, each of them characterizing response of particular subsystem to the perturbation, the researcher faces a task to find parameters (amplitudes and characteristic times) of particular exponential functions constituting the signal. There is no common method to find these parameters in general case because the problem is ill-conditioned.

In particular cases the task may be solved by linear regression. We develop the method of spectral multi-exponential approximation (SMEA) [1], in which characteristic times of exponential functions are taken over fixed logarithmic scale, and non-negative least square solver is used to find pre-exponential factors. These factors (amplitudes) constitute discrete spectrum. To obtain scale-independent transform, for any arbitrary characteristic time we define the integral amplitude as a partial sum of estimated amplitudes corresponding to characteristic times less than this arbitrary time. Integral amplitude is a step function, and its plot against time provides a pictorial representation of the SMEA transform. A heatmap visualization of the integral amplitude with characteristic times coded by color is suitable for representation of a large sample of signals.

This method was applied for analysis of chlorophyll fluorescence transient in ecological and biotechnological studies. The measurement of the kinetics of chlorophyll fluorescence transient of algae and plants is a widely used method for determining the state of photosynthetic apparatus. The time dependence of the fluorescence intensity is a complex multiphase curve, which depicts the various stages of the electron transfer in the electron transport chain of chloroplasts. SMEA allows to formalize phase identification, to estimate quantitative characteristics of individual phases of the induction curve (amplitudes and characteristic times), and to reveal hidden phases of the curve. Occurrence of additional phases on the induction curve points to a change in the functioning of the photosynthetic

apparatus in response to changing growth conditions. A high sensitivity of SMEA allows to suggest it for detection of early cell response to stress. SMEA decomposition and visualization techniques may find broad application in various signal processing tasks, especially in the analysis of the response of complex biological systems to external impact.

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MODELING THE QUARKS' HELICITY FLIPPING STIMULATED BY THEIR CONFINEMENT POTENTIAL

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The proton spin puzzle is known since 1988 after measurements of quarks' helicity contribution to the proton spin [1]. In spite of all efforts applied, the problem remains an unresolved enigma of high-energy physics till now (see [2] and references therein). It has been recently shown that the confinement of quarks induces a change of their helicities together with a simultaneous alteration of orbital momenta, so that the total angular momentum of each quark is conserved [3]. As a necessary consequence, a superposition of states with opposite helicities of quarks should appear. Thus, contribution of quarks helicities to the proton polarization may be much less than it is expected on the ground of the conventional picture of entirely free partons. In principle, this mechanism might be considered as a solution to the proton spin puzzle.

In present communication, such a scenario is verified on basis of the Dirac equation written in the cylindrical coordinates. Firstly, a resulting system of differential equations was tried to be solved numerically with MAPLE assisted standard methods such as Runge-Kutta-Fehlberg algorithm (the rkf45 procedure) and a finite difference technique with the Richardson extrapolation (the bvp procedure). Unfortunally, none of them was able to reproduce the confinement of quarks in the usual linearly increasing attractive potential. A method of numerical solution of the system describing the quarks' helicity flipping as well as their confinement is proposed in this report.

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EXTRAPOLATION OF FUNCTIONS OF MANY VARIABLES BY MEANS OF METRIC ANALYSIS

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We consider a problem of extrapolating functions of several variables. It is assumed that the values of the function of m variables are given at a finite number of points in some domain *D* of the *m*-dimensional space. It is required to restore the value of the function at the points outside the domain *D*. To solve the extrapolation problem, we propose a scheme which is based on a metric analysis approach. This scheme consists of two stages. At the first stage, using the metric analysis, the function is interpolated to the points of the domain *D* belonging to the segment of the straight line connecting the center of the domain *D* to the point M in which it is necessary to restore the value of the function. At the second stage, based on the autoregression model and the metric analysis, the function values are predicted along the above straight-line segment beyond the domain *D* up to the point *M*. We present some numerical examples which demonstrate the efficiency of the proposed scheme.

MODELLING OF THE HIGH TEMPERATURE SUPERCONDUCTORS AT NONEQUILIBRIUM CONDITIONS

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Nonequilibrium effects in layered superconducting materials that appears as a result of injection of a stationary current are actively studied in recent years [1-3]. An experimental proof of the existence of a nonequilibrium effect in intrinsic Josephson junctions was given in [4] and was explained by the charge imbalance in the superconducting layers, which arises as the result of injection of the quasiparticle current.

In our work, we provide a detailed numerical simulations of intrinsic Josephson junctions of high temperature superconductors under external electromagnetic radiation taking into account the charge imbalance effect [5]. We demonstrate that the charge imbalance is responsible for a slope of the Shapiro steps on the current-voltage characteristic. The value of slope increases with a nonequilibrium parameter. Coupling between junctions leads to a distribution of the slope's values along the stack. The nonperiodic boundary conditions shift the Shapiro step from the canonical position determined by a frequency of external radiation. This fact makes ambiguous the interpretation of the experimentally found Shapiro step shift by the charge imbalance effect [6].

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NUMERICAL MODELLING OF NORMAL AND SUPERCONDUCTING PROPERTIES OF THE DOPED GRAPHANE

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The normal properties of graphane with various degrees of doping are calculated with the help of the generalized Eliashberg theory. Within the theory of strong electron-phonon interaction, a superconducting order parameter of the doped graphane has been found. The classical approach for determining the critical temperature of a superconducting transition as a result of a strong electron-phonon interaction does not involve calculating the renormalization of the density of electronic states and the chemical potential. In this work the critical temperature of superconductivity of graphane has been calculated as a function of the doping degree taking into account the renormalization of the electron mass, the chemical potential, and the density of electronic states.

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ASYMPTOTICS FOR PENALIZED SPLINES

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Algorithmic complexity is a very important topic in computer science. Knowing the complexity of algorithms allows you to answer questions such as “How long will a program run on an input?”, “How much space will it take?” and “Is the problem solvable?”. These are important bases of comparison between different algorithms. An understanding of algorithmic complexity provides programmers with insight into the efficiency of their code.

We perform an asymptotic analysis of penalized spline estimators. We compare P-splines and splines with a penalty of the type used with smoothing splines. A P-spline and a smoothing spline are asymptotically equivalent provided that the number of knots of the P-spline is large enough, and the two estimators have the same equivalent kernels for both interior points and boundary points. We consider the convergence of the algorithm as well as the uniqueness of its solution.

Also, we develop asymptotic theory with quasi-solution for penalized spline estimators in generalized additive models. Our purpose is to establish the asymptotic bias and variance as well as the asymptotic normality of the penalized spline estimators proposed by Marx and Eilers.

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MINIMUM PERIOD OF ROTATION OF MILLISECOND PULSARS AND EQUATIONS OF PULSAR MATTER STATE

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The astrophysical data is indicative of the presence of a minimum period of rotation of millisecond pulsars. Now this period is 1.396648 ms.At that, the indicated value is reached long before pulsar destruction under the influence of centrifugal forces. This phenomenon is easily explained by the fast growth of angular momentum losses near the bifurcation point of pulsar configuration due to intense pulsar gravitational radiation.

Based on the findings of our previous studies of fast-rotating Newtonian magnetized polytropies, we found the relation between a minimum pulsar rotation period, a value of pulsar central density, and a polytropy index. Due to this relation we drawn a conclusion that a value of minimum central density of a pulsar with a peak period was $2.5088 \cdot 10^{14}$ g/cm^3.

THE CALCULATION OF MULTICOMPONENT MIXTURE PHASE DIAGRAM, USING THE EQUATIONS OF STATE OF THE VAN DER WAALS TYPE

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Hydrocarbon mixtures filtration process simulation development has resulted in use of cubic equations of state of the van der Waals type to describe the thermodynamic properties of

natural fluids under real thermobaric conditions [1]. Two- and three-component hydrocarbon systems allow to simulate the fluids of different types of reservoirs qualitatively, what makes it possible to carry out the experimental study of their filtration features. Exploitation of gas-condensate reservoirs shows the possibility of existence of various two-phase filtration regimes, including self-oscillatory one, which occurs under certain values of mixture composition, temperature and pressure drop [2]. Plotting of the phase diagram of the model mixture is required to determine these values. A software package to calculate the vapor-liquid equilibrium of multicomponent systems using cubic equation of state of the van der Waals type has been created. Phase diagrams of gas-condensate model mixtures have been calculated.

This work is supported by RFBR (project № 17-08-01270).

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PARALLEL IMPLEMENTATION OF NUMERICAL SOLUTION OF FEW-BODY PROBLEM USING FEYNMAN'S CONTINUAL INTEGRALS

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Modern parallel computing algorithm has been applied to the solution of the few-body problem. The approach is based on Feynman's continual integrals method implemented in C++ programming language using NVIDIA CUDA technology. Calculations were performed on the NVIDIA Tesla K40 accelerator installed within the heterogeneous cluster of the Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna. A wide range of few-body bound systems has been considered including nuclei described as consisting of protons and neutrons (e.g., 3,4He), nuclei described as consisting of clusters and nucleons (e.g., 6He), as well as quark systems. The correctness of the results was checked by the comparison with the experimental data and the results obtained within other approaches. Parallel implementation of Feynman's continual integrals method significantly increases the speed of calculations, which, in certain cases, enables calculations impossible before. In addition, it allows one to reduce the mesh step in calculations of wave functions as well as obtain good statistics, which increases the accuracy of calculations.

MOLECULAR DYNAMIC SIMULATION OF WATER VAPOR INTERACTION WITH BLIND PORE OF DEAD-END AND SACCATE TYPE

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One of the varieties of pores, often found in natural or artificial building materials, are the so-called blind pores of dead-end or saccate type. Three-dimensional model of such kind of pore has been developed in this work. This model has been used for simulation of water vapor interaction with individual pore by molecular dynamic method [1]. Special investigations have been done to find dependencies between thermostats implementations and conservation of thermodynamic and statistical values of water vapor-pore system. The all types of evolutions of water-pore system have been investigated: drying and wetting of the pore. Full research of diffusion coefficient, diffusion velocity and other diffusion parameters has been made. Simulation results analysis demonstrates an importance of the investigation of the water vapor interaction with individual pore from point of view the control of water penetration into building material and protection of building material from wetting.

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JOINT ANALYTICAL AND NUMERICAL INVESTIGATION OF BLOW-UP IN SOME MATHEMATICAL MODELS

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In some models (for example, in plasma physics and semiconductor physics), the blow-up phenomenon occurs, i.e. the solution's norm tends to infinity as time tends to a finite moment. There exist some methods to detect blow-up analytically: Pokhozhaev and Mitidieri's test function method, Levine's method, and Samarskii and Galaktionov's similarity solutions method. These methods typically provide us with an estimation of the blow-up moment. The numerical algorithm (based on N.N. Kalitkin and co-authors' ideas), however, allows us to specify the moment and the process of the solution's blow-up by using Richardson's effective accuracy order. In particular, one can obtain the blow-up moment with the accuracy up to mesh interval. Some numerical experiments will be presented in order to demonstrate the effectiveness of the method.

THE BOUNDARY VALUE PROBLEM FOR ELLIPTIC EQUATION IN THE CORNER DOMAIN IN THE NUMERICAL SIMULATION OF MAGNETIC SYSTEMS

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The formulation of the boundary value problem arises in magnitostatics when finding the magnetic field distribution by the method of two scalar potentials in the domain comprising ferromagnetic and vacuum. The problem nonlinearity is stipulated by the dependence of the medium properties (magnetic permeability) on the solution to be found. In connection with that the solution of such a problem has to be found by numerical methods, a question arises about the behavior of the boundary value problem solution around the angular point (the intersection of two environments-vacuum/iron) of the ferromagnetic. The upper estimate for the acceptable growth of the magnetic field in the vacuum region near the corner point of the ferromagnet has been obtained. It is shown that under certain conditions imposed on the magnetic permeability, the magnetic field within the vacuum region in the vicinity of the corner points is limited. An algorithm of thickening differential grid near the corner point has been developed. It allows one to significantly reduce the computation time and simultaneously to increase the accuracy of the solution of the boundary value problem. The results of modeling the magnetic system containing corner points are presented. The problems of creating a homogeneous map of the field of possible solenoid-type magnetic systems of the NICA installation are analyzed. The computations were performed with the help of two software products, i.e. TOSCA and MFC (Magnetic Field Calculation) developed by the authors.

ESTIMATION OF MAGNETIC FIELD GROWTH AND CONSTRUCTION OF ADAPTIVE MESH IN CORNER DOMAIN FOR MAGNETOSTATIC PROBLEM IN 3-DIMENSIONAL SPACE

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A magnetostatic problem arises in searching for the distribution of the magnetic field generated by magnet systems of many physics research facilities, e.g., accelerators. The domain in which the boundary-value problem is solved often has a piecewise smooth boundary. In this case, numerical calculations of the problem require the consideration of the solution behavior in the corner domain.

Based on the estimate is obtained by E.E. Perepelkin in his previous works, we propose

a method of condensing the differential grid near the corner domain of vacuum in case of 3-dimensional space. An example of the modeling problem calculation in the corner domain is given.

INVESTIGATION OF THE ENTROPY OF A SYSTEM OF MANY PARTICLES WITH GRAVITATIONAL INTERACTION

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This paper is devoted to the study of entropy of a system of many particles with gravitational interaction. The study of entropy behavior is based on the Vlasov kinetic equation, using both numerical and exact solution. In view of the special laboriousness of the computation, parallel algorithms using CUDA technology are implemented in this paper. A parallel algorithm for solving the Vlasov equation by the particle method is presented. The time dependence of entropy is obtained, its analysis is carried out.

A COMPUTATIONAL ALGORITHM FOR COVARIANT SERIES EXPANSIONS IN GENERAL RELATIVITY

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We present a new algorithm for computing covariant power expansions of tensor fields in generalized Riemannian normal coordinates introduced in some neighborhood of a parallelized k-dimensional embedded submanifold $\left(k = 0,1,\ldots < n\right)$; the case $k = 0$ corresponds to a point. The algorithm is applicable for nonmetric connections, possibly with the torsion. The power series coefficients of an arbitrary real analytic tensor field are expressed in terms of its covariant derivatives and covariant derivatives of the curvature and the torsion. We discuss different ways to reduce normal polynomial expansions to the irreducible form, enumerate the number of summands in the coefficients, and evaluate the computational complexity of the algorithm.

GENERALIZED DARCY'S LAW IN FILTRATION THEORY

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We study the hydrodynamics of flow in porous medium modeling the grain filling in filters. Using the lattice approximation, we derive the structure of the current in porous medium and obtain the transverse diffusion coefficient D which proves to be proportional to the diameter d of the grain. We consider the axially-symmetric stationary flow with the velocity components $u_z = u(\rho, z),\ u_\phi = w(\rho, z)$ in cylindrical coordinates $\rho,\ \phi,\ z$. The current density $\vec{j}$ of the liquid takes the form

$$j_\rho = w - D\partial_\rho u,\ \ u_z = u,$$

with the density of the liquid being unit. Solving the corresponding continuity equation $\mathrm{div}\vec{j} = 0$ and neglecting the radial velocity $w \ll u$ one can explain the so-called "near-wall" effect for the case of cylindrical filter, resulting in large value of velocity near the wall [1] of the filter tube.

To find the profiles of the velocity $\vec{u}$ and the pressure p, it is necessary to solve also the Euler equation

$$(\vec{u}\nabla)\vec{u} + \nabla p = \vec{f} = \vec{g} - k_D\vec{u},$$

where the force density $\vec{f}$ includes the gravity acceleration $\vec{g}$ and the Darcy force $\vec{f}_D = -k_D\vec{u}$. In the simplest approximation the Darcy coefficient k_D appears to be constant: $k_D \approx k_0 = \mathrm{const}$, but in general it should be some function of the velocity and pressure. We suggest a generalization of the Darcy law by including in k_D the natural invariant $I = (\vec{u}\nabla p)$ in the simplest linear form: $k_D = k_0 + k^* I$. We analyze the dependence of the filtration process on the coefficient k^*.

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ALGORITHM FOR THE ORTHOGONAL FAST DISCRETE SPHERICAL BESSEL TRANSFORM ON A UNIFORM GRID

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We propose an algorithm for the orthogonal fast discrete spherical Bessel transform on a uniform grid. Our approach is based upon the spherical Bessel transform factorization into the two subsequent orthogonal transforms, namely the fast Fourier transform and the orthogonal transform founded on the derivatives of the discrete Legendre orthogonal polynomials. The method utility is illustrated by its implementation for the numerical solution of the three-dimensional time-dependent Schroedinger equation.

VARIATIONAL SOLUTION OF THE SCHRÖDINGER EQUATION IN AN INHOMOGENEOUS CENTRAL FIELD AS APPLIED TO EMISSION PROBLEMS

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The present work is devoted to the supercomputer modelling of the emission processes from the surface of nanostructures that are perspective for modern applications. Within the subject emission processes from single-wall nanotubes with diameters of nanometre range are of particular interest. These devices can be successfully used in nanolithography and non-destructive sounding of nanomaterials. However, for their practical realization the emission processes are needed a detailed study, considering quantum effects. One of essential elements of such analysis is studying the properties of the nanotube surface at the atomic level. In the present paper, we use the fact that the fragment of the nanotube surface is a layer of graphene. A hydrogen-like atom model is used for a detailed consideration of the properties of this object. Earlier, we solved this problem without taking into account the inhomogeneity of the ion field. This research was made with considering the influence of the inhomogeneity of the ion field on the solution of the ground state of a weakly bound electron of a hydrogen-like carbon atom in a graphene lattice. It is shown that the use of the virial theorem in an inhomogeneous field essentially affects the variational solution of the Schrödinger equation.

GROUND STATE OF THE ELECTRON-HOLE LIQUID IN QUANTUM WELLS

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The study of the properties of electron-hole systems is one of the rapidly developing areas of modern condensed matter physics. At present, most attention is paid to low-dimensional electron-hole systems, in which the role of the Coulomb interaction increases. Recently, electron-hole liquid (EHL) was found in SiO2/Si/SiO2 quantum wells [1] and in Si/Si1-xGex/Si heterostructures [2].

The aim of this work is to find the energy and equilibrium density of a quasi-two-dimensional EHL. The ground states of quasi-two-dimensional EHL are studied by the density functional theory. The nonlinear Schrödinger equations for electrons and holes are numerically solved. The wave functions and energy levels of electrons and holes field are found. The binding energy of the electron and hole for different surfaces of silicon is calculated. The calculated values of the equilibrium density are in good agreement with the experimental values [2].

The work was supported by the RFBR and Administration of the Krasnodar Region (Project No. 16-42-230280).

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NUMERICAL SIMULATION OF THE HYDRATED ELECTRON STATES FORMATION

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A method and a complex of computer programs are developed for the numerical solution of the system of nonlinear partial differential equations describing a formation of the polaron states in condensed media [1,2]. Parallel implementation is based on the MPI technique and on the utilizing of the partition algorithm [3].

Numerical simulation of the photoexcited electron states formation in water under the action of the ultraviolet range laser irradiation is carried out. Our approach allows one to reproduce the experimental data on the hydrated electrons formation [2,4]. The model was modified to account for the time-dependence of the absorption band width of the hydrated electron. This modification improves an agreement of numerical results with experimental data.

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ON INTERPOLATIONAL APPROXIMATION OF NONLINEAR DIFFERENTIAL OPERATORS OF THE SECOND ORDER IN PARTIAL DERIVATIVES

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We consider the differential operators $F: C^2(T \times S) \to Y$ of the second order in partial derivatives of the form

$$F(x) = f\left(t,s,x(t,s),x'_t(t,s),x'_s(t,s),x''_{t^2}(t,s),x''_{t,s}(t,s),x''_{s^2}(t,s)\right), \quad (1)$$

where $x'_t(t,s)=\dfrac{\partial x(t,s)}{\partial t}$, $x''_{t^2}(t,s)=\dfrac{\partial^2 x(t,s)}{\partial t^2}$, $x''_{t,s}(t,s)=\dfrac{\partial^2 x(t,s)}{\partial t\partial s}$, the derivative $x''_{t,s}(t,s)=x''_{s,t}(t,s)$, the space $C^2(T\times S)$ is the space of two times continuously differentiable on $T\times S\subseteq R^2$ functions $x(t,s)$, the function $y=f(t,s,u_0,u_1,...,u_5)$ is defined on a rectangle $\Omega=T\times S\times T_0\times T_1\times\cdots\times T_5$, T_i are sets of the number line $(i=0,1,...,5)$ and *Y* is a function space.

Here is the Lagrange interpolation formula for the operators (1):

$$L_n(F;x)=F(x_0)+\sum_{k=1}^{n}\int_0^1\sum_{i,j=0;i+j\le 2}^{2}\frac{\partial}{\partial\left(\dfrac{\partial^{i+j}\upsilon_k}{\partial t^i\partial s^j}\right)}F(\upsilon_k(t,s,\tau))\times$$
$$\times\frac{\partial^{i+j}}{\partial t^i\partial s^j}\left\{\frac{l_{n,k}(x(t,s))}{\sigma_n(x(t,s))}(x_k(t,s)-x_0(t,s))\right\}d\tau \qquad (2)$$

where the functions $\upsilon_k=\upsilon_k(t,s,\tau)=x_0(t,s)+\tau(x_k(t,s)-x_0(t,s))$ $(k=1,2,...,n)$, $l_{n,k}(x)$ are fundamental polynomials of the *n*-degree with respect to the Chebyshev system of functions $\{\varphi_k(x)\}_{k=0}^{n}$, $l_{n,k}(x_j)=\delta_{kj}$ is the Kronecker symbol $(k,j=0,1,...,n)$, and $\sigma_n(x)=\sum_{k=0}^{n}l_{n,k}(x)$ is a constant or a variable value. The polynomial (2) satisfies to the following interpolation conditions:

$$L_n(F;x_k)=F(x_k),(k=0,1,...,n).$$

For the interpolation error $r_n(x)=F(x)-L_n(F;x)$, where $L_n(F;x)$ is interpolation polynomial (2), the following representation holds:

$$r_n(x)=\sum_{k=1}^{n+1}\int_0^1\sum_{i,j=0;i+j\le 2}^{2}\frac{\partial}{\partial\left(\dfrac{\partial^{i+j}\upsilon_k}{\partial t^i\partial s^j}\right)}F(\upsilon_k(t,s,\tau))\times$$
$$\times\frac{\partial^{i+j}}{\partial t^i\partial s^j}\left\{\left(\frac{l_{n+1,k}(x(t,s))}{\sigma_{n+1}(x(t,s))}-\frac{l_{n,k}(x(t,s))}{\sigma_n(x(t,s))}\right)(x_k(t,s)-x_0(t,s))\right\}d\tau,$$

where $x_{n+1}=x$, $l_{n,n+1}(x)\equiv 0$ 1_{n,n+1}.

Some other interpolation formulas for the operator (1) are also constructed.

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MATHEMATICAL METHODS FOR COMPLEX SYSTEMS

BEYOND THE PHENOMENOLOGY OF THE BCS MODEL

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By a reevaluation of the grandcanonical partition function, we show that the phenomenology of the BCS model is much richer than previously known: the phase transition may be discontinuous (the energy gap has a jump at the phase transition temperature), there may be two solutions for the energy gap at the same temperature, etc. We present both zero temperature [1] and finite temperature results [2].

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ELASTIC FORM FACTORS FROM SEPARABLE KERNEL

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The method of construction of bound systems (deuteron, pion) based on the separable kernels of interaction is discussed. Also the work describes a way of studying the EM characteristics of such the systems, including elastic form factors. The questions of gauge-invarience are discussed. Comparison with the experimental data is carried out.

PERCOLATION PROCESS IN THE PRESENCE OF VELOCITY FLUCTUATIONS: TWO-LOOP APPROXIMATION

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Critical behaviour of directed bond percolation is studied in presence of an advective velocity field [1,2]. The velocity field is modeled by Kraichnan ensemble [3]: time-decorrelated compressible Gaussian velocity field. The model is studied by means of field-theoretic approach. Renormalization group (RG) method is used in order to analyse asymptotic large-scale behaviour of the model near its critical point and to calculate perturbatively all fixed RG points and critical exponents in the framework of double-expansion scheme [4,5]. We classified possible asymptotic regimes corresponding to infrared stable fixed points of the RG equations which have been calculated up to the two-loop approximation.

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LATTICE STUDY OF EFFECTIVE GLUON MASS AT VARIOUS BOUNDARY CONDITIONS

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We extract effective gluon mass from zero-momentum gluon correlators in the SU(2) lattice Quantum Chromodynamics (QCD). Lattice simulations of these correlators have been done both for (i) periodic and (ii) so-called “open” boundary conditions. We found that the results for effective mass obtained in cases (i) and (ii) get closer when the lattice size increases. Nonzero effective gluon mass found for zero-momentum gluon correlators can be viewed as additional confirmation of “decoupling”, or “massive”, solution found in lattice simulations of momentum-dependent gluon correlators, accomplished both in SU(2) and SU(3) QCD.

APPROXIMATE FORMULAE FOR EVALUATION OF EXPECTATIONS OF RANDOM FUNCTIONALS BASED ON CHAOTIC DEVELOPMENT WITH RESPECT TO MULTIPLE ITO INTEGRALS

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The report is devoted to numerical evaluation of mathematical expectations of functionals defined on trajectories of stochastic processes. Our approach is to use quadrature formulas exact for functional polynomials of the trajectories of the process, as it was considered in [1,2]. Construction of this type of formulas is strongly dependent on way of giving the stochastic process. In [1,2] the quadrature formulas are built in the cases where the characteristic functional of the process is known in explicit form. Some results are received in the cases where the process is the solution of Ito stochastic differential equation [1-3]. Application of chaotic expansions of one class of functionals defined on the trajectories of Gaussian processes with respect to functional Hermite polynomials is considered in [4]. In this report we use chaos expansion with respect to multiple Ito integrals to construct quadrature formulae for calculating of nonlinear functionals of one class of stochastic Levy process

containing continuous and discontinuous components. The formula is exact for symmetric functional polynomial of third degree, so we use in the construction the product formula of multiple Levy-Ito integrals [5].

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TURBULENT MIXING OF A CRITICAL FLUID: THE EXACT RENORMALIZATION

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Non-perturbative Renormalization Group (NPRG) technique is applied to a stochastical model of non-conserved scalar order parameter near its critical point, subject to turbulent advection. The compressible advecting flow is modelled by a random Gaussian velocity field with zero mean and correlation function $\left\langle \upsilon_j \upsilon_i \right\rangle \sim \left(P_{ji}^{\perp} + \alpha P_{ji}^{\parallel} \right) \Big/ k^{d+\zeta}$. Depending on the relations between the parameters ζ, α and the space dimensionality d, the model reveals several types of scaling regimes. Some of them are well known (model A of equilibrium critical dynamics and linear passive scalar field advected by a random turbulent flow), but there is a new nonequilibrium regime (universality class) associated with new nontrivial fixed points of the renormalization group equations. We have obtained the phase diagram $\left(d,\ \zeta \right)$ of possible scaling regimes in system. The physical point $d = 3,\ \zeta = 4/3$ corresponding to three-dimensional fully developed Kolmogorov's turbulence where critical fluctuations are irrelevant, is stable for $\alpha \lesssim 2.26$. Otherwise, in the case of "strong compressibility" $\alpha \gtrsim 2.26$, the critical fluctuations of the order parameter become relevant for tree-dimensional turbulence. Estimations of critical exponents for each scaling regimes are presented.

RENORMDYNAMICS (RD) AND GENERALIZED ANALYTIC FUNCTIONS (GAF)

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Concise introduction in RD and GAF with some applications.

ANOMALOUS SCALING IN COMPRESSIBLE KAZANTSEV-KRAICHNAN MODEL WITH SPATIAL PARITY VIOLATION

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The field theoretic renormalization group and the operator product expansion are used for the investigation of the inertial-range anomalous scaling behaviour of the single-time correlation functions of the weak magnetic field within the framework of the compressible Kazantsev-Kraichnan rapid change model with spatial parity violation of the corresponding conductive turbulent environment. Two-loop expressions for the critical dimensions of the leading composite operators in the operator product expansion are found as functions of the compressibility and helicity parameters. Their influence on the hierarchy of the anisotropic contributions to the anomalous dimensions is discussed and it is shown that the crucial role is played by the composite operator near the isotropic shell in agreement with the Kolmogorov isotropy restoration hypothesis. It is shown that the presence of the helicity as well as that of the compressibility of the electrically conductive turbulent environment can have a nontrivial impact on the scaling properties of the correlation functions of the passive magnetic field, namely, to make the anomalous scaling more pronounced than in the incompressible and non-helical case.

THE NUMERICAL EVALUATION OF UNIVERSAL QUANTITIES OF DIRECTED BOND PERCOLATION: THREE-LOOP APPROXIMATION

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Universal quantities (anomalous dimensions and critical exponents) of directed bond percolation are calculated by the renormalization group method in higher order perturbation theory. We put forward a renormalization procedure for a numerical calculation in which the quantities are expressed in terms of irreducible renormalized Feynman diagrams. The procedure is based on the perturbative renormalization scheme in formally small parameter ε, where $\varepsilon = 4 - d$ denotes a deviation from an upper critical dimension. Numerical calculation of integrals has been performed using Vegas algorithm from CUBA library. Main results of our approach is a calculation of the dynamical exponent z and the critical exponent η to the third order in ε expansion.

FINITE SIZE EFFECTS IN THE THERMODYNAMICS OF A FREE NEUTRAL SCALAR FIELD ON THE LATTICE AND IN THE CONTINUUM

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The exact analytical lattice results for the partition function of the free neutral scalar field in one spatial dimension in both the configuration and the momentum space were obtained in the framework of the path integral method. The symmetric square matrices of the bilinear forms on the vector space of fields in both configuration space and momentum space were found explicitly. The exact lattice results for the partition function were generalized to the three-dimensional spatial momentum space and the main thermodynamic quantities were derived both on the lattice and in the continuum limit. The thermodynamic properties and the finite volume corrections to the thermodynamic quantities of the free real scalar field were studied.

COMPARISON OF OPTIMAL CONTROL PROPERTIES FOR LINEAR FRACTIONAL-ORDER SYSTEMS DESCRIBED BY EQUATIONS WITH DIFFERENT TYPE OF FRACTIONAL DERIVATIVE

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Linear time-invariant fractional-order systems with lumped parameters considered in several cases, which differ from each other by fractional derivative type in system dynamics equation. The Caputo, Riemann-Liouville and Hadamard derivatives used. Two kinds of optimal control problem are investigated: the problem of control with minimal norm and the problem of control with minimal time at given restriction on control norm. Admissible controls allowed to be the p-integrable functions $(p>1)$ at half-interval. The optimal control problem studied by moment method. The correctness and solvability conditions for the corresponding moment problem are derived. For several special cases the optimal control problems stated are solved analytically. Some analogies pointed for results obtained with the results which are known for integer-order systems. Comparative analysis results represented for fractional-order systems describing by equations with Caputo-, Riemann-Liouville- and Hadamard-type derivatives.

NONLINEAR SPINOR FIELD IN NON-DIAGONAL BIANCHI TYPE SPACE-TIME

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Within the scope of non-diagonal Bianchi cosmological models we have studied the role of spinor field in the evolution of the Universe. Unlike in diagonal Bianchi models such as I, III, V, VI0 and VI where spinor field distribution along the main axis is isotropic and becomes zero for linear spinor field, in case (non-diagonal) Bianchi models such as II, VIII and IX, spinor field distribution along the main axis is anisotropic and does not vanish in absence of spinor field nonlinearity. The equation for volume scale V in case of diagonal Bianchi models can be resolved exactly and the corresponding solution can be presented as quadrature. In case of non-diagonal Bianchi models the corresponding equation contains a term with the firs derivative of V explicitly and does not allow exact solution in quadrature.

In absence of non-diagonal components of energy-momentum tensor non-diagonal Bianchi spacetime becomes locally rotationally symmetric. Inclusion of spinor field does not change the situation as well.

It was found that depending on the sign of coupling constant the model allows either an open Universe that rapidly grows up or a close Universe that ends in Big Crunch singularity.

ON THE GENERALIZED SUNDMAN TRANSFORMATIONS AND INTEGRABLE LIÉNARD-TYPE EQUATIONS

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In this talk we discuss applications of the generalized Sundman transformations for finding families of integrable Liénard-type equations. Under integrable equations here we understand equations for which we can construct the general analytical solution. Employing connections, given by the generalized Sundman transformations, between Liénard-type equations and equations of the Painleve-Gambier type we demonstrate a possibility of finding new integrable Liénard-type equations. We consider connections between Liénard-type equations and type I-III Painleve-Gambier equation. As a result, we obtain nine criteria for the integrability of the Liénard-type equations. We also consider applications of this approach for finding autonomous Lagrangians, Jacobi multipliers and first integrals for Liénard-type equations.

DISTRIBUTED AND PARALLEL COMPUTING AND TOOLS FOR SCIENTIFIC COMPUTING

NEW HYBRILIT CLUSTER MODULE DEVOTED TO GRAPHICAL APPLICATIONS

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The heterogeneous cluster HybriLIT [1] enables high performance computing (HPC) in JINR by means of a modular architecture involving multi-core processors, coprocessors and graphical accelerators. A lately acquired HybriLIT module – the virtual desktop infrastructure (VDI) – secures the coverage of another vital need, the resource intensive graphical applications.

The VDI implementation merges both cloud services and HPC resources within two kinds of virtual desktop solutions. The QUVE/KVM [2] based solution answers the cases when no dedicated GPU resources are requested. The XenServer [3] with Citrix Xen software [3] enables the use of high performance GPU resources as well.

The present paper provides technical details of the VDI implementation. Typical scenarios enabling remote access to the graphic applications are described. They allow the SaaS (software as a service) use of HPC resources by the end users.

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TESTS OF DIFFERENT MPI IMPLEMENTATIONS IN HPC/KVM CLUSTER

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The work explored the possibility of combining Cloud and High-performance computing (HPC) cluster into a single system. Message Passing Interface (MPI) is the most popular programming technology used for parallel calculations conducted on HPC cluster. The solution of the problem of combining Cloud and HPC cluster is of interest to investigate the efficiency of MPI technology when it is used on virtual machines.

In this paper various MPI implementations (IntelMPI, OpenMPI) were tested on virtual machines based on Kernel Virtual Machine (KVM) [1] hypervisor. The test polygon was placed on the Dell PowerEdge FX2 server which consists of 8 computing units with 2x CPU Intel Xeon E5-2680 v3, 256 GB RAM. Each computing unit was connected to others by integrated 10 Gbit/s switch.

During the tests all available combinations of connections to local network and types of virtual network card supported by KVM hypervisor were investigated. For each combination the test of network's bandwidth and processor load were measured.

Testing was carried out for two cases: 1) when virtual machines were placed on different physical computing units; 2) when virtual machines were placed on the same physical computing unit.

Various MPI implementations were used following tests: Intel MPI Benchmarks [2], the program for calculating CVC in Long Josephson Junctions [3], science package GIMM_FPEIVE [4] and so on. The results of the efficiency of MPI-tasks performed in HPC/KVM cluster are presented.

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ANALYSIS OF POLYDISPERSED VESICULAR SYSTEMS STRUCTURE: PARALLEL IMPLEMENTATION OF THE SEPARATED FORM-FACTORS METHOD

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The separated form factors method (SFF) is an effective approach to obtain information about a structure of vesicular systems from the small angle scattering data. Parameters of vesicular system are determined by means of minimization of a discrepancy between experimental data on intensity of small angle scattering and the results of respective SFF-based calculations. The minimization procedure is based on the least square method which was employed in the code FUMILI from the library JINRLIB. In this contribution, we utilize the parallel MPI-version of this code. Effectiveness of parallel implementation is tested on the cluster HybriLIT. Results of numerical analysis of small angle neutron scattering data on polydispersed population of phospholipid vesicles are presented.

The work is supported by the Russian Scientific Foundation (project No. 14-12-00516).

MACHINE-LEARNING ALGORITHMS FOR CLASSIFICATION AND SEPARATION OF NOISY SIGNALS

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The main goal of this paper is to investigate the applicability of machine learning methods for processing and classifying experimental data obtained from the DEMON detector, as well as a comparative analysis of their effectiveness.

Detectors of the DEMON type are one of the basic measuring elements in the ATLAS and ALICE experiments and are usually used for detecting neutrons and gamma quanta.

The standard software package for this detector allows you to convert all events into energy diagrams that are recorded and saved for later statistical and mathematical analysis. The main problem of statistical processing of the obtained data is the separation and identification of events corresponding to neutrons and gamma/quanta. The double integration method used to solve it in the framework of standard software does not allow us to clearly identify and separate these events at certain energy intervals.

This fact motivated us to apply modern methods of machine learning to this problem.

SHOWERS SIMULATION STUDY OVER CAUCASUS REGION BY WRF MODEL BASED ON GRID COMPUTING

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The main goal of this paper is investigation of some singularities and specific features of atmosphere flows above the complex terrain of the Georgian territory, for prediction a regional scale dangerous events (heavy rains, hails) formation by different cumulus parameterization (CPSs) and micro physics (MP) schemes. To achieve the specified goal, we have used 3-D non-hydrostatic, non-stationary Whether Research Forecast – Advanced Researcher Weather (WRF-ARW) version 3.6 model. We have configured the WRF-ARW nested grid model for Caucasus region considering geographical-landscape character, topography height, land use, soil type and temperature in deep layers, vegetation monthly distribution, albedo and others. Investigations required High Performance Computer systems. That is way we have ported the WRF-ARW application to the GRID site GE-01-GRENA in Georgia which is located at Georgian Research and Educational Networks Association (GRENA). As GRENA connected in European GRID infrastructure so it was a good opportunity for running model on larger number of CPUs and storing large amount of data on the grid storage elements. The ability of the WRF model in prediction precipitations with different set of these MP and CPSs was examined using two precipitation events occur on the territory of eastern Georgia for warm season of 2015. Two set of domains with horizontal grid-point resolutions of 6.6 and 2.2 km are chosen to represent complex topography in

current research WRF v.3.6 model. Accumulated total (24 h) precipitations are evaluated by careful examination of meteorological radar and radio zoned data and simulated fields. Some results of the numerical calculations performed by WRF model are presented.

PARALLEL CALCULATIONS IN OPTIMAL CONTROL PROBLEM

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We consider the problem of choice of angle of attack and bank by a device which is slowed down in the atmosphere for the flight on the minimum of maximum heat with constraints on the value of full loading factor. The solution of mentioned problems allows to determine maneuver abilities of the device. The constraints on full loading factor (control-state constraint), the lift force coefficient (control), constraints on the bank, typical device area, the drag force coefficient, mass, the boundary conditions are parameters. For the solution proposed problem we use two stages approaches. On the first stage we determine geometry of optimal trajectory on inequality constraints. Here we solve a non-linear programming problem with the help of factor analysis. On the second stage we verify received solution by the maximum principle in the form of Dubovitsky-Milyutin. For all proposed algorithms we use parallel calculations.

WEB PLATFORM FOR SHARING MODELING SOFTWARE IN THE FIELD OF NONLINEAR OPTICS

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We present a web platform intended for sharing of software programs for computer modeling of nonlinear optics phenomena. Nonlinear optic is a rapidly evolving area of modern physical research and engineering with many important applications such as fiber-optic communications, nonlinear spectroscopy, diagnostic of non-stationary and inhomogeneous processes in plasma and gas phases, laser biomedicine, etc. Successful development of optical devices requires complicated modeling of physical processes that occur in components of devices and comprehensive database of optical properties of used materials (see e.g., [1]). Many developers of application software, including those for computer modeling, have the intention to share their products for use by other researchers. However, individual developing and maintaining hardware and software infrastructure supporting the delivery of a product is disadvantageous from a financial point of view and from the point of view of time spent on its creation. Therefore, a very important task is to develop a web platform where users of application software, presented in the form of web services, and their providers be able to directly interact.

The suggested platform is build on the top of the HUBZero open-source middleware

(http://hubzero.org) [2]. It provides services for application software installation and includes a set of tools for simplifying the interaction between the software developers and resource administrators. In particular, the platform comprises tools for transforming application software (with allowance for certain rules for API) into software as a service (SaaS). It also provides facilities for supporting communities of users (including on-line seminars, network conferences, storages of domain-specific information, etc.). General architecture of the web platform has the three-layer architecture. The first layer is the frontend that provides the user web interface; the second layer consists of the platform engine responsible for job submitting, obtaining results, the system of remote software deployment, the administration system (responsible for user management, tool configuration, etc.); the third layer is a resource manager that exposes data and compute resources to the preceding layer. The web platform uses the technology of virtual machines [3], which provide both security (software isolation) and an operating system required for a given application software. Users can interact with the platform through the web browser interface.

Such a resource has no analogues in the field of nonlinear optics and will be created for the first time, therefore allowing researchers to access high-performance computing resources that will significantly reduce the cost of the research and development process.

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MOCK DATA CHALLENGE FOR THE MPD/NICA EXPERIMENT ON THE HYBRILIT CLUSTER

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The simulated data processing before receiving first experimental data is an important issue in the high-energy physics experiments. This work presents Mock Data Challenge (MDC) for the MPD experiment at the NICA accelerator complex. It uses the ongoing simulation studies to exercise in a stress-testing distributed computing infrastructure and experiment software in the full production environment from simulated data through a physical analysis. The current Event Data Model of the MPD experiment will be shown, and the MpdRoot software of the experiment based on this model will be noted. The report briefly describes a hardware part – the current structure of the heterogeneous computations cluster HybriLIT of the Laboratory of Information Technologies. In addition, software for parallelization of the MPD data processing is noted. The MDC presented in the work allows one to test the full processing chain (simulation, reconstruction and following physical analysis) for the MC data stream parallelized by the MPD scheduling system on the HybriLIT cluster and helps to identify its potential issues.

APPLICATION OF SLURM, BOINC AND GLUSTERFS AS SOFTWARE COMPLEX FOR SUSTAINABLE MODELING AND DATA ANALYTICS

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Modern numerical modeling experiments and data analytics problems in various fields of science and technology reveal wide variety of serious requirements for distributed computing systems. Many scientific computing projects sometimes exceed allowed resource pool limits, requiring extra scalability and sustainability. In this paper we share the experience and findings of our own on combining power of SLURM, BOINC and GlusterFS as software complex for scientific computing. Especially, we suggest a complete architecture and highlight important aspects of systems integration.

APPLICATION OF METHODS OF MACHINE LEARNING AND DATA MINING TO PROBLEMS OF INSTITUTIONAL ECONOMICS

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Methods of machine learning and data mining are widely used now in many tasks of physics, chemistry, biology, medicine and in some other areas. Such techniques allow to obtain reliable results in poorly formalized areas. The last several years we used these methods for search of regularities in panel data of the statistical indicators, characterizing the institutional economy of different countries of the world. Consideration of influence of institutional characteristics of the countries connected with features of the legislation (for example, the property rights), traditions, habits of citizens of the concrete countries on indicators of economic development is important for borrowing of their experience, including, economic. Our analysis is based on variety of machine learning tools including some original techniques. For verification of the identified regularities the methods based on permutation tests, which do not demand aprioristic assumptions of the nature of probabilistic distributions, and allowing correct application at the small data set. Panel data researches usually are associated with analysis of a large number of the factors, characterizing relative dynamics of economic indicators. So they demand adequate accounting of multiple testing problem.

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ASTROPARTICLE DATA LIFE CYCLE INITIATIVE

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Nowadays the exponential growth of the amount of experimental data can be observed. While there was 1-10 Tb of data per year in astrophysics 10-15 years ago, new experimental facilities generate data sets ranging in size from 100's to 1000's of terabytes per year.

It's obvious that various activities must be performed continually across all stages of the data life cycle to help support effective data management: the collection and storage of data, its processing and analysis, refining the physical model, making preparations for publication, and data reprocessing taking refinement into account. An important topic for modern science in general and astroparticle physics in particular is open science, the model of free access to data. This approach is especially important in the age of Big Data, when a complete analysis of the experimental data cannot be performed within one collaboration.

The present project will strive to develop an open science system to be able to collect, store, and analyze astrophysical data having the TAIGA and KASCADE experiments as the examples.

This is an innovative approach that will be used in astroparticle physics research for the first time. Plans are underway to expand the number of experiments by exporting data from other scientific collaborations, it will rapidly advance the research of fundamental properties of matter and the universe.

ANALISYS OF THE DISTRIBUTION OF THE BEAM IN PARTICLE ACCELERATORS

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In particle accelerator physics the problem is that we cannot see what is going on inside the working machine. There are a lot of packages for modelling the behaviour of the particles in numerical or analytical way. The idea is to provide scientists with a problem-solving environment, which can not only do some numerical calculations, but show the changes of the particle distribution as a motion 3D picture.

DDS – THE DYNAMIC DEPLOYMENT SYSTEM

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The Dynamic Deployment System (DDS) is a tool-set that automates and significantly simplifies a deployment of user-defined processes and their dependencies on any resource management system (RMS) using a given topology.

A number of basic concepts are taken into account in DDS. Namely, DDS implements a single responsibility principle command line tool-set and APIs. The system treats users' tasks as black boxes – they can be executables and scripts. DDS doesn't depend on RMS and provides deployment via SSH, when no RMS is present. It doesn't require pre-installation and pre-configuration on the worker nodes. DDS deploys private facilities on demand with isolated sandboxes. The system provides a key-value property propagation service for tasks. DDS provides a rule-based execution of tasks.

In this report detailed description, current status and future developments of the DDS will be presented.

CONCEPT OF A CLOUD SERVICE FOR DATA PREPARATION AND COMPUTATIONAL CONTROL ON CUSTOM HPC SYSTEMS IN APPLICATION TO MOLECULAR DYNAMICS

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The development of computer technology greatly expanded the possibilities of computational experiment. At the present stage it is already possible to study the properties and processes in complex systems at the molecular and even atomic level, for example, by the means of molecular dynamics (MD). The most interesting are problems related with the study of complex processes under real physical conditions.

Solving such problems requires the use of high performance computing systems of various types, for example, GRID systems and HPC clusters. For parallel calculations using the MD methods it is necessary to create an initial structure of computational domain, which describes the starting conditions, types and properties of the particles involved in the simulation.

Also, considering long-time computational tasks, there is a need for software of automatic monitoring such tasks and data relocation from HPC to the user storage.

Most of these actions today a scientist performs manually.

Authors will present the concept and the prototype of cloud service KIAM MolSDAG, intended for design of atomistic systems of large volume for further detailed molecular dynamic calculations. The main objective of the service is to provide a user the interface for designing an atomistic structure and then the preparation of input data for its numerical analysis using a variety of MD simulators. The second task of this service is to deploy, monitor and relocate the calculation-related data on the user-defined HPC system.

The individual elements of the service have already been implemented and confirmed the effectiveness of the overall service concept.

WEB SERVICE FOR ANALYSIS OF EXPERIMENTAL DATA ON HPC PLATFORMS USING PACKAGE ROOT

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Scientists get large amount of raw experimental data when conducting experiments. These data are analyzed using package ROOT. Processing of large data requires high-performance computers; thus, analysis of experimental data is performed on high-performance clusters.

Conducting data analysis on cluster requires some preparatory work: it is necessary to download files to the cluster, write macros, download results, etc. Also, it is important to note that users work remotely and this might cause some problems, in particular, slow response time of GUI.

For a more efficient work on the cluster and optimization of the process of experimental data analysis, a dedicated web service has been developed. This web service allows computing users tasks on high-performance cluster while visualizing results on the client computer. The web service communicates with task manager and distributed file system of the computing complex.

Users can create, delete, start and stop tasks on cluster. The web app has several templates for different types of user tasks that makes it possible to quickly create new task and submit it for computation on the cluster. Users can also browse directories and open files on the file system of the cluster using web interface.

RO-14-ITIM, UPGRADES FOR A DISKLESS SITE

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Grid site are a challenging job, but in they can modify for the greater good. They can become from full Grid sites just to simple processing units or simple storage systems. Everything depends on financial support or financial and human support. At the National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM) Cluj-Napoca, there is such a Grid site which in the last time because of lack of financial support and low storage capacity has to change his status from a full site to a diskless site for the ATLAS processing experiment. This paper will present the last year thinking and solution for upgrading the site to a strong processing system for single and multi-core jobs from around the world.

IMAGE CLASSIFICATION BY SHALLOW AND DEEP NEURAL NETWORKS

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The paper intends to demonstrate the advantages of deep learning approaches over ordinary shallow neural network (NN) on their comparative applications to image classifying. An autoassociative neural network is used as a standalone program realized the nonlinear principal component analysis (NLPCA) for prior extracting the most informative features of input data for neural networks to be compared further as classifiers. Two special studies devoted to the optimal choice of activation function, the normalization transformation of input data and to denoising properties of our NLPCA algorithm demonstrate its efficiency even on noisy data. Three types of neural networks are compared: feed-forward NN with one hidden layer, deep NN with several hidden layers and deep belief NN with several pretraining RBM layers. The number of hidden layer and the number of hidden neurons in them were chosen by cross-validation procedure to keep balance between number of layers and hidden neurons and classification efficiency. Results of our comparative study demonstrate the undoubted advantage of deep networks, as well as denoising power of autoencoders. In our work we use both GPU and cloud services to speed up our calculations.

COMPUTER MODELING OF A DISPERSED STORAGE SYSTEM FOR PRIVATE DATA ON PUBLIC RESOURCES IN P2P NETWORKS FOR DETERMINING THE OPTIMAL VALUES OF ITS PARAMETERS

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We present a project devoted to a development of a reliable, secure, and convenient dispersed storage system for private data on public resources in the Internet based on peer-to-peer (P2P) networks [1,2], as an alternative to centralized solutions, including clouds. Novelty of the offered project is the research of the behavior of dispersed storage system (DSS) and determining the optimal parameters of its operation under the conditions of high volatility of resources within a P2P network. The proposed method of solving the problem is the computer modeling and analysis of the various algorithms of routing of private data between its owners and the providers of the resources based on computer modeling, and multi-objective optimization of the parameters of information dispersal algorithms (IDA) [3] under the conditions of dynamically changing P2P network. In particular, effective integration of IDA in DSS implies mutual optimization of the choice of a particular variant of IDA, type (structured, unstructured, hybrid) of topology of the overlay P2P-networks, search and data routing algorithms, techniques for checking retrievability of undistorted data stored on a particular node of the network as well as the timely restoration of lost fragments in dynamically changing network.

There is a number of approaches and methods for the solution of tasks of such multi-objective optimization [4]. In particular, in the project it is supposed to use the adapted version of a method of the weighed sums (in more general context such approach is called a scalarization of the multi-objective optimization). Up to now these methods were not applied to assessment of efficiency of data stores on the basis of peer-to-peer networks. The parameters of DSS operation will be optimized for different external conditions and dynamic change of a network, in particular at different speeds and types of nodes disappearing (churn, failure, crash), and also joining of the network by new nodes. The study of the functioning of the network and the search for the optimal parameters of its operation will be based on computer simulation that will estimate functionality, performance, scalability and reliability of the DSS.

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MODIFICATION OF ADAPTIVE ARTIFICIAL VISCOSITY FOR SOLUTION OF GASDYNAMIC PROBLEMS ON PARALLEL COMPUTER SYSTEMS

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In work the modified method of adaptive artificial viscosity so-called AIV method is considered. Earlier developed AIV method belongs to schemes a predictor – corrector type. In the procedure of this method between a predictor and the proofreader there is a stage of definition of areas of physical ruptures of the solution, in particular, of areas of an arrangement of shock waves and numerical oscillations. In these areas artificial viscosity which provides monotony of the numerical decision is entered. At the solution of concrete problems on parallel computer systems this method demanded unfairly large number of transfers of data between subareas of computational domain. The modified AIV method is developed for overcoming this problem. The new variant of the AIV method consists of two stages. At the first stage the analysis of the numerical solution on the previous temporary layer is made and amendments to flows for the purpose of ensuring monotony of the solution are calculated. The second stage is responsible for calculations of all physical quantities on the following temporary layer. The modified AIV method has been applied to the solution of the equations of gas dynamics in the presence of shock waves. The carried-out calculations have shown that on a shock wave the quantity of intervals for resolution of her front can increase all by unit. In other areas, in particular, on a depression wave the numerical decision even approaches the exact solution of a task closer. Thus, the offered modification doesn't worsen the AIV method, and at realization on parallel computer systems significantly reduces the overhead costs connected with introduction of adaptive artificial viscosity.

MATHEMATICAL METHODS AND SOFTWARE FOR EXPERIMENTAL DATA PROCESSING

TIME-BASED GLOBAL TRACK RECONSTRUCTION IN THE CBM EXPERIMENT

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CBM ("Compressed Baryonic Matter") is an experiment being prepared to operate at the future Facility for Anti-Proton and Ion Research (FAIR) in Darmstadt, Germany. CBM will explore the high-density region of the QCD phase diagram by investigating nuclear collisions from 2 to 45 GeV beam energy per nucleon. Its main focus is the measurement of very rare probes (e.g. charmed hadrons), which requires interaction rates of up to 10 MHz. A specific feature of the experiment will be the free-running data acquisition fashion, without a hardware trigger. It differs from the traditional event-based approach, and demands taking to account the measurements time-coordinate in track reconstruction, and using smart approaches to cope with an enormous combinatorics.

Physical studies in the CBM experiment are planned to based on the the so called "global" track reconstruction – which means the reconstructed tracks comprise data, obtained from different detectors. Before the authors started their work, the only time-based track reconstruction component, available in the CBM software repository, was an STS-tracks reconstructor L1. The existing CBM global tracking facility Littrack worked only in the event by mode.

Efforts were applied for making the Littrack library be able to work in the time-based mode, as well as to the development of a stand alone time-based solution for creating the global tracks, basing on the already available STS reconstructed track and measured hits in the Time of Flight (ToF) detector.

4-DIMENSIONAL RECONSTRUCTION OF TIME-SLICES

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Traditional latency-limited trigger architectures, typical for conventional experiments with a hardware trigger, are inapplicable for CBM. Instead, the experiment will ship and collect time-stamped data into a readout buffer in a form of a time-slice of a certain length with no isolated collisions, and deliver it to a large computer farm, where online event reconstruction and selection will be performed. Grouping of measurements into physical collisions must be performed in software and requires reconstruction not only in space, but also in time, the so-called 4-dimensional track reconstruction and event building. The tracks, reconstructed with 4D Cellular Automaton track finder, are combined into event-corresponding clusters according to the estimated time at the target position and its errors. The obtained events were given as an input to the KF Particle Finder package for reconstruction of short-lived particles.

J/Ψ→E$^+$E$^-$ DECAYS SELECTION CRITERIA WITH TRD IN CBM EXPERIMENT

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Currently the CBM experiment is being developed in GSI (Darmstadt, Germany) at the FAIR accelerator complex of an international collaboration with JINR. One of the main aims of the experiment is the study of charmonium production in nuclear-nuclear collisions at high energies. The key task in this problem is fast and reliable electron-positron identification using the energy losses of charged particles in the Transition Radiation Detector (TRD). The current paper presents effective algorithm of the trajectories reconstruction in TRD based on the Cellular Automaton model. The comparision of the different electron identification methods is also given.

GLOBAL ALIGNMENT OF BM@N DRIFT CHAMBERS

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Drift chambers (DCH's) constitute an important part of the tracking system of the BM@N experiment designed to study the production of baryonic matter at the Nuclotron energies.

The method [1,2] of particle hit and track reconstruction in the drift chambers has been already proposed and tested on the BM@N deuteron beam data.

In this study the new approach to global alignment of DCH's is introduced and applied in order to correct the systematic errors of experimental data caused by the detectors misalignment. The approach is based on the GEANT backward extrapolation of DCH reconstructed deuteron beam to a position prior to being affected by the BM@N magnetic field. The difference between the extrapolated and the assumed beam position is subsequently used to globally align both the drift chambers.

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BM@N ONLINE MONITORING

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The BM@N experiment is the crucial stage in the technical development of the NICA project. In order to effectively maintain experiment it is extremely important to have uniform

for all detectors, fast and convenient tool to monitor experimental facility. The system implements decoding of the incoming raw data on the fly, preprocessing and visualization on the webpage. Users can monitor any detector subsystem, select specific detector's plane/station, time or strip profile histograms in 1/2/3D view. The system is developed as a part of the BmnRoot package with the use of the CERN jsROOT library. The lighttpd webserver is used.

SIMULATION OF ANTI-MATTER–MATTER INTERACTIONS IN GEANT4

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One of the most exciting puzzles in cosmology is connected with the question of the existence of anti-matter in the Universe. A number of dedicated cosmic ray experiments aim to search for anti-nuclei. Also, anti-nuclei have been observed in nucleus-nucleus and proton-proton collisions by experiments at the RHIC and LHC accelerators. To support the experimental studies of the anti-nuclei a Monte Carlo simulation of anti-nuclei interactions with matter is implemented in the Geant4 toolkit. Geant4 is a software toolkit for the simulation of the passage of particles through matter. Simulation codes for antiptoron and antinucleus interactions with matter were implemented in the FTF model of Geant4. The implementation combines practically all known theoretical approaches to the problem of antinucleon-nucleon interactions. Main components of the simulation algorithm of antiptoron and antinucleus-nucleus interactions in Geant4 will be presented. Good agreement with simulation results and corresponding experimental data is reached.

STRANGE PARTICLES RECONSTRUCTION BY THE MISSING MASS METHOD

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The main goal of modern heavy-ion experiments is a comprehensive study of the QCD phase diagram, in a region of Qaurk-Gluon Plasma (QGP) and possible phase transition to QGP phase.

One of possible signals of QGP formation is enhanced strangeness production. Reconstruction of Σ particles together with other strange particles completes the picture of strangeness production. Σ+ and Σ- have all decay modes with at least one neutral daughter, which cannot be registered by the CBM detector.

For their identification the missing mass method is proposed:

a) tracks of the mother (Σ-) and the charged daughter (π-) particles are reconstructed in the tracking system;

b) the neutral daughter particle (n) is reconstructed from these tracks;

c) a mass constraint is set on the reconstructed neutral daughter;

d) the mother particle is constructed of the charged and reconstructed neutral daughter particles and the mass spectrum is obtained, by which the particle can be identified.

The method can be applied for other strange particles too. In total 18 particle decays with neutral daughter are now included into physics analysis.

SPEED UP APPROACHES IN THE CELLULAR AUTOMATON TRACK FINDER

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Tracking procedure is an important part of event reconstruction in high energy physics experiments. One of the fastest and efficient track finding algorithm is a cellular automaton (CA). It is used in various experiments including CBM at FAIR and STAR at RHIC. CBM and STAR CA track finders have similar implementations. But standard track finding procedure may be not fast enough for online calculations, especially in case of high particle multiplicity.

In this work we consider several methods to speed up CA track finders in STAR and CBM. Different approaches were implemented and investigated. For instance, grid structure allows us to seriously reduce the number of calculations when hits are combined into segments. Using of multimap for merging of neighbouring segments help us quickly exclude impossible combinations. In addition, CA track finder was vectorized taking into account scalability for CPUs with SSE and AVX instructions (128 and 256 bit registers). Appropriate data structures provide to reduce combinatorial calculations and optimise memory usage, which leads to nice speed up for vectorized calculations.

Most of used approaches are common and can be easily applied to different versions of CA tracking algorithms.

STUDY OF THE GEM DETECTOR PERFORMANCE IN BM@N EXPERIMENT

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Gas Electron Multiplier (GEM) detector is developed for modern purposes in elementary particle physics. In the actual BM@N experiment a GEM system is used for trajectories reconstruction of charged particles. The investigation of GEM performance (efficiency and spacial resolution) is presented.

A SCIENTIFIC WORKFLOW SYSTEM FOR SATELLITE DATA PROCESSING WITH REAL-TIME MONITORING

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Fully automatic processing of satellite data is a dream for every space weather scientist. In fact, a streamlined scientific workflow system that can process satellite data automatically and track the details of the data processing history is critical for the efficient handling of fundamental routines used in space weather research. The information that describes the details of data processing history is referred to as "provenance" which plays an important role in most of the existing workflow management systems and also space weather models that use data provided by such systems. The proper scope, representation, granularity, and implementation of a workflow management system can vary from domain to domain and pose a number of challenges for an efficient pipeline design. This paper provides a case study on satellite data processing, storage, and distribution in the space weather domain by introducing the SDDS system. The approach proposed in this paper was evaluated through real-world scenarios and addresses the provenance scope, representation, granularity, and implementation issues related to satellite data processing. Although SDDS is used as a primary data provider for space weather models at SINP MSU, the system can potentially be adapted to a wide range of data processing scenarios in other fields of physics.

LIGHT ION BEAMS FOR ENERGY PRODUCTION IN ACCELERATOR DRIVEN SYSTEMS

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A comparative study of the energy efficiency of proton beams with an energy from 0.5 GeV to 4 GeV and light ion beams (7Li, 9Be, 11B, and 12C) with energies from 0.25 AGeV to 1 AGeV in natural and enriched quasi-infinite U target is presented. The numerical results on the particle transport and interaction are obtained using the code Geant4. The following target optimization issues are addressed: the beam window dimensions, the coolant, the possibility to use a core from low Z materials. The best solution for ADS from the point of view of the energy gain and miniaturization is obtained for 7Li or 9Be beam with an energy of 0.35-0.4 AGeV and a target with Be core.

STABILITY ANALYSIS OF THE IBR-2M PULSED REACTOR IN AN AUTOMATIC REGULATED REGIME AT THE DIFFERENT LEVEL OF AVERAGE POWER

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The IBR-2M pulse reactor is characterized by a high level of reactivity fluctuations and, as a consequence, a high level of fluctuations in the regulated parameter-the amplitude of the power pulses. Fluctuations of the regulated parameter relative to the average level in the standard stabilization regime usually fall within the range of 20% with possible emissions up to 40%, which is close to the limits of the emergency protection operation (50%). Taking this into account, special and contradictory requirements are imposed on the automatic regulator. In this paper, the results of stability analysis of the IBR-2M reactor in the automatic regulating regime at the different level of average power are presented.

PRIMARY DATA TREATMENT SOFTWARE FOR POSITION-SENSITIVE DETECTOR OF SMALL-ANGLE NEUTRON SCATTERING SPECTROMETER IN ISOTROPIC PATTERN SCATTERING CASE

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The modern trends in use of the small-angle scattering method consist in varying a sample environment, e.g. temperature, pressure, magnetic or electric fields. The objects under investigation can be oriented in the field or by the flow of a liquid. In this case the need for the position-sensitive detector (PSD) arises.

The position-sensitive detector of the new type has been created for the YuMO spectrometer. Currently, this spectrometer has a two-detector system with coaxial ring detectors with a central hole [1] and does not have azimutal angle sensitivity. And the SAS package [2-4] is used for its data treatment. PSD is planned to be mount either in the place of one of YuMO detectors, or in addition to them (turning it into three-detector system). And the problem of PSD data processing is actual.

Due to small size of PSD cells statistics in them is often poor. That fact negatively impacts on data treatment. On the other hand, in most of the experiments one needs isotropic pattern of scattering only, when objects in a sample are not oriented. Thus in most cases is possible to combine PSD cells into concentric rings what first improves statistics and finally makes applicable the algorithms already used for data processing in SAS.

To implement this task of data reduction ROOT framework [5] was choosen. The final script [6] allows one to choose the number of rings, to correct their common center if needed, to visualize and to control all the data at every stage of the conversion. The crossection area of a cell and the resulting ring is taken into account. And the next step will be implementing it as the SAS module for reading PSD data directly.

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COMPARING THE EFFECTIVENESS OF PROOF WITH OTHER METHODS OF PARALLELIZM FOR THE EXPERIMENTAL DATA PROCESSING

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The modern scientific research requires careful modeling of experiments, as well as the fast and qualitative processing of a large amount of data. Under that the comparison of the used models and the optimization of the program code are performed. Optimization implies both algorithmic code improvement and the usage of high-performance and parallel technologies.

In high-energy physics, the standard of data analysis and visualization has become ROOT – the object-oriented framework been developed at CERN. ROOT based software is used in most of modern experiments. ROOT provides several options for parallelism. First, it contains PROOF [1] – Parallel ROOT Facility – ROOT extension, which performs interactive analysis on large sets of ROOT files in parallel on multiprocessor machines. Secondly, it allows the use of technologies OpenMP and MPI.

In current paper we compare the effectiveness of all ROOT methods for parallelizing computations, depending on the type of experimental data analysis, on their volume and on the computing platform.

The PROOF cluster is built according to the standard master-workers scheme. Due to the multi-level architecture, which allows creating a hierarchy of master and submaster nodes, this approach can be easily adapted to a wide range of virtual clusters. The user, working in the ROOT session, can start the processes communicating with the PROOF-cluster and submit requests for job processing. Upon receiving request for job processing, a special ROOT application – proofserv – starts on the wizard and on the working nodes for each user session. The process executed on the master coordinates the work between the work nodes and combines the results. At work nodes, the proofserv process does performed the computational work itself, processing individual jobs.

Parallel calculations can also be implemented with the TThread class. A single process can have multiple threads. The actual work is done in the class TThreadImp (or TPosixThread or Twin32Thread).

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NUCLOTRON BEAM MOMENTUM RECONSTRUCTION USING MULTIWIRE PROPORTIONAL CHAMBERS AND DRIFT CHAMBERS IN THE BM@N EXPERIMENT

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Relativistic heavy ion collisions provide the unique opportunity to study nuclear matter under extreme density and temperature. If the energy density in the formed fireball is sufficiently large the quark-gluon substructure of nucleons becomes visible. Theoretical models, however, suggest different possible scenarios to describe these features of strongly interacting matter. New experimental data with high resolution and statistics are needed in order to disentangle different theoretical predictions [1,2]. The BM@N is a fix-target experiment that is meant to fulfil this need.

The BM@N project is considered as a 1st phase of NICA Mega science project. The energy of the beam will vary from 1 to 6 GeV/u. The beams delivered by Nuclotron will be of different types from simple protons to heavy Au. The ability to reconstruct the beam momentum with high precision is one of the methods for showing that the tracking detectors are tuned in the right way and the reconstruction procedure performs well.

The quick overview of the experimental setup is given in the work along with the description of the main tracking detectors. The performance parameters of the detectors and reconstruction algorithms are brought up. The beam momentum reconstruction procedure is described and the results of this procedure are presented for different values of beam energy.

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RADIOACTIVITY REGISTERED WITH A SMALL NUMBER OF EVENTS

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A significant amount of the human knowledge of Nature is based on the evidence which the rigorous mathematics would have called insufficient. However, in some cases (very important ones indeed) the increasing of data statistics is hardly implementable, added to which once such problem has been overcome in one field of the research investigations there appear another ones with the same problem. Radioactivity is a very proliferic source of the information about the atomic and subatomic world, but in some cases it is just an example of the above situation, e.g., experiments on the synthesis of superheavy elements, the outcome of which is always small. The report discusses the different aspects of the data analysis under unfavorable conditions: low statistics, incomplete observation data etc. and their impact on the parameter estimation and the hypothesis testing which in case of the exponential distribution are very unfavorable to the low statistics, since here its most probable event is very far from the expected one. A special attention is given to criteria for an optimum test by its different merits: minimal confidence interval length, maximum covering probability, the most "natural" interpretation, etc.

MATHEMATICAL METHODS AND APPLICATION SOFTWARE COMPLEXES FOR MODELING COMPLEX SYSTEMS AND ENGINEERING

WAVELET-BASED NUMERICAL AND SEMIANALYTICAL METHODS OF LOCAL STRUCTURAL ANALYSIS IN ENGINEERING

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Numerical or semianalytical solution of problems of structural mechanics with immense number of unknowns is time-consuming process. High-accuracy solution at all points of the model is not required normally, it is necessary to find only the most accurate solution in some pre-known domains. The choice of these domains is a priori data with respect to the structure being modeled. Designers usually choose domains with the so-called edge effect (with the risk of significant stresses that could lead to destruction of structures) and regions which are subject to specific operational requirements. Stress-strain state in such domains is important. Wavelets provide effective and popular tool for local structural analysis.

Operational and variational formulations of problems of structural mechanics with the use of method of extended domain are presented. After discretization and obtaining of governing equations, problems are transformed to a multilevel space by multilevel wavelet transform. Discrete wavelet basis is used and corresponding direct and inverse algorithms of transformations are performed. Due to special algorithms of averaging, reduction of the problems is provided. Wavelet-based methods allows reducing the size of the problems and obtaining accurate results in selected domains simultaneously. These are rather efficient methods for evaluation of local phenomenon in structures.

THE DISCRETE-CONTINUAL FINITE ELEMENT METHOD IN ENGINEERING

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Development, research and verification of correct mathematical models and methods of structural mechanics are the most important aspects of ensuring safety of structures and buildings. Finite element method (FEM) is the most popular method of structural analysis. The field of application of discrete-continual finite element method (DCFEM) comprises structures with regular (in particular, constant or piecewise constant) physical and geometrical parameters in some dimension ("basic" direction). Considering problems remain continual along "basic" direction while along other directions finite element approximation is presupposed.

After discretization within DCFEM we obtain resultant multipoint boundary problem for system of ordinary differential equations with piecewise constant numerical coefficients. Solution of such problems is accentuated by numerous factors. They include boundary effects (stiff systems) and considerable number of differential equations. Moreover, matrices of coefficients of a system normally have eigenvalues of opposite signs and corresponding

Jordan matrices are not diagonal. Special method of solution of such multipoint boundary problems of structural analysis has been developed. Its major peculiarities include universality, computer-oriented algorithm, computational stability, optimal conditionality of resultant systems and partial Jordan decomposition of matrix of coefficient, eliminating necessity of calculation of root vectors.

Combinations of DCFEM and FEM are considered as well.

LINEAR APPROXIMATION OF VOLUME INTEGRAL EQUATIONS FOR SOLVING MAGNETOSTATICS PROBLEMS

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Volume integral equations method is considered for calculation of magnetic systems. We discuss an approach, based on finite element linear approximation of unknown vector field variables. Initially a three-dimensional domain is represented as a combination of standard macro-blocks with two-dimensional mesh on the boundaries. This allows to generate three-dimensional mesh in each individual block. Cubature formula methods are used for matrix coefficient calculations. We introduce a special procedure for evaluating matrix elements in a singular case. The results of various magnet systems simulations based on this approach are shown.

SIMULATING FLUID FLOW WITH COMPLEX PHYSICS IN ARBITRARY SHAPED DOMAINS BY CFD CODE FLOWVISION

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FlowVision software is designed for automation of engineering calculations in industrial computational fluid dynamics (CFD). It has a capability to solve complex non-tradition problems involving different physical processes. The paradigm of complete automation of labor-intensive and time-taking processes like grid generation makes FlowVision attractive for many engineers. FlowVision includes an advanced graphical interface, the system for specifying a computational project as well as the system for flow visualization by different methods – from planar to volume visualization.

The software is based on the finite-volume approach to approximation of the partial differential equations describing fluid motion and accompanying physical processes. It provides explicit and implicit methods for time integration of these equations. FlowVision has own split-based method for solving Navier-Stokes equations allowing to solve incompressible as well as supersonic gas flows existing simultaneously in one computational domain. The software includes automated generator of unstructured grid with capability of its local dynamic adaptation and resolving boundary layers. The solver involves two-level parallelism which allows calculations on computers with distributed and shared memory (coexisting in the same hardware). FlowVision incorporates a wide spectrum of physical

models: different turbulence models, models for mass transfer accounting for chemical reactions and radioactive decay, several combustion models, a dispersed phase model, an electro-hydrodynamic model, an original VOF model for tracking moving interfaces. It should be noted that turbulence can be simulated within URANS, LES, and ILES approaches. FlowVision simulates fluid motion with velocities corresponding to all possible flow regimes: from incompressible to hypersonic. This is achieved by using an original all-speed velocity-pressure split algorithm for integration of the Navier-Stokes equations.

FlowVision enables solving multi-physic problems with use of different modeling tools. For instance, one can simulate multi-phase flows with use of the VOF method, flows past bodies moving across a stationary grid (within Euler approach), flows in rotary machines with use of the technology of sliding grid. Besides that, the software solves fluid-structure interaction problems using the technology of two-way coupling of FlowVision with finite-element codes. Some industrial examples of solving challenging problems in the FlowVision software are demonstrated in this paper. The first one is splashdown of a spacecraft after deceleration by means of jet engines. The second problem is simulation of the work of a human heart with artificial and natural valves designed on the basis of tomographic investigations with use of a finite-element model of the heart.

NUMERICAL DAMPING OF OSCILLATIONS OF BEAMS BY USING MULTIPLE POINT ACTUATORS

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Forced transverse oscillations of an elastic beam are described by the equation:

$$y_{tt} = -a^2 y_{xxxx} + g(t,x), \quad 0 \le t \le T, \quad 0 \le x \le l, \quad a = const.$$

The initial conditions: deviation and velocity – are known:

$$y(0,x) = h_0(x), \quad y_t(0,x) = h_1(x). \tag{1}$$

On the boundary of a beam imposes fixing conditions:

$$y(t,0) = y(t,l) = y_{xx}(t,0) = y_{xx}(t,l) = 0.$$

The problem of damping is: to find the control function $g(t,x)$, which allows to get the state of a beam from initial state (1) to final state for the minimum time *T*:

$$y(T,x) = 0, \quad y_t(T,x) = 0.$$

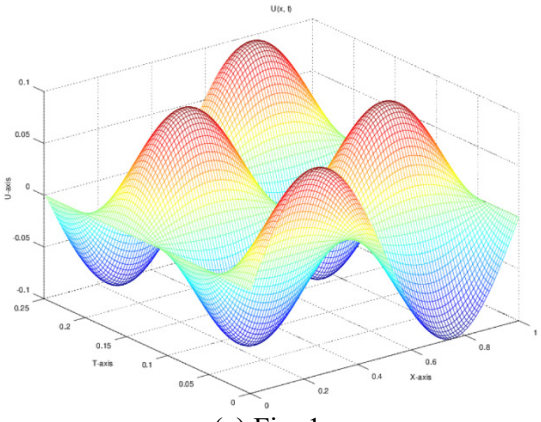
In [1], to solve this problem, there was considered usage of functions specified in the form $g(t,x) = W(t) f(x)$, simulating point actuators, where $f(x)$ is a known function, and $W(t)$ – control function. However, in the case of a static point actuator, the solution of the problem may not exist if actuator is placed in the node of standing waves (Fig. 1).

In this report we consider the damping of oscillations of a beam by using multiple point actuators. The function $g(t,x)$ is considered in the form:

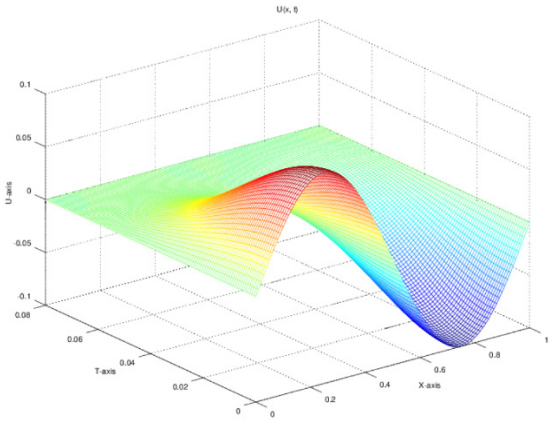
$$g(t,x) = \sum_{i=1}^{n} W_i(t) \delta(x - x_i),$$

where x_i – the points on a beam where actuators are placed, $\delta(x-x_i)$ is Dirac delta function and $W_i(t)$ are control functions. To find the required control functions we use the second order Marquardt minimization method for finding the unconditional minimum of the corresponding functional.

Example. Let us consider a damping of oscillations of a beam with $l=1$, $a=1$ by using one and two point actuators, which are placed at $x_1=0.5$ and $x_1=0.25$, $x_2=0.75$ respectively. The initial conditions (1) are $h_0=0.25\sin\left(\pi x/l\right)$, $h_1(x)=0$, $\varepsilon=10^{-4}$. Figures 1 and 2 show process of damping oscillations of $y(t,x)$.



(a) Fig. 1



(b) Fig. 2

In Fig. 1, 2, respectively, solutions obtained with the single actuator placed at point $x_0=l/2$ (undamped oscillations), and using two actuators (the problem was solved by time $T=0.08$).

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USER SOFTWARE FOR NUMERICAL STUDY OF JOSEPHSON JUNCTION WITH MAGNETIC MOMENTA

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Presented user software is aimed at the field of science research. Potential users are physicists who study Josephson junction with magnetic momenta. Computer implementation has been done by means of Wolfram Mathematica using the extensive capabilities of this system to create interactive dynamic objects. It enables to analyze the problem in amending all relevant physical parameters. The accuracy of the results is controlled. The users can choose a

method for solving the ODE. Advantage of the developed software is the creation of a programming model that implements the method of Runge-Kutta-Fehlberg method in which a predetermined accuracy of calculation is ensured. The results can be displayed in different ways depending on what is needed to the user. The resulting graphs and tables can be used by physicists in their study, articles and presentations.

METHODS OF INVESTIGATION OF EQUATIONS THAT DESCRIBE WAVES IN TUBES WITH ELASTIC WALLS AND APPLICATION OF THE THEORY OF REVERSIBLE AND WEAK DISSIPATIVE SHOCKS

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Different models of tube with hyper elastic walls are investigated. They are tube with controlled pressure, tube filled by incompressible fluid, tube filled by compressible gas. Complete membrane model and non-linear hyper elastic model are used for walls of tube. Linear model of plate is used in order to take bending resistance of walls into account. Equations are solved numerically. Walls of the tube are treated as incompressible. Compressibility of material of walls and viscosity of material and gas of fluid may be taken into account. Simplified hyperbolic equations and Boussinesq-type equations are derived. Stability of solitary waves for the case of controlled pressure is investigated. Analysis of solutions of Riemann problem is made for all models. It is opened that in all cases typical non-dissipative shock structures are predicted by the theory of reversible and weak dissipative shocks. Three-layer centered time and space reversible numerical scheme and similar two-layer space reversible numerical scheme with approximation of time derivatives by Runge-Kutta method are used. It is opened that in the case controlled pressure both methods give good results. But in the case of fluid-filled and gas-filled tube numerical edge instability appears. Numerical scheme based on Runge-Kutta method was used in these cases. It was opened that this scheme possesses non-correct scheme dissipation. Increase of disturbances is observed for long-time calculations. It was opened that there are no such increase if predictor-corrector method with predictor for complete time step is used. In the case of Runge-Kutta method predictor is calculated for half of time step. Hence the same program may be used. But this method is method of first order approximation. It possesses essential numerical viscosity. Non-dissipative shocks become weak dissipative shocks if this method is used. Method of correction of numerical schemes by inclusion of terms with high-order derivatives was developed. Order of approximation of numerical scheme is not changed. Good results for tubes filled by inviscid fluid and gas were obtained. It seems that such approach may be used in all cases of models with evolutional equations. Result of the investigation is a step to development of general approach of calculations of equations with dispersion.

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NUMERICAL SIMULATION OF AEROHYDRODYNAMIC AND AEROHYDROELASTICITY PROBLEMS

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Aerohydrodynamics and aerohydroelasticity problems (also known as Fluid-Structure Interaction (FSI) problems) cause big and uninterrupted interest in science, industry, biomedicine and other applications. Preconditions for a detailed study of the nature of aerohydrodelasticity and the search for methods that let to predict consequences of strong wind impact and solve coupled problems related to the civil engineering were a series of tragic cases of collapse and dangerous structural vibrations as a result of the occurrence of aerodynamic instability (like vibrations of bridges and flexible building structures interacting with wind flow), as well as the destruction of thin-walled metallic tanks with liquid under intense seismic loads. Mentioned problems, characteristic and scientifically significant for very diverse technical applications are still far from their exhaustive solution and require scientific and methodological and program-algorithmic research and development. Present work gives an overview of the existing techniques for solving the considered problems; demonstrates developed numerical technique, based on effective mathematical models and numerical methods; deals with the verification and approbation of the developed numerical technique.

OPTIMISATION OF AIR POLLUTION DISPERSION AND DEPOSITION MODELS

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Gaussian plume models are commonly used class of mathematical models used in the air pollution dispersion and/or deposition modelling. The goal of the study was to optimize computations with the Gaussian model Symos'97 to significantly improve the speed of computations and to migrate computations from proprietary software (ArcGIS, SW implementation of the model for PC) to unified, platform-independent and open source platform via the Python programming language. The result is the Python script module which has been able to speed up whole modeling process by several order of magnitude thanks to more optimal code and parallel processing and make it more user friendly for modelers.

The modelling toolset is going to be used in studies evaluating air quality and studying effectivity of potential air quality remedies within vast regions in a detail scale.

FITTING BY ORTHOGONAL POLYNOMIALS OF SILVER NANOPARTICLES SPECTROSCOPIC DATA

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Our original Orthonormal Polynomial Expansion Method (OPEM) [1] in one-dimensional version is applied for first time to describe the silver nanoparticles spectroscopic data [2,3]. The experimental errors in variables are included in weights for approximation – different in every point. In this way we construct orthogonal (orthonormal) polynomials for presenting the curve. The corridors of given data by the help of the weights define the optimal behavior of sought for curve with the help of some criteria.

We have received four experimental curves in thousands points for analysis. We have chosen one subinterval in one of them. The most important subinterval of spectra data is investigated, where the minimum (surface plasmon resonance absorption) is looking for.

The received results from our numerical experiments are compared with other theoretical curves for the data. We hope that with our description we have pointed the experimental work to regular direction.

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TIME DISCRETIZATION IMPACT ON THE TARGET LOCALIZATION PRECISION USING UWB RADAR

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UWB radar technology enables a target localization of an object, e.g., man behind a wall of known material consistency, e.g., concrete. If exact values of TOA (Time of a signal arrival from a transmitting antenna to a receiver) are known, it is possible to achieve high precision of localization. In the paper an influence of a time quantization on the localization precision will be studied and discussed.

MULTILANE TRAFFIC FLOW MODELLING USING CELLULAR AUTOMATA THEORY

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The paper deals with mathematical modelling of traffic flows on urban road networks. The presented model relates to microscopic approach, i.e. each car is considered separately and is described by its own set of parameters.

The model is based on cellular automata theory and presents generalization of Nagel-Schreckenberg model [1] to a multilane case [2]. The computational domain is a 2D lattice, where two directions correspond to road length and width. A number of cells in the transverse direction corresponds to a number of lanes. Each cell of the lattice can be either empty or occupied by one vehicle. This approach allows vehicles to change lanes and to overtake one another. The algorithm of cell state update is formed by two components: lane change (if it is necessary and possible), movement along the road by the rules of Nagel-Schreckenberg model.

Numerical realization of the model is represented in a form of the program package CAM-2D, that consists of two modules: User Interface and Visualization module (for setting initial conditions and modelling parameters and calculations visual representation) and Computation module (for calculations).

Computations are carried out for each element of the road (i.e. T or X type intersection, strait road fragment) separately and in parallel, that allows performing calculations on various complex road networks.

Computations show that CAM-2D can be used to set up optimal traffic lights regimes on complex road fragments. Besides that, the program package allows to predict the consequences of various decisions regarding road infrastructure changes, such as: number of lanes increasing/decreasing, putting new traffic lights into operation, building new roads, entrances/exits, road junctions.

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QUASI-VECTOR MODEL OF PROPAGATION OF POLARIZED LIGHT IN A THIN-FILM WAVEGUIDE LENS

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In [1], a scalar model of the propagation of electromagnetic radiation in a thin-film waveguide lens is described. The applicability of the model to the approximate description of the depolarization process in a thin-film waveguide lens is investigated. In this paper, based on the ideas underlying the model, we propose an approximate vector model. The proposed model explicitly uses the slow dependence of the Maxwell equations on the transverse horizontal independent variable y and the rapid dependence on the two remaining ones *x*, *z*. In Cartesian coordinates related to the geometry of the regular waveguide on which the thin-film waveguide lens is based, taking into account the small parameter of the ratio of slow and fast variables, we obtain a system of zero order equations for *TE*-polarization and *TM*-polarization.

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MODELING OF STATIC ELECTRIC FIELD EFFECT ON NEMATIC LIQUID CRYSTAL DIRECTOR ORIENTATION IN SIDE-ELECTRODE CELL

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Two-dimensional model of Fredericks effect was used for the investigation of the static electric field influence on nematic liquid crystal director orientation in the side-electrode cell.

The solutions were obtained by finite-difference methods. The programs for numerical solution of two-dimensional parabolic partial differential equation were developed by using both FORTRAN and C++. Fredericks transition threshold for the central part of the cell, as well as dependencies of the distribution of the director orientation patterns on the electric field and location were obtained. The results of the calculation were compared to the experiment.

HIDDEN ATTRACTORS IN BUBBLE CONTRAST AGENT MODEL

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In this work we studied a model, describing dynamics of a spherical gas bubble in a fluid. The bubble is oscillating close to the wall of finite thickness under the influence of external field pressure. This model is a generalization of the well-known Rayleigh-Plesset equation describing dynamics of gas filled bubble in an incompressible fluid. In the model considered in this work, the fact that gas bubble is close to an elastic wall of finite thickness is taken into account. Thus, the model depicts a bubble contrast agent, oscillating in a neighborhood of a blood vessel wall. Besides, in the model being studied, compressibility and viscosity of the fluid are taken into consideration. In earlier works, dedicated to the dynamics of gas bubbles in a fluid, the possibility of existence of hidden attractors was not taken into account. In this work we investigated different motion modes of the bubble oscillations. We used perpetual points method to seek for hidden attractors. We have shown that in the system under investigation there are hidden chaotic attractors and co-existing periodic attractors. Also, we have given an example of existence of hidden chaotic attractor, when the parameters of the system are physically realistic. As well, it was shown that in the range of parameters where this attractor exists, if we vary frequency of the external force, system can unexpectedly switch from periodic motion to chaotic and vice versa. The example mentioned above shows importance of finding of hidden attractors for applications. If chaotic behavior is undesirable, parameters should be choosen in a way avoiding ranges where hidden attractors exist.

ONE PRINCIPLE FOR THE IDENTIFICATION OF SHAPE OF AN OBJECT

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Process of recognition of the shape of graphic objects consists of several stages. At the first stage as a result of processing images some set of characteristic properties of some object are extracted. On the second one, identification of object is made by comparison of these properties with properties of the sample. Presence of noise on real graphical images often distorts quality of characteristic properties. This article describes methods for the extraction of characteristic properties of graphical objects and presents methods for the identification of

object's shape with partly-present or distorted characteristic properties. The advantage of the described methods is their invariance to affine transformations of the shape of object, and also high speed of identification independent on complexity of the object being identified.

HIGH PRECISION COMPUTER SIMULATION OF CYCLOTRONS

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Effective and accurate computer simulations are highly important in accelerators design and production. The most difficult and important task in cyclotron development is the magnetic field simulations. It is necessary to achieve the accuracy of the model that is higher than the tolerance for the magnetic field in the real magnet. An accurate model of the magnet and other systems of the cyclotron allows us to perform beam tracking through the whole accelerator from the ion source to the extraction. While high accuracy is necessary in the late stages of R&D works, high performance of the simulations and ability to swiftly analyze and apply changes to the project plays the key role in the early stages of the project. Techniques and algorithms for high accuracy and performance of the magnet simulations have been created and used for development of the SC202 cyclotron for proton therapy, which is under production by collaboration between JINR (Dubna, Russia) and ASIPP (Hefei, China).

FEATURES OF PLASTIC FLOW LOCALIZATION IN HOLLOW CYLINDER

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The process of plastic flow localization in hollow cylinder which is made from high-strength steel undergoing the torsion deformation is considered. The mathematical model of the process of plastic flow localization is formulated taking into account the cylindrical symmetry of the problem. The transition of the proposed model to a mathematical model describing the processes of plastic flow localization in the plane case is discussed. Numerical algorithm which allows one to simulate the fully localized plastic flow in cylindrical case is proposed. The influence of the geometry of the problem on the processes of plastic flow localization is considered. In particular, the effect of the value of the internal radius of the cylinder on the processes of localization of plastic deformation is studied. It was found that a decrease in the radius of the inner cylinder leads to a substantial change in the solution and to the displacement of the region of localization of the deformation to the inner surface of the hollow cylinder. The effect of nonuniform heating of the sample on the localization of plastic deformation is also investigated. The obtained results are compared with the limiting case, namely, the process of localization of plastic deformation under shear deformations of the plate.

NUMERICAL METHODS FOR THE PREDICTION AND OPTIMIZATION OF THE CRYOSURGERY OPERATIONS

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In this talk we consider the problem of planning and optimization of the cutaneous cryosurgery operations. The method of the additional heating and freezing elements mounting is studied as an approach to optimize the cellular necrosis front propagation. Mathematical modeling is used for the effectiveness improvement of the method under consideration. An explicit scheme based on the finite volume approximation of phase averaged Pennes bioheat transfer model is applied. The flux relaxation method is used for the stability improvement of scheme.

TRANSPORT DESCRIPTION OF HEAVY ION FRAGMENTATION REACTIONS AT ENERGIES OF 35-140 MEV

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Fragmentation reactions are of interest for the production of exotic beams and for accelerator driven applications. They have been well parametrized by empirical methods, but a microscopic understanding of the mechanism is of great interest. One such method is the transport approach which describes the collision as a Hamiltonian mean field propagation together with a dissipative two-body collision term of the Boltzmann-type including Pauli blocking factors. The propagation is treated in the Euler method, while the collision term is simulated stochastically. Here we present a comparative study of such collisions for light and intermediate mass systems in the energy range from Fermi to intermediate energies in relation to experimental data from the FLNR, Dubna, and other laboratories. The primary fragments obtained from the transport calculation are still excited by several MeV/A and the consideration of their de-excitation is important for the comparison to experiment. This is done using statistical multi-fragmentation approach, where the input of the excitation energies of the primary fragments is calculated consistently with the transport method. We discuss the isotope yield distributions as well as the energy or velocity distributions of the isotopes.

From the evolution with incident energy one sees an evolution of the mechanism of the fragmentation reactions. At the lower energies a substantial direct component is seen, which is not well described by the transport approach, while at higher energies the process is dominantly dissipative and is reasonably well reproduced by transport. This evolution is seen particularly in the velocity distributions, which at lower incident energies display an undamped component, probably due to direct transfer-type processes. The main dissipative

component is well described by transport, however, the strongly damped tail of the velocity distribution is not well accounted for. Here most likely fluctuations around the mean field evolution of the system are responsible, the implementation of which is one of the current developments in transport theory.

NUMERICAL ALGORITHM FOR OPTIMIZATION OF POSITIVE ELECTRODE IN LEAD-ACID BATTERIES

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The positive electrode in lead-acid batteries is one of the most sensitive parts of the battery, that is affected by aggressive chemical processes during its life. Therefore, an optimal design of the positive electrode of the battery may have as effect a dramatic improvement of the properties of the battery – such as total capacity or endurance during its life. Numerical optimization of electrodes covers a range of rather complex tasks, from the analysis of the graphical representation of the current distribution to numerical solution of differential equations. We integrate all these in a software package that can be used for the development of optimized electrodes. We present the principles of our analysis as well as several guiding rules to be used for the electrode's design.

MODELING HYSTERETIC EFFECTS IN PEROVSKITE SOLAR CELLS

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Dynamic J-V hysteretic effects [1] are consistently described by the dynamic electrical model (DEM) introduced in Ref. [2]. DEM explains the dependence of the hysteresis amplitude and short circuit current on the bias scan rate. It also reproduces the current

overshoot experimentally observed in the reverse characteristics and its dependence on bias pre-poling. The basic assumption is that the rather slow ion migration process (typically in the order of seconds) governing the time evolution of the polarization charge is described in the single relaxation time approximation, however the steady state polarization charge being a bias dependent quantity. Using DEM we obtain the time dependent solution of the coupled differential equations that govern the dynamic J-V characteristics. Furthermore, analytical extensions are considered.

We investigate here the dynamic J-V characteristics of perovskite solar cells obtained by successive spin-coating deposition of TiO2 thin and meso-porous layers, CH3NH3PbI3-xClx mixed halide perovskite and spiro-OMeTAD on comercial glass/FTO substrate, with Au electrodes [3]. We report the occurrence of normal hysteresis (NH) and inverted hysteresis (IH) in the J-V characteristics in the same device structure, the behavior strictly depending on the pre-poling bias (Vpol).

Using a three step measurement protocol, which includes the stabilization of the open circuit bias (Voc), bias pre-poling at Vpol for a time interval tpol, followed by a reverse-forward scan starting from Voc as actual measurement, we introduce a unified description of the dynamic hysteresis, which can be tuned from NH (Vpol>Vvoc) to IH (Vpol<0) [4]. We also analyze comparatively reverse-forward and forward-reverse scans, with different pre-poling conditions. In this context we discuss the conditions for a correct evaluation of the solar cell power conversion efficiency (PCE).

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APPLICATION OF ARTIFICIAL NEURAL NETWORKS AND SINGULAR-SPECTRAL ANALYSIS IN FORECASTING THE DAILY PASSENGER'S TRAFFIC IN THE MOSCOW METRO

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In this paper, we developed a methodology for the medium-term prediction of daily volumes of passenger traffic in the Moscow Metro. It includes three variants of the forecast:

1) on the basis of artificial neural networks: a multilayer perceptron (MLP) was used, on the input of which a set of factors affecting the daily volume of passenger transportation was supplied;

2) using the singular-spectral analysis implemented in the package "Caterpillar"-SSA: in this case, only the data of the time series of daily passenger traffic were analyzed;

3) joint use of the MLP and the "Caterpillar"-SSA approach: to the input of the neural

network, in addition to the above factors, the forecast data computed using the package "Caterpillar"-SSA were supplied. The developed methods and algorithms allow one to conduct with an acceptable accuracy a medium-term forecasting of the passenger traffic in the Moscow Metro.

SIMULATION OF COLLECTIVE EXCITATIONS IN THE STACK OF LONG JOSEPHSON JUNCTIONS

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We consider the generalized model of the system of coupled long JJs [1] which takes into account the inductive and capacitive coupling and the diffusion current [2,3]. Numerical investigation of phase dynamics of long JJs stack is based on the parallel simulation algorithm which provides an essential acceleration of simulation procedure [4]. Using the developed numerical approach, we demonstrate a creation of charge travelling wave in the system of coupled LJJs. Another important result is related to the demonstration of the coexistence of the charge travelling wave with the standard fluxon mode. This fact indicates an appearance of a new unique collective excitation in the system of coupled Josephson junctions, namely, a composite state of the Josephson current, electric field, and vortex magnetic field. We have demonstrated the effect of this collective excitation on the power of the electromagnetic radiation from the stack of long JJs.

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DIFFUSION PROCESSES IN A MODEL OF VECTOR ADMIXTURE: TURBULENT PRANDTL NUMBER

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One of the most important characteristics of diffusion processes in fluids is the Prandtl number as a ratio of the coefficient of kinematic viscosity to the coefficient of the

corresponding diffusivity. The numerical values of various Prandtl numbers, in general, depend on the microscopic structure of the fluids at low Reynolds numbers. The situation changes when the Reynolds numbers obtain very high values, i.e., in the so-called fully developed turbulence regime. Here, the Prandtl numbers obtain universal values which are known as "effective" or "turbulent" Prandtl numbers. Recently, the turbulent Prandtl numbers were studied in various models of passive admixtures (scalar or vector) in fully developed turbulence given by the stochastic Navier-Stokes equation using the field theoretic renormalization group technique in the second order of the perturbative expansion (two-loop approximation) [1-4].

In the present work the behavior of the turbulent vector Prandtl number is investigated as the function of the spatial dimension $d > 2$ in the framework of the general A model of passively advected vector field, where three important and physically interesting cases, namely, kinematic MHD $(\mathrm{A} = 1)$, linearized Navier-Stokes equation $(\mathrm{A} = -1)$ and admixture of a vector impurity by the N-S turbulent flow $(\mathrm{A} = 0)$, are included. The behavior of the turbulent Prandtl number is studied in the model with the Navier-Stokes fully developed turbulence. Using the field theoretic renormalization group approach in the two-loop approximation we analyzed the dependence of the turbulent vector Prandtl number on the parameter A as well as on the spatial dimension *d*. For detailed analysis and results see [5].

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REDUCTION OF NETWORK TRAFFIC TO POINT IMAGES FOR THE ANALYSIS OF ITS BEHAVIORAL STRUCTURE

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In Cisco Guard XT technology under the protection against DDoS attacks, along with filtering and active verification, uses anomaly detection. In this case, all traffic that is not stopped by the filtering and active verification modules is monitored, and this traffic is matched against the basic behavior recorded for a certain period of time.

In this paper, we propose an approach based on the reduction of numerous parameters of network traffic into point images that form the corresponding time trajectories in 3D and 2D spaces. Initial parameters of the network traffic are obtained from the information generated by the NetFlow protocol (Cisco). In the future, the resulting trajectories can be easily used both at the learning stage and at the stage of anomalies recognizing of network traffic, since it becomes possible both for visual and automatic marking of 3D and 2D spaces to normal and abnormal areas.

Examples of visualization of network traffic are presented, which simplify the analysis of its behavioral structure.

MATHEMATICAL MODELING OF AIR PROLUSION AND APPROACH TO ESTIMATING AND FORECASTING HEALTH INDICATORS OF POPULATION OF ULAANBAATAR CITY

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In this report we considered research results based on mathematical modeling approach to estimating and forecasting health indicators of population of Ulaanbaatar city from influenced of air pollution distribution in the atmosphere.

In particular of the research, the present situation of air pollution sources in the districts on UB's have been broadly reviewed and health impact analysis how it's influenced for health of 0-14, 15-60, over old person's ability to breath. The main sources of air pollution in UB, in no particulate order, include ger district, blast-furnace of low pressure, power plants, means of transports. We forecasting that reduction of air pollution from this main sources by 10, 20, 30 per should decrease illness respiratory way.

SYMBOLIC AND NUMERICAL MODELING OF NONLINEAR DYNAMICS OF PARTICLES IN ACCELERATORS

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The actual task of accelerator physics is the preliminary modeling of particle beam dynamics in an accelerator (including polarized ones). The search for optimal parameters of the control system that provides the necessary functionality of the particle beam particle control system is a resource-intensive problem, which leads to the need to use appropriate mathematical models which naturally allow parallelization and distribution of the corresponding computational procedures. At present, the main tool are software packages based on a numerical of trajectory description of the particle beam, which significantly reduces the efficiency of finding optimal parameters for control elements. In this paper, we consider a method that allowing us to form a map generating by the control system in terms of special matrices and ensure the performance of the necessary properties (for example, symplecticity).

The similar approach makes it possible to effectively use the methods of symbolic computation, which makes it possible not only to significantly reduce the time spent and simplify the analysis procedure, and also to provide the possibility of varying the parameters that ensure the necessary properties of the beam.

In this paper, we present a mathematical method that allows us to construct the necessary solutions, taking into account the symplecticity of the system with a given accuracy. Examples of the solution of such problems are given.

EVOLUTION OF CONTINUUM-ATOMISTIC APPROACH FOR THE MODELING OF IRRADIATION OF METALS BY HEAVY IONS

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Research in the field of materials irradiation by high energy heavy ions (HEHI) has been actively made for several decades. The experiments in this area are labor-consuming and expensive. Therefore, the improvement of existing mathematical models and the development of new ones based on the experimental data of interaction of HEHI with materials is of current interest. Currently, there are used two models for studying these processes: a thermal spike (TS) model [1] and a method of molecular dynamics (MD) [2]. Combining two these models (continuous-atomistic model (CAM)) will give the opportunity to investigate more thoroughly the processes of irradiation of materials by HEHI.

The work presents the evolution of using the CAM when irradiating metal targets with heavy ions of different energies. The applicability of CAM and the essential points of the model are discussed. A software package has been developed to solve the CAM equations and to test the block of MD of the software complex on the heterogeneous HybriLIT cluster [4]. The results of modeling the processes of interaction of uranium ions with different energies with a nickel target are obtained.

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ANALYTICAL SOLUTION FOR EXPERIMENTAL DATA APPROXIMATION BY SOLVING LINEAR DIFFERENCE EQUATIONS WITH CONSTANT COEFFICIENTS

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This paper proposes an analytical method for approximating experimental data points X*(j) by the curves representing the solutions of linear difference equations with constant coefficients, in particular, by the curves of the exp*cos class (for the second-order equation –

in form of

$X(j) = c1 \cdot X(j - 1) + c2 \cdot X(j - 2) + b)$.

As for coefficients of such approximation (c1, c2 and b) – they can be calculated as a solution of system equations just the same as Yule-Walker system of equations. To find the initial conditions (X0 and X1) it is necessary to solve the system of two linear equations based on recurrently calculated values A(j), B(j) and C(j):

For j=0 A(0) = 0, B(0) = 1, C(0) = 0;

For j = 1, A(1) = 1, B(1) = 0, C(1)=0; and for j>=2 as:

$A(j + 1) = c1 \cdot A(j) + c2 \cdot A(j - 1)$;

$B(j + 1) = c1 \cdot B(j) + c2 \cdot B(j - 1)$;

$C(j + 1) = c1 \cdot C(j) + c2 \cdot C(j - 1) + b$;

where c1, c2 and b – primarely finded coefficients (solution of system of Yule-Walker type).

The proposed approach minimizes the root mean square (RMS) deviation. The analysis of two possible sources of noncorrect behaviour of approximating curve was done. The method is tested on some examples.

PERIODIC SOLUTIONS IN ISOTHERMAL PROBLEMS FILTRATION OF HYDROCARBON MIXTURES

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An oscillatory flow regime of the formation fluid is sometimes observed at the operating gas-condensate reservoirs which entails unbalance of the well operation and leads to unstable work of the well. Both external impact of periodic factors and monotonous energy inflows into the system could be the reasons for observed pulsations. The system converts the incoming energy into vibrations due to its nonlinearty. Therefore, investigation of the wave filtration regime, which is discovered during the development of oil and gas-condensate fields, is relevant.

The possibility of occurrence of periodic solutions in the filtration process is associated both with the stability loss of stationary solutions of the general two-phase multicomponent filtration equations and with the transformation of the resolving equation for pressure into wave equation with certain combination of numerical values of its parameters. The solution of the wave equation makes it possible to describe mathematically the conditions for the occurrence of such oscillatory flow regimes for a gas-condensate system in a first approximation.

The paper focuses on a mathematical description of the wave filtration process, obtainment of the periodic solutions of the isothermal two-phase filtration problem and calculation of the period of these oscillations depending on the parameters characterizing the mixture and the porous medium. It is shown that periodic solutions can be obtained not for any values of these parameters, but only for their certain combination.

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NEW METHODS OF DETECTION IN COMPUTER VISION

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The construction of event detectors is still a relevant task, due to dynamic developments in the field of computer vision. We present the new approaches which we developed to achieve superior detection performance for realistic tasks, such as detection of objects, detection of motion and detection of behaviors. These are then successfully implemented in detectors, which can be integrated in real life projects – such as smart cities, security monitoring, safe cities.

ALGORITHM OF THE EXPLICIT TYPE FOR POROUS MEDIUM FLOW SIMULATION

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Development of mathematical fundamentals and software for simulation of complex fluid flows in the subsurface is one of urgent tendencies of industrial mathematics. Among applications of such flow modeling there are oil-and-gas industry problems, in particular, the development of perspective hydrocarbon recovery technologies, as well as ecological problems concerning the soil and groundwater contamination.

The present work is devoted to elaboration of an original mathematical model of porous medium flows constructed by analogy with the quasigasdynamic system of equations and allowing implementation via explicit numerical methods [1]. The model is generalized to the case of multiphase multicomponent fluid and takes into account possible heat sources. It also accounts for gravitational and capillary forces.

The distinguishing feature of the model is modification of phase continuity equations: they get regularizing terms and second order time derivatives with small parameters. The equations' type is changed from parabolic to hyperbolic, consequently they can be approximated by the three-level explicit scheme with rather a mild stability condition; convective terms are approximated by central differences. As the temperature of all phases and the rock is identical the system involves a single equation of the total energy conservation approximated also by an explicit scheme.

To ensure the critical accuracy of the solution of some large-scale oil-recovery problems it is necessary to execute computations with a very small space step what constrains a time step strictly. Then explicit schemes can gain in terms of the total computational time in comparison with implicit schemes. Besides algorithms of the explicit type are preferable as they can be easily adapted to modern HPC systems.

The proposed approach is verified by a number of test predictions. High parallelization efficiency is achieved on a hybrid supercomputer.

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MODELING THERMAL EFFECTS IN METALS IRRADIATED BY COPPER NANOCLUSTERS

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One of the promising and important areas in condensed matter physics is the study of the interaction of nanoclusters with various metallic targets [1]. When nanoclusters interact with a metal target in a small volume, there is a huge energy release per unit volume and this leads to structural changes. The origin of the structural changes can be a consequence of thermal processes or elastic interactions (repulsion of target atoms). In experimental studies, one can only see the effect of structural changes in targets when irradiated with nanoclusters, and the application of mathematical modeling techniques allows one to "see" the entire cycle of the target irradiation process with nanoclusters.

In this paper we investigate thermal processes in metals irradiated with nanoclusters by the molecular dynamics method and within the thermal speak model [2,3]. In the framework of the molecular dynamics method, the wave effects of heat transfer are obtained, what is not observed when the thermal peak model is used. The results of simulation of the structural changes in irradiated targets of different sizes are also obtained depending on the energy of nanoclusters. When processing results, the fractal analysis method [4] is used.

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BIOINFORMATICS AND COMPUTATIONAL BIOPHYSICS

SPECTRAL PHOTOSENSITIZATION OF OPTICAL ANISOTROPY IN POLY(VINYL CINNAMATE) SOLID FILMS

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We observed possibilities and properties of sensitized photo induced optical anisotropy formation in amorphous poly (vynyl-cinnamate) films (PVCi) and its derivant poly (vynyl-4-methoxy-cinnamate) (PVMCi) under polarized light, including the one which is not absorbed by the supermolecules of the polymeric material. The effect of the induced optical anisotropy involves transferring the energy of electronic excitation from the donor molecules (Michler's ketone or 2-benzoyl-methylene-3, methyl-β-naphthosol) to the scavenger's molecules – PVCi or PVMCi) and photo-topochemical ring formation of cinnamate units in polymeric supermolecules. The discovered photo-induced anisotropy in solid PVCi and PVMCi films provides sensitized photo orientation of low-molecular thermotropic liquid crystals.

MODELING OF CHARGE DYNAMICS IN HOMOGENEOUS CHAIN WITH DEFECT

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Various results of numerous biophysical experiments on charge transfer along DNA fragment have demonstrated that different transport mechanisms are possible in DNA. The transfer rate depends not only on the length of the chain along which the transfer occurs, but also on its sequence [1].

We have studied the simple 1D-model based on the semi-classical Holstein Hamiltonian for a discrete chain of sites (for DNA sequence, the site is a complementary base pair) with temperature T (Langevin-type equations). Recently, using the computer simulation, it has been shown that the charge distribution in homogeneous chains in thermodynamic equilibrium (TDE) depends not only on the temperature, but also on the length of the chain.

When the energy of the classical chain Ecl = Nk_BT (N is the length of the chain) is less than the critical value E*, the charge is in the polaron state. When Ecl > E*, the charge is in a delocalized state [2].

For homogeneous DNA fragments, in TDE the polaron state exists at low temperatures, less than 5 Debye temperature, below which the semiclassical approximation is inapplicable. We have investigated the TDE states in the case when a trap-site with negative electron energy is placed in the middle of a homogeneous chain. Computational experiments were carried out for parameters corresponding to polyA fragments.

A qualitative picture of the total energy E, averaged by set of samples, for homogeneous chain with a trap is the same as for the chain without defect. The temperature stability of polarons in a chain with trap-site increases in comparison with the case of a homogeneous chain. For oligonucleotide AAAAGAAAAA (N = 10), the critical temperature T*~E*/N ~ 400 K is in the region of biological temperatures, and for the 40-site chain of adenine with guanine in the center T* <175 K.

The simulation results demonstrate that as the length of the chain increases, the type of charge distribution changes. In short chains, the charge is in the polaron state, and its transfer occurs slowly by hopping mechanism [3]. In long chains at the same temperature, the charge is in delocalized state, and the transfer process is more rapid.

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MODELING OF T-CELL POLARIZATION

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The repositioning of the microtubule organizing center is a part of many fundamental biological processes. It occurs in T-cell lymphocyte immediately after antigen presenting cell is recognized by T-cell. The Dynein's effort to walk to the minus end of the microtubule while being anchored at one place results in microtubule's sliding, and, hence in the repositioning of the microtubule organizing center and in the rotation of the whole microtubule structure. This process was experimentally observed, but its inner dynamics and key features remained poorly understood. We developed a physical model of microtubules and their organizing centre. By taking account of the cell's inner geometry, various forces acting in the cell and contact between microtubules and other organelles, we achieved to perform realistic simulation of the repositioning. The output of the model is in compliance with experimental observables. The results can cast a new light on the intracellular dynamics that is a key part of many biological processes. The influence of the rotation of microtubule structure on the intracellular patterns of concentration of calcium ions is explained.

HOLTER MONITORING DATA-BASED INSTANTANEOUS CARDIAC RHYTHM SPECTRUM. RESONANCES AND ANTIRESONANCES

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The report contains the instantaneous cardiac rhythm (ICR) frequency (y) distribution functions $f(y)$ determined on the basis of the Holter monitoring data using MAPLE programs. There was identified a multimodal behaviour of the distribution function $f(y)$. It was shown

that the ICR spectrum consisted of a solid component, resonances and antiresonances. The resonances are peaks *f(y)* determined by peak height h and peak width *Γ*. The antiresonances are dips *f(y)* determined by peak dip depth h and width *Γ*. The most of the time an ICR is in resonance states, and the rest of the time – in antiresonance states.

INSTANTANEOUS CARDIAC RHYTHM RATE SPECTRUM BASED ON HOLTER MONITORING DATA AND ITS FEATURES

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Together with frequency characteristics of instantaneous cardiac rhythm (ICR), characteristics related to the ICR change rate v are of great value for studies in cardiology. According to the data from day-long Holter monitoring, we constructed the ICR change rate (v) distribution function $f(v)$. It was demonstrated that for different patients the function had both the unimodal and the polymodal characters. In many cases the $f(v)$ is approximated accurately by the Laplace distribution $f(v)=(\varkappa/2)\exp(-\varkappa|v-v_0|)$. In general, the $f(v)$ is approximated with the plenty high enough accuracy by the linear combination of Laplace's and Gaussian functions.

DENSITY BASED CLUSTERING OF BROWNIAN DYNAMICS TRAJECTORIES REVEALS PREDOMINANT ENERGETICALLY FAVORABLE ORIENTATIONS IN PROTEIN-PROTEIN INTERACTIONS

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Protein-protein interactions are of central importance for virtually every process in living matter. Simulation of protein association dynamics is crucial for understanding their functionality. In Brownian dynamics proteins are considered as rigid bodies subjected to electrostatic and random Brownian forces. This rough approximation is rather accurate when protein surfaces do not touch each other, and in combination with molecular dynamics used to simulate close contact of molecules this simulation technique provides complete reconstruction of protein-protein interaction over large temporal and spatial scales.

Brownian dynamics is not so computationally expensive as molecular dynamics, thus allowing exhaustive sampling of relative orientations of protein molecules approaching each other in a virtual reaction space. Long-range electrostatics is the major factor effecting molecule orientation on encounter. To gain some understanding of the role of electrostatic

interactions at successive stages of protein-protein complex formation we need to detect and somehow describe intermediate metastable states on the association pathway. To do so we sample frames if electrostatic attraction energy between proteins is above some predefined threshold and analyze similarity of sampled structures in terms of root-mean-square deviation (RMSD) of their atomic positions in aligned to each other structures. Density based clustering technique [1] allows to find if all sampled structures constitute a single group, or they can be classified into several distinct clusters, and obtain characteristics of such groups (clusters).

We performed a comparative study of diffusional encounter of photosynthetic electron transport proteins cytochrome *f* and plastocyanin from two species of cyanobacteria (Phormidium and Nostoc) and higher plants. Cytochrome *f* is an exposed to thylakoid lumen subunit of a large transmembrane cytochrome b6f complex, its redox center is a type C heme. Plastocyanin is a copper-containing mobile carrier performing shuttle electron transfer from cytochrome *f* to photosystem I. Spatial structures of these proteins are similar, but the amino acid sequences significantly vary. Thus electrostatic properties of the binding sites in all three protein pairs are rather different.

For cyanobacterial proteins formation of structures with electrostatic attraction energy of 4kT or greater is a very rare event (k_{on} is less than 10^7 M-1 s-1). Several electrostatically favorable binding modes were identified by density based clustering for these species. However, Phormidium plastocyanin always approaches cytochrome *f* far from its redox center (heme), thus electron transport is very unlikely in these orientations. So we can suppose that electrostatic interactions should not play any significant role in formation of Phormidium plastocyanin-cytochrome *f* functionally active complex. This can be confirmed by the fact that experimentally obtained reaction rate for these proteins does not depend on solution ionic strength. Salt ions screen protein charges thus addition of salt weakens electrostatic interactions between proteins whereas for Phormidium proteins it does not change the reaction rate.

On the contrary, Nostoc plastocyanin in most cases binds directly to the heme location in two predominant orientations (43% and 40% of all sampled structures). Copper atom is turned toward cytochrome *f* in all these structures, thus we conclude that electrostatic interactions facilitate the formation of final complex capable of electron transport. Indeed, in experiments we can see strong dependence of electron transfer rate from the ionic strength.

In higher plants, formation of structures with attraction energy of 4kT or greater is much more frequent (k_{on} is above 10^9 M-1 s-1). The structures constitute one uniformly dense group, in which plastocyanin is located nearby heme of cytochrome *f*, but its copper atom is turned from the contact area. However, plastocyanin retains noticeable rotational freedom around its center of mass. We sampled protein orientations with even higher energy threshold of 8kT, and k_{on} still remained rather high (more than 10^7 M-1 s-1), but two distinct groups of plastocyanin orientations were detected. In 57% of structures a flexible single-point joint is formed by oppositely charged areas of two proteins, thus allowing thermal motion to rotate plastocyanin molecule into electron-transfer-capable orientation without breaking electrostatic link. In remaining structures binding of plastocyanin is much more tight, and its orientation suppresses electron transfer. We suppose that in higher plants the process of final complex formation involves at least two stages: the first is diffusive entrapment of plastocyanin by cytochrome *f*, and the second is orientation adjustment in the transient complex.

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ROADMAP FOR COMPUTER-AIDED MODELING OF THERANOSTICS AND RELATED NANOSYSTEMS

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The key impact of nanotechnologies on many areas of research and development has become prominent in recent years. Biomedicine belongs to the most influenced fields by nanotechnology, for example thanks to the introduction of theranostics (systems for combined diagnostics and therapeutic utilization). These systems can be composed from metallic core nanoparticles functionalized with monolayer-covered bio-active molecules. Despite the recent "state of the art" level of molecular modeling methodologies and the number of articles published annually on noble-metal nanostructures, this particular field is still in discovery phase [1]. In addition, detailed understanding of interactions of such nanoparticles with biological membranes, macromolecules and other entities of the living cell has crucial importance for elucidation of the mechanisms governing biological actions of these nanosystems. Insights into molecular details how these nanomaterials interact with subcellular nano-machinery of the cells can facilitate design and engineering of new generation of nanoparticles [2]. We were interested in building and modeling thiolate-protected gold clusters and compute their static and dynamic properties, using our in-house hardware and software resources. In order to compare the performance issues for modeling of such complex nanosystems, we performed comprehensive testing of available software protocols.

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PHASE SPACE OF INSTANTANEOUS CARDIAC RHYTHM IS A FRACTAL

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In this paper we present the instantaneous cardiac rhythm (ICR) function $y(t)$ and its difference derivative $v(t)$ constructed based on the data of day-long Holter monitoring. These functions contain complete patient cardiovascular system state information. In order to analyze the behavior of these functions, there was introduced a concept of phase space (PS) of ICR the points of which had coordinates $y(t)$ and $v(t)$ in space R^2 and moved along the

phase trajectories. In order to visualize the ICR dynamics, there was introduced a concept of extended phase space (EPS) of ICR. The examples of PS and EFS of ICR for specific patients of the Tver Cardiology Health Center are shown visually.

Within 24-48 hours we calculated the volumes of PS and EFS filled with the phase trajectories of ICR with different sizes of cells covering the phase trajectories. The calculation results showed that a phase volume of ICR had a power law dependence on cell size within the accuracy of 1-2%. That established the fractality of PS of ICR.

Taking into account the fractal properties of PS of ICR, volume Γ of PS of ICR is introduced. Γ is a volume filled with the phase trajectories of ICR in the D-dimensional space. As in statistical physic, the $\log \Gamma$ can be referred to as fractal entropy S of ICR.

We undertook a study of $\Gamma(t)$ and $S(t)$ behavior dynamics for several patients the results of which are given in the tables.

We argued in favor of use of parameters Γ and S as cardiovascular system state markers.

CRITICAL POINTS OF EXTENDED PHASE SPACE OF INSTANTANEOUS CARDIAC RHYTHM AS CARDIOVASCULAR SYSTEM STATE MARKERS

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One of the most effective instantaneous cardiac rhythm (ICR) imaging methods is application of extended phase space (EPS) of ICR. In this space, the ICR state is described by a point in the R^3 with coordinates $y(t)$, $v(t)$, $n(t)$, where $y(t)$ – ICR rate, $v(t)$ – ICR change rate, $n(t)$ – retry equal values y and v in different time moments.

We wrote down and implemented the MAPLE programs allowing the real-time monitoring of the dynamics of EPS of ICR. In this work, we demonstrate the actual examples of this dynamics based on the results of Holter monitoring of patients of the Tver Cardiology Health Center.

It was demonstrated that the EPS structure corresponded with the patient statuses determined by standard cardiology methods.

There were found critical points of EPS of ICR representing the centres of attraction of phase trajectory. Geometrically this appears as high and narrow EPS peaks. Near the peaks, the phase point spends sufficiently long time thus giving deterministic tone to ICR. The critical points of EPS of ICR are determined by cardiovascular system state features, and undoubtedly can be its markers.

FRACTIONAL LANGEVIN EQUATION MODEL FOR CHARACTERIZATION OF ANOMALOUS BROWNIAN MOTION FROM NMR SIGNALS

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Nuclear magnetic resonance (NMR) is non-destructive and one of the best developed tools to study random motion of spins in different systems, including soft tissues such as the brain, heart and muscles. In the long-time limit the current mathematical description of the experiments allows proper interpretation of measurements of normal and anomalous diffusion. The all-time dynamics is correctly considered only in a few works that however do not go beyond the standard Langevin description of the Brownian motion (BM). In the present contribution, the attenuation function $S(t)$ for an ensemble of spins in a magnetic-field gradient is calculated by accumulation of the phase shifts in the rotating frame that result from the motion of spin-bearing particles. The found $S(t)$, expressed through the particles' mean square displacement (MSD), is applicable for any kind of stationary stochastic dynamics of spins with or without a memory. We have studied in detail the model of the fractional BM and obtained in a simple way the MSD of particles trapped in a harmonic potential. The solution is used for the calculation of $S(t)$. In the limit of free particles coupled to a fractal heat bath, the results compare favorably with experiments acquired in human neuronal tissues.

SIMULATION OF RADIATION DAMAGE TO NEURAL CELLS

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Radiation damage to the central nervous system (CNS) has been an on-going challenge for the last decades primarily due to the issues of brain radiotherapy and radiation protection for astronauts during space travel. Although recent findings revealed a number of molecular mechanisms associated with radiation-induced impairments in behaviour and cognition, some uncertainties exist in the initial neuronal cell injury leading to the further development of CNS malfunction. As usual, these initial stages of neuronal injury are hardly accessible to experimental measurements. Many events cannot be investigates experimentally at all. In this regard, development of computation methods for assessing these early stages of radiation damage to CNS is of great interest.

To help in understanding the physical and biological mechanisms underlying effects of cosmic and therapeutic types of radiation on CNS, we have developed an original microdosimetry application based on the Monte-Carlo Geant4 toolkit, in particular, its biophysical extension of Geant4-DNA [1,2]. The applied simulation technique provides a tool for simulation of physical, physico-chemical and chemical processes (e.g. production of water radiolysis species in the vicinity of neurons) in realistic geometrical model of neuronal cells

exposed to particle radiation. The present study is performed to evaluate microscopic dose depositions and water radiolysis species yields within a detailed structure of individual neurons taking into account such cell components as soma, dendrites, axon and spines. To demonstrate benefits of the developed approach, the calculations were made for proton, 12C and 56Fe of different energy within a relatively wide range of linear energy transfer values from a few to hundreds of keV/μm. Simulation results indicate that the neuron morphology is an important factor determining the accumulation of microscopic radiation dose and water radiolysis products in neurons. The estimation of the radiolytic yields in neural cells suggests that the observed enhancement in the levels of reactive oxygen species may potentially lead to oxidative damage to neuronal components disrupting the normal communication between cells of the neural network.

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RADIATION DAMAGE TO NERVOUS SYSTEM: DESIGNING OF OPTIMAL MODELS FOR REALISTIC NEURON MORPHOLOGY

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A quantitative study of early mechanisms of the central nervous system (CNS) disorders induced by high-energy heavy ions at the molecular and cellular levels is one of urgent problem of modern radiobiology. The present study is focused on the development of optimal models of neuronal morphology for Monte Carlo microdosimetry simulation of initial radiation-induced events of heavy charged particles in the specific types of cells of hippocampus, which is most radiation-sensitive CNS structure. The applied simulation technique is based on the Geant4-DNA toolkit. The calculations were made for beams of heavy ions with doses corresponding to real fluxes of galactic cosmic rays. Simple compartmental model and complex model with realistic morphology extracted from experimental data were constructed and compared. We estimated distribution of energy deposition events and production of reactive chemical species within developed models of CA3, CA1 pyramidal neurons, DG granule cells and interneurons of hippocampus. Similar distributions of energy deposition events were obtained in both simplified and realistic neuron models. The results demonstrate that neuron morphology is an important factor determining the accumulation of microscopic radiation dose and water radiolysis products in neurons.

SAAS PLATFORM FOR TIME SERIES DATA HANDLING

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There is a cloud based resource MathBrain which provides users with tools for time series analysis. The most of methods is dedicated to magnetic- and electro encephalography (MEG, EEG) analysis which originally contains big amount of data to calculate. These methods of brain analysis are noninvasive, and the process looks like a registration of electro-magnetic activity. During the procedure, magnetic encephalograph device registers a magnetic field for several minutes, in hundreds of channels. Thus, as a result of these experiments specialists have big amount of data with complex structure. The resource suggests spectral methods, quantitative analysis, principal component analysis, independent component analysis and inverse problem solution [1]. From mathematical prospective the analysis is based mostly on Fourier transform method [2]. From technical side, Software as a Service platform gives such advantages as operating system independency, hardware capacity and opens a way for revising solutions in data-handling problems field [3, 4]. These pros are available, because the tool is provided as a "thin" client and user doesn't have to install any application on local computer. The architecture of this resource contains several layers of abstraction which help to share hardware between tasks and can be used for balancing the load. The engine of the resource which handle data is written on Python language. The task queue works on JSON-RPC listener/task-dispatcher scripts. Such approach allows not to overload the hardware during the complex calculations.

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REDUCED MODEL OF ELECTRON TRANSFER IN PHOTOSYSTEM II INHIBITED BY DCMU

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Photosystem II (PSII) is one of the cue protein complexes involved in photosynthesis. It carries out the transfer of electrons from oxygen evolving complex (OEC) to the plastoquinone in the time range from picoseconds to hundreds of milliseconds. The fluorescence emitted by the antenna pigments of PSII is an important marker of the photosynthesis activity. Different phases of fluorescence transient reflect definite stages of electron transfer in PSII, but the interpretation of fluorescence transient is not fully clear because of the complexity of PSII. To get more simple system for studying the inhibitor DCMU, which blocks transfer of electron to plastoquione, is used.

In this work we developed the detailed model of electron transfers in PSII treated with DCMU. The model describe transitions of different states of PSII, which mediate electron transfer from OEC to primary quinone. The model possesses 24 ordinary differential linear equations. Time hierarchy of processes allowed us to apply Tikhonov's theorem and reduce this system to three ordinary differential linear equations. The parameters of novel reduced model are the expressions that consists of original parameters of the fully model. We derived the analytical solution of the reduced model as the sum of three exponential functions. The final three-exponential expression describes three slow stages of electron transfer: light-dependent stage and two stages of electron transfer by OEC. This analytical solution allowed us to get single-valued fitting of experimental curves and analyze some changes in PSII of algae growth under different light conditions.

PARALLEL EVOLUTIONARY OPTIMIZATION ALGORITHMS FOR PEPTIDE-PROTEIN DOCKING

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In this study we examine the prospect of using evolutionary optimization algorithms in protein-peptide docking. We present the main assumptions that reduce the docking problem to the continuous global optimization problem and provide a way of using evolutionary optimization algorithms. The Rosetta all-atom force field was used for structural representation and energy scoring. We describe the parallelization scheme and MPI/OpenMP realization of the considered algorithms. We demonstrate the efficiency and the performance for some algorithms which were applied to a set of benchmark complexes.

PARTIAL SPECTROSCOPY OF ALPHA-RHYTHM AND PATHOLOGICAL ACTIVITY OF THE HUMAN BRAIN

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The new method to study human brain activity was developed [1]. This method aims to determine spectral characteristics, specific to various regions and structures of the human brain. Said method combines two completely different sources of information: 1) anatomical information, obtained from magnetic resonance imaging(MRI); 2) information about human brain activity, obtained by multichannel magnetic encephalograph. To find activity sources from magnetoencephalogram functional tomography method is used [2]. Functional tomography finds corresponding unique spatial location for each coherent elementary oscillation. Spatial information about regions of interest(ROI) is extracted from MRI either by semi-automatic segmentation, or by direct selection. Combining these ROIs with functional tomogram one can obtain set of the field sources, corresponding to selected ROI. Frequencies and Fourier coefficients of these sources form partial spectrum of the studied region or structural element of the human brain. From this partial spectrum, multichannel time-series can be reconstructed, thus giving us partial encephalogram, produced by region of interest. Further analysis of such encephalograms can be used to determine connectivity between different regions and structures of the brain.

For verification, the method was applied to the records of the human brain spontaneous activity obtained from healthy subjects and from subjects with certain pathologies (multiple sclerosis and neuralgias of different genesis). The results obtained show good correlation with the generally accepted ideas about the localization of sources of such activity.

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MODELING THE BEHAVIOR OF VIRTUAL SYSTEMS WITH ENDOGENOUSLY SHAPING PURPOSES

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The problem of constructing a choice model of an agent endogenously shaping purposes of his evolution is under debate. It is demonstrated that its solution requires the development of well-known methods of decision-making while taking into account the relation of action mode motivation to an agent's ambition to implement subjectively understood interests and the environment state. The latter is submitted for consideration as a purposeful state situation model that exists only in the mind of an agent. It is the situation that is a basis for getting an insight into the agent's ideas on the possible selected action mode results. The agent's ambition to build his confidence in the feasibility of the action mode and the possibility of achieving the desired state requires him to use the procedures of forming a model-representation based on the measured values of the environment state. This leads to the gaming approach for the choice problem and its solution can be obtained on a set of trade-off alternatives.

COMPUTER ALGEBRA AND QUANTUM COMPUTING WITH APPLICATIONS

THE DIPOLAR RELAXATION OF MULTIPLE QUANTUM COHERENCES AS A MODEL FOR AN INVESTIGATION OF DECOHERENCE PROCESSES IN MANY-QUBIT CLUSTERS IN MULTIPLE-QUANTUM NMR

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Quantum decoherence is one of the most important problems for creation of quantum devices which outperform their classical counterparts [1]. The performed investigations demonstrate [2] that the decoherence time decreases when the number of qubits in the coherent cluster increases.

We used methods of multiple-quantum (MQ) NMR [3] for the investigation of the decoherence processes in many-qubit clusters forming in the course of the MQ NMR experiment. One-dimensional systems are very suitable for the considered problem because the consistent quantum-mechanical theory for MQ NMR dynamics was developed [4] only for one-dimensional systems. It was shown [4] that only MQ coherences of zeroth and plus/minus second orders emerge in a one-dimensional chain, initially prepared in the thermodynamic equilibrium state, on the preparation period of the MQ NMR experiment in the approximation of the nearest neighbor interactions [5]. We developed a theory describing the dipolar relaxation of the MQ coherences of zeroth and second orders in the finite spin chain on the evolution period of the experiment which follows immediately after the preparation period [6]. The dependencies of the intensities of the MQ NMR coherences of the zeroth and second orders on the evolution period are obtained for various numbers of spins in the chain. It is shown that the MQ NMR coherence of the zeroth order does not decay completely in the relaxation process.

The size of the coherent clusters forming on the preparation period is expressed via the duration of this period and the space dimension. The dependence of the relaxation time on the number of spins in the formed cluster is obtained. Considering the dipolar relaxation of the MQ NMR coherence of the second order as a simple model of the decoherence process in the many-qubit system, we found that the decoherence time slowly decreases with the increase of the number of spins in the correlated cluster.

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AUTOMATION OF STOCHASTIZATION ALGORITHM WITH USE OF SYMPY COMPUTER ALGEBRA LIBRARY

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To describe models where the intensity of the interaction between components depends on the concentration of a component, one can use the scheme of interaction from chemical kinetics:

$$\sum_{i=1}^{n} N_i^s X_i \leftrightarrow [k_s^-]\, k_s^+ \sum_{i=1}^{n} M_i^s X_i, \quad s = 1,\ldots,S.$$

Here X_i represents the number i-th component, matrices $\mathrm{M} = \left[M_i^s \right]$ and $\mathrm{N} = \left[N_i^s \right]$ are called the system state matrices and specify the number of interacting components of the system at each stage of the reaction k_s^+ and k_s^- – are coefficients of interaction in direct and reverse reactions.

One can use such schemes to describe models of chemical reactions, biological and ecological systems. From these diagrams we can derive a system of ordinary differential equations describing the change of variables $X_i(t)$ over time.

Our research group has been generalized the stochastization method, which allows write out stochastic differential equation based on deterministic model. The original data reported in the interaction scheme, it is enough to get stochastic differential equations. For systems of large dimension, the stochastization method requires a large amount of routine work. However, it is possible to automate it. This paper describes this automation, by using Python language and SymPy library for symbolic computations.

Created program allows from the array of the coefficients of the interactions to obtain at the output the system of ODE and vector drift and the diffusion matrix for the system of SDEs in human-readable form and in other formats suitable for direct numerical solution.

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QUANTUM CORRELATIONS IN REMOTE STATE CREATION. INFORMATION EXCHANGE WITH VANISHING ENTANGLEMENT

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The formation and evolution of quantum correlations is one of the central problems of quantum information. Although quantum correlations are necessary to provide advantages of quantum information devices in comparison with their classical counterparts, the appropriate measure of these correlations is not well-established yet. Quantum entanglement [1] was

considered as a suitable measure for a long time. However, recently the quantum discord was introduces [2,3] as an alternative measure which can be valuable in systems with vanishing entanglement.

We assume that quantum correlations can be classified (with possible overlaps among different classes) so that a given quantum process is governed by a certain class of quantum correlations rather than by all of them. In our work we are aimed on revealing those quantum correlations that are responsible for remote creation of a one-qubit state in a spin chain [4], which is the further development of the problem of end-to-end quantum state transfer along a spin chain [5].

We study the dependence of quantum correlations between the two remote qubits (sender and receiver) connected by a transmission line (homogeneous spin-1/2 chain) on the parameters of the sender's and receiver's initial states (control parameters) [6]. We consider two different measures of quantum correlations: the entanglement [1] (a traditional measure) and the informational correlation [7] (based on the parameter exchange between the sender and receiver). We find the domain in the control parameter space yielding (i) zero entanglement between the sender and receiver during the whole evolution period and (ii) non-vanishing informational correlation between the sender and receiver, thus showing that the informational correlation is responsible for the remote state creation. We demonstrate that, among the control parameters, there are the strong parameters (which strongly effect the values of studied measures) and the weak ones (whose effect is negligible), therewith the eigenvalues of the initial state are given a privileged role. We also show that the problem of small entanglement (concurrence) in quantum information processing is similar (in certain sense) to the problem of small determinants in linear algebra. The particular model of the 40-node spin-1/2 communication line is presented.

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MODERN APPROACHES TO SYNTHESIS, STABILITY ANALYSIS AND VERIFICATION OF NONLINEAR STOCHASTIC MODELS OF NATURAL SCIENCE

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The modern approaches to the nonlinear stochastic models synthesis, stability analysis and verification are characterized in the current work. One of the approaches is related to the self-consistent stochastic models constructing technique. Based on this technique, the interaction schemes are constructed that includes the symbolic record of the possible interactions between the system elements. Then, using the system state operators and the state change operator, the stochastic models structure is described and the transition to the corresponding Fokker-Planck vector equation is performed, and the rules for the transition to the multidimensional stochastic differential equation in Langevin form are formulated. The specified approach allows us to estimate the influence of the stochastic injection on the properties of the models [1]. For the models under study, it is possible to carry out a numerical experiment with the application of the developed software package that allows us to solve the stochastic differential equations systems taking into account the features of the described transition from the deterministic case to the stochastic case. The second approach is based on the transition from the deterministic description of the model to the stochastic description and on the principle of the stability problem reduction of the differential inclusion solutions to the stability problem for other types of the equations [2,3]. In the framework of this approach, the usual, fuzzy and stochastic Lyapunov functions are applied and from the unified point of view the stability properties of the solutions of differential inclusions, fuzzy and stochastic differential equations are studied. For obtaining the stability conditions, we use both the properties of Lyapunov functions and the divergence properties of the vector fields determined by the right-hand sides of the differential equations [4]. Based on the combination of the specified approaches, nonlinear mathematical models of the populations interactions are constructed and studied [5,6]. The results can be used in the modeling problems of the various classes of stochastic systems, and also for comparing the qualitative properties of the natural science and technics models in deterministic and stochastic cases.

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ON DIFFERENCE SCHEMES OF SECOND ORDER FOR KORTEVEG-DE VRIES EQUATION

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We consider the classical Korteveg-de Vries equation in the following form

$$f = 0,\ f := u_t + \alpha u u_x + \beta u_{xxx},\ \ u = u(t,x),\ \ \alpha,\beta \in \mathbb{R}. \tag{1}$$

In the present talk we apply to equation (1) our approach described in [1] and based on the methodology of paper [2]. As a result, we obtain the following difference scheme

$$\begin{aligned} \tilde{f} = 0,\ \tilde{f} := \frac{u_j^{n+1} - u_j^n}{\tau} + \alpha \frac{\left(P_{j+1}^{n+1} - P_{j-1}^{n+1}\right) + \left(P_{j+1}^n - P_{j-1}^n\right)}{8h} + \\ + \beta \frac{\left(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + 2u_{j-1}^{n+1} - u_{j-2}^{n+1}\right) + \left(u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n\right)}{4h^3}. \end{aligned} \tag{2}$$

Here $u_j^n := u(\tau \cdot n, h \cdot j)(n, j \in \mathbb{Z})$ is the grid function approximating $u(t,x)$ on the Cartesian solution grid with spacings $\tau := t_{n+1} - t_n$, $h := x_{j+1} - x_j$ and $P_j^n := \left(u^2\right)_j^n$. The scheme (2) has accuracy $O(\tau^2, h^2)$ and is consistent with (1). Besides, the scheme is implicit and, hence, unconditionally stable. Therefore, it is *convergent*.

Then we compare, on the exact soliton solution

$$u_{\text{exact}} = \frac{2k_1^2}{\cosh\left(k_1\left(x - 4k_1^2 t\right)\right)^2},$$

the numerical behavior of scheme (2) with that of two schemes of the same order of approximation used in the literature [3] and show that our scheme provides substantially better numerical accuracy.

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COMPUTATIONAL ASPECTS OF BRADED AND MULTIPLE ZETA FUNCTIONS

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In *q*-deformed geometry braded zeta functions for any rigid object in a ribbon braided category have defined by Majid and Tomasic, and others. By the category of realizations multiple zeta values have defined by Goncharov, by Furusho, by Unver and other. In the communication we present ontology and computer algebraic aspects of braded and multiple zeta functions.

HIGH-ACCURACY FINITE ELEMENT METHOD FOR ELLIPTIC BOUNDARY-VALUE PROBLEMS

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High-accuracy finite element method for elliptic boundary-value problems is presented.

The basis functions of finite elements are high-order polynomials, determined from a specially constructed set of values of the polynomials themselves, their partial derivatives, and their derivatives along the directions of the normals to the boundaries of finite elements.

Such a choice of the polynomials allows us to construct a piecewise polynomial basis continuous on the boundaries of elements together with the derivatives up to a given order. In present talk we show how this basis is applied to solve elliptic boundary value problems in the limited domain of multidimensional Euclidean space, specified as a polyhedron.

The efficiency and the accuracy order of the finite element scheme, algorithm and program are demonstrated by the example of exactly solvable boundary-value problem for a triangular membrane, depending on the number of finite elements of the partition of the domain and the number of piecewise polynomial basis functions.

SYMBOLIC-NUMERICAL MODELING OF THE INFLUENCE OF DAMPING MOMENTS ON SATELLITE DYNAMICS

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The dynamics of a satellite in a circular orbit under the influence of gravitational and active damping torques, which are depend on the projections of the angular velocity of the satellite is investigated [1]. Such active damping torques are proportional to the projections of

angular velocities onto the axes of the satellite body coordinate system and can be provided by using the angular velocity sensor. Computer algebra methods for determination of all equilibrium orientations of the satellite in the orbital coordinate system with given damping torque and given principal central moments of inertia are used. The equilibrium orientations are determined by real roots of the system of nonlinear algebraic equations. An algorithm for construction of the Groebner basis for solving the problem was applied.

The conditions of the equilibria existence depending on three damping parameters were obtained by the analysis of real roots of algebraic equations from the constructed Groebner basis.

The conditions of asymptotic stability of the satellite's equilibria were determined as a result of the analysis of linearized equations of motion using Routh-Hurwitz criterion. The integration of the differential equations of satellite attitude motion has been done numerically. The transition decay processes of spatial oscillations of the satellite at different damping parameters have been studied.

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ON THE WIGNER QUASIPROBABILITY FUNCTION FOR N-LEVEL QUANTUM SYSTEMS

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According to the Stratonovich-Weyl correspondence there is mapping between operators on the Hilbert space of a finite-dimensional quantum system and functions on the phase space of its classical mechanical counterpart. This map is given by the Wigner quasiprobability distribution and can be implemented with the aid of the Stratonovich-Weyl operator kernel which satisfies a number of lucid physical postulates. In the present report, applying this formulation to a generic N-level quantum system, we propose the k-fold family of Wigner functions defined on the complex flag manifolds $F_N^{N-k} := U(N)/\big(U(N-k)\times U(k)\big)$ with $k \le \lceil (N-1)/2 \rceil$ and present explicit expressions for kernels of few low-dimensional Wigner function.

ON GENERATION OF RANDOM ENSEMBLES OF MIXED STATES FOR QUANTUM BIPARTITE SYSTEMS

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Two methods of generation of random ensembles of mixed quantum states of different ranks are discussed. The first method exploits the Ginibre ensemble of complex square random matrices, while the second one is based on the singular value decomposition of

density matrices. Distribution properties of the "probability of entanglement" in composite systems consisting from qubit-qubit and qubit-qutrit pairs are studied using both approaches to generate random Hilbert-Schmidt and Bures ensembles of quantum states of all possible ranks.

ON STRATIFICATIONS OF X-STATE SPACE OF TWO QUBITS

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We are considering the state space of two qubits formed from the X-states. Its decompositions with respect to two groups actions are studied. The first decomposition is constructed in accordance with the types of orbits of the invariance group G_X of X-state space. The second decomposition arises considering the action of the subgroup LG_X of invariance group G_X, the so-called "local group of invariance" of X-states, every element of which is given by the tensor product of mutually independent unitary transformations acting on each qubit. The equations and inequalities, determining all components of both stratifications, are given in terms of the corresponding group invariants.

The primary stratification classifies the X-state space in accordance with the properties of two-qubit system as a whole, while the secondary stratification provides complete information on non-local characteristics of the given composite system.

COMPUTER ALGEBRA ALGORITHMS OF SIMPLIFICATION OF TENSOR EXPRESSIONS

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Will be presented the computer algebra algorithms of simplification of tensor expressions which based on group-theoretical properties of tensor monoms and multilinear identities like Bianchi.

AN APPLICATION OF GEOMETRIC METHODS TO THE ONE-STEP PROCESSES STOCHASTIZATION

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When modeling different physical and technical systems, they can often be modeled in the form of one-step processes. Our group has been developing a formalism of stochastization

of one-step processes for quite a long time. We investigated a variety of representations of both the one-step processes, and methods of their stochastization. We have considered representations in the state vectors (combinatorial approach) and in the occupation numbers (operator approach) [1]. With stochastization of systems with control, we use a geometric approach to control theory. It would be useful to consider the geometric approach also to the methods of stochastization of one-step processes.

We have considered various variants of geometrization of the process of stochastization of one-step processes and stochastic differential equations. Approaches were considered both on the basis of Riemannian quadratic metrics [2-3] and on the basis of a more general approach of Finsler geometry [4-8].

Different approaches to geometrization of stochastic systems are considered in the paper and comparison with other methodological approaches is made.

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ENTANGLEMENT AND QUANTUM STATE TRANSFER IN SPIN CHAINS WITH XY-HAMILTONIAN

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We investigate quantum state transfer [1] and quantum entanglement [2], emerging in this process, in spin chains. We consider a quantum system, consisting of N spins, connected by the XY-Hamiltonian in the approximation of the nearest neighbor interactions [3]. Initially the spin chain is in the thermodynamic equilibrium state. Magnetic resonance methods allow us to create a pure state of the first chain spin, which is called the sender. As a result of the

evolution under the action of the XY-Hamiltonian, the pure quantum state transmits along the chain to its end. The last chain spin is called the receiver. A quality of the quantum state transfer is estimated by fidelity [4]

$$F=\langle\psi|\chi|\psi\rangle \quad (1)$$

where $|\psi>=a|0>+b|1>$ is the transmitted quantum state $(a, b$ are complex numbers, $|a|^2+|b|^2=1)$, χ is the reduced density matrix over all spins besides the receiver. We evaluate analytically a quality of the transferred state with fidelity between the sender state and the receiver one.

We found also that the quantum entanglement between the sender and the receiver emerges in the transmission process. We investigate numerically the dependencies of entanglement on parameter $|b|$ and the temperature by simulations with the computational program "Mathematica". We use concurrence [5] for the estimation of quantum entanglement in the system. We found the critical temperature of emerging entanglement. We established that the critical temperature depends on the polarization of the initial pure state. It is shown that the critical temperature decreases with increasing parameter $|b|$ at small $|b|$. However, the critical temperature increases with increasing $|b|$ at large values of $|b|$. A break point between regions of increasing and decreasing the critical temperature does not depend on the number N of spins in the chain.

Time of emerging entanglement grows with increasing N in the considered quantum system.

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A NEW APPROACH TO WEIGHT MULTIPLICITY IN REPRESENTATIONS OF COMPACT LIE GROUPS

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The multiplicity of a weight of an irreducible finite-dimensional representation of a complex semisimple Lie algebra can in principle be evaluated by using the celebrated Kostant multiplicity formula, which employs summation of values of Kostant partition function over

the Weyl group of the algebra. While Kostant's formula is quite elegant, it is usually not suitable for computations due to the size of the Weyl group. From the computational point of view, storing all data about the Weyl group consumes an enormous amount of space. In practice, computer methods based on the recursive method of Freudenthal are usually implemented. Another inductive formula is that of Racah, which also uses summation over the Weyl group. The new direct approach to weight multiplicity suggests a method for computing the weight multiplicity that does not use summation over the Weyl group and is not recursive. The method is based on localized partition functions.

FINITE DIFFERENCE SCHEMES AS ALGEBRAIC CORRESPONDENCES BETWEEN LAYERS

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Modern development of computer science revived the old investigations about the solvability of differential equations in the finite terms. There are remarkable differential equations which can be integrated in CAS. In our work we want to speak about remarkable differential equations in another sense: for these equations there are finite difference schemes which conserve algebraic properties of solutions exactly. It should be noted that these classes of differential equations are very similar.

As was shown by Painlev'e, all ordinary differential equations which can be integrated in classical transcendental functions have a common algebraic property, namely, general solution of such differential equation depends on integration constant algebraically. So we can construct a version of Galois theory without fixation of allowed transcendental operations [1,2].

In term of Cauchy problem this property means that the differential equation defines an algebraic correspondence between initial and terminal values. For example, Riccati equation $y' = p(x)y^2 + q(x)y + r(x)$ defines one-to-one correspondence between initial and terminal values of y on projective straight line. However, standard finite difference scheme doesn't conserve this algebraic property of exact solution. Furthermore, the scheme, which defines one-to-one correspondence between layers, truly describes solution not only before but also after mobile singularities and conserves algebraic properties of equations like the anharmonic ratio [3].

When the differential equation has a form $F(x, y, y') = 0$ we reduce it to equation of 2nd degree and then apply the finite difference method. In so doing, the expression $F(x, y, y')$ is the integral of the differential equation of 2nd degree and thus its quantity is conserved on approximate equation only with some small error. However if the equation $F(x, y, y') = 0$ defines one-to-one correspondence between initial and terminal values we can try to find the difference scheme which define one-to-one correspondence between layers, that is between algebraic curves. For curves with the genus $p > 0$ such correspondence can be constructed by pure algebraic way and at the same time periodical functions appear here naturally without any references on exact solution. In our talk such schemes will be presented.

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DIFFRACTION OF ELECTROMAGNETIC WAVES ON A WAVEGUIDE JOINT

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Consider a waveguide of a constant simply connected cross-section S with ideally conducting walls. The axis Oz is directed along the cylinder axis, the normal to ∂S will be denoted as $\vec{n}$, the tangent vector perpendicular to $\vec{e}_z$ as $\vec{\tau}$. Let the filling ε, μ of this waveguide have the jump at $z=0$ so this plane is the joint of two waveguide. For a while we will not make any assumptions about the dependence ε, μ on x, y.

For a basis we take the system of Maxwell's equations, from which we exclude E_z and H_z. A two-dimensional analogue of the Helmholtz decomposition makes it possible, without loss of generality, to seek a solution in the form

$$\vec{E}_\perp = \nabla u_e + \nabla' v_e, \quad \vec{H}_\perp = \nabla v_h + \nabla' u_h,$$

where

$$\nabla = (\partial_x, \partial_y)^T, \quad \nabla' = (-\partial_y, \partial_x)^T.$$

The four scalar functions introduced here will be called potentials, and we'll always assume that they satisfy the boundary conditions

$$u_e = u_h = n \cdot \nabla v_e = n \cdot \nabla v_h = 0.$$

The boundary conditions for the field are automatically satisfied and Maxwell's equations give a system of four equations on the potentials. The solution of this system we consider as functions of variable z with values in appropriate Sobolev spaces. Thus Maxwell's equations give for vector $w=(u_e, u_h, v_e, v_h)$ the ordinary differential equation

$$B\frac{dw}{dz} + ikAw - \frac{1}{ik}Cw = 0,$$

where A, B, C are bounded operators. Any solution of this equation at $z<0$ and at $z>0$ can be represented as the superposition of normal modes with respect to the eigenvalue problem

$$\beta Bw = Aw + \frac{1}{k^2}Cw,$$

so the solving of diffraction problem is reduced to the matching of both solutions.

In our talk we want to show how to calculate the eigenmodes and to make the matching in Sage partially by the analytic way.

PROVABLE PROGRAMMING OF ALGEBRA: ARITHMETIC OF FRACTIONS

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It is described a certain provable program for a generic arithmetic of fractions. This is a small part of the project DoCon-A of provable programs for a computer algebra library. In this system, functional programs for known algebraic methods are written together with proofs, and proofs are automatically checked by the compiler (see the Coq and Agda systems). The used language (Agda) is purely functional and includes the feature of dependent types. This paper describes provable programming of arithmetic of fractions over arbitrary ring with gcd.

EVOLUTION OF QUANTUM STEERING OF TWO BOSONIC MODES IN A SQUEEZED THERMAL ENVIRONMENT

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Einstein-Podolsky-Rosen steerability of quantum states is a property that is different from entanglement and Bell nonlocality. We describe the time evolution of a recently introduced measure that quantifies steerability for arbitrary bipartite Gaussian states in a system consisting of two bosonic modes embedded in a common squeezed thermal environment.

We work in the framework of the theory of open systems. If the initial state of the subsystem is taken of Gaussian form, then the evolution under completely positive quantum dynamical semigroups assures the preservation in time of the Gaussian form of the states.

It was shown that the thermal noise and dissipation introduced by the thermal environment destroy the steerability between the two bosonic modes. In the case of the squeezed thermal bath we show the dependence of the Gaussian steering on the squeezing parameters of the bath and of the initial state of the system. A comparison with other quantum correlations for the same system shows that, unlike Gaussian quantum discord, which is decreasing asymptotically in time, the Gaussian quantum steerability suffers a sudden death behaviour, like quantum entanglement.

NEAR-PERFECT MATCHINGS ON CYLINDERS $C_M \times P_N$ OF ODD ORDER

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The problem of counting near-perfect matchings on cylinders $C_m \times P_n$ is discussed when both parameters m and n are odd. A distinctive feature of these matchings is the presence of

exactly one node which is left unmatched. This node will be called vacancy.

This combinatorial problem is directly related to the dimer problem, one of the classical lattice models of statistical physics. If at least one of the lattice parameters is even, then maximum matchings often turn out to be perfect matchings. But if the order of the graph is odd, then maximum matchings are usually near-perfect matchings. The generating function for the number of near-perfect matchings is identical to generating function for the dimer model when activities of all dimers are the same.

The methods known to date are able to find closed-form expressions for the number of near-perfect matchings on $C_m \times P_n$ graphs only when the vacancy is located on the boundary [1]. Summation over all possible vacancy locations for arbitrary values of parameters m and n is beyond the scope of available analytical tools.

In our work, a counting problem is considered for a fixed value of the parameter m. Under this condition, generating functions $G_m^P(z)$ for the number of perfect matchings in the graphs $C_m \times P_{2n}$ and $G_m^N(z)$ for the number of near-perfect matchings in the graphs $C_m \times P_{2n+1}$ rational. These generating functions can be reconstructed from sufficiently long initial segments of sequences, the elements of which are numbers of near-perfect matchings in graphs for fixed values of m and changing n.

The implementation of the method by Wilf [2] in computer algebra system Maple allowed us to obtain a set of recurrence relations and generating functions for the number of near-perfect matchings for fixed odd values of the parameter $3 \le m \le 13$. The coefficients of the asymptotic expansions are calculated for $3 \le m \le 19$.

The study of generating functions $G_m^N(z)$ made it possible to establish a close connection between their denominators and the denominators $G_m^P(z)$. For all values of m studied in our research, the denominator $G_m^N(z)$ had been always the square of the denominator $G_m^P(z)$.

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CREATING DEVELOPMENT ENVIRONMENT AND BASED ON IT VERSIONS OF THE COMPUTER ALGEBRA SYSTEMS AXIOM, REDUCE AND MAXIMA

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It is created the minimal development environment for computer algebra systems AXIOM, REDUCE and MAXIMA, which includes compilers from C and FORTRAN, standard libraries libc, libm, …, utilities lex, yacc, awk, …, and COMMON LISP interpreter, which is complete and closed.

It is based on sources of libraries and compilers of the middle of 90-th, available in internet and belonging to classical software. Mainly it is from System V Release 4 sources of

the UNIX System Laboratories, and COMMON LISP interpreter from Lucid.

This, from one side, allows again to provide numerical computations from symbolic session, dynamically loading needed object files.

From another side, it is possible to works with the same environment in different operating systems.

At present it is worked under Linux.

THE STANDARD SCHEME OF THE ANALYSIS OF A STABILITY THROUGH LIE SYMMETRIES AND CONSERVATION LAWS: A NONLINEAR SCHRÖDINGER EQUATION

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Many natural phenomena are described by a system of nonlinear partial differential equations (PDEs) which is often difficult to be solved analytically, as there is no a general theory for completely solving of the nonlinear PDEs.

One of the most useful techniques is the Lie (classical) symmetry method and to obtain the invariant solutions, we focus on the physically interesting situations which admit potential symmetries. Then by using the partial Lagrangian approach, we find conservation laws.

In the study of PDEs, conservation laws are important for investigating integrability and linearization mappings and for establishing existence and uniqueness of solutions. They are also used in the analysis of stability and global behavior of solutions.

The common scheme (worksheet) presented for known example: nonlinear Schrödinger equation.

IVC CALCULATION PROBLEM FOR JOSEPHSON JUNCTION STACKS. ON ASYMPTOTIC CONSTRUCTION NEAR THE BREAKPOINT

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A detailed investigation of the IVC breakpoint and the breakpoint region width gives important information [1,2] concerning the peculiarities of stacks with a finite number of intrinsic Josephson junctions. In [3] IVC for a stack of n Josephson junctions is defined numerically using the fourth-order Runge-Kutta method. The current voltage characteristic has the shape of a Hysteresis loop. On the back branch of the Hysteresis loop, near the breakpoint I_b, voltage $V(I)$ decreases to zero rapidly. In addition, in numerical modelling (non-periodic boundary condition) IVC branching is observed near I_b. It is interesting to study this phenomenon analytically developing asymptotic methods. A numerical-analytical method was proposed in [4]. The general scheme of suggested numerical-analytical method of

the hysteresis loop calculation is following: the right branch of the hysteresis loop and the back branch (not nearing some finite distance to I_b) are calculated using the "asymptotic" formulas. The rest points $\left(I;V\left(I\right)\right)$ of the hysteresis loop are calculated numerically using the fourth-order Runge-Kutta method. This method showed good results in IVC branching calculation in particular. I succeeded to calculate analytically the whole hysteresis loop in the case of periodic boundary conditions. The approximate solution at the breakpoint region had been developed using the Bogolyubov-Krylov method [5].

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FINDING THE SPECTRAL CHARACTERISTICS FOR SYSTEMS WITH CONTROL

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We are studying the process of global synchronization in systems with control. As a control system, we study the continuous model of the active control module of the type RED [1-3]. We apply the method of harmonic linearization. To simplify the model, we applied the following:

- The model is written in moments;
- The model describes only the phase of avoiding overloading of the TCP Reno protocol;
- In the model, only the reset is considered when obtaining 3 consecutive ACK acknowledgments.

To determine the region of occurrence of auto-oscillations, we use the Routh-Hurwitz criterion, and to determine the self-oscillation parameters, the Mikhailov criterion.

Next, we use the Fast Fourier Transform method to obtain the spectral characteristic. Verify the model with NS2.

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HIGH-ACCURACY FINITE ELEMENT METHOD FOR THE 2D PARAMETRIC ELLIPTIC BOUNDARY-VALUE PROBLEMS

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High-accuracy finite element method for solving the 2D parametric elliptic self-adjoint boundary-value problems is presented. The triangular elements and new high-order fully symmetric Gaussian quadratures with positive weights, and no points are outside the triangle (PI type) is applied. The program calculates with the given accuracy the eigenvalues, the surface eigenfunctions and their first derivatives with respect to the parameter of the BVP for parametric self-adjoint elliptic differential equation with the mixed Dirichlet-Neumann type boundary conditions on the 2D polygonal domain, and the potential matrix elements, expressed as integrals of the products of surface eigenfunctions and/or their first derivatives with respect to the parameter. We demonstrated an efficiency of finite element schemes and program by means of benchmark calculations the 3D boundary-value problem for Helium atom bound states in the framework of Kantorovich method.

THE SYSTEM OF N-ORDER RICCATI EQUATIONS: DERIVATION, SOLUTIONS, APPLICATIONS

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An algorithm of reduction of n-order differential equation into the system of n-order Riccati-type equations is constructed. Solutions of the system of Riccati equations are roots of the polynomial coefficients of which are given by the set of linear independent solutions of n-order differential equation. Interrelations with the Poincare model of hyperbolic space and the general complex algebra are established. The physical interpretation of the obtained system of Riccati equations is given via dynamics of the generalized classical mechanics.

COMPUTING GRÖBNER AND INVOLUTIVE BASES FOR LINEAR SYSTEMS OF DIFFERENCE EQUATIONS

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In this paper the author will talk about the problem of computing involutive bases and Gröbner bases of linear systems of difference equations, its importance, applicability for physical and mathematical problems and the algorithm for solving it.

An implementation of the computation algorithm in C will be presented, calculation times will be compared with the competing programs. The parallel version of this implementation and its scalability will be considered.

INFORMATION PROCESSING BY QUANTUM INTELLIGENCE NETWORKS

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A scheme of functioning of a quantum intelligence is suggested. The main difference between quantum and classical intelligences is that the former acts on the basis of quantum decision theory, evaluating prospects by quantum probabilities [1-5]. Owing to the quantum nature, a quantum probability is a sum of two terms, utility factor and attraction factor. Several quantum intelligences compose a quantum intelligence network, where the quantum intelligences play the role of quantum agents interacting with each other by exchanging information. Evolution of opinions in the network depends on the type of agent memory. Dynamics of opinions for short-term and long-term memories are studied numerically.

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CUNNINGHAM NUMBERS IN ACCELERATED MODULAR ARITHMETIC AND APPLICATIONS

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For certain modular algorithms, the modulus need not be a prime, and implementers are left with more freedom to choose moduli. One suggestion, made by Knuth [3], is to use integers of the form $2^n - 1$. A similar choice is $2^n + 1$. Numbers of these forms are Cunningham numbers for the special case of the base $b = 2$. We discuss suitability of these types of moduli for standard computer algebraic modular algorithms. Different schemes of choice of these types of moduli are analyzed along with algorithms for conversion of arbitrary precision integers into the modular representation. In particular, this leads to division free linear time conversion to modular representation, and multiplication free reconstruction of the result from modular images. Experimental implementation of the described algorithms along with applications in multi-precision linear algebra and evaluation of rapidly convergent hypergeometric series are discussed. For very high bit lengths, over 10 000 bits, a modular representation using these Cunningham moduli outperforms both the standard binary representation as well as a modular representation using small prime moduli.

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POSTER SESSION

FILE SYSTEM ACCESS SPEED TEST

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In this paper the method for estimating the file system access speed in a virtual machine environment is considered. During the research tests of Linux's family various file systems were tested. All tests were conducted with continuous read/write modes in a certain area of physical medium. Read/write operations were performed in sequential and random modes at state of disk cache turned off. The conclusion was made about the method of estimating the file system access speed is applicable.

DEVELOPMENT OF SWARM OPTIMIZATION METHODS FOR THE STRUCTURAL BIOINFORMATICS PROBLEMS ON THE BASIS OF THE MODEL PROBLEM OF GRAPH DRAWING

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Our research is related to the problems of predicting the spatial structure of polypeptide molecules and their complexes. Our approach is based on the solution of the corresponding optimization problem, in which the objective function is the potential energy of the corresponding atomic ensemble, and the parameters of optimization are such geometric characteristics as bond lengths, valence and torsion angles. Distinctive features of this kind of optimization tasks are their high dimension and a long calculation time of the objective function, which determines the high requirements to the speed of convergence of the optimization algorithm. Our preliminary studies have shown that the absolute majority of existing optimization algorithms solve this task very badly. The development of new algorithms (or optimization of existing ones) is obstructed by the high computational complexity of the problem itself – typical calculation time is measured in hours and even days. In addition, the calculation of the objective function (energy) requires the installation of very serious software. For these reasons, we proposed to use the simpler related problem of graphs drawing to develop new optimization algorithms. The results of numerical investigation of several classical algorithms of swarm and evolutionary optimization are presented on the solution of such a model problem.

GPU SIMULATIONS OF BLOOD FLOW IN CT BASED DOMAINS

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Arterial aneurysms are dilations of arterial walls that can grow over time and, in case of rupture leads to dangerous hemorrhage.

Computer simulations of the blood flow and its interaction with the surrounding vessel tissue enables physicians to estimate rupture risks by calculating the distribution of blood pressure, velocity and wall stresses in the aneurysm, in order to support the planning of clinical interventions.

For the numerical simulation, the computational domain is extracted from medical image data of the patient's vascular system. The blood is modeled as an incompressible Newtonian fluid, and the surrounding vessel wall as an isotropic linear elastic material.
Both the Navier-Stokes equations for the fluid domain and the Navier-Lame equations for the solid domain are handled with a finite element method, and the resulting linear equation systems are solved via and algebraic multigrid algorithm. Implicit coupling between blood flow and wall elasticity is achieved using an iterative fluid-structure interaction technique deforming the fluid mesh according to the wall displacement in each step. For the efficient solution of the resulting large-scale problem, we exploit efficient numerical methods and high performance computing on advanced heterogeneous CPU-GPU parallel architectures.

NONLINEAR WAVE SIMULATION ON THE XEON PHI KNIGHTS LANDING PROCESSOR

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A finite difference scheme for solving systems of 2D Sine-Gordon equations is constructed. A parallelization strategy with both thread and SIMD levels of parallelism is proposed and an OpenMP program is realized. The program is tested on two different Intel architectures: 2x Xeon E5-2695 v2 processors, (code-named "Ivy Bridge-EP") in the Hybrilit cluster and on Xeon Phi 7250 processor (code-named "Knights Landing" (KNL)). As a result, we achieve good performance scalability on both architectures and better performance on KNL processor. A numerical example of a standing nonlinear wave is given.

NEW METHODS FOR CALCULATION OF COMPLICATED FUNCTIONAL INTEGRALS

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We present an elegant method for calculation of complicated integrals by using the Mellin representation. In this paper, the passage to a complex plane plays a vital role in obtaining universal formulas for taking enormous number of integrals from sign variables functions.

SIMULATION OF TRANSPORT TRAFFIC AT URBAN CROSSROADS USING EXTENDED PETRI NETS

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Our work is devoted to the construction and numerical study of low-level models of urban traffic based on extended Petri nets. We describe the basic principles for constructing such models. We propose an algorithm for automatic conversion of a given graph description of a road network into a Petri net taking into account the resolution of conflict situations (on the basis of traffic rules). As an example, we consider in detail the simulation of one of the most complex intersections in the Dubna town. The results of a numerical study of the throughput capacity of this intersection are presented, taking into account the different modes of traffic.

STUDY ON POSSIBILITY FOR REDUCING THE SLOW FLUCTUATIONS OF THE THERMODYNAMIC PARAMETERS OF THE COOLING SYSTEM OF THE COOLING SYSTEM OF THE IBR-2M REACTOR

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The problem of predicting the oscillations of the main thermodynamic parameters of the core in the first loop of the sodium cooling system of IBR-2M reactor is examined. Attention is focused mainly on the prediction of the temperature and sodium flow at the entry into the core as well as the thermal power. It is shown that the prediction makes it possible to reduce by a factor of 3 the influence of slow oscillations of reactivity on the power and thereby reduce the operational requirements for the automatic power stabilization system. Neural-net

prediction using nonlinear autoregression nets with feedback is proposed. The results agree with experiment to within ~5%.

THE PROBLEM OF OPTIMAL MOTION CONTROL FOR DYNAMICAL SYSTEMS OF FRACTIONAL ORDER

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The problem of optimal motion control for one-dimensional and two-dimensional systems of fractional order is considered. To search the analytical solutions of the problem the method of moments was applied. The properties of optimal controls depending on the index of fractional index, the control time, initial and final conditions were analyzed.

USING OF MACHINE LEARNING ALGORITHMS TO THE PROBLEM OF RECOGNITION OF VEHICLES TRACKS

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Within the framework of our project on modeling of urban transport traffic, we consider the following task. There is a mobile application that continuously records the geographic coordinates of the mobile device and data from its other sensors (for example, an accelerometer). These data form a “loaded” track – the trajectory of the movement of the device, the points of which are assigned additional information. Our goal is to automatically extract from this raw track those parts of it that correspond to the movement of the device on the vehicle (car, taxi, bus). Collected in this way, “transport” tracks in the future should be combined into a single network – a scheme of traffic in a certain area. To solve this problem, it is proposed to use algorithms of machine learning. We collected a database of training data – short tracks (10 seconds) with a known type of traffic – “car” and “no car”. These data were used to construct a logistic regression to predict the likelihood that a given track corresponds to movement on a car. A method for improving recognition is proposed, taking into account the connectedness of individual tracks (neighboring tracks should most likely belong to the same type). The results of testing the proposed approach for the analysis of traffic tracks in the Dubna town are presented.

ADAPTATION OF SWARM OPTIMIZATION ALGORITHMS TO THE SWARM ROBOTICS CONTROL PROBLEMS

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The work is devoted to the development of algorithms for control of robot swarms. The complexity of this problem lies in the fact that we should program the behavior (identical) of the individual robot, and the programming goal is the collective behavior of the entire swarm. At the same time, there are a number of search-type problems, for example, the problem of finding the source of pollution, which can be considered as optimization problems. To solve such problems, there is a well-designed class of algorithms called swarm optimization algorithms (particle swarm optimization algorithm, bacterial foraging optimization algorithm), which were originally designed on the basis of swarm behavior. However, direct application of such algorithms in swarm robotics is impossible due to the use of mechanisms that cannot be supported by real robots (instantaneous movement of robots to any point in the decision space, reproduction and selection). In addition, the very task of searching for a particular object inside given area can limit even the usual behavior of robots – for example, the presence of obstacles (walls) prevents the movement of robots even a short distance. Such limitations in optimization problems are usually absent. The purpose of our research is to adapt the algorithms of swarm optimization to solving search problems by swarm robots. We consider the model problem of searching for the source of a certain signal, describe the adapted versions of several classical algorithms of swarm optimization, and present the results of a numerical study of the efficiency of the developed algorithms. We use NetLogo integrated environment as a modeling tool.

ON A METHOD OF INVESTIGATION NONLINEAR SELF-CONSISTENT EIGENVALUE PROBLEM WITH THE GROWING POTENTIALS

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Success in solving multiparticle problems is in many cases connected with the choice of an adequate model. As a simple example, we can cite the concept of a polaron as a problem of an autolocalized electron in an ionic crystal. At present, there are a large number of physical examples [1-3], the theory of polarons, bipolarons, a strong-coupling binucleon model, a generalized polaron model, etc. The effect of autolocalization in liquids leads to the formation of solvated electrons in them, which play an important role in many chemical processes [4,5]. Similar problems arise in the nonrelativistic potential model at the description of the spectrum of heavy quarkonia [6]. To study such problems, one can involve methods of self-consistent description of multiparticle systems.

A method is proposed for investigating the properties of solutions of a nonlinear self-consistent boundary value problem with increasing potentials of even and odd powers. A comparative analysis of the solutions of the linear boundary value problem for a quadratic growing potential with a nonlinear self-consistent boundary value problem for this potential is carried out. Formulas are obtained which allow us to calculate the shift of the eigenvalues. If the distances between the levels of a linear problem are equidistant, then in a self-consistent problem this property is also satisfied. In addition, when investigating problems with potentials above the quadratic one, new growing potentials appear to a lesser degree in the self-consistent problem than the original potential.

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GENERATING FUNCTIONS METHOD FOR CONSTRUCTING NEW ITERATIONS

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In this paper we propose a generating function's method for constructing new two and three-point iterations with $p\,(3 \le p \le 8)$ order of convergence. This approach allows us to derive a new family of optimal order iterative methods that includes well known methods as a special cases. The necessary and sufficient conditions for *p*-th order convergence of proposed iterations are given in term of parameters τ_n and α_n. Several numerical results are given to demonstrate the efficiency and performance of the presented methods and compare them with some other existing methods.