Contents

A fast parallelized Kalman filter based reconstruction of charge particle trajectories for the CBM experiment on a manycore server at LIT JINR

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The task of a charge particle trajectories reconstruction is one of the most important tasks of the CBM experiment (GSI, Germany). The experiment assumes a full on-line event reconstruction, that requires development of fast algorithms, which utilize the potential of modern CPU and GPU architectures in the most efficient way. In the current work the results of analysis of the Kalman filter based track reconstruction algorithm, which is implemented using different parallelization approaches, are presented and discussed. For the analysis a manycore server with two Intel Xeon X5660 CPUs and a NVidia GTX 480 GPU at LIT, JINR was used.

On the width of full rank linear differential systems with power series coefficients

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We consider the following problem: given a linear ordinary differential system of arbitrary order with formal power series coefficients, decide whether the system has non-zero Laurent series solutions, and find all such solutions if they exist (in a truncated form preserving the space dimension). If the series coefficients of the original systems are represented algorithmically (thus we are not able, in general, to recognize whether a given series is equal to zero or not) then these problems are algorithmically undecidable ([2]). However, it turns out that they are decidable in the case when we know in advance that a given system is of full rank. Our proof is based in part on [1, 4, 4].

We prove additionally that the width of a given full rank system S with formal power series coefficients can be found algorithmically, where the width of S is the smallest non-negative integer w such that any l-truncation of S with $l \geq w$ is a full rank system. An example of a full rank system S and a non-negative integer l such that l-truncation of S is of full rank while its $(l+1)$-truncation is not, is given in the paper; however it is shown as well that the mentioned value w exists for any full rank system.

We propose corresponding algorithms and their Maple implementation, and report some experiments.

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Sharpening local error estimates using redundancy in Bayesian automatic adaptive quadrature[1]

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The possibility of the implementation of redundancy-based features within Bayesian automatic adaptive quadrature (see, e.g., [1] and references therein, and [2]) is discussed. On a hardware environment characterized by multi-core processors, *local quadrature rules* yielding $(q, e > 0)$ outputs (where q denotes the computed approximate value of the integral of interest, while $e > 0$ denotes its associated local error estimate) are

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proposed taking advantage of the possibility of computing independently a pair of high order quadrature sums on different cores. The obtained result, while keeping the most accurate quadrature sum output for q, allows the derivation of a dramatically sharpened $e > 0$ estimate without increasing, however, the computational cost of the procedure.

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The volume integral equations method in magnetostatics problems

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Applications of the volume integral equations method for calculations of magnetic systems are considered. A GFUN program based on this method applies a method of collocations and piecewise constant approximations of unknown variables in the elements for discretized equations. Limitation of this approach is related to singularity of the integral equations kernel. Alternative to the collocation method is integrating over discretization elements. This allows one to use the higher order approximations for unknown variables. A piece-wise constant and linear approximations of unknown variables are considered. The matrix

elements calculation problems and the methods for solving nonlinear systems of discretized equations are discussed. The results of the dipole magnet simulations using different versions of the volume integral equations discretization are given.

Cellular automaton track finder at high track multiplicities

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The CBM experiment at FAIR is being designed to study heavy-ion collisions at extremely high interaction rates. The event selection has to be done online, therefore fast and efficient reconstruction algorithms are required. The Cellular Automaton (CA) track finder is fast and robust and thereby is used both for the online and offline track reconstruction in CBM. Since the CBM beam will have no bunch structure, but continuous, the reconstruction of time slices rather than events is needed. Measurements in this case will be 4D (x, y, z, t). In order to study the worst case scenario with no time measurement taken into account a number of minimum bias events (up to 100) was grouped into one, which was treated by the track finder as one event. The study has showed that CA track finder is stable with respect to track multiplicity: the efficiency of the algorithm decreases only by 4% for 100 minimum bias events in one group. The speed of the algorithm behaves as a second order polynomial with the number of track.

MPI algorithm realization for 3D-computation of phase transitions in materials irradiated by ions beams in frames of thermal spike model[1]

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A parallel algorithm implemented on the basis of MPI technology has been developed for 3D computations of the evolution of temperature fields and the dynamics of phase transitions in materials irradiated by heavy ions and ion beams. Description of the interaction of ion beams with matter is based on a modified nonlinear thermal spike model [1]. The computational scheme is based on the finite- difference scheme described in [2], while simulation of the dynamics of phase transitions is performed in frames of the enthalpy approach [3]. Using the developed MPI/C++ program, the phase transitions in the nickel target irradiated by 700 MeV uranium ions and in the iron target exposed to a 300 keV pulsed carbon ion beam have been investigated. A comparison was performed of the calculated size of the melting region with known experimental data and computations presented in [4], where phase transitions are not taken into account.

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A new software complex for modeling thermophysical processes in materials irradiated with heavy ion beams on HPC systems[1]

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A new software complex for modeling thermal processes in materials irradiated with heavy ion beams has been developed. The complex includes programs which implement parallel algorithms for numerical calculations of coupled thermal equations which are a basis of the thermal spike model.

The developed algorithms were realized on the basis of MPI and CUDA technologies for computations on hybrid computer systems containing multi-core processors (CPU) and graphic accelerators (GPU). The created complex meets the following requirements: possibility of the complex use on different computing platforms with various operating systems; possibility of parallel algorithms launching on multi-core systems and on systems with graphic accelerators; possibility of program modules launching which implement various numerical algorithms of problems solution; a possibility of complex expansion by adding physical characteristics of new materials to the database, as well as a possibility of adding of program modules which implement other algorithms.

For convenient editing and adding the new physical characteristics of the materials stored in the XML database, corresponding program interfaces have been developed.

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Modeling of thermal processes in materials irradiated with heavy ion beams with the use of parallel algorithms on HPC complexes[1]

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Parallel algorithms of numerical solution of coupled equations of heat conductivity which are a basis of the thermal spike model have been developed. Implementation of the developed algorithms realized on the basis of MPI and CUDA technologies for calculations on HPC complexes with multicore processors (CPU) and graphic accelerators (GPU) NVIDIA. Patterns on organization of parallel computing depending on the dimension of the computational domain and characteristics of computational elements have been worked out. A research on the efficiency of parallelizing according to the grid dimension and the number of CPU and GPU in use has been carried out.

Computational experiments have been held on the JINR CICC parallel cluster, on the cuda.jinr.ru hybrid cluster and the hybrid computer complex, M.V. Keldysh Institute for Applied Mathematics.

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Simulation of eddy current and electromagnetic loads in ITER conducting structures

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A modelling technique has been developed to efficiently predict electromagnetic (EM) loads in conducting structures of the ITER machine. An integral set of models has been developed in the course of activities requested and supervised by ITER Organization. Detailed models were built for the system "vacuum vessel (VV), cryostat, and thermal shields (TS)" which enable description of its complex multiply connected thin-walled structures with required accuracy. A shell model of the system implements an integral-differential formulation, and a single unknown is determined in terms of the vector electric potential taken at the nodes of an FE mesh on a shell surface. The EM transients are simulated through the space and time variations of the toroidal plasma current, halo current, the toroidal magnetic flux, and the coil currents, that covers practically all field sources. These data are derived from results of MHD simulations. This enables simulations for all plasma scenarios and operating modes. Reasoning from the simulation efficiency, first, induced eddy currents are simulated in the global system "VV+cryostat+TS" that has crucial EM effect on other structures. EM loads on in-vessel and out-vessel structures are simulated with the use of local FE models, based either on the 3D solid-body or shell approximation. In-time field sources can be described via a set of basic functions. As an alternative to direct integration over the entire operation scenario, a generalized

solution for any scenario is obtained as a superposition of individual solutions. The mathematical formulation is implemented in terms of vector potentials or through a field vector. In the Cartesian coordinates, a separation of variables (vector components) is applicable. Parallel computations enable solving the problem in both formulations during the same runtime. An efficiency of these solutions is compared. Combined computations with different models provide cross-checking within common procedures. Integration with other computer codes is feasible that improves reliability of simulations. The proposed computational technique has been applied to EM analyses to support ITER design activities. The results have been included in the project documentation. Developed computational models enable cost-and time effective computations at further activity.

Computer simulation of electrical activity in the sinoatrial node[1]

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We have simulated a 3D propagation of the action potential in the sinoatrial node to study the heart rhythm initiation. We have found that the leading center inside the sinoatrial node is formed by a group of cells, appears spontaneously under normal conditions, and migrates as acetylcholine is applied. The leading center drifts toward the center of the sinoatrial node, if we consider the effect of the surrounding atrial tissue [1].

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We have studied the dynamics of vortex-like rotation (reentry) inside the sinoatrial node and found that reentry is unstable at high intercellular conductance. Rotating reentry induces a slow migrating crescent shaped functional block near the SAN boundary [2].

In a chain of sinoatrial pacemaker cells connected via gap junctions we simulated the dynamics of phase of oscillations and show that Burgers equation is adequate to describe phase dynamics in the sinoatrial node. We show that propagating action potential bears properties of either trigger waves or phase waves, which depends upon its wave number. We propose a definition of the safety factor that is applicable to an oscillatory tissue of the sinoatrial node and show that the maximum of the safety factor relates to the boundary case separating phase waves and trigger waves [3].

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Investigation of solutions of quasistationary states for the quasipotential equation [1]

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Investigation of the solutions of quasistationary states is carried out for the quasipotential equation [1] with piecewise-constant potentials at various values of parameters of the problem. A comparative analysis of the solutions of a quasipotential equation with the solutions of Schrodinger equation is performed.

In our previous papers [2-4] boundary-value problems have been investigated for a quasipotential equation with different methods and a comparative analysis of the solutions to similar problems with solutions for the Schrodinger equation is performed. Similar studies are important for the identification of relativistic effects.

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Mathematical modeling of beam dynamics for estimation of operating modes of isochronous cyclotron[1]

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The work presents the equations of motion and the numerical results of estimating the quality of the isochronous magnetic field calculated for the main operating mode of the AIC-144 multipurpose isochronous cyclotron located at the Institute of Nuclear Physics, Polish Academy of Sciences and intended for the carrying out of proton radiotherapy of eye melanoma. The main operating mode of the AIC-144 cyclotron is simulated using a new technique [1]. After the successful realization of the current variant of the specified operating mode on the AIC-144 cyclotron in July, 2012 and fine tuning of the amplitude of central bump of formed magnetic field in October, 2012, the beam dynamics was calculated using the programs developed at the Laboratory of Nuclear Problems of the Joint Institute for Nuclear Research [2].

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[2]Work is supported by RFFR grant No 13-01-00595-a.

Scheme of splitting with respect to physical processes for a model of heat and moisture transfer[1]

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A difference scheme of splitting with respect to physical processes for a model of heat and moisture transfer is proposed. The model involves three physical processes - heat, liquid and saturated vapor transfer in the porous material. The density of the saturated vapor and the transfer coefficients of liquid and vapor moistures depend on temperature. At the same time, the heat capacity and conductivity of the porous material depend on moisture. On the basis of the proposed scheme of the model, a numerical simulation of the heat and moisture transfer for a drying process has been performed.

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Modeling the track formation in amorphous iron alloys exposed to high-energy heavy ions [1]

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An important process in the fundamental radiation in solid state physics and in applications is the process of the track formation at irradiation by high-energy heavy ions of different in their physical and chemical properties materials. The development of modern methods of analysis and studies of the structure of extended defects stimulates initiation of the new experimental and theoretical research in this area. The track diameters 11.1 MeV/amu ion 132Xe, 152Sm, 197Au and 8.2 MeV/amu 238U ions in a number of amorphous alloys of iron and boron were measured using a small angle scattering of synchrotron radiation [1]. In this work, a three-dimensional model of the thermal spike [2] modified with phase transitions of the fusion was introduced and used to estimate the diameter of tracks all of the above ion-target combinations whose values were compared with experimental data [1]. Accounting the phase transitions made in this work to evaluate the tracks diameters significantly improves the agreement of the simulation results with experimental data [1].

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Optimization of currents in ITER correction coils

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In tokamaks non-axisymmetric magnetic field perturbations (error fields) can induce locked modes in plasma and cause plasma disruptions. In ITER the main contributor to error fields is assembly and manufactory errors of the magnet system of the machine.

To suppress intrinsic error fields and guarantee the expected plasma performance ITER is provided with the proper correction coils (CC).

The paper is related to optimization of CC currents. The optimization takes into account as constraints both CC current capacities and the allowable level of error fields.

The transition from the error field statistics to that of CC currents allows us to describe more precisely the Monte Carlo model and improve the accuracy of probability estimations.

As a result, the maximum CC currents, observed in the Bottom CC, reduce from **250 kAt** to **164 kAt** at the **99.9%** probability criterion on minimizing the root-mean square norm of currents.

The transition in optimization from the root-mean square norm of currents to the vector norm of the lowest of a set of the maximum current values allows us a further reduction of the maximum value of current in the coils from **164 kAt** (Bottom CC, 99.9% confidence) to **130 kAt** (all coils, 99.9% confidence).

Solutions to nonlinear ODE's by means of power geometry algorithms

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We consider author's computer programs for calculations by power geometry algorithms [1]. These programs and algorithms allow to calculate power expansions with integer and fractional power exponents of solutions to nonlinear ODE's. By means of the programs we calculate terms of Laurent Laurent-Puiseux expansions with rational power exponents of solutions to the Euler-Poisson ODE's, that describe motion of the rigid body with a fixed point [2]. As results of calculations we obtained constraints on parameters of the considered ODE's, including all constraints for known solutions [3] to the Euler-Poisson equations. Also we obtained some new expansions.

Suggested programs are implemented by C++ language and CAS Maxima.

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Modelling of superfluid helium in forced-flow cooling circuits with VENECIA code

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Extremely high thermal conductivity of superfluid helium HeII makes it very attractive for the use in magnet cooling systems. The superfluid-helium technology has been developed in this field quite intensively from the first milestone application for the TORE SUPRA machine, Cadarache, France in 1988 to the Large Hadron Collider, Lausanne, Switzerland, 2008. One of key point of practical demand is development of software tools and computational models capable of adequate description of fluid dynamics and heat transfer in forced-flow circuits. A numerical formulation is presented for the superfluid helium model implemented in the thermal hydraulic code VENECIA. The model is based on the Gorter-Mellink law for heat transfer in superfluid helium represented in 1D approximation. Such model gives solutions with fairly good accuracy for engineering of HeII cooling systems. To validate the model a set of test simulations has been compared successfully to experimental data.

Algorithms for mathematical modeling of thermal processes for design a technical device[1]

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Multiparameter control problem for heat equation is proposed to design the cryogenic cell pulsed (millisecond range) feeding the working gases into the electron-stringed source of multiply charged ions [1].

For solving multiparameter control problem algorithms for numerical solving the direct mixed problem for a heat equation with discontinuous coefficients are developed and presented [2-4].

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Stable computer modeling of thin-film generalized waveguide Luneburg lens

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The method of adiabatic guided modes models the propagation of the waveguide radiation when taking into consideration the exact tangential boundary conditions. The results of using the method developed and its descriptions are published in [1,2]. Stable algorithms for the calculation of the dispersion relations and the electromagnetic fields of guided modes by adiabatic waveguide modes method are implemented in a complex of programs and published in [3,4]. Examples of the device in the description of which and especially in the numerical design of which such consideration is required, are thin-film generalized waveguide Luneburg lens. It is an important part of many integrated optical systems and processors, it performs (with a proper design and manufacture) a generalized amplitude-phase Fourier transform. The work presents computer simulations of polarized electromagnetic radiation from entering the thin-film generalized waveguide Luneburg lens to its focal plane.

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Application of functional polynomials to approximation of matrix-valued functional integrals

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One approach to approximate evaluation of functional integrals is approximation of the original integrand functional by functional polynomials. Another approach to evaluation of functional integrals is the construction of approximate formulas that are exact for a class of functional polynomials of a given degree [1-3].

There are different types of functional integrals because there are different spaces, measures and ways to define the functional integrals. Functional polynomials and formulas with given degree of accuracy are widely used to approximate evaluation of integrals with respect to Gaussian measure.

We propose to use the functional polynomials to approximate evaluation of matrix-valued integrals, generated by solutions of Dirac equation. These integrals are widely used in relativistic quantum mechanics for investigation of particle in electromagnetic field [4-5].

The method of evaluation of matrix-valued integrals is based on the expansion of functional in a series. Terms of a series have the form of a product of linear functionals with increasing total power. In case of Gaussian integrals the series of integrals of the product of linear functionals converges for a narrow class of functionals. In case of matrix-valued integrals the series converges for a wide class of functionals.

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Application of the perfect match problem to the track-match problem

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A question of the track-match problem of the elementary particle (track) trajectory recognition is reduced to to solving the problem of existing a perfect match in a two-particle graph.

Methods of numerical analysis for reversible shocks in media with complex dispersion [1]

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Reversible shock structures (kinks) are observed in numerical solutions of equations corresponding to non-dissipative and low-dissipative models with complex dispersion and nonlinearity. Effective method for investigation of such shock structures is analysis of arbitrary shock split problem (Riemann problem). These solutions consist of regions of homogeneous states and wave zones. Wave zones and homogeneous states are separated by shock structures. Wave zones may be described by averaged equations. For non-dissipative case regions of wave zones are increasing with time. For the case of regular solutions after enough long period of time envelope for such wave zones becomes homogeneous or self-similar. For low-dissipative case wave zones after a long period of time become stationary. Stationary reversible shock structures that are transitions between uniform or periodic states are analyzed. Some periodic states may be treated as a result of interaction of two waves with integer ratio between spacial periods (resonance solutions) [1]. Averaged equations based on resonance solutions may be derived for this states also as based on one-wave states. These equations are the special case of averaged equations based on non-stationary solutions [2]. Condition of evolutionality (the necessary condition to be mathematical problem well-posed) is analyzed. For some structures evolutionality takes place for both direct and reversed shock and for others only direct shock is evolutional and the reversed shock is overdetermined [2]. New classification of shock structures according to number of free parameters is made [2]. This classification is made for periodic and solitary waves also. Methods of numerical analysis based on solution of ordinary travelling wave equations are developed. One of them is analysis of pictures of brunches of periodic stationary solutions. This method gives effective way to determine stability of these solutions and predict possible type of shock structures [1].

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A method of local improvements for lower bounds on valuations of solutions of linear difference systems with polynomial coefficients

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We present a method to improve lower bounds on valuations of meromorphic solution components of an arbitrary-order difference system

$$A_r(x)y(x+r) + \cdots + A_1(x)y(x+1) + A_0(x)y(x) = b(x),$$

$A_0(x), A_1(x), \ldots, A_r(x) \in \mathrm{Mat}_m(\mathbf{K}[x])$, $b(x) \in \mathbf{K}[x]^m$, $\mathbf{K}$ is a numeric field. The method is based on associating valuations of coefficients of equations with given bounds on valuations of solutions. The method can be used as an auxiliary for known computer algebra algorithms for finding lower bounds on valuations [1]. Such bounds are needed, e.g., for constructing rational solutions of a given system [2, 3].

For any system of the described form the known algorithm EG_σ constructs embracing systems of the same form [4]. The solutions set of embracing system

contains all the given system solutions. After that, the linear constraints encountered during the work of the algorithm can be used to discard "parasitic" solutions. The proposed method allows to use some analogues of linear constraints for improvements of lower bounds on valuations of the given system solutions.

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Comparative study of cluster and neural network methods in the problem of protein structure analysis

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This work continues the previous study [1] where the important problem of automatization of differentiation methods of the genetic protein structures according to their electrophoretic spectrums (EPS) was considered. The multicriterion problem of the agriculture cultivar identification by their spectra

caused the idea of its solution by an artificial neural network (ANN) trained on an expert data base [2].

In the given paper peculiarities of the neural net use as well as the purposefulness of cluster analysis applications for the EPS classifying are studied.

A special model of multidimensional vectors adequately imitating the most essential characteristics of real data obtained after EPS digitalization, denoising and normalization is developed. A numerical experiment is fulfilled on such simulated data stream to study the influence of contamination and distortion factors on the ANN efficiency in order to suppress those factors and improve ANN functioning.

Various methods of cluster analysis [3] are also applied to simulated multidimensional data as either an ANN alternative or more soundly as a prior stage of a coarse data classification in some set of detached cultivar groups to be classifying next by ANN.

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Simulation of interaction of a colliding nanoclusters beam with solid surface[1]

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Simulation of impact processes of colliding metal nanoclusters with a metal solid surface is fulfilled by molecular dynamics methods [1] and suitable software [2]. A preliminary procedure is a transformation of the impact nanoparticles with a face-centered cubic structure to nanoclusters with an icosahedral structure. The goal is to investigate a penetration depth of the metal clusters into the solid metal surface in dependence on a beam energy, a number of particles in clusters and a frequency of the impulsive nanoclusters source. The analysis of simulation results demonstrates importance of the investigation of the surface deposited layer thickness as a function of the nanoclusters beam parameters. It is shown that realization of one of the choice of the nanoclusters surface interaction (soft landing, droplet spreading and implantation) should be controlled by means of changing both the nanoclusters beam energy and the number of atoms in the clusters. The investigation results should be of interest in various fields of technologies developing nanomaterials with new physical and chemical properties.

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Global optimization algorithms for data analysis

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Algorithms for the global optimization of functions are not yet widely used for data processing.

The goal of our study is to demonstrate the potential of these algorithms for obtaining new information based on spectroscopy, material science and geophysics.

Genetic algorithms [1] provide an example of stochastic global optimization. They are based on the idea of natural selection or perfection of a species by transmitting the best genes to the offspring. The environmental adaptability function of individuals is determined on a variety of individual chromosomes formed as a sequence of unities and zeros that represent numbers in the Gray code. The smaller the function value, the more environmentally adaptive the individual. A genetic algorithm retrieves the global minimum of this function, beginning with an arbitrary set of individuals selected as a population. At each iteration, the individuals are paired and an offspring is produced by crossing-over: chromosome tail exchange and mutation — random value inversion in a random number rank. Individuals are selected for a new population with regard for the adaptability of the offspring and the parents. The algorithm is considered convergent, if the new population does not differ from the previous one. Genetic algorithms have some advantages: they need not be continuous and differentiated; they are not sensitive to being in local minima; they are capable of multi-criterion optimization; their convergence is more rapid than random search; and they are readily used in computer mathematics systems. They have some disadvantages: the use of biological terms makes them hard to understand and the global extremum is too inaccurate. However, it can be made more accurate by executing the algorithm several times and selecting the most adaptable extremum value.

A search algorithm based on a pattern, i.e. a set of points in the form of the peaks of an n-dimensional cube which expands or compresses, depending on whether the template point value is smaller than the current function value, is less labour-intensive than genetic algorithms. The minimum size of the pattern provides the basis for the termination of the search.

The algorithms ga and patternsearch, used to reconstruct signal and noise structure in the maximum entropy method, are consistent with the methods for the optimization of Matlab, a computer mathematics system, Matlab (Fig.1) [2].

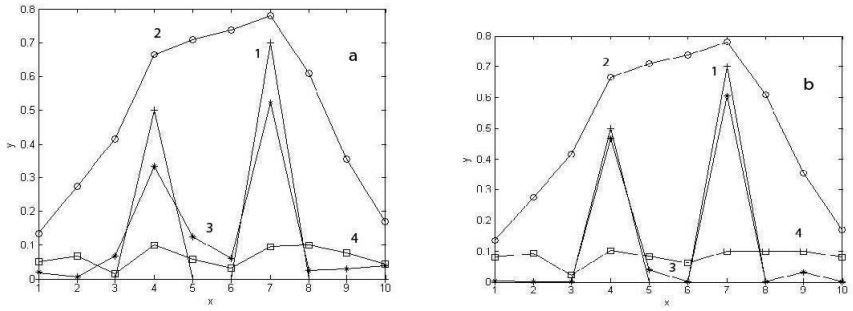

Fig.1: Results of the reconstruction of signal and noise structure by the maximum entropy method, using global optimization algorithms ga () and patternsearch (b) of the Matlab System: 1 – original signal; 2- data processing signal; 3-estimation of the original signal; 4- noise estimation

A simulated signal was produced by blurring two δ-peaks by a 1.41-wide Gaussian and adding white noise in the range [0;0.1]. An entropy functional was constructed from original function and noise estimates. Limitations in the form of linear equations which connect the signal observed, the blurring function, original function and noise estimates and inequalities which set the variable variation range were introduced into the command line of the algorithm. Signal and noise estimates were obtained by skipping an intermediate stage in the finding of the Lagrange multiplier.

Real spectra were processed using global optimization algorithms in the maximum entropy method to reveal the hidden spectrum structure [3] and in the least square method to estimate the parameters of its components.

The algorithms described were employed to analyze the rapidity distribution structure of high-energy particles; the characteristics of structural phase transitions were revealed; and the possibility of selecting gravity and magnetic anomalies upon gravimetric and magnetometric data processing was shown. The positions, amplitudes and widths of the complex contour decomposition components make it possible to re-interpret monitoring and experimental data and can facilitate the construction of adequate matter models and can make analysis of spectra and distributions informative.

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The inverse problem for the Grad — Shafranov equation with application to magnetic field computation in tokamak [1]

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The well–known model [1] of magnetic field in tokamak reduces to solving the Grad — Shafranov equation $\Delta u(x) = au(x) + b$ in the cross–section G of plasma coil with homogeneous Dirichlet condition on its boundary Γ, which is supposed to be piece-wise $C^{3,\alpha}$–smooth; constants a, b are unknown. In [2] this

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statement was supplemented with the non–local condition $\int_\Gamma \partial_\nu u(x)\, ds = 1$, which physically means prescribing the value of full current; here ds is length element of arc Γ, ∂_ν is normal derivative to Γ. The non–local condition states an explicit relation $b = b(a)$ between parameters a and b of the equation, and so makes the problem stated above depending only on parameter a. The inverse problem for the Grad — Shafranov equation with non–local condition consists in finding parameter a via the value of normal derivative $\partial_\nu u(x)$ in any point x belonging to special subset $\widetilde{\Gamma}$ of boundary Γ. In the present work the necessary and sufficient conditions of unque solvability of the inverse problem are stated. An effective analytic–numerical method is elaborated for finding parameter a, including an algorithm of constructing subset $\widetilde{\Gamma}$. Those results were obtained by the use of the multipole method [3] that ensures high precision computation of normal derivative $\partial_\nu u(x)$ and by the use of asymptotics [4] as $a \to \infty$ for $\partial_\nu u(x)$ and $\frac{d}{da}\, \partial_\nu u(x)$, $x \in \Gamma$.

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A method for statistical comparison of histograms

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We propose an approach for testing the hypothesis that two realizations of the random variables in the form of histograms are taken from the same statistical popu- lation (i.e. that two histograms are drawn from the same distribution). The approach is based on the notion "significance of deviation". Our approach allows also to estimate the statistical difference between two histograms.

Extremal dynamics of the system of three coupled singularly perturbed equations with two delays

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We consider model-system, applied in neurodynamics and population's biology, consist of three linked in a hoop singularly perturbed oscillators with two delay

$$\dot{u}_j = \lambda\big[-1 + f_1(u_j(t-h_1)) + f_2(u_j(t-h_2)) + \varepsilon^3 u_{j-1}\big]u_j. \tag{1}$$

where $j = 1,2,3, \lambda > 0$, $h_1, h_2 > 0$ – parameters, $f_j(u)$ – sufficiently smooth functions, ε– small parameter. Suppose, that (1) has only one non-zero tranquillity u_* such that $f_1(u_*) + f_2(u_*) = 1$. Suppose also, the functions of the right side of (1) expanded at u_* in the series $f_i(u) = a_{i0} + a_{i1}u_*(u-1) + a_{i2}u_*^2(u-1)^2 + a_{i3}u_*^3(u-1)^3 + \mathcal{O}\big((u-1)^4\big)$, here $u = (u_1, u_2, u_3), i = 1,2$. The problem (1) will study in a singularly perturbed case when

$$\begin{aligned} &h_2 = \varepsilon\gamma h_1,\ a_{11} = -1/2 - \mu,\ a_{21} = -1/2 + \mu, \\ &\gamma = const > 0,\ \varepsilon = 1/\lambda,\ 0 < \varepsilon, \mu << 1, \end{aligned} \tag{2}$$

Also assume that the parameter γ is fixed and satisfies $\gamma < 1$.

Realized for (1) linear analysis shows that the assigned bifurcation problem is close to the infinite: when $\varepsilon, \mu \to 0$ to the imaginary axis seeks a countable number of roots the characteristic equation, and in this situation, to study the dynamics of the original system we has to resort to the so-called method of quasi-normal forms [1], by means of which one can construct a quasi-normal form of the system (1), representing the following parabolic boundary value problem

$$\begin{aligned} &\frac{\partial \xi_j}{\partial s} = 2(1-\gamma)\frac{\partial^2 \xi_j}{\partial \tau^2} + 4\beta\xi_j + d\xi_j^3 + 2a_{31}\xi_{j-1}, \quad \xi(s, \tau+1) \equiv -\xi(s,\tau), \\ &j = 1,2,3, \end{aligned} \tag{3}$$

where s is playing the role of time, τ is the spatial variable, $d = 2(a_{23} - a_{13}) + 4(a_{22}^2 - a_{12}^2)$. Investigation of (3) allowed to show that for any positive integer n, one can choose the parameters of the system in such way that the original system will co-exist exactly n stable attractors.

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Modeling of the behavior of European options in the cloud computing system

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Considerable interest in the problems of financial mathematics is defined due to the needs of huge derivatives markets, and the ability to use physics approaches which are well developed for these purpose.

The principle feature of the problem from a computational point of view is the need in a short period of time (10-15 min.) to obtain solutions with a large set of initial data (hundreds of thousands).

Since these calculations are only required for certain situations with a great turbulence in the markets [1], approach based on cloud technologies looks very attractive, when at the peak of the calculations we can collect the required resources, and pay only for the actually used one.

We propose the algorithm that allows to hold mass calculations European options [2] in real-time using cloud technology. In addition, the requirements for building virtual computer systems have been formulated. Complex calculations can be performed on the base of these computer systems.

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New approximation results for data with errors in both variables

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We introduce the new data from mineral water probe /Lenovo Bulgaria/, measured with errors in both variables [1]. For this case we apply our Orthonormal Polynomial Expansion Method (OPEM) [1], based on Forsythe recurrence formula [2] to describe the data in the new error corridor [3]. It receives the approximating curves and their derivatives including the errors in both variables by weighting approach. The developing of our numerical method and approximation results are presented and discussed. The special criteria are carried out for orthonormal and evaluated from it usual expansions.

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Qusiclassical methods for perturbed KDVB equation

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The solution of nonintegrable nonlinear equations is very difficult even numerically and practically impossible by standard analytical technic. We shall give some examples of such analysis on the base of nonlinear waves evolution study in multiphase media with chemical reaction [1]. It was shown, that for one dimensional gas dynamic problem, described by Navier-Stockes equation, equation of state, and simple linear relaxational equation after expansion up to the second order near the equilibrium state one gets for the velocity nonlinear evolution equation of the form

$$\nu_t + \nu\nu_x + \alpha\nu_{xx} + \beta\nu_{xxx} = \gamma\ I(\nu),$$

with α being the measure of dissipational effects, β being the measure of dispersion, γ is the measure of interphase interactions and $I(\nu)$ is the integral operator. Computations were realized by implicit MacCormack scheme with flux-corrected procedure. Special attention was given to behavior in asymptotic region and appearance of nonintegrable effects like tails and nonlinear soliton interactions.

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Functional integration as a tool for mathematical modelling and high performance algorithms creation

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We propose the approach for generation of the representation for solution of PDE based on functional integration. The representation is the integral representation over subspace of coordinate space and under the integral the functional is determined by solution of four first order PDE. This opens excellent possibilities both for study of peculiarities of solutions and for generation of parallel computational algorithms. As examples we study scattering problem and kinetic equation.

On 2D and 3D localized solutions with nontrivial topology

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Localized topological solutions can be divided into 2 classes: topological solitons (TS) and topological defects (TD). We exemplify and compare stationary TSs and TDs in 2 and 3 spatial dimensions.

Using multi-threading in the relevant LP-inference method

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LP structures, that are actually one of the algebraic system classes are used in various research areas and their further extension - an enhanced backward inference method provides serious improvements when working with data queries. The strategy of a relevant backward inference is aimed at minimization of a number of queries to the external information source (either to a database or an interactive user). The queries whenever possible are sent for those facts that are truly necessary for the inference. A negative answer to a unique query eliminates all subsequent queries about the elements of a subset of facts. Along with a significantly reduced number of queries, when using LP inference, the preference is given to testing the sets of facts of a minimal cardinality.

The proposed theory provides new opportunities for research, optimization and verification of knowledge bases and creates basis for an integrated framework that can be used for the development of production logical systems. In some of its parts the framework uses an object-oriented class LPStructure, which is aimed for searching logical reductions and solutions of the production logical equations. Multi-threading is a fundamentally new element in the implementation, which allows speeding up the process of constructing sets of facts that are required in the inference, and their further processing. The benefits of its use are confirmed experimentally and the results are processed by statistical methods which show that the proposed approach increases the efficiency of a backward inference by 30%.

Parallel 3D PIC code for the numerical simulations of ultrarelativistic charged beams in supercolliders[1]

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We present a parallel fully 3D algorithm for simulation of beam-beam effects in super-colliders, where colliding beams have superhigh densities and high relativistic factors. The beams undergo strong compression (pinching) and even disruption of the beam may appear.

The most commonly used algorithms for such problems are based on a quasi-three-dimensional model ("slice" model) in which a beam is represented by a sequence of thin two-dimensional slices. The longitudinal motion is simulated by "rearrangement" of the slices and cause difficulties for complete taking into account the longitudinal effects and crossing angle beam-beam effects.

In our 3D algorithm we employ the Vlasov-Liouville equation for the distribution function of beam particles, the three-dimensional set of Maxwell equations and new methods for initial and boundary conditions calculations[1], which automatically account for such difficulties. We solve these equations by using the particle-in-cell (PIC) method and the leap-frog scheme[2].

The parallel code is based on the domain decomposition along the transversal direction: every processor group gets its own part of the subdomain grid and all the particles of the subdomain. We additionally employ particle parallelization: within the group every processor gets its own set of particles[3]. This method allows to increase appreciably the scalability and to overcome the high restrictions on particle number due to the highly non-linearity of the density distribution and the limited computer memory: for 6 processors and $100\times100\times100$ grid the limit is $2\cdot10^6$particles, what means quite small for PIC method particle number in cell.

In the report we present the parallel performance, strategies to increase the parallelization efficiency and demonstrate some results of numerical experiments on the focused beam dynamics.

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Structural, electronic and optical properties of CdS1-xTex ternary semiconductors

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Structural, electronic and optical properties of several CdSxTe1-x ternary alloys were studied using ab initio calculations. The structural optimization of the zinc-blende CdSxTe1-x lattices constant are calculated using the Broyden-Fletcher-Goldfarb-Shanno minimization. Good agreement with theoretical and experimental studies for the structural properties was found. All alloys compositions show that the maximum of valence band is situated on the point and that the minimum of the conduction band is also situated on this point Γ. Ternary alloys are within a direct gap $E(\Gamma - \Gamma)$ for all x values. However, only good agreement with theoretical studies for the electronic properties was evident. Very interesting properties were found using new calculation methods.

Open geoinformation internet system for the air pollution modeling

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This report describes a hybrid GIS that Combines the spatial analysis methods of geographic information systems with modules for mathematical modeling air pollution. The architecture of the developed system has been designed to provide an opportunity for professionals to use different modeling technologies on different data and different territories.

Parallelized procedure for the determination of the fully differential cross section for $(\gamma, 2e)$ photo-double ionization of N_2 molecule

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We have determined a multiply differential cross section (MDCS) of the vertical photo-double ionization of diatomic nitrogen with coincidence detection of the ejected electrons, for fixed and random orientations of the internuclear axis, using a correlated product of two two-center continuum coulomb functions for the description of the two ejected electrons, which satisfy exact asymptotic conditions. To verify our procedure, we have applied it to the photo-double ionization of diatomic hydrogen for which many experimental and theoretical results are available. Our results show the influence of the initial state correlation. In the case of the double ionization of the $3\sigma_g$ orbital of nitrogen, our results confirm the symmetry properties of the MDCS and give the optimal ejection angles. The MDCS are expressed as 2+6-dimensional integrals.

The corresponding 2D+6D integrals encountered in the procedure are calculated using an adaptive subdivision algorithm in its author's version for parallel computers. The parallel FORTRAN code with MPI has been tested for several multidimensional integration examples, and it demonstrated its high efficiency.

Analysis of a piecewise linear trend of average surface temperature of the Northern Hemisphere of Earth in the 2^{nd} and the beginning of the 3^{rd} Millennium in the mathematical model of multifractaldynamics

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In this work the model of variations of average annual temperature of the Northern Hemisphere of the Earth is constructed. And on its basis research of the main regularities of temporary variability of temperature from 1000 till 2010 with application of methods of the multi-fractal dynamics, which are described in work [1]. For 1010 it was allocated 26 periods and for each of them it is settled an invoice fractal dimension of D. Also the schedule of jumps of a difference h=D-D_0 (where D_0 is equilibrium value of fractal dimension), which gives an evident idea of dynamics of fractal dimension for the studied period was constructed.

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Mathematical and computer modeling of oil spill pollution in shallow water[1]

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A new mathematical and computer model for prediction oil spill behavior is presented. The features of the model are based on the use of Mervin Fingas' evaporation equations [1] adopted to shallow water. To build a difference scheme with good properties the Gröbner bases method [2] is used.

Several methods are to be analyzed for parallelization of numerical computation based on the difference scheme obtained.

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Searching automorphisms using computer algebra and its applications in coding theory[1]

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A method of error correcting codes automorphisms finding based on solving an operator equation is presented. To solve the operator equation it is transformed to system of algebraic Boolean equations. The system includes linear equations derived from the code parity check and generator matrices. Also it includes nonlinear equations representing conditions satisfied by the rows and columns of permutation matrices. An algorithm of the system solving using the properties of Boolean symmetric polynomials is presented [1]. The working of the method is demonstrated on the family of Hamming and Reed-Muller codes [2].

A comparison of our method with method presented in [3] is performed. Slightly modified, our method can be used to determine interleaver function [4] for intercepted binary sequence encoded by error correcting code.

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Hydrodynamic pressure computation under real sea surface on basis of autoregressive model of irregular waves

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Determining the impact of external excitations on a dynamic marine object such as ship hull in a seaway is the main goal of simulations. Now such simulation is most often based on approximate mathematical models that use results of the theory of small amplitude waves. The most complicated software for marine objects behavior simulation LAMP IV (Large amplitude motion program) uses numerical solution of traditional hydrodynamic problem without often used approximations but on the basis of theory of small amplitude waves. For efficiency reasons these simulations can be based on autoregressive model to generate real wave surface. Such a surface possesses all the hydrodynamic characteristics of sea waves, preserves dispersion relation and also shows superior performance compared to other wind wave models. Naturally, the known surface can be used to compute velocity field and in turn determine pressures in any point under sea surface [1]. The resulting computational algorithm and its derivation is presented and evaluated in the paper.

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Особенности построения вычислительных экспериментов в гидромеханике с использованием явных численных схем и функциональных алгоритмов тензорной математики

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Трехмерная тензорная математика представляется в виде аналитического обобщения численных решений прикладных задач гидромеханики, основанных на конечноразностных моделях метода крупных частиц (конечного объема). Основные физические законы определяются в рамках элементарной частицы сплошной среды с помощью линейных формализаций скалярных, векторных и тензорных полей, строго контролируемых внутри пространственного симплекса в отношении всех ближайших – смежных узлов и граничных элементов. Построение прямого вычислительного эксперимента проводится на основе разделения решений по физическим процессам с использованием явных численных схем, что позволяет распараллеливать все вычислительные потоки до уровня независимого контроля состояния каждого тензорного объекта, в том числе с возможностью динамического выбора наиболее адекватных законов гидромеханики, в зависимости от локальных оценок реологического состояния сплошной среды и аппроксимационных особенностей тензорного описания трансформаций и взаимодействия тензорных объектов.

Главное внимание уделяется особенностям непротиворечивого проектирования новых численных алгоритмов и возможности сквозной физической интерпретации всех вычислительных объектов и операций, обобщаемых в форме гибридных численных схем с адаптивным применением тензорных выражений в соответствии с физической и логической обоснованностью математических моделей для режимов течения в локальных областях и в особых зонах вычислительных экспериментов, что особенно важно при моделировании нестационарных процессов.

The method of stochastization of one-step processes

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Usually at stochastization of mathematical models stochastic term is introduced as the external noise. This action can only characterize the environment, but not itself system under study. There is a need introduce the stochastic term in concert with deterministic, that is, to receive both parts of one and the same first principles. A method is presented stochastization of models describing the single-step processes (birth-death processes) [1, 2]. The method allows to obtain deterministic and stochastic components from first principles that allows us to consider these pieces matched with each other. For equations used notation of chemical kinetics. In addition to simple the law of mass action can be used trophic functions. Application of the method demonstrated by the environmental [3] and telecommunication models.

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Point vortices and nonlinear polynomials of the Sawada–Kotera and the Kaup–Kupershmidt equations[2]

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Special polynomials associated with the Painlevé equations and their higher–order analogues have been attracting much attention during recent decades. It was shown that these polynomials possess a certain number of interesting properties. For example, their roots form highly regular structures in the complex plane.

In this talk we present the connection between equilibria of point vortices and special polynomials associated with rational solutions of the Sawada – Kotera equation, the Kaup – Kupershmidt equation, their hierarchies, and some other integrable partial differential equations including the Fordy – Gibbons equation.

We obtain that stationary equilibria of point vortices with arbitrary choice of circulations can be described with the help of the Tkachenko equation, while translating relative equilibria of point vortices with arbitrary circulations can be constructed using a generalization of the Tkachenko equation. We prove that roots of any pair of polynomials solving the Tkachenko equation and the generalized Tkachenko equation give positions of point vortices in stationary and translating relative equilibrium accordingly. These results remain valid even if the polynomials inside a pair possesses multiple or common roots.

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Algorithms for $J/\psi \to e^+e^-$ selection registered with CBM setup in Au+Au collisions at 25 AGeV

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The problem of fast $J/\psi \to e^+e^-$ event selection registered in AuAu collisions at 25 AGeV beam energy is considered. The key task here is a fast and reliable electron/positron identification using the energy losses of particles in the Transition Radiation Detector. Two methods are used to solve this problem: the former is based on the artificial neuron network (ANN), while the latter is a modified nonparametric goodness-of-fit w_n^k-criterion. Our analysis shows that the two approaches give similar results for the $J/\psi \to e^+e^-$ yield and the signal to background ratio. Compared with the w_n^k criterion, the method based on ANN has a number of disadvantages which are analyzed in detail. Taking into consideration the very simple software implementation of a w_n^k algorithm, it can be used for the real time J/ψ mesons selection.

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Piecewise approximation and smoothing by high degree polynomials using the basic element method

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Problems of polynomial approximation and smoothing are solved within the basic element method (BEM) in which the n^{th} degree polynomial is expressed in the form of *four* basic elements [1, 2, 3]. The main feature of the BEM-polynomial is *a fusion* of the properties of Taylor polynomial and a second degree Lagrange polynomial on *a three-point grid*. The efficiency of methods and algorithms of the 12^{th} order piecewise approximation and smoothing is shown. The efficiency of segmentation includes *an accuracy* and *uniformity* of approximation on *an extended* interval, *stability* of calculations (conditionality problem), *high* order smoothness, *reduced* computational complexity and *robust* smoothing. Examples of quite complicated tests and comparisons with known methods [4, 5] are given as well.

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Numerical investigation of the dynamics of fluxon lattices in long Josephson stacks

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We study numerically the fluxon dynamics in multistacked Josephson junctions by using the unified model of Machida and Sakai [1]. This model captures both the inductive and the capacitive coupling between junctions. The influence of the capacitive coupling on the fluxon dynamics is analyzed and a comparison with the case of only inductive coupling [2] is carried out. We study as well the influence of a magnetic field, applied along the layer direction, on the generation of Josephson vortex (fluxon) lattices. The corresponding system of coupled sine-Gordon equations is solved numerically by using finite difference methods. The investigation is made for different geometric and physical parameters of N stacked Josephson junctions. Some physical quantities that can be measured in real experiments are calculated numerically.

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Operational calculus approach to explicit solving of initial and boundary value problems

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Local and non-local boundary value problems for the classical equations of Mathematical Physics in rectangular domains traditionally are solved by Fourier method or some of it extensions intended for the non-local case.

We elaborate the Fourier method combining it with an extended Duhamel principle for the space variables. We use non-classical operational calculi, custom-tailored for the specific problem. Thus we obtain explicit solution of the considered problem.

Methods and tools for organic crystal structure prediction[1]

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The crystal structure prediction is a methodology of numerical simulation of the ground equilibrium states of crystalline matter by global potential energy minimization - the key step toward the physical properties of yet unknown solid materials: enthalpy of sublimation, density, elasticity moduli, equations of state, etc. This talk introduces the following aspects of molecular crystal structure prediction with mathematical algorithms and program tools for their treatment in practical calculations [1]:

- Description of crystal structures in terms of rigid molecular fragments;
- The strategy for enumeration of crystallographic space groups;
- Symmetry of global potential energy landscapes;
- Semiempirical potential functions for van der Waals, electrostatic, hydrogen bonding, harmonic, and torsion terms contributed to lattice energy;
- Advanced point-charge and distributed-multipole molecular models by treatment of molecular QM electrostatic potential with program FitMEP;
- Solution of *inverse* structure prediction problem with program FitPTL;
- Parallel algorithms for global energy minimization with program PMC;
- Comparison of structures with program CRYCOM for crystal similarity search, identification of symmetry and phase transition evolution paths.

Examples of successful structure predictions for both the (a) known crystals and their phase transformations, undertaken to assess a theoretical method and (b) for previously unknown crystals will be presented.

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Numerical simulation of flows in highly heterogeneous porous media

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We shall present an overview of some solution strategies developed in [1-4] for numerical treatment of flows in highly heterogeneous porous media. Our main goal is derivation, study, and testing of numerical methods that work well for both, Darcy and Brinkman equations and could be used either as (1) a stand-alone numerical upscaling procedure (see, [2, 5]), or (2) robust (with respect to the high contrast of the media) iterative solvers for the finite element approximation on a fine-mesh spatial scale [1, 4].

The approximation methods involve the recent achievements in the area of discontinuous Galerkin finite element methods and their hybridization and the multiscale finite elements, while the preconditioners are based on overlapping domain decomposition technique. The robustness with respect to the contrast is achieved via special construction of a coarse grid space that includes patched together eigenfunctions corresponding to the smallest eigenvalues of properly weighted local spectral problems. This approach has a natural abstract framework which we shall discuss as well.

The main target of our applications are numerical upscaling and simulation of fluid flows in highly heterogeneous media modeled by Brinkman, Darcy, and/or steady-state Richards' equation, including Haverkamp, exponential, and van Genuchten relations for the relative permeability as discussed in [3].

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Evaluation of expectations of random functionals [1]

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The numerical evaluation of mathematical expectations of functionals defined on stochastic processes is an important issue in many areas of science and technology. As a rule, Monte Carlo methods are used for this purpose. At the same time, there exist a lot of deterministic numerical methods for evaluation of expectations of functionals defined on trajectories of stochastic processes [1-3]. A combined use of these two approaches, in many cases, provides more accurate results and control the computational error.

Using a deterministic approach in the case where there is a functional dependence of the additional random parameter was not considered. In this report we propose an approach to the calculation of this kind functionals of the form

$$F(W) = \int_0^T a(s, W) X_s(W) ds,$$

where $a(s, W)$ and $X_s(W)$ are stochastic processes given as nonlinear functionals of Wiener process $W = W_t$, $t \in [0, T]$. The Wiener chaos expansion of these functionals [4, 5] and formulas exact for functional polynomials [1-3] are used.

Special cases when X_s is the solution of the stochastic differential equation, $a(s, W)$ is a functional polynomial or given by its Fourier transform are presented in more detail.

A possible generalization of the method to the cases of Gaussian and other processes that allow a chaotic expansion is considered.

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Modeling of speech features via simulated annealing algorithm

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In many speech recognition systems various spectral techniques are used to obtain features which describe input utterance. Mel - Frequency Cepstral Coefficients or Perceptual Liner Prediction coefficients are examples of such features. Unfortunately, due to differences in length of vocal tracts of different speakers such features can poorly describe a given phoneme.

Alternative way is to use speaker independent features such as that obtained using Auditory Image Model (AIM) to describe input utterance. In our work we propose AIM based features which are calculated using simulated annealing algorithm. We also propose different ways to calculate these features.

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Discrete modeling using stochastic cellular automata

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This paper is devoted to the problem of discrete low-level modeling of the various natural systems and processes [1]. Classic tools in this area are cellular automata [2], Lindenmayer systems [3], membrane systems [4] etc. A new approach to simulation modeling of such systems based on the use of block stochastic cellular automata is suggested.

The notion of two-dimensional Markov automaton is introduced and illustrated by the examples of modeling of different physical, chemical and biological systems. These examples demonstrate the simplicity and easy of use of the suggested approach. It is shown that under certain conditions behaviour of the automaton can be described by the system of differential equations. On the other hand this kind of automata permits algorithmically complex behavior, example of parallel binary adder is given.

Application of the Markov automata to the modeling of neurons, synapses and neural networks [5] is considered. The automata model of an excitable medium and the mechanism of inhibition are described. Simple feedforward neural networks are constructed and numerically analyzed.

Issues of the parallel (MPI and CUDA) implementation of the Markov automata are considered.

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Two-spin correlations in a system of nuclear spins s=1/2 in a nanopore in a strong magnetic field[1]

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Dynamics of the spin system of a gas of spin-carrying molecules (atoms) in a strong external magnetic field is studied. Fast molecular motion in nanopores does not average the dipole-dipole interactions (DDI) of nuclear spins completely and the residual DDI is described by one coupling constant which is the same for all pairs of interacting spins [1]. As a result, it is possible to investigate spin dynamics analytically. Reducing the density matrix (which describes the time evolution of the system with residual DDI) for all spins except the chosen pair, we can obtain information about all two-spin correlation functions. All these correlation functions are calculated [2].

The pair entanglement and the quantum discord [3] are investigated on the basis of the obtained correlation functions. It is important that the reduced density matrix is a centrosymmetric one [2]. As a result, we obtained an analytical expression for entanglement in an arbitrary two-qubit system. We show that xx- and yy-correlation functions equal to zero at regular time intervals. Since the quantum discord can be expressed through the obtained correlation functions, it equals to zero periodically. It means that the quantum discord in considered systems has the "flickering" character and disappears periodically in the course of the time evolution of the system.

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Parallel computations using Maple 17

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We present different type of parallel computations using Maple 17 on 16 processor super computer. Specific results obtained for some physical models will be also presented.

Application of ZDD diagrams for solving SAT problems [1]

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Boolean Gröbner basis have shown their practical efficiency for diffirent problems. Among them are algebraic cryptoanalysis, boolean satisfiability problem (SAT) and modeling of quantum computing.

We introduce Zero-suppressed Decision Diagram (ZDD) [1, 2] as data structure for boolean polynomials. Furthermore, we apply ZDD for computing Gröbner basis [3] with using of involutive algorithm [4] and make several series of computation of 3CNFSAT problems with using our own C++ ZDD package.

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Ionization dynamics of atoms exposed to strong laser pulse: semi-analytical model at low field frequencies

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Low field frequencies are the most difficult for the numerical solution of a time-dependent Schrödinger equation (TDCS). To have some estimations of the expected effect of low field frequencies on the ionization dynamics of atoms, we propose a simple model of an atom based on a separable presentation of the Coulomb potential in the momentum space. Both the length and velocity gages are considered. It is proved that the Strong Field Approximation (SFA) works well, and the results can be interpreted like pure tunneling.

Computer algebra aided numerical solving KdV-like PDEs[1]

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We consider a four parameter family of nonlinear partial differential equations which contains the Korteveg-de Vries equation and the modified Korteveg-de Vries equation [1]. To solve equations in this family numerically, we follow the procedure suggested in [2] and based on combination of the finite volume method [3], numerical integration and computer algebra based difference elimination by means of Gröbner bases [4]. As a result, we obtain a discretization of PDEs that is valid for the whole family. Then we apply it for numerical solving. To analyze quality of the obtained discretization we found an exact solution and compared dynamics of the numerical solution and its exact counterpart. We implemented numerical procedure for construction of a solution in Python with the use of package SciPy [5].

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On the inequalities defining the entanglement space of 2-qubits[1]

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The issue of description of the *entanglement space* $\mathcal{E}_2$, i.e., the orbit space P_+/G, where P_+ - the space of mixed states of the pair of qubits, $G = U(2) \otimes U(2)$ - a group of the so-called local unitary transformations [1], is discussed. Within the geometrical invariant theory, using the integrity basis for the ring of G-invariant polynomials, the derivation of equations and inequalities [2] that determine the entanglement space E_2 are outlined. For these purposes we discuss the algorithm for reduction of a matrix to the Smith normal form [3] wich may work when the entries of a matrix are multivariate polynomials.

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Development of the distributed computing system for the MPD experiment at the NICA collider, analytical estimations

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Experimental data processing and storing are topical issues in the present experiments in high energy physics. Development of the distributed cluster based on server farm of Laboratory of high energy physics was started to accomplish these tasks in the MPD experiment at the NICA accelerating complex. This report describes the approaches and methods of cluster development for storing and processing data obtained at the multipurpose detector. The current cluster scheme and structure are presented; software for building data storage and parallelization of the MPD event processing is noted. The presentation introduces two methods to parallelize data processing: using PROOF software tool of ROOT environment and scheduling system developed by author. Analytical estimations of the required computing power and prediction of future cluster efficiency are presented particularly.

Modeling of 3D classical spin glasses under influence of external electromagnetic fields

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We study statistical properties of a 3D classical spin glass layer of certain width and length. The 3D spin glass is represented as an ensemble of disordered 1D spatial spin-chains (SSC) where interactions between spin-chains (nonideal ensemble of 1D SSCs) are random too. It is proved that at the limit of Birkhoff's ergodic hypothesis performance 3D spin glasses can be generated by Hamiltonian of disordered 1D SSC with a random environment. The disordered 1D SSC is defined on a regular lattice where one randomly oriented spin is put on each node of the lattice. It is supposed that each spin randomly interacts with the six nearest-neighboring spins (two spins on lattice and four in the environment). The recurrent transcendental equations are obtained on the nodes of spin-chain lattice. These equations combined with the Silvester conditions allow one step by step to construct a spin-chain in the ground state of energy where all spins are in minimal energy of classical Hamiltonian. On the basis of these equations an original high-performance parallel algorithm is developed for a 3D spin glasses simulation. Distributions of different parameters of unperturbed spin glasses are calculated. In particular, it is analytically proved and by numerical calculations shown that the distribution of the spin-spin interaction constant in Heisenberg nearest-neighboring Hamiltonian model, as opposed to widely used Gauss-Edwards-Anderson distribution, satisfies Lévy alpha-stable distribution law which have no variance. A new formula is proposed for construction of a partition function in kind of one-dimensional integral on the energy distribution of 1D SSCs.

Calabi-Yau-type varieties over fields of finite characteristics and their applications

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The subject matter of this communication lies in the area between Arithmetic and Algebra and has applications in physics. More specifically, I want to discuss the relations between the arithmetic of Calabi-Yau type varieties [1-2] and orbifolds over fields of finite characteristics and dualities in the varieties and orbifolds and their applications to physics. The topics of the arithmetic of Calabi-Yau type varieties and dualities in the varieties are intimately related and I will try to show that the cooperative study both two first topics is of great importance for the development of some results of mathematical physics. We investigate dualities (generalized symmetries) and other symmetries of CY type varieties over finite, global and local fields of mixture or finite characteristics [3-5]. We will consider cases of CY type varieties that are elliptic curves, two dimensional abelian varieties and K3 surfaces, three dimensional abelian varieties and CY threefolds.

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Relaxation self-oscillations in circular chains of unidirectionally coupled Hopfield neurons[1]

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We consider singularly perturbed non-linear system of differential-difference equations with delay which simulates the functioning of a circular network of m ($m \geq 3$) Hopfield neurons (see, for example, [1])

$$\dot{u}_j = -\mu\, u_j + \lambda[1 - (a+1)f(u_j(t-1)) - b\, g(u_{j-1})],\ \ j = 1, \ldots, m. \quad (1)$$

Here $u_j(t)$ stand for the membrane potentials of the neurons, $u_0 = u_m$, $\mu = \text{const} \geq 0$, $a = \text{const} > 0$, $b = \text{const} > 0$, and the parameter $\lambda > 0$ is assumed to be large (from the point of view of biophysics, this means that the electrical processes in a neuron are rapid). We assume that the functions $f(u), g(u) \in C^\infty(\mathrm{R})$ satisfies the asymptotic representations

$$f(u) = \sum_{k=1}^{\infty} \frac{c_k^-}{u^k} \ \text{ as } \ u \to -\infty, \ \ f(u) = 1 + \sum_{k=1}^{\infty} \frac{c_k^+}{u^k} \ \text{ as } \ u \to +\infty.$$

$$g(u) = \sum_{k=1}^{\infty} \frac{d_k^-}{u^k} \ \text{ as } \ u \to -\infty, \ \ g(u) = 1 + \sum_{k=1}^{\infty} \frac{d_k^+}{u^k} \ \text{ as } \ u \to +\infty,$$

which remain valid after differentiating arbitrarily many times with respect to u. It is proved that, under an appropriate choice of the parameters μ, a, and b and for any $\lambda \gg 1$, the number of finitely many co-existing stable relaxation cycles in the system (1) can be prescribed arbitrarily. In other words, the buffer phenomenon is realized in this system (see [2,3]).

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Краевые задачи с уравнением Грэда-Шафранова в моделировании магнитных ловушек

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Реализация управляемого термоядерного синтеза связана с проблемой удержания плазмы магнитным полем. В исследовании эффективности удержания с целью оптимизации параметров соответствующих установок существенную роль играют математическое моделирование и расчет. Плазмостатические модели ловушек, обладающих симметрией (плоской, осевой, винтовой) строятся в терминах двумерных краевых задач с уравнением Грэда-Шафранова [1, 2]– скалярным полулинейным дифференциальным уравнением эллиптического типа. Представляет интерес перспективный класс тороидальных ловушек – галатей, предложенных А.И. Морозовым [3, 4] в которых проводники с электрическим током, создающие магнитное поле, погружены в плазменный объем. Проблемы моделирования равновесных конфигураций плазмы и магнитного поля, достаточно общие для галатей, рассмотрен на примере распрямленного в цилиндр аналога ловушки "Пояс"с двумя параллельными оси проводниками. Распределение плазмы, поля и электрического тока в равновесии определяется в процессе численного решения краевой задачи с уравнением Грэда-Шафранова итерационными методами типа установления, которые встречаются с нетривиальными вопросами существования и единственности. Эти вопросы, общие для широкого класса моделей взаимодействия реакция и диффузии (например,

теория горения), связаны со спектральными свойствами дифференциального оператора линеаризованного уравнения [5]. В докладе представлены новые результаты расчетов "Пояс" в терминах первой краевой задачи, относящиеся к конфигурациям в областях с прозрачными для магнитного поля границами. Решение краевой задачи с граничными условиями второго рода описывает зависимость конфигурации от полного электрического тока в ловушке.

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About singularity of calculating a higher orders derivative at identification of the form of graphic objects

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Identification of graphic objects on the basis of a methods of linear correlation [1] demands reception of zero k-jet. It, in turn, demands calculation of derivatives of the k-th order. Application of the procedure of numerical differentiation is usually caused by necessity to differentiate not analytical function. Such functions, in the form of a set of coordinates usually turn out as a result of preliminary image processing and feature set allocation.

When a contour of the investigated object will close, there is a considerable quantity of the methods founded on the signature analysis and methods of geometrical correlation [2]. However, in real images the object contour often happens damaged and the signature analysis is inapplicable in this case. In [3] the method founded by use of zero k-jet has been offered. However, the description has not been given how to calculate positions of zero k-jet.

In the report, some features of various methods of calculating derivative high orders (app to 7) are considered and some questions of the accuracy of their calculation are discussed.

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About one model of computer control on the basis of gaze tracking

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There are some circumstances in which it is necessary to interact with a computer without a physical contact. These include situations of a human being with physical disabilities of computer interaction or an operator controlling some settings when both hands are busy, etc.

For such cases, a contactless interaction model based on video stream capture from a human face was developed. The pupils are detected on each video frame and their condition analysis for the control action elaboration. The main feature of the current method is the use of infrared illumination, which allows one to eliminate noise and interference.

A model of the non-contact human operator interaction with a computer is considered in the report. The images fragments at different stages of processing are demonstrated. The moment of two pupils capture is shown. Various system features are highlighted.

Numerical solution of time-independent Schrödinger equation for quantum dots

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The work focuses on the eigenvalue problem for time-independent Schrödinger equation, with the pseudopotential function that imitates a semiconductor heterostructure, with the use of supercomputer Blue Gene /P. The programs written in the work are based on the libraries PETSc and SLEPc.

Identifying protein-DNA recognition rules using a database of amino acid-nucleotide contacts in protein-DNA complexes [1]

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In the course of our previously published studies of protein-DNA recognition [1,2] we identified frequently occurring amino acid-nucleotide contacts in interfaces of the protein-DNA complexes, allowing to find consistencies in the protein-DNA recognition. We found that only allowance for at least three properties of these contacts, namely the physicochemical characteristics, positions of the participating amino acids and nucleotides in the chains of the protein and the DNA, respectively, as well as conservatism of these contacts allows to derive rules for protein-DNA recognition. To systematize those highly heterogeneous data, we have developed a database of amino acid-nucleotide contacts ANTPC (Amino acid Nucleotide Type Position Conservation) [3] following the archetypal example of the proteins in the homeodomain family. We show that it can be used to compare and classify interfaces of the protein-DNA complexes.

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KANTBP 3.0: New version of a program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel adiabatic approach [1]

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A FORTRAN 77 program for calculating energy values, refection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach is presented [1].

In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on a finite interval with the homogeneous boundary conditions of the third type at the left- and right-boundary points for continuous spectrum problem, or a set of first, second and third type boundary conditions for discrete spectrum problem. The resulting system of these equations containing the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method.

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Efficiency of the schemes proposed is demonstrated on an example of solution of quantum transmittance problem for a pair of coupled ions through the repulsive Coulomb barriers [2]. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions for the two-dimensional problem with different barrier potentials.

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POTHEA: a program for computing effective potentials, energy levels and wave functions in the coupled-channel hyperspherical adiabatic approach [1]

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A FORTRAN 77 program for calculating effective potentials, energy values, and corresponding wave functions in a coupled-channel approximation of the hyperpherical adiabatic approach is presented [1].

In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on a finite interval with a set of first, second and third type boundary conditions for discrete spectrum problem [2]. The resulting system of these equations containing

[1] This work is supported by grants 13-602-02 JINR, 11-01-00523 and 13-01-00668 RFBR.

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the effective potentials, i.e., the potential matrix elements and first-derivative coupling terms, is solved using high-order accuracy approximations of the finite element method [3].

Efficiency of the schemes proposed is demonstrated on an example of solution boundary value problem for the Helium like atom or exciton models. As a test desk, the program is applied to the calculation of the potential matrix elements and first-derivative coupling terms, energy values of ground and excited states and corresponding wave functions of a Helium atom.

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Use of GEANT4 in brachytherapy

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Brachytherapy is the radiation therapy given at a short distance, when the radioactive source is implanted directly into the tumor. In determining the parameters of the sources used in brachytherapy, according to the conventional formalism TG43U1, their mathematical modeling with Monte-Carlo method is a must. GEANT4 can be used as a program code to implement the Monte Carlo method. GEANT4 is a system of libraries for computer simulation of the passage of elementary particles through matter, developed by an international collaboration with the center at CERN. Large functionality allows its

use for solving various problems, including use in medicine and in brachytherapy for instance. The goal of this paper is to show the possibility and benefits of GEANT4 use to calculate the required parameters of brachytherapy microsource. Cobalt-60 is taken as a radioactive source. The geometric part of the work is to build a "grid" of concentric rings of equal thickness. The centers of the circles lie on one axis disposed along the linear radiation source. The geometry of the source is a cylinder of Cobalt-60 sheathed in stainless steel. All rings are logical volumes, from which the following data are taken: the energy absorbed in the volume and KERMA in the volume. The main advantage of using the software package GEANT4 is the possibility of an independent determination of the absorbed dose. In most of the program codes only the calculation of KERMA is made, while the absorbed dose is equated to it, implying the presence of electron equilibrium in the calculated volume.

Simulation of electron emission from nanostructure surfaces[1]

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Now computer modeling of electronic processes in silicon and carbon micro and nanostructures is an integral part of production of electronic components of new generation [1, 2]. With transition to the nanometer range of the sizes of active elements of electronic schemes requirements to the accuracy of mathematical models and numerical methods of their analysis significantly raised. As a result calculation even the ordinary silicon transistor with sizes of lock of ten nanometers and less turns into a serious problem. It is connected with that the mathematical model of the transistor adequate to physical conditions comprises not only classical, but also quantum descriptions. Numerical realization of similar models needs performance of large volume of calculations and can't be executed on the ordinary personal computer in acceptable time limits any more. Therefore for the solution of such tasks powerful clusters or

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even supercomputers with hybrid architecture are used. Development of parallel algorithms and technologies of programming for such calculators also is a pressing problem.

In represented work approaches to the solution of actual problems of a nanoelectronics on modern computer facilities are discussed. As an example one of the perspective directions of the nanoelectronics, connected with development of vacuum autoemission devices with sizes of active elements (cathodes) about 15 nanometers and less is chosen. Such devices are applied to creation of systems of display of information (displays of ultrahigh permission and a color rendition), sources of the microwave radiation (nanolithograph), devices of electronic sounding of surfaces (an electronic tunnel microscope of high resolution) [1 ,2]. Recently use of emission devices for realization of supercompact sources of current, quantum transistors and elements of memory of computers is considered. As cathodes the most various materials, including metals (copper, vanadium, etc.), semiconductors (silicon, compounds of gallium with arsenide, India with phosphorus, etc.), and also the nanomaterials showing metal and semiconductor properties (allotropic forms of carbon, nitrogen, phosphorus oxide) can be applied. Supercompact and superfast elements of computers and communication systems which will allow to pass to the terahertz range of frequencies at essential decrease in total energy consumption can become result of application of these materials.

In the work problems of modeling of processes of electronic autoemission on a surface of the nanostructures being in vacuum are considered. As specific objectives field electronic emission from a surface of silicon autocathodes and the carbon nanotubes having the nanometer sizes of an active element (an edge or an edge) is considered. The parallel computing technology of modeling of such problems, focused on use of hybrid architecture is offered. Elements of the technology were presented in [3, 4]. With the help of the technology numerical simulation of emission processes on a surface of the silicon microcathode, a graphene edge and the closed carbon nanotube was executed.

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Dimer problem on cylinders: recurrences and generating functions

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We consider the problem of counting the number of perfect matchings in $C_m \times P_n$ grid graphs (cylinders) when parameter $m \geq 3$ is fixed. The properties of recurrences and generating functions associated with the sequences arising in the problem are discussed. The obtained results made it possible to find out the essential dependence of the recurrence order growth on the parity of m. In the similar grid graph family $P_m \times P_n$ analogous dependence does not exist.

If m is odd the upper bound of the order of a recurrence agrees with the Stanley conjecture [1]. For even values of m the order of a recurrence grows rather slower. The recurrences found for each $3 \leq m \leq 30$ permit us to assume that the order of the recurrences is bounded above by the quantity

$$\begin{cases} 2^{(m-1)/2}, & \text{if } m \text{ is odd,} \\ 3^{m/4}\Big(1 + \big(\frac{2}{\sqrt{3}} - 1\big)\delta\big(\frac{m}{2}\big)\Big), & \text{if } m \text{ is even,} \end{cases}$$

where $\delta(k)$ is equal to 1 for odd k and 0 otherwise.

The denominator $Q_m(x)$ of generating function has several interesting symmetry properties. In the case of odd m it satisfies the same equality which exists for a lattice grid graph $P_m \times P_n$, that is $Q_m(x) = x^{q_m} Q_m(1/x)$ where $q_m = \deg Q_m(x)$. There is no unified relation for even m. The available results are summarized in the following table.

$m \bmod 8 = 4$	$Q_m(x) = x^{q_m} Q_m(1/x)$
$m \bmod 8 = 0$	$Q_m(x) = -x^{q_m} Q_m(1/x)$
$m \bmod 4 = 2$	$Q_m(-x) = -x^{q_m} Q_m(1/x)$

Similar properties have been detected for the numerators $P_m(x)$ of the generating functions. In particular, if m is odd then $P_m(x) = -x^{p_m} P_m(1/x)$, where $p_m = \deg P_m(x)$, was true in all available cases.

From the computational point of view the recurrences are much more efficient than the explicit formulas, obtained in [2] by means of the pfaffian method.

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Multioperator models[1]

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The theory of multioperator models (equations)

$$b\mathbf{y} = a\mathbf{u}$$

connected pair vectors (arithmetical vectors, functions or vector-functions) ($\mathbf{u}$, $\mathbf{y}$), belonging to some Euclidean space E, is constructed. Here $a{:}E \to E$, $b : E \to E$ – elements of free commutative algebra (named multioperator algebra), generated by one or more operators $g_i{:}E \to E$.

The method of multioperator models constructing for finite dimensional Euclidean space E is described. This method is generated the method of Krylov sequences constructing.

It can be used for system identification in control and for constructing theoretical or experimental models.

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Monte Carlo simulation of gamma scattering for density variation measurement[1]

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Back-scattered gamma-rays nowadays have been used widely in many different fields of science and technology. One of its useful applications is for checking the density fluctuations of concrete thickness of newly constructed highways. This report studies the possibility of using backscattered gamma radiation for this purpose by means of Monte Carlo simulation. A computer program named NUCLGAUGE has been written in Visual Basics language. The program simulates a transportation of gamma-rays emitted by a radioactive source to a concrete layer of highway and scatter back to a NaI detector. The different gamma-ray sources of different energies and strengths as well as different measuring configurations have been used to simulate the number of backscattered gamma-ray recorded by the detector. Our computer program should be useful for optimal designing the density gauges. Furthermore, the results of our simulations also confirmed that the resolution for density variation measurement of concrete layer of newly constructed highways is quite good.

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A software for simulation of efficiency of HPGe detectors[1]

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A computer software named GE_EFF for calculation of detection efficiency of High Purity Ge detectors recently developed by us is presented. A Monte-Carlo method has been used for simulation. The software is written in Visual Basic language. The calculated efficiencies for our detectors are in agreement with the measured values using a standard gamma-ray sources. The software has been used at our laboratory of nuclear physics of the Institute of Physics for gamma radiation measurements.

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Non-steady mathematical model of fluid flow in a thin drop [1]

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There are several effects, which may be observed during desiccation of droplets. For-example, coffee ring effect [1] or protein on the edge of the roller [2]. These phenomena are explained theoretically by existence of radial flow with using quasi-steady models [3, 4]. But quasi-steady approach has a restriction connected with consideration of slowly evaporation only. It is important to prepare a "platform" for switching over to the quantitative description of the process. Therefore it is necessary to considerate a non-steady approach. Non-steady model was developed to compare results with a quasi-steady model. More information about this comparison see in [5]. For the first time one-dimensional motion equation of fluid in a drop is proposed from a momentum conservation law. Inward flow is possible on the edge of drop [5]. It was not described theoretically earlier with using one-dimensional models. Inward flow was explained by existence of stagnation points in [1].

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Finite difference schemes for Boussinesq equation

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In this talk we compare several finite difference schemes for Boussinesq equation with respect to approximation errors, stability, rate of convergence, existence of conserved quantities.

These properties are discussed both theoretically and from numerical implementation point of view. Our numerical study covers not only one dimensional but also two dimensional problems.

Coulomb three-body problem and precision spectroscopy of light atoms and molecules

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It is known that the Coulomb three-body problem in the nonrelativistic quantum mechanics has no analytical solution. In our presentation we want to show that for stationary states this problem may be solved numerically with about arbitrary precision and for a wide variety of physical systems in high vibrational and/or rotational states. A variational method is described, which is based on simple exponential basis functions (Slater germinals), and which allows to study with very high precision light atomic and molecular systems as well as exotic atoms. In our presentation we demonstrate application of the aforementioned variational method to various problems of physics of fundamental constants. Among them are: 1) Determination of the fine structure constant

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via precision spectroscopy of the fine structure splitting in the $2P_3$ state of helium; 2) Determination of the antiprotonic mass via precision spectroscopy of the antiprotonic helium; 3) Improved determination of the proton-to-electron mass ratio via ro-vibrational spectroscopy of the positive hydrogen molecular ions H_2^+ and HD^+. There results were used by CODATA in the 2010 year adjustment of the values of the fundamental physical constants.

Signs of dibaryon detection in D+D→X+D reaction

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It is established that quasi-resonant peaks observed in the two-proton effective mass distribution from reactions np→pp$\pi^-m\pi^0$ and np→pp$\pi^+\pi^-\pi^-m\pi^0$, $m = 0, 1$ (see [1,2]), were also detected though unrecognized in a more earlier paper [3] in D+D→X+D reaction. This fact increases significantly the reliability of existence of dibaryons described in [1,2]. Besides, data of paper [3] hint at a possibility of existence of dibaryons with $I = 0$ and masses in the vicinity of 2.4 and 2.5 GeV/c^2 which were predicted in the frame of a 6-q bag model [4].

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The dynamical Casimir effect in two nucleon systems

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Arguments for observation in [1-3] of a quantum phenomenon of a similar nature as the theoretically predicted, but still unobserved experimentally, Hawking effect are given. An analog of the Hawking radiation in this case is a bound π-meson field in a generalized coherent state corresponding to the dynamical symmetry group $SU(1,1)$ (quantum π-condensate). Just like Migdal's π-condensate, this field emerges in dense nucleon systems, but at a slightly smaller pion binding.

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Computational studies of glycan-protein interactions[1]

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Computational modeling of complex biological macromolecules on atomic level is a complex task that requires HPC resources. This is due to number of atoms, environment (solvent molecules), simulation time and temperature, as all of these variables need to be accounted for realistic outcomes. This is especially valid for glycans (oligo- or polysaccharides) that are either linear or branched molecules. Glycans can be found in cells as unique entities or attached to other biomolecules, such as glycoproteins, proteoglycans, glycolipids, *etc.* Upon addition of glycan to proteins, the complexity is vastly increased. For example, when using the 20 amino acids as building blocks, there are around 6.47×10^7possible molecules of hexapeptides (with only 6 amino acids in length) that could be produced. In the case of glycans, the total number of modeled glycan-hexasaccharide structures, assuming equivalent number of 6 building blocks, could be as high as 1.44×10^{15} [1]. Comparable to proteomics, glycomics deals with the structure, function and interactions of glycans [2]. The increasing importance of glycomics to medicine was outlined by Shiver *at all* [3]. Our recent interest in the field is concentrated on the use of microarray technologies, on both, experimental and computational level [4].

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Clustering data for coordinate detectors in the CBM experiment

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Clustering algorithms are an important part of the event reconstruction in high energy physics, in particular, in the CBM experiment. These algorithms translate fired strips and pads into space coordinates - hits - which are later used in the track reconstruction algorithms. In this paper we discuss a clustering problem for the Micro Vertex Detector (MVD) and Muon Chamber (MUCH). A high interaction rate and a large amount of data lead to high requirements to the clustering algorithms, which have to perform fast and efficient and be able to deal with a high track multiplicity.

Currently two different approaches are under discussion. In the first case, each fired pad has information about its charge. In the second case, a pad can be either fired or not, thus the separation of overlapping clusters becomes a difficult task.

For clustering with charges, we have developed an algorithm which works by the following rule: every pad with local maximum of charges forms a separate cluster. Pads that are not local maximum are attached to the neighbors with the highest charges. This approach allows defining clearly expressed clusters (with their own local maximum of charge) and does not require complex calculations.

For clustering without charges, we used an algorithm based on the single linkage method. According to this algorithm, every group of neighboring fired pads has to be combined into one cluster. In this approach, clustering is very fast, but the separation of overlapped clusters is not possible.

The developed algorithms have been integrated into CBMROOT and tested on various types of simulated events (p-C, C-C, Au-Au). The algorithms show their high efficiency and accuracy.

Theoretical concept of integrated microfluidic system for magnetic cell separation, electroporation, and transfection[1]

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For the purposes of a successful *ex vivo* gene therapy we have proposed, modeled and analyzed a new concept of an integrated microfluidic system for combined magnetic cell separation, electroporation, and magnetofection, using computational simulations.

For the analysis of magnetic and electric field distribution (given by the Maxwell equations) as well as dynamics of magnetically labelled cell and transfection complex, we have used finite element method directly interfaced to the MATLAB routine solving Newton dynamical equations of motion as single particle problem, considering magnetic force and Stokes drag force. Microfluidic chamber has been modelled as a channel with height and length 1 mm and 1 cm, respectively, as planar model in longitudinal section. Bottom electrode consisted of 100 parallel ferromagnetic straps and the upper electrode was plate of diamagnetic copper.

From the dynamics of magnetic particle motion we have found that the characteristic time-scales for the motion of magentically labelled cells (mean capture time $\sim$ 30 ms) and gene complexes (mean capture time $\sim$ 4 s), when permanent magnets are used [1], are in the range suitable for efficient cell separation and gene delivery [2]. The largest electric field intensity ($\sim$ 10 kV/m) was observed at the edges of the microelectrodes, in the close proximity of magnetically separated cells, which is optimal for subsequent cell electroporation.

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Analysis of the efficiency of classificators based on ADABOOST algorithm

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ADABOOST [1,2] allows to combine a set of weak classifiers to form strong decision rules. It is quite important, especially in case of computer vision, that computational complexity should be as less as possible. Most preferably to use such simple things as threshold decision rules or Haar-features [3] as weak classifiers, because their computational cost is very low. However, in such cases, in practice, ADABOOST as greedy algorithm does not always give an effective combination of classifiers. In this paper we propose a two-step approach to getting an effective classification: stage one - ADABOOST, which will determine a set of simple weak classifiers, and stage two - an artificial neural network, with one or two layers. The neural network is trained on the results of classifiers determined by ADABOOST, allowing to combine them more effectively.

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Separation of the deterministic components and forecasting of time processes

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An approach to predict the chaotic time processes based on preliminary exclusion of anomalous and chaotic components from the analyzed series and subsequent application of one of the forecasting methods to the deterministic component is presented [1, 2]. To isolate the deterministic component, we apply robust schemes implemented on the basis of orthogonal polynomials, robust splines, singular spectrum and metric analysis [3,5]. The provided examples demonstrate the effectiveness of the proposed forecasting schemes.

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The optimal control problem for linear dynamical systems of fractional order

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The optimal control problem (OCP) for n-dimensional linear (lumped) dynamical systems of fractional order formulated and investigated. The method of moments used for OCP investigation and solving which allow to operate with discontinuous controls and obvious restrictions on control norm. Possibility of statement and solvability for problem of moments analyzed and corresponding conditions derived. Some special systems considered for n=1 and n=2. In these cases an explicit solutions obtained for control with minimum norm at given time interval and for control with minimum transient time at given norm restriction. Behavior of control norm, transient time and phase trajectories at different orders of integrators studied. Its demonstrated that analogous derivations can be realized for distributed systems of fractional order.

Thus, in this work some classical basic results and procedures of optimal control theory generalized on the case of fractional order systems. Obtained results can be useful for modeling and control of any complex systems such as non-regular (fractal) capacitors, electrochemical cells, viscoelastic materials etc.

Simulation of the gravitational mixing on GPU

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The problem of Rayleigh–Taylor instability (RTI) [1, 2] development in 2D and 3D geometries is investigated. This kind of instability is observed in a wide range of phenomena, both natural and man-made as well as in a wide range of scales – from supernova explosion to few millimeters capsule compression in ICF. In this regard, a detailed study of the evolution process of the instability at all time scales is of considerable interest. Accurate description requires significant computational resources and thus the development of new parallel algorithms for hybrid cluster systems is a prospective direction here.

As the initial numerical method for modeling the mixing induced by RTI, has been chosen [3], which is based on Godunov's method [4] with the introduction of anti-diffusion flow limiters. As is known, the resulting difference scheme is explicit, and the fluxes through the edges of the cells are found by solving the Riemann problem on each one. In this case, an algorithm scaling on massively parallel architecture such as a GPU, where one thread handles one counting cell, is allowed.

This work shows the different implementations of the parallel algorithm, and the resulting graphs of speed-up on the number of cells per dimension compared to the sequential version that runs on a cluster type processors Intel Xeon X5670 [5]. The dependence of speed-up on the size of the block and the grid is also analyzed. The optimal block size and the number of blocks in the grid was obtained for the chosen numerical method. These values reflect the balance between the computational complexity of the tasks for each thread (solution of the Riemann problem) and the number of threads per block.

Numerical calculations of the gravitational mixing problem in different geometries were performed with the help of the developed algorithm on the video card nVidia Fermi C2050 [6], a comparison of characteristics was made.

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Оценка устойчивости уровня психической реакции человека при информационном воздействии на него

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В статье представлено исследование устойчивости уровня психической реакции с личностными характеристиками человека и с силой информационного воздействия на него. Метод сопряженных уравнений позволяет найти положения равновесия, проверить будет ли иметь место устойчивость невозмущенного состояния. Также проведено исследование на основе метода Ляпунова по первому приближению, в результате представлены условия устойчивости уровня психической реакции с личностными характеристиками человека и с силой информационного воздействия на него.

Применение метода сопряженных уравнений к исследованию процесса потери устойчивости оболочек при действии подвижных нагрузок

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В статье проведено исследование процесса потери устойчивости уравнений, описывающих математические модели грунтовых массивов и оснований. Эти модели отражают характер работы грунтов под нагрузкой, строятся на законах строительной механики и теории упругости.

Для исследования процесса потери устойчивости был применен метод сопряженных уравнений, который позволил найти положения равновесия и проверить будет ли иметь место устойчивость невозмущенного состояния. Также было проведено исследование на основе метода Ляпунова по первому приближению, в результате получены условия устойчивости оболочек при действии подвижных нагрузок.

Multifractal dynamics and mathematical modelling of natural, social and economic processes

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In this report the mathematical model of multifractal dynamics on the basis of the principle of self-similarity for multifractal systems is constructed. One of the key moments of this approach is possibility of the description of the crisis phenomena in natural, social and economic systems. Within model multifractal dynamics new schemes of classification and the forecast of evolution of natural and social and economic systems are given. On its basis the analysis of dynamics of exchange rates and market indexes, prices of oil, growth of the population, tendencies of global warming, the crisis phenomena of agriculture of the Tver region is carried out.

Waves of fractal dimension of global temperature of the Earth, world economic crises and Kondratyev's cycles

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In this report existence of the lengthiest waves of fractal dimension of global temperature of an Earth's atmosphere for the period, since 1850, lasting period of 61 year is established. It is shown that all main world economic crises fall on the negative values of the function h describing these waves. Communication of these waves with the Kondratyev cycles which average period made 41 years, for the same period of time is discussed.

Self-organization of adiabatic shear bands in cooper and steel

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The self–organization processes of adiabatic shear bands (ASB) formation in OFHC cooper and HY-100 steel are considered taking into account the strain hardening. We proposed a numerical algorithm for analyzing this processes. The method presented allows to study the processes of adiabatic shear bands formation from the moment of their initiation till the stationary state. It was found that the processes of ASB formation in material at high rate shearing deformations are quasi periodic (Fig. 1). It was shown that in the localization areas there is a sharp jump in the temperature to 6-12 times (Fig. 1) and in the strain to 50-100 times.

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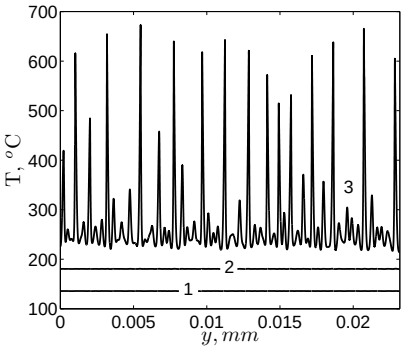

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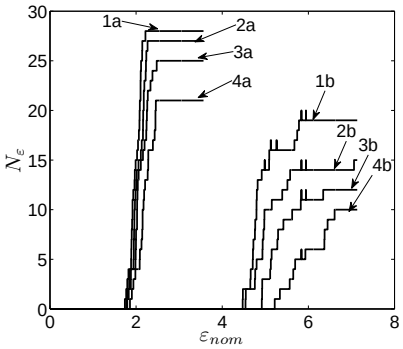

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Using this algorithm we study the influence of the strain hardening on the processes of ASB formation. We present the evolution of the average stress, temperature and plastic deformation with time. Using the results from [1] we give the estimation of the distance between ASB. We show that the strain hardening process leads to an increase of the localization time and reduces the number of totally formed bands, see Fig. 1.

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Mathematical modeling of heat frozen earth[1]

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In the talk, a mathematical model of heating permafrost are considered taking into account the Stefan condition at the boundary melting [1]. We proposed numerical algorithm for analyzing this processes. Computation module is produced on an open architecture with the use of object-oriented programming language OpenFOAM [2]. Verification of the computation module carried by the known exact solutions of simplified tasks. We present the evolution of permafrost melting in the case of one, three and four cylindrical heaters.

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Nonlinear waves on shallow water under an ice cover. Higher order expansions

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Propagation of long wave with small amplitude on shallow water surface under ice sheet is considered. The ice sheet is assumed to be thin infinite homogenous plate with constant thickness under bending and stretching forces.

The closed equation system [1] for water perturbation level and velocity potential is given. In dimensionless form system has five small parameters, defined by problem geometry and ice properties. All parameters is supposed to be the same order. Compatibility condition for system and perturbation theory gives the nonlinear 9-order equation for water perturbation level [2].

Periodic solution in terms of elliptic Weierstrass function is obtained [3]. Modification of simplest equation method gives way to find solitary waves solution expressed via the logistic function [4]. It is shown that two forms for both periodic and solitary waves solution exist.

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Extended evolution equations for nonlinear waves in liquid with gas bubbles [1]

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Nonlinear waves in a liquid with gas bubbles are studied. We take into account liquid viscosity, inter–phase heat transfer, surface tension and weak liquid compressibility in the mathematical model. Higher order terms with respect to the small parameter are taken into account in the derivation of the equations for nonlinear waves. Nonlinear differential equations are derived for long weakly nonlinear waves. These equations are extensions of the Burgers, Korteweg–de Vries–Burgers and Kuramoto–Sivashinsky equations. Normal forms of these equations were constructed with the help of the near–identity transformations. Some exact solutions of the nonlinear equations were found. The nonlinear waves are numerically investigated as well.

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Geometrization of electromagnetic waves

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In the problems of transformation optics have to solve extremely complex macroscopic Maxwell equations [1]. To simplify the calculations, instead of macroscopic Maxwell equations in the plane space-time is proposed to write vacuum Maxwell equations in curved space-time. For this tensor polarization-magnetization geometrized in the sense of the field theory of gravity [2, 3]. As an implementation of this method calculates the lenses.

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Smooth approximation of functions of two variables

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An inductive algorithm is presented for smooth approximation of functions of two variables, based on the Tikhonov regularization method. The discrepancy principle is used for estimation of the regularization parameter. The principle of heuristic self-organization is applied for assessment of some parameters of the approximating function.

Mathematical modeling of charge dynamics in molecular chains [1]

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Consideration is given to general properties of a charge motion in molecular chains. When modelled mathematically, a charge motion is described quantum-mechanically, while the motion of oscillatory degrees of freedom of the chain is treated both classically and quantum-mechanically. Modelling is reduced to numerical integration of quantum-classical dynamical nonlinear equations of charge transfer in a molecular chain with random force and random potential and the solutions found are used to calculate the conducting properties of the chain. A new approach to finding the conducting properties of molecular nanowires is developed. It implies calculation of the charge mobility by

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Kubo formulae which involve averaged over realizations squares of charge displacements obtained by solving a discrete chain of dynamical quantum-classical equations with a random force simulating the source of temperature fluctuations. A typical picture of charge transfer at low temperatures represents a polaron or soliton transfer. In the framework of Holstein model an analytical solution is obtained for the dependence of the particle velocity on the electric field intensity which is analyzed by numerical modeling. Special attention is given to the case of a charge motion in rigid chains. Calculations of the band structure of Hamiltonians spectra are carried out for regular polynucleotide chains. It is shown that in one-chain periodical polynucleotides whose period is determined by the number m of nucleotides in a unit cell, the spectrum consists of m non-overlapping energy bands. Consideration is given to the dynamics of polaron states formation in Holstein chain, the polaron motion in an electrin field, the role of dispersion, Bloch oscillations of a soliton and breather states [1]-[7].

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Quality Assurance for simulation and reconstruction software in CBMROOT

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The software framework of the CBM experiment at FAIR - CBMROOT - has been continuously growing over the years. The increasing complexity of the framework and the number of users require improvements in maintenance, reliability and in overall software development process. In this report we address the problem of the software quality assurance (QA) and testing. Two main problems are considered in our test suit. First, a test of the build process (configuration and compilation) on different systems. Second, a test of correctness of the simulation and reconstruction results. The build system and QA infrastructure are based on CMake, CTest and CDash. The build process is tested using a standard above-mentioned set of tools. For the simulation and reconstruction tests a set of tools has been developed which includes base classes for reports, histogram management, simulation and reconstruction QA classes and scripts. Test results in form of the user-friendly reports are published on the CDash and on dedicated web-server where the developer can browse, for example, the tracking performance two weeks ago in order to fix the bug. The described QA system considerably improves the development process and leads to a faster development cycles of CBMROOT.

Selected event reconstruction algorithms for the CBM experiment at FAIR

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Development of fast and efficient event reconstruction algorithms is an important and challenging task in the Compressed Baryonic Matter (CBM) experiment at the future FAIR facility [1]. The event reconstruction algorithms have to process terabytes of input data produced in particle collisions. In this contribution, several event reconstruction algorithms, which use available features of modern processors, namely, SIMD execution model, are presented. Optimization and vectorization of the algorithms in the following CBM detectors are discussed: Ring Imaging Cherenkov (RICH) detector, Transition Radiation Detectors (TRD) and Muon Chamber (MUCH). In RICH event reconstruction includes ring finding (based on Hough Transform method), fitting (based on circle or ellipse fit methods) and association of reconstructed rings and tracks. In TRD and MUCH track reconstruction algorithms are based on track following and Kalman Filter methods. All algorithms were significantly optimized to achieve maximum speed up and minimum memory consumption. Obtained results showed that a significant speed up factor for all algorithms was achieved and the reconstruction efficiency stays at high level.

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Locality enhancement of parallel algorithms for numerical solution of quasi-linear two-dimensional parabolic equations

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Parallel implementations of locally one-dimensional method for the numerical solution of linear and quasi-linear two-dimensional parabolic equations are proposed in [1, 2]. The implementations for distributed memory parallel computers are based on the natural parallelism of the method. Computational processes at each time step can be executed independently, but the transition to a new layer is required large overhead for communication operations. In this paper, we propose to abandon the use of part of the natural parallelism and obtain parallel algorithms with improved locality. The locality of the parallel algorithm designed for implementation on distributed memory computers, characterizes the communication costs.

Hamiltonization of the dynamical systems and the theory of quanputers

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A short introduction in the Hamiltonization and the Nambu-Poisson formulation of the dynamics with several applications to (in)finite dimensional problems of mechanics, hydrodynamics, M-theory and quanputing is given.

Local dynamics of a pair of FitzHugh-Nagumo oscillators with asymmetric interaction[1]

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The dynamics of two coupled oscillators FitzHugh– Nagumo considered:

$$\begin{aligned} \dot{x}_1 &= x_1 - {x_1}^3/3 - y_1 + \gamma_1 x_2\,, \quad \dot{y}_1 = \varepsilon(x_1 + a_1)\,, \\ \dot{x}_2 &= x_2 - {x_2}^3/3 - y_2 - \gamma_2 x_1\,, \quad \dot{y}_2 = \varepsilon(x_2 + a_2)\,. \end{aligned} \tag{1}$$

Variables $x_1(t)$, $x_2(t)$ — are normalized membrane potentials of neurons, parameters $\gamma_1 > 0$, $\gamma_2 > 0$ characterize the relationship between them, value $\varepsilon > 0$ is fixed and small. System (1) has an unique equilibrium state

$${x_1}^* = -a_1,\ {x_2}^* = -a_2,\ {y_1}^* = {a_1}^3/3 - a_1 - \gamma_1 a_2,\ {y_2}^* = {a_2}^3/3 - a_2 + \gamma_2 a_1. \tag{2}$$

We choose the parameters a_1 a_2 close to the critical values, when the characteristic polynomial of task (1), linearized by (2), has two pairs of purely imaginary roots $\pm i\omega_1$, $\pm i\omega_2$. Assume $a_1 = \sqrt{2-\mu}\cos\varphi$, $a_2 = \sqrt{2-\alpha\mu}\sin\varphi$, where $0 < \mu \ll \varepsilon$.

We use the method of normal forms to study the local dynamics of system (1).Run the standard replacement

$$(x_1 - {x_1}^*, y_1 - {y_1}^*, x_2 - {x_2}^*, y_2 - {y_2}^*)^T = \sqrt{\mu}u_0(s,t) + \mu u_1(s,t) + \mu^{3/2}u_2(s,t) + \ldots, \tag{3}$$

where $j = 1, 2$, $u_0(s,t) = z_1(s)\exp(i\omega_1 t)\mathbf{c}_1 + z_2(s)\exp(i\omega_2 t)\mathbf{c}_2 + ..$, $z_1(s)$, $z_2(s)$ — complex amplitudes, $s = \mu t$ — slow time, at .. means the complex conjugate of this expression in the same bracket, $\mathbf{c}_1$ and $\mathbf{c}_2$ are eigenvectors of the matrix of linear part of the system (1), corresponding to the eigenvalues $i\omega_1$ and $i\omega_2$.

We get the following normal form at the third step of the algorithm:

$$\xi_1' = \varphi_1\xi_1 + (a_{11}\xi_1^2 + a_{12}\xi_2^2)\xi_1\,, \quad \xi_2' = \varphi_2\xi_2 + (a_{21}\xi_1^2 + a_{22}\xi_2^2)\xi_2, \tag{4}$$

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the prime denotes the derivative with respect to s, $\xi_1 = |z_1|$ and $\xi_2 = |z_2|$ — absolute values of z_1, z_2.

There are 2 situations at the normal form (4) for different values of the parameters. **At the first case** there are 4 coexisting equilibrium states: unstable zero, equilibrium saddle in the first quadrant of the plane (ξ_1, ξ_2), its stable manifold separates the region of stability of the other 2 equilibrium states lying on the axes. They correspond to coexisting periodic oscillations in (1) with frequencies ω_1 and ω_2. **Second case** associated with the co-existence of the zero unstable equilibrium and 2 equilibrium states at the axes, one of them is stable. In this case at $\mu > 0$ single frequency mode branches from the equilibrium in the system (1).

Population dynamics: limits of predictability

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I give a review of the case studies, which demonstrate mechanisms responsible for limitations of population dynamics predictability. Specifically, the results obtained testify that competition between different dynamical regimes can make predictability of the population dynamics more complicated than that of chaotic dynamics. In the case that the structure of the basins of attraction to each of the competing dynamical regimes is fractal, estimation of the horizon of predictability can even lose its significance.

Resonances in ultracold collisions confined by atomic traps

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By using our computational technique for ultracold scattering in low-dimensions [1,2] we have developed and analyzed a theoretical model which yields the shifts and widths of Feshbach resonances in atomic waveguides [3]. This model permits quantitative investigation of Feshbach resonances with different tensorial structure and having broad, narrow and overlapping character. We have calculated the shifts and widths of s-, d-, and g-wave magnetic Feshbach resonances of Cs atoms emerging in harmonic waveguides as confinement-induced resonances T(B_r)=0 at the field strengths B_r and resonant enhancement T(B*)=1 of the transmission T(B) at zeros a(B*)=0 of the free-space scattering length a. We have found the linear dependence of the width $\Gamma = \Delta k a_\perp^2/a_{bg}$ of the resonance at the magnetic field B* on the longitudinal atomic momentum k and quadratic dependence on the waveguide width $a_\perp$ (here Δ= B*-B_{r0} is the width of the Feshbach resonance at the field B_{r0} and $a_{bg}$is the background scattering length in free-space).

The found effect could potentially be used experimentally. Actually, one can control the width $\Gamma = \Delta k a_\perp^2/a_{bg}$ of the resonance by varying the trap width $a_\perp$. From the other side, by measuring the width Γ one can extract from the obtained formulae the longitudinal colliding energy E (k=$\sqrt{mE}/\hbar$, m is the mass of Cs atom) and estimate the temperature of the atomic cloud in the trap.

We have also found that the relationship $a = 0.68 a_\perp$ for the position of the confinement-induced resonance in a harmonic waveguide (where T(B_r)=0) is fulfilled with high accuracy for the Feshbach resonances of different tensorial structure which holds in spite of the fact that this property was originally obtained in the framework of the s-wave single-channel pseudopotential approach [4]. Note, that this property was recently experimentally confirmed for d-wave Feshbach resonances in a gas of Cs atoms transformed in atomic traps into confinement-induced resonances [5].

Our model opens novel possibilities, which we briefly discuss, for quantitative studies of the scattering processes in ultracold atomic gases in traps, particularly, the appearance of dipolar confinement-induced resonances [6].

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Particle-In-Cell simulation of kinetic instability of an electron beam in plasma

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In this work parallel 3D numerical model is created on the basis of Particle-In-Cell method. The model is designed for simulation of relaxation processes of the warm electron beam in plasma. Growth saturation of a separate unstable mode is studied in different regimes. The two methods for diagnostics of the instability are proposed. The comparative analysis of this methods of increment calculation is carried out and "less noisy" one is chosen.

The numerical solution of three-dimensional Vlasov-Maxwell system is usually performed by Particle-In-Cell methods. In Particle-In-Cell method the discreteness of model particles can bring the energy loss, self-heating and self-force occurrence and other non-physical effects called "noise" . The reasons for noise occurrence are various. Often it is difficult to define the influence of various non-physical factors on the solution as they interact and cooperate with each other. At the present time, there is no uniform approach to solving the noise

problem. Sometimes the particle form-factor are modified, or an optimal time and spatial steps are selected. Also, a "quite start" algorithm, Fourier filtering and smoothing algorithms are used. But such algorithms leads to increasing algorithm complexity and can cut or damp physical effects.

More often, the number of particles is increased, but that is not always possible because of limitation of computer resources. Therefore it is necessary to define sufficient number of particles. For our model the results accuracy dependance on model particle number is determined. Minimal model particle number for correct instability increment calculation in weak electron beam-plasma interaction is defined. The results of 3D PIC simulation are in good agreement with theoretical predictions. It is shown by instability increment values computation and also by phase plane analysis for both cold and warm beam relaxation.

Description of peripheral heavy ion collisions at Fermi energies with transport theory

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Peripheral heavy ion collisions in the Fermi energy range are a successful method to produce exotic isotopes far from the stability line at the same time exploring the equation-of-state of nuclear matter. At least two mechanisms contribute to these reactions as can be seen by analyzing velocity distributions of projectile-like fragments. To model the collision of two ions transport approaches have been extensively used [1]. The primary fragments at the freeze-out time are obtained in the Boltzmann–Nordheim–Vlasov (BNV)

approach, that gives us a set of differential equations which are solved numerically. To compare with experiment we use the Statistical Multifragmentation Model (SMM) [2] to describe the de-excitation of the excited fragments. We calculate the excitation energy and its fluctuations in the BNV model and also discuss the effect of the fluctuations on the results. The transport description only provides a reasonable description of the dissipative part of the reaction. Isotope and velocity distributions are compared with the experimental data for the reaction of 40Ar projectiles on 9Be targets at 36.5A MeV measured by using the double achromatic fragment-separator COMBAS at FLNR [3,4].

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Application of clustering approach in the UrQMD fragmentation model for nuclear collision for relativistic energies

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Heavy ion collisions, besides of particle (protons, neutrons, mesons, hyperons, etc) production, are accompanied by a nuclear spallation with the nuclear fragments formation. Nuclear spallation is a challenging task for theoretical models. The Quantum Molecular Dynamic (QMD) model [1,2] was more or less successful for calculations of isotopes generation for energies less than 0. 4 GeV [3]. However, its version for higher energies, Ultra Relativistic Quantum Molecular Dynamic, UrQMD, [4] does not include nuclear fragmentation. Our aim is to develop the UrQMD describing nuclear fragmentation by dynamical clusters formation. Calculations consist of several steps. On the first step, realized in the framework of the UrQMD, time evolution of spatial distributions of nucleons and mesons (pions, kaons, etc) is traced.

On the next step the nuclear fragments are shaped from nucleons and clusters, and their kinetic energies and masses are calculated. The clusters or nuclear fragments are generated via dynamical forces between nucleons during their evolution in coordinate and momentum space. This evolution of cluster formation is described by the visual representation.

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Watershed on vector quantization for the Big Data clustering

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A method for clustering large amounts of data is presented which is a sequenced composition of a two algorithms: the former builds a partition of input space into Voronoi regions and the latter partitions them. First, a model of clusters as high-density regions in input space is presented, then it is shown how a Voronoi tessellation and its topological map (a) can be built and (b) used as a low complexity approximation of the input space. During the (b) step, the usage of "watershed" algorithm is presented which was previously used for image segmentation, but it is its first use for the data space segmentation that is known to the authors.

Chaotic dynamics of solitons in classical Heisenberg antiferromagnet model

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In this paper we study the chaotic dynamics [1] of breather-like solutions of classical Heisenberg model in the presence of dissipation and pumping by variable external magnetic fields. Numerical approach based on stereographical projection allows us to avoid singularities on the poles of the Bloch sphere. Parameters of dissipative breather regime formation are determined. Analysis of the phase portrait of the system, i.e. the dependence of soliton energy density in the center on its total energy, shows that the phase trajectories densely fill a finite region of space - the so-called "strange attractor", which is an indication of chaotic dissipative soliton formation [2]. Fourier analysis demonstrates the presence of three main harmonics of the dynamics of breather solutions.

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Dynamics of two-dimensional breathers in O(3) vectorial nonlinear sigma-model

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In this paper we present an algorithm numerical code for simulation of particle-like localized perturbations in two-dimensional O(3) nonlinear sigma-model. The algorithm of the finite difference schemes uses stereographic projection, which avoids the singularity at the poles.

By the numerical solution of Couchy problem with the specially chosen perturbation to the solution of two-dimensional sine-Gordon equation [1-3] as initial condition we obtained new stationary and dynamic breather solutions of the two-dimensional O(3) vectorial nonlinear sigma-model which possess the dynamics of isospin vector in Bloch sphere. Numerical simulation demonstrates the stability of obtained solution.

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Quark correlations and discrete symmetry of nuclear structure

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Starting with a quark model of nucleon structure, elaborated by one of the authors (G.M.), in which the valence quarks are strongly correlated with one another within the nucleon, the light nuclei are constructed by assuming similar correlations with the quarks of neighboring nucleons [1]. Applying the model to larger collections of nucleons reveals the emergence of the face-centered cubic (FCC) symmetry at the nuclear level. The FCC model of nuclear structure which is isomorphic to the shell model and, moreover, composes the features of the liquid drop and cluster models has been proposed by N.Cook [2]. The visual interface for graphical representation of the discrete symmetry of nuclear structure was created.

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Magnetic field and entanglement control in vertical two-electron quantum dots

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Two-electron quantum dots (QDs) have drawn a great deal of experimental and theoretical attention in recent years [1]. Since almost all parameters of QDs can be varied in a controlled way, they are considered as a tiny laboratory allowing direct investigation of fundamental properties of charge and spin correlations at the atomic scale. Another strong motivation for studying the properties of QDs is due to a rapid development of the field of quantum computing, because the entangled states of electrons confined in a quantum dot may give a natural realization of a quantum bit or "qubit". Using a three-dimensional parabolic approximation for confining potential, two-electron quantum dots in magnetic field are studied for various strengths of electron-electron interaction. We analyse the entanglement for the ground and for a few excited states [2,3]. We find that these states become more entangled when the electron-electron interaction becomes stronger. As a general trend, we also observe that the entanglement of the eigenstates tends to increase with the states's energy. There are, however, entanglement level-crossings where the entanglement of a state becomes larger than the entanglement of other states with higher energy. In particular, at a specific magnetic field value the dot attains a spherical symmetry. The transition from the axial to the spherical symmetry manifests itself as a drastic change of the entanglement of the lowest state with zero angular momentum projection. The entanglement of this state, being first a decreasing function of the magnetic field, starts to increase after the transition point with the increase of the magnetic field. This behaviour is associated with a geometrical phase transition from the lateral to the vertical localization of the two-electron probability density for this state in the QD. Varying the magnetic field around the transition point, one can control the increase/decrease of the entanglement in QDs.

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Density waves in Bose-Einstein condensates

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In this talk I will review experimental and theoretical results on the emergence of Faraday and resonant density waves in cigar-shaped Bose-Einstein condensate with contact interactions and will discuss in detail a novel variational model for dipolar (i.e. long-range) Bose-Einstein condensates.

Numerical investigation of IWZ(k) preconditioner

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The work is devoted to numerical investigation of effectiveness of IWZ(k) preconditioner [1] when used with BiCG iterative method [2] for solving large sparse systems of linear algebraic equations. Test cases originated from different problems of mathematical physics. Results for sequential and parallel version of the preconditioner are presented.

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Scrutiny of some data sets concerning the cuprate superconductivity under selective copper substitution with metallic ions[1]

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Scattered data found in 29 references dealing with the derivation of direct experimental evidence concerning the role of the copper-oxygen CuO_2 layers in the occurrence of high-temperature superconductivity in cuprates were collected together.

The investigations dealt with two optimally doped cuprates belonging to the LMCO and YBCO classes respectively ($La_{1.85}Sr_{0.15}CuO_4$ and $YBa_2Cu_3O_{6.84}$). Different metal ions M characterized by effective ionic radii close to those of the Cu^{2+} ions in the CuO_2 layers were added in controlled proportions during sample preparations. The M ions were found to substitute the copper in the CuO_2 layers and the measured superconducting critical temperature T_c showed M-ion-dependent monotonic decreases with the concentration y of the M-ion.

In order to accommodate with each other the data reported by various authors on a given cuprate for a same M-ion, data processing was performed using L_p ($p = 2$ and $p = \infty$) metrics.

The analysis of the uniquely resulting $T_c(y_i)$ distributions for different M-ions was then performed by data smoothing using Gramm-Schmidt orthogonal polynomial sets up to a maximum degree $m \geq 1$ at which a stochastic distribution of the residuals was achieved.

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Undecidability of existence of certain solutions of partial differential and difference equations

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We consider algorithmic decidability of the existence problem for certain kind non-zero solutions of homogeneous partial linear differential or difference equations with polynomial coefficients. We prove that this problem is undecidable for solutions in the form of rational functions [1] and formal Laurent series. Proofs are based on undecidability of this problem for polynomial and monomial solutions [6, 2] and on Davis-Putnam-Robinson-Matiyasevich theorem [3]. Note that there are methods that solve this problem in some cases [4, 5], however there are no universal algorithms for this.

We show as well that this existence problem is decidable for monomial solutions with real exponents in the differential case and describe an algorithm for finding such solutions.

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Parallel LU-SGS numerical method implementation for 3-dimensional gas dynamics problems on GPU-accelerated computer systems

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An effective algorithm for calculation of gas dynamics problems by using GPU-accelerated multiprocessor computing systems is presented. The algorithm is based on the implicit-explicit scheme that leads to large-size linear systems with sparse matrices, which are solved with the method of LU-SGS (Lower-Upper Symmetric Gauss-Zeidel) approximate factorization [1,2,3]. Geometry model is represented in terms of volume of fluid and immersed boundary methods [4,5]. The parallel algorithm exactly copies the work of the successive one and possesses a high-level of scalability[6].

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Model of dynamics of the IBR-2M pulsed reactor for analysis of fast transients

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On the basis of the program system MATLAB the nonlinear dynamics model of the IBR-2M pulsed reactor which links values of variables at discrete moments (at moments of appearance of power pulses) is established. The testing by means of modeling calculated processes in the IBR-2M shows the correctness of the model. A preliminary estimate of the transfer coefficient of the linear part of the automatic regulator is obtained.

Simulations of magnetostatic problems with an "angular point" in ferromagnetic region

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The design and construction of magnetic systems of electrophysical installations require preliminary mathematical simulations. A mathematical modeling is required in the process of adjustment and a subsequent exploitation of the installation. Although the calculations of the fields of magnetic systems were performed on the basis of solving direct magnetostatic problems, they are related to a class of inverse magnetostatic problems, since they actually include search for an optimal design of current elements and an iron yoke for a predetermined magnetic field distribution. A peculiar feature of the modeled magnet is

that the region in which the magnetostatic problem is solved, has the so-called 'angular points' in a vicinity of which the border is formed by crossing two smooth curves. The work deals with formulation of a boundary-value problem of magnetostatic and a computational procedure with research on the behaviour of the solutions in a vicinity of the "angular point". The purpose of this investigation is to find out whether there are solutions to the boundary-value problem of magnetostatic with indefinitely growing in a vicinity of the "angular point" and, if such solutions exist, then to construct a difference scheme which takes into account the character of the behaviour of the solution with the purpose of increasing the accuracy of numerical computations.

With the help of the Legendre nonlinear transformation the research on the nonlinear magnetostatic problem in the area of ferromagnetic is reduced to the consideration of the properties of a boundary-value problem for a linear differential equation. The existence of solutions with unlimitedly growing in a vicinity of the ferromagnetic angular point is shown. The properties of such solutions are investigated. For the boundary-value Dirichlet problem in the area with a corner, a difference scheme giving a substantial improvement of the accuracy of the solution has been constructed. Calculations of the model problem were performed with the use of the methods received.

3D simulation of filamentation instability in laser interaction with overdense plasma with CFHall code [1]

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The efficiency of laser pulse energy conversion to electron acceleration in fast ignition scenario is known to be impeded by filamentation (Weibel) [1] instability. As the accelerated electrons pass through the cold plasma the classical

[1]This work is supported by RFBR grant 12-01-00708-a

condition for the instability, namely, anisotropic particle velocity distribution, is formed. This leads to formation of "filaments" in charge currents and growth of the magnetic fields that are transverse to the fast electron stream.

Due to the complexity of the system, the theoretical analysis provides only rough estimates for the instability growth. The accurate numerical simulation would predict the ratio of pulse energy transfer to magnetic field generation dependence on the laser pulse and plasma parameters.

The simulation serving such purpose should take into account the three dimensional nature of the phenomena, have enough spacial and time resolution to show the fastest growing instability modes and be able to cover the size of a characteristic laser-plasma system in question.

In the current work we show the ability of CFHall code [2] to provide accurate simulation results of laser interaction with plasma in the aforementioned scenario.

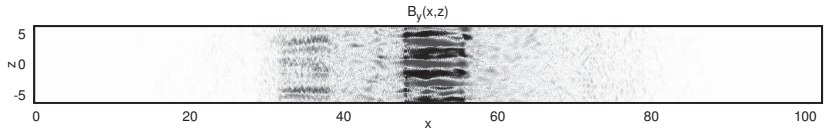

Figure 1: An x-z slice at $y \sim -6.5$ of the 3D distribution of B_y magnetic field component. The filamentary structure of the developing instability is observed. ($t = 153.6$)

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Localization of gas-dynamic fields singularities and adaptation of grid to singularities position[1]

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Shock capturing methods are widely used in the calculations of gas-dynamic flows. They universality is incomparable because they can do without information on the position of discontinuities. At the same time, this approach leads to the erosion of discontinuities which may have a negative affect on the accuracy of a calculation. Moreover, it is the position of shock waves in the flow that often is of a special interest. Thus an inverse problem, i.e., to localize and classify the discontinuities in the field obtained in the calculation, arise. At present, there is a need for algorithmic localization directly during calculation, in order to build adaptive grids and increase the quality of the calculation. The algorithms used for these purposes should be universal, and should not need individual adjustment for each class of flows. Method for the localization of the gas-dynamic fields' singularities has been developed in [1]. As input data algorithm gets fields of physical values of density and pressure assigned in the nodes of the computation grid. As a result of the detection each grid node is associated with a natural number that characterizes the flow around this node. Feature of the method is so that it does not require fine tuning (the same threshold sensitivity and filter sets can be effectively used for many different tasks), that allows to use it in automatic mode. One of the ways to use the detector for adaptation of the calculation to the position of the discontinuities is presented and tested. The use of adaptive method improved the quality of calculation by reducing the erosion zones of discontinuities.

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Parallel MD-simulation of gas mixture in microchannels[1]

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In this work we consider the modeling of gas mixtures flow when the Knudsen numbers close to applicability limit of the continuum [1-4]. We propose combined approach for simulation of supersonic binary gas flow. Macroscopic approach is based on the quasi-gasdynamic equations (QGD) and the correction of the flow parameters is performed by molecular dynamic method (MMD) [4,5]. The numerical algorithm uses a splitting into physical processes [6, 7]. QGD system is a generalization of quasi-gasdynamic equations for the case of the gas mixture. They are solved by finite volume method. The system of molecular dynamic equations is used as a sub-grid algorithm. Within the MMD algorithm the interactions of particles are described by the Lennard-Jones potential, which is determined by the properties of the mixture components and their thermal conditions. The MMD allows us to get information about processes on molecular scale, and at times of a few nanoseconds.

We have studied the (N_2+H_2) system. Number density and temperature in the zone of silence of supersonic jets (N_2,H_2), and their mixtures (N_2+2H_2) and (2N_2+H_2), at p_0=1 bar and T_0=295 K, have been investigated.

For calculations a hybrid computing system was used. The constructed parallel numerical algorithm is based on Domain decomposition technique. Parallel code utilizes MPI, OpenMP technologies and it is optimized for modern hybrid architecture clusters. The system has a central processing units (CPU) and graphic processing units (GPU). A decomposition of the computational domain on the nodes of the computing system was realized. This decomposition is a grid that is similar to used computational mesh. As a result, each node of a computer system processes some subset of cells. Macro parameters calculation of the the gas flow is performed by CPU threads. Correction the obtained gas dynamic parameters is produced by molecular dynamic method on GPU.

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Self-adaptation in swarm optimization algorithms

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Almost all swarm optimization algorithms are based on some simple nature-inspired idea. However, these basic ideas usually engender a set of different advanced rules (heuristics), which are controlled by one or more parameters.

As a result every swarm optimization algorithm becomes dependent on a large number of parameters which affect the efficiency of work and the speed of convergence of this algorithm. Unfortunately, it is impossible to adjust these parameters case by case. This paper is devoted to the description of the self-adapted method for adjusting parameters of swarm optimization algorithms, such as Bacterial Foraging Optimization Algorithm [1] and Bees Algorithm [2].

The idea of self-adaptation is following. In the background of the main optimization algorithm we run genetic algorithm [3] with tournament selection, which performs adjusting parameters of the main algorithm. The objective for this additional algorithm is maximization of the convergence speed of the main algorithm. Initial values for parameters participating in genetic selection are established randomly.

The proposed self-adaptive algorithms were numerically tested on standard benchmark functions suggested in the special session of Congress of Evolutionary Computing [4]. The results of this testing are given.

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Method of artificial viscosity on unstructured grids[1]

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The method of adaptive artificial viscosity (AAV) was proposed for the solution of gas dynamics equations on orthogonal grids; in our work, this method is extended to unstructured grids.

The method of AAV for the solution of gas dynamics equations consists of three stages. At the first stage the predictor solution is found using the explicit difference scheme with allowance for the Lax–Wendroff corrections but without dissipative terms with artificial mathematical viscosity at time layer $t_{n+1} = t_n + \tau_n($ τ_n is the time step of the grid). Note that on the orthogonal grid and in the regions of solution smoothness, Lax–Wendroff corrections result in the difference schemes with time approximation τ_n^2. The difference scheme is constructed by the balance method. The desired functions belong to the cell centers, triangles or tetrahedrons. Schemes are constructed using the support operators method [1] (the construction of the grid operator $grad^h$ is based on the grid operator div^h). In constructing the approximations, techniques are employed developed during the construction of fully conservative difference schemes [2].

The second stage, we introduce into the difference scheme the dissipative terms with the same artificial viscosity for all equations. The artificial viscosity is obtained from the requirement of the maximum principle condition under the frozen coefficients of the scheme ensuring the monotony of the grid solution. The artificial viscosity is introduced adaptively to the solution, i.e., $\mu^{n+1} = \mu^n_{\min}$ on the shock wave (SW) and compression wave (CW), and $\mu^{n+1} = \mu^n_{\max}$ in the area of the solution oscillations (OSC), $\mu^{n+1} = 0$ on the contact discontinuity (CD) and the rarefaction wave (RW). The areas occupied by SW (CW), OSC, CD, and RW are determined by the verification of the well-known inequalities [3] for the derivatives of the predictor solutions. The derivatives are found by the linear fulfilment of the predictor solution.

At the third stage, the predictor solution is smoothed by the introduction of dissipative terms into the difference scheme. The absence of the artificial

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viscosity on the CD and low artificial viscosity on the (CW) do not lead to their significant blurring as the CD is only blurred by the internal viscosity of the difference scheme [4] and the SW is blurred on 3–4 grid intervals. The dissipative terms are only noticeable in the vicinity of the discontinuities.

Here, we present the numerical calculations of the two-dimensional (2D) test problems on orthogonal grids from [5] and compare them with the computations on the triangular grids obtained in this study. Both the calculation results proved to be close.

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Modeling of telecommunication processes in an overall complex system[1]

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An approach for modeling of telecommunication processes in an overall complex system is presented. It includes conceptual, mathematical and computer methods.

Main overall network teletraffic tasks are described and, for Virtual Networks (VNETs) with Quality of Service (QoS) guaranties, the performance prediction and re-dimension tasks are considered. The coordinated use of different methods and software tools, as well as the integration of computer algebra systems and computer modeling and simulation tools in uniform platforms is discussed.

We hope that the presented results, ideas and program tools allow development of a more general approach and program systems for solving design and re-dimensioning problems in complex systems.

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Few-body simulation in atomic and molecular physics

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The main difficulties in the research of few-body problems are bounded with the really many-channels and multidimensional nature of the these problem, impossible applied many well known theories such as adiabatic, impulse, coupled channels, etc.

For this reason we proposed new method for the investigation of the different few-body processes used the mathematically rigorous formalism based on the treatment of collision processes as many body processes, using Faddeev-Yakubovsky equations [1] (FYE) in integral and differential forms. In particular techniques based on FYE have been used successfully in studies of the dynamics of few-particle systems (bound-state properties and elastic, reactive and breakup scattering) [2]. That is why we applied this formalism for the theoretical investigation of the dynamics of the different processes in atomic and chemical physics. The following results are presented and discussed [2].

Calculation of low-energy characteristics in scattering processes like scattering length, effective range parameter, amplitude, cross section etc. in processes $p + d$, $n + d$, $p + He$, electron + molecule etc. for the verification of the fundamental principal of the atomic and chemical interaction.

The theoretical investigation of the quasibound, virtual and resonances states in few-body systems such as $p+d$, $n+d$, $e+H$, $e+He$, $p+H$, $p+He$.

Scattering the electrons, protons on the few-centers targets (atoms, molecules etc.) and the estimation the role of many center scattering in these cases.

The calculations of the excitation, rearrangement and ionization H and He atoms and its ions by the electrons and protons impact.

The investigation of the influence of the long range part of pair-wise potentials in FYE on the scattering in few-body systems.

The study on the correlation between low-energy characteristic in few-body scattering.

Scattering electrons by two atomic (H_2, HD, D_2, N_2, Cl_2, F_2, Br_2, J_2, HF, DF, HJ, DJ, HCl, DCl, HBr, DBr,$RbCl$, $RbBr$, $CsCl$, $CsBr$, KI) and few atomic molecules (CO_2, O_3, NF_3).

The investigation the theory of quasimolecule (electron + molecule), the ionization mechanism in quasimolecule and the main characteristics of

quasimolecule autoionization states, determination of the bound between these states, the resonance states, potential energy surface (PES) and dynamics of the chemical reaction.

The scattering atoms with two ($O + CS$, $H + H_2$, $O + N_2$, $O + O_2$) and few atomic ($O + CF_3J$, $O + CS_2$, $O + OSC$, $HCl + HCl$) molecules, the many particles interactions, orientations of the reacting molecules etc. on the reactions dynamic, the confection between the interactions in FYE and PES, the investigation of the resonances, virtual states and threshold phenomena in chemical reactions.

The studding the unusual dynamical threshold phenomena in chemical reactions such as Efimov states based on FYE. This research may be obtain the information of the reaction mechanism, PES etc. and may have a strong influence on the scattering observable. Hence the careful studding of these states may be provide better understanding of the control and management of the chemical reaction processes.

The investigations of the possibility of the analytical solution of FYE in the different approximations, the construction of the solvable model in FYE approach are presented.

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Simulation of the scattering hydrogen halide molecules by slow electron

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The electron scattering by hydrogen halogen molecules has been the subject a large number of experimental and theoretical papers [1, 2]. If the energy of scattering electron is slow hydrogen halogen molecules HX (X is halogen atom) may be considered consisting of an proton and negative ion of halogen because electron affinity halogen atom is much more than the affinity of hydrogen atom [2]. In this assumption the processes of the collisions slow electron with hydrogen halogen molecules is treated as four-body process:

$$e + (H^+, X^-) \rightarrow \begin{cases} e + (H^+, X^-) & (1) \\ e + (H^+, X^-(v, j)) & (2) \\ H + X^- & (3) \\ H + X + e & \\ H^+ + X^- + e & (4) \end{cases}$$

The interaction of the electron with the hydrogen halogen molecule is replaced approximately by the pair-wise interaction with each component consisting hydrogen halogen molecule (H^+, X, e) as if they are simple field centers. In this case two-body potentials have form of sum the long-range part and short-range one. In this approach we consider all processes of the scattering of the electron by molecule such as elastic scattering (1), ro-vibrational excitation (2), dissociative attachment (3), ionization (4) simultaneously. This approximation seems reasonable as long as the energy of incident electron is below the threshold of electronic excitation of hydrogen hyalogen molecule. To calculate the cross section of the processes (1)-(4) we use the modified Faddeev-Yakubovsky equations (FYE) [3]. It is well known that the FYE are the most consisting and concise way of treating multiple scattering effect in few-body problems as well as the resonances connected with arbitrary number and location of the centers [4]. For the numerical solution of FYE we used the technique developed in [3,4]. Using this model the calculations of the electron scattering HF, DF, TF, HCl, DCl, TCl, HBr, DBr, TBr, HJ, DJ, TJ molecules of the processes (1)-(4) are presented and discussed. The results of this calculations are compared with the available experimental data and other calculations [1, 2, 4].

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Memory effects for fast electron transport in open systems:photosynthetic reaction centers

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The effect of environment on transport properties of quantum systems is a highly topical problem in atomic, nuclear and condensed matter physics. Markovian approaches have been successfully used to study various phenomena in open systems, when the past memory of the system is neglected. The advent in ultrafast laser-pulse technology, quantum information processing, synthesis of new superheavy elements in cold and hot-fusion reactions are requiring a resolution of quantum dynamics, when a system is far from equilibrium. Analogous processes can be found in biological systems as well as in nanoscale devices.

Although there are wide structural and functional differences, the laws, that govern quantum solar energy conversion to chemical energy or electricity in biological systems and semiconductor solar cells, share many similarities. In these systems the conversion processes proceed from the creation of elect ron-hole pairs (exitons) by a photon of light, followed by charge separation to produce the required high-energy product. The efficiency of solar cells may be

increased due enhanced multiple exciton production in semiconductor quantum dots, which is essentially created extremely fast upon absorption of high-energy photons. In the photosynthetic reaction center (RC), after excitation the electron transfer is so fast that there can exist unrelaxed vibrational modes in the primary stage of electron transfer. Creation of electron or exciton by external fields in a system with initially statistically independent unrelaxed vibrational modes leads to an initial condition term. The problem of nonequilibrium transport of electrons in a quantum system with the initial condtional term (IT) is a highly nontrivial task, and still is in its infancy. We proposed the microscopic approach to study the effect of the ITs on the electron transfer in a RC with initial conditions being far from equilibrium. The contribution of this term in the time convolution generalized master equation approach is studied in second order of the perturbation theory for electron-phonon coupling in the parth integral formalism. We found that the IT impact depends in the RC mainly on the amount of energy stored in the initially unrelaxed phonon modes and also on the lifetime of the electron in the system. If the electron lifetime is much longer than the phonon relaxation time, the ITs do not affect the quantum yields of electron transfer via possible pathways. In systems, where this condition is not fulfilled, the ITs can cause the electron transfer via channels which are closed in the case without the ITs.

Evolutionary optimality in structured systems and its applications in medical and biological problems

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The direction of the natural selection in the competition conditions brings to formation of structures, which can be considered mathematically as ones to be stable. As an example of the simplest model one can consider the competition of a finite number of biological species $\frac{dx_i}{dt} = x_i f_i(x)$, $i = 1, \ldots, n$, $x = (x_1, \ldots, x_n)$. The necessary condition for stability of an equilibrium of

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the form $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_m, 0, \ldots, 0),\ \bar{x}_i > 0,\ i = 1, \ldots, m$ here is an equality $f_i(\bar{x}) = \max(f_j(\bar{x})),\ 1 \le i \le m,\ 1 \le j \le n$, having the character of an extreme relationship, whereas it is called *the evolutionary optimality principle*. Its biological sense is in the species which manage to survived in a stable equilibrium are obliged to have the maximal values of Maltusian parameters amongst all potentially possible ones, which may be computed at the equilibrium. These factors characterize the "power" of species in its Darvin's understanding if bear in mind wording of the principle about survival of the most strong.

Since in the equilibrium the species with senior numbers are absent, they may to be considered as virtual ones, i.e. we can add to their collections any other species, which have hypothetical possibility to turn out to be in initial set. Herewith their distinguishing parameters can have a free nature and, in particular, can be chosen from a certain area in the space of parameters, so the optimization problem will already to be solved with respect to it. Such an expansion allows to find the isolated values of parameter, under which the equilibrium turns out to be stable. On this way one can built the methods of the calculation of parameters values for (quasi)stationary biological systems, for determination of which the natural measurement can turn out to be impossible or difficult.

In mathematical model of the concrete structured biological systems the most difficult is the construction of functionals, which ought to play the role of Maltusian functions in the considered example. During their construction the analogues of the result stated above can be got from the general theory of relationship between stability and optimality for the case of structured quasilinear systems [1,2]. As an example one can consider its application to systems with continuous age or spatial structures. The last one bring about the theory of correlation adaptometry, allowing to evaluate the degree of badness in biological group on the basis of distributions of its representatives in the region of the parameter measured [3].

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Evaluation of spinors in computer algebra

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The qualitative analysis of models of evolution of the Universe begins with deriving evolution equations by computer algebra tools and continues with constructing a characteristic equation, finding special points in a phase space, analysis of their type and presentation of phase portraits. Performance of all these operations by computer algebra within a differential geometry package is considered as a token of the logic integrity of modelling.

The formulations of models including spinor fields [1, 2] use the algebra with noncommutative factors. Preserving this symbolics over all of the analysis is preferable for understanding the modelling results.

For the solution of these problems by means of the commutative computer algebra two approaches are used. The former is the transition to symbolical matrix representations of noncommutative terms in formulas, then transformations of the formulas by the substitutions set by the user, and back transition in resulting formulas.

The letter is real evaluations in a matrix representation and back transition to a symbolical one in a corresponding matrix basis.

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Analytical solutions of linear homogeneous thermal spike model

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For the linear homogeneous Thermal Spike Model (TSM) with constant coefficients, a set of nontrivial symmetry operators (SO) is obtained. Efficiency of the application of these SO is confirmed by several examples of concrete infinite series of analytical solutions of TSM.

On the separability problem for quantum composite systems [1]

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The presentation aims to discuss the so-called *"separability/entanglement"* problem, the mathematical issue that lies in the foundations of quantum theory [1], [2] and computationally is classified as NP-hard [3]. The separability problem consists in the elaboration of effective computational methods allowing one to determine whether the given state of the composite quantum system admits representation in a product form with the factors corresponding to each subsystem. Here we discuss the probability aspects of this problem. Using the

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method based on the measurement theoretical point of view (cf. [4], [5], [6]), the probability distributions of diverse characteristics of the entanglement have been computed. The results of analytic and numerical studies of the geometric probability of the mixed separable/entangled states in quantum systems composed from 2-qubits and qubit-qutrit pairs will be given.

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Volatility in classifications[1]

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The idea of duality of system dynamics and statics (sometimes named as idea of canonic ensemble) is one of the most essential ideas of natural sciences. This idea is especially important near phase's transitions, bifurcation points, etc. However, in investigation of socioeconomical systems this approach is comparatively uncommon.

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The main concern is focused on formalization, exact definition and calculation of the important property of subsets of the given initial set that describes their stability, exactness, validity - in essence, their possibility (or impossibility) to be selected as classes. This property is named volatility, which is determined formally for separate classes as well as to the whole classification problem.

The goal of the presented work consists in the construction of the new classification algorithm that finds the classes with arbitrary levels of volatility (including the conventional case of zero volatility). One of examples describes volatility of party fractions in the 3rd State Duma near essential bifurcation point - creation of the new party "United Russia" (01.12.2001). The significantly different levels of volatilities of the two parties involved in the union process underlines their different roles in this process: zero level of party "Unity" and high level of party OVR. The other analysis of the same period was done in book [1].

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Structure of topological solitons in nonlinear spinor model[1]

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We consider nonlinear spinor model based on 8-spinor Brioschi identity resulting in description of baryons and leptons as topological solitons. The model suggested [1] includes as particular cases the well-known Skyrme model (baryons) and Faddeev one (leptons), the particles in these models being described by the soliton configurations endowed with topological charges of the

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degree kind or Hopf index respectively. The corresponding topological phases can be fixed via the Higgs mechanism by the inclusion of the Higgs potential of the special stricture in the Lagrangian of the model. The Higgs potential appears to depend on the spinor current squared, which can be represented, due to Brioschi identity, as the sum of corresponding bispinor quantities squared. The structure of the soliton configuration is shown to depend on the type of topological invariant. In particular, the lepton configurations are similar to the closed twisted strings. For the appropriate description of the latter configurations the toroidal coordinates are used. The simple approximations of these configurations are suggested to estimate the mass, the spin and the magnetic moment of the particle-soliton in question. In the baryon sector with the unit charge there appears typical for the Skyrme model hedgehog configuration, the main contribution to the mass of the state being determined by the Yang – Mills gauge field. It is worth-while to underline the important difference in mirror symmetry between lepton and baryon sectors, the leptons being realized as the states invariant under the space reflections and the baryon states being invariant under the combined reflections in the coordinate and isotopic spaces.

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Anisotropic dark energy model with varying EoS parameter

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The latest discoveries of astrophysics suggest that our Universe is expanding with acceleration. This discovery of late time accelerating mode of expansion in one hand leads to a major breakthrough in observational cosmology, on

the other it sets a major task of theoretically explaining this newly found phenomenon to cosmologists. One of the ways to explain this accelerated mode of expansion is to introduce dark energy into the system.

Given the fact that the WMAP shows some temporal anisotropy in the microwave background radiation, we consider an anisotropic Universe filled with perfect fluid and dark energy. This anisotropic universe is given by the Bianchi type-VI cosmological model.

To get the deterministic model of Universe, we assume that the shear scalar (σ) in the model is proportional to expansion scalar (ϑ). It was found that if the proportionality condition is used, this together with the non-diagonal Einstein equation leads to the isotropic distribution of energy momentum tensor, i.e., $T_1^1 = T_2^2 = T_3^3$. This fact allows one to solve the equation for volume scale V exactly. The behavior of EoS parameter ω is thoroughly studied.

The EoS parameter for dark energy as well as deceleration parameter is found to be the time varying functions. Using the observational data qualitative picture of the evolution of the universe corresponding to different of its stages is given. The stability of the solutions obtained is also studied. It is found that the solution becomes stable as the Universe expands.

Modeling of hydrodynamics processes with phase transitions

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The new method of numerical simulation for heterogeneous fluid dynamics with take of phase transitions like graphite-diamond will be presented. Heterogeneities of the fluids are considered as small drops or particles of one fluid

within other fluid. Total number of the drops can be large enough and the drops may have phase transitions. Thus, simulations of the main fluid with small transited drops dynamics are discussed.

The method is a combination of Harlow's particle-in-cell method and Belotserkovskii's large particles method (see, for example, [1]). The method is based on a discretization of conservation laws for masses, momentums, and energies in integral forms. The discretization is natural and numerical simulations are realized as direct computer experiments for the dynamics with phase transitions like graphite-diamond.

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

The method seems to be perspective for numerical simulations of other absorption and diffusion processes in plasma dynamics [2] and complex fluid dynamics [3,4].

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Mathematical modeling of gyrostat satellite dynamics using methods of computer algebra systems

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Dynamics of the gyrostat satellite in a circular orbit is investigated[1]. Computer algebra and numerical methods for determination of all equilibrium orientations of the gyrostat satellite in the orbital coordinate system with given gyrostatic torque and given principal central moments of inertia is proposed. The equilibrium orientations are determined by real roots of the system of nonlinear algebraic equations. Computer algebra method based on the algorithm for construction of the Groebner basis and the resultant concept for solving the problem is used.

Evolution of domains with fixed number of equilibria is investigated numerically in dependence of four dimensionless system parameters.

For each equilibrium orientation of the gyrostat satellite sufficient conditions of stability are obtained as a result of generalized energy integral analysis. The stability of the equilibrium orientations are analyzed numerically.

It is shown that the number of equilibria of the gyrostat satellite in general case is not less than 8 and no more than 24 and number of stable equilibria changes from 4 to 2. All calculations were implemented with the computer algebra systems Maple and Mathematica 8.0.

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Solving the hysteresis loop calculation problem for Josephson junction stacks

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A detailed investigation of the IVC breakpoint and the breakpoint region width gives important information concerning the peculiarities of stacks with a finite number of intrinsic Josephson junctions. In [1] IVC for a stack of n Josephson junctions is defined by a numerical solution of a system of n nonlinear differential equations. The numerical solution was obtained using a fourth-order Runge-Kutta scheme. Solving the Cauchy problem on the interval $[0, T_{max}]$ for different I values, we obtain IVC (graph $V(I)$) as a Hysteresis loop. On the back branch of the Hysteresis loop, near the breakpoint I_b, voltage $V(I)$ decreases to zero rapidly. The goal of this work is to accelerate the computation of the current-voltage characteristics. It was proved in [2] that in the case of periodic boundary conditions and non-periodic boundary conditions with $gamma = 0$, the IVC computation problem reduces to solving a single unique equation. For the solution of this equation with given initial data long time asymptotic formula was derived. $V(I)$ values found by using this formula are in a good agreement with numerical values up to a small vicinity of I_b. The following numerical-analytical method was suggested in [2]: the right branch of the Hysteresis loop and the back branch (not nearing some finite distance to I_b) are calculated using the asymptotic formula. The rest points $(I, V(I))$ of the Hysteresis loop are calculated numerically using the fourth-order Runge-Kutta scheme. This method was tested on Hysteresis loop calculations for a stack of 9 Josephson junctions. The results obtained are in a good agreement with numerical results, and the computation time was reduced more than five times. The question of choosing a change-over point from "analytical" to numerical calculation, when we have no results of numerical calculations, was open. In testing computations the change-over point was taken equal to $2I_b$. In [3] an equation, determining the approximate location of I_b, was obtained. We proved in [2] as well that in the case of non-periodic (with $gamma = 1$) boundary conditions the calculation of the current-voltage characteristic (IVC) for a stack of n intrinsic Josephson junctions reduces to solving a system of $[(n + 1)/2]$ non-linear differential equations instead of n original ones. This moment we succeeded to develop an algorithm determining the approximate value I_b and simultaneously to improve the mixed numerical-analytical algorithm of IVC

calculation for a stack of Josephson junctions developed in [2]. The efficiency of the improved algorithm is shown by the calculation of IVC for a stack of 19 intrinsic Josephson junctions. A good agreement with the results of numerical computations has been received. The computational time reduced more than 9 times. All calculations were performed using the REDUCE 3.8 system.

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Verification of Kuryshkin-Wodkiewicz mathematical model for quantum measurement

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Quantum mechanics was created as a theory able to explain a series of the experimental data not covered by the framework of classical physics. Conventional quantum mechanics connects the probability of quantum objects detection to the square-wave function independent of orientation, bandwidth and other parameters of the filter and the detector. To perform analysis of the experimental results of quantum objects observations we need a theoretical model

of quantum measurements. The Kuryshkin-Wodkiewicz model implements operational approach to quantum measurements and the principle of quantum estimation in the phase space representation. The Weyl-Kuryshkin quantization rule specifies measured quantum observables in the form of pseudo-differential operators as a function of the quantum states density matrix parameters of the measuring device. Recovered from the experimental spectral data, the parameters of the density matrix, and hence of the pseudo-differential operator in the framework of the Kuryshkin-Wodkiewicz model, allow predicting the probability of radiation transitions in order to verify the model.

Optimal regression model selection with least angle regression

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Optimal model selection is a crucial and difficult part of a successful data analysis. Selection model methods are computationally intensive and time consuming. Efron et al. [1] proposed Least Angle Regression (LARS), a computationally fast variable selection procedure based on pair wise correlations which is closely related to forward selection and LASSO regression procedures.

Nearly we presented some algorithms to construct a new modification of least angle regression method, which is based on a robust correlation estimates by extending one-dimensional H-estimators [2] to the bivariate one and than using bivariate M-estimators [3]. The main aim of our algorithms is the construction of the optimal range of most effective predictors from wide set of them, from which an optimal model can be selected.

In this talk we further explore the adopted models by applying them to the wide rows of real data sets and comparing their effectiveness.

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Application of the Fourier series for particle dynamics simulation in the periodic magnetic fields

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Proposed procedures originated in studies of synchrotron radiation properties in the cyclic accelerators. In this case for discrete magnetic systems there was a need to describe the continuous trajectory of charged particles. For this purpose the alternating field gradient or components of magnetic fields were expanded in the Fourier series. Then the transversal electron oscillations were characterized by the modified Hill equations. With the aim of determining of their solutions were used the Bogoliubov-Mitropolsky higher-order method and original technique of perturbation theory.

Computer model of a qubit

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The computer model of a qubit is constructed. We have considered a number of key experiments in physics of the quantum information: (i) distribution of values of quantum observables for a single qubit; (ii) correlation functions in a quantum singlet state of two qubits; (iii) Einstein-Podolsky-Rosen paradox; (iv) violation of Bell inequality; (v) quantum state teleportation; (vi) fidelity of teleportation. In all these cases the proposed model regularly reproduces results of quantum measurements without use of adjustable parametres.

The distributed monitoring system of a compute cluster and the state of the user tasks

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The article is devoted to the research of the author as part of the MpdRoot software for MPD / NICA project. The paper considers a distributed monitoring system of a compute cluster nodes and the state of the user tasks. Such monitoring can objectively evaluate the distribution of the load on the cluster nodes, and also shows what types of tasks are calculated, and how much time they take. The monitoring system has a web interface that integrates into existing MpdRoot software web site and allows evaluating the state of the cluster at the moment.

Simulation of the IRON OXIDES complexes magnetic field parameters for the biomedical applications[1]

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The iron oxide nano-complexes produced by living systems have a big potential in biomedicine, especially in the diagnostics of the pathological processes. In humans, it is mainly the iron storage proteins such as ferritin and hemosiderin, but also the magnetite nanoparticles, which have been found in the human brain tissue. Ferritin and hemosiderin are involved in the formation of the so called "iron-overloaded" disorders, such as cirrhosis, diabetes and heart disease [1]. Elevated levels of the magnetite nanoparticles are usually connected with the neurodegenerative processes in the human brain [2]. Magnetic properties of these particles make them "visible" by magnetic resonance imaging (MRI), so they have a potential to become a biomarker for the noninvasive diagnostics of the above mentioned disorders. However, there still remain the unresolved questions. The most important is, in what concentration and spatial distribution are they able to alter the MRI signal sufficiently for the detection by the clinical tomographs. We bring a simple simulation method, based on so called "Cube model" [3], which allows the calculation of the magnetic field parameters of the biogenic iron oxides complexes. This allows the theoretical determination of the minimal concentration and spatial distribution of the iron oxides still detectable by the MRI techniques. The nanoparticles magnetic field was calculated with use of the analytical expressions for the magnetic field of a current loop, adjusted to the cube particle [4]. We showed that only specific regions (thin, near-surface rings around the particles in the planes perpendicular to the direction of the particle magnetic moment) are able

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to affect the relaxation time of the protons and cause the desired MRI signal changes. Furthermore, we provide the theoretical analysis of the quantitative imaging feasibility in clinical practice.

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Multi-configurational time-dependent Hartree for bosons method: efficiency of the hybrid MPI&CUDA parallelization schemes

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To describe statics and highly non-equilibrium quantum dynamics of trapped ultra-cold atomic clouds one has to solve the time-dependent many-body Schrodinger equation (TDSE). The MCTDHB is a parallel OpenMP/MPI package [1-3] capable of solving TDSE numerically exactly [4]. To improve numerical efficiency of the package one has to explore different combination of the parallel technologies. The main goal of the present work is to include into the MCTDHB package novel hybrid parallel technologies combining multi-core CPU and GPU-accelerators. We have implemented the MPI+CUDA (MPI+PGI CUDA) parallelization schemes in the program modules where the Fast Fourier transform (FFT) algorithms are involved. In this report we show how efficiency of the parallelization depends on the dimension of the FFT grid and on the number of GPU used.

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Generalized recurrence relations and dimensional recurrences for Feynman integrals

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Theoretical predictions needed for comparison with experimental results obtained on the running LHC experiment as well as for the future experiments require evaluation of huge amounts of complicated Feynman diagrams. The most advanced techniques for calculating Feynman diagrams are based on recurrence relations. In the present talk detailed description and further development of the method of generalized recurrence relations proposed by the author in Ref. [1] is given. Two methods for deriving such relations are proposed. Explicit formulas of generalized recurrence relations for scalar integrals with arbitrary number of loops, arbitrary masses and external momenta are given. Explicit form of all these relations for arbitrary integral is determined by two Symanzik polynomials and their derivatives. Explicit formula for generating function for tensor integrals is given. A method for derivation of dimensional recurrence relations proposed in Ref. [1] described in detail. Application of the Laplace method for determining asymptotic behaviour of the integral needed for finding periodic function in the solution of dimensional recurrence relations is illustrated on several examples.

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Temperature map in power transformer: model and experimental data[1]

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Magnetic liquids or ferrofluids are new technological materials which are of great interest for applications. One from the application is the cooling and isolative medium in power transformer where the magnetoconvection effect is present. This work is devoted to the analyzing the cooling effect of transformer oil based magnetic fluid in 10 kW power transformer with power frequency 50 Hz. For analyzing the cooling effect of magnetic fluid, the finite element method was used and results were compared with the real experimental data collected from experiment on fully loaded transformer.

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Splines without diagonal matrices

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The question of basis functions is crucial in LS smoothing with splines. Nevertheless, the B-splines are local, in LS techniques [1-3] they are used in a global way. We show that B-splines are not the only splines that possess basis functions. We succeeded in deriving basis functions for clamped cubic splines uncovering of one of the Hermite splines' hidden properties.

The new basis functions can be used in both approximating and interpolating data points. In the case of the latter there is no need for solving three-diagonal matrices since the spline formula is given explicitly.

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Asymptotic solutions of boundary problems for singular perturbated infinite order differential equations

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The boundary problems for the singular perturbated infinite order differential equations are studied. Using the small parameter methods solutions for these problems are obtained. Using this approach the solutions of the boundary value problem for the one-dimensional relativistic Schrödinger equation with the quarkonium quasipotentials are built. The convergence of these solutions to the solutions of the boundary value problem for the non-relativistic Schrödinger equation with the same quasipotentials is shown. These results are compared with the solutions of the boundary value problem for the one-dimensional non-relativistic Schr?dinger equation with the quarkonium quasipotentials.

Modeling of surface patterning arising from the nonuniform evaporation of a colloidal film or droplet[1]

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When a colloidal film or sessile droplet desiccate on a hydrophilic substrate, non-uniform evaporation and surface tension produce a fluid flow. The solute in the drop is dragged to the contact line by this flow, where it accumulates,

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the deposit remains after complete evaporation of the liquid [1]. If the film is covered by a "mask" with holes, evaporation primarily occurs under the holes so that surface tension drives a flow of liquid to replenish this loss. The solid film after evaporation is a set of hills that match the locations of the holes [2]. In other situation, an obstacle placed above the film surface and solid film has a dip surrounded by a rim at the place below the obstacle [3].

The proposed model explains the redistribution of component in the film arising from the non-uniform evaporation under a mask or a disk. Calculations of spatial-temporal dynamics of volume fraction of the colloidal particles have been performed using the models described in details in [4].

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Numerical simulation of the hydrated electron formation[1]

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The polaron model considered in [1] has been modified for numerical simulation of the formation of the solvated electron from the initially delocalized state in a polar medium under action of subpicosecond laser. Numerical approach is based on the finite-difference scheme presented in [1]. Results of numerical simulation are discussed in comparison with experimental data [2] and theoretical estimations [3].

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About workgraphs, typical for representation of computable models in the network library

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The complexity of simulation models encourage to create network libraries of computable models with easy access to the models for the partially competent users.

For computable models and numerical methods on the basis of the reactive distributed systems with a graphic interface the concept and the architecture of network component-oriented information libraries are discussed. Calculation of modelling situations is driven by the events and workflow constructed by the user using components saved in library and their data [1].

Shown as an arithmetic expression is cast to the oriented graph of computing work, and then aggregated in a generalized workgraph. Examples of decomposition of the complex models into workgraphs of the components - domain concepts of the model are discussed. A method is described for the downward refinement of the components by subordinate worksubgraph and the method of conjugate refinement that allows to synthesize models. An example of the model driven by the finite difference method and the sweep method to recursive workgraph is discussed [2].

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Transient processes in the plasma flow in a diverging magnetic field[1]

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This problem relates to the possibility to create an effective rocket engine based on the acceleration of plasma in a magnetic field flux with a flow separation from the magnetic force lines of a plasma generator.

The idea is as follows [1]. If the magnetic field is trapped in a high-temperature plasma confined by transverse expansion pressure of the magnetic field, the magnetic field in a divergent field pressure will decrease faster than the plasma pressure. In the process of removing plasma clot at a considerable distance from the thruster pressure of the field will not be able to slow down and keep the plasma flow. As a result the rocket with the thruster will get a significant boost with a relatively small flow of the rapid plasma.

In the work 2d3v particle-in-cell method in cylindrical coordinates with realistic electron-proton mass ration is used in order two simulate plasma behavior in a diverging magnetic field. Magnetic reconnection is observed. Some quasi-stationary regimes are obtained.

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Solution of n-order Riccati equation and applications

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We present solutions of n-order Riccati equation in terms of generalized trigonometric functions. The summation formula for solutions is obtained. Connection with geometry and relativistic physics is presented.

Evaluation of parallel computations of Gröbner and involutive bases on the massive SMP computer[1]

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In previous papers two different approaches to parallelization of computation of Gröbner and involutive bases of polynomial systems with benchmarking on the 8-cores SMP computer were given: a reduction-level parallelism with coefficients of polynomials in $\mathbb{Z}$-ring [1] and a basis-level parallelism using modular basis computation and lifting [2]. In this work further development of this algorithms is described, benchmarking results and maximal speedup achieved on the massive 32-cores computer are presented, scalability differences of the algorithms are investigated.

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Interpolation functional polynomials for nonlinear ordinary differential operators[1]

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We consider the ordinary differential operators of the form

$$F(x) = f\left(t, x(t), x^{(1)}(t), x^{(2)}(t), ..., x^{(n)}(t)\right), \tag{1}$$

that are given on the space $C^{(n)}(T)$ continuously differentiable n times on $T \subseteq R$ functions $x(t)$, where the function $y = f(t, u_0, u_1, ..., u_n)$ of variables $t, u_0, u_1, ..., u_n$ is defined on a rectangle $\Omega = T \times T_0 \times T_1 \times \cdots \times T_n$, T_i are sets of the number line $(i = 0, 1, ..., n)$. Let the operator $F : C^{(n)}(T) \to Y$, where Y is a function space. Interpolation formulas of the Lagrangian and Hermite type for differential operator (1) have been constructed. Let $x_0(\tau)$ and $x_1(\tau)$ be the interpolation nodes, vectors $a(\tau) = (a_0(\tau), a_1(\tau), ..., a_n(\tau))$, $b(\tau) = (b_0(\tau), b_1(\tau), ..., b_n(\tau))$ are such that the difference $a_k(\tau)x_1(\tau) - b_k(\tau)x_0(\tau)$ is

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not equal to zero on $T = [a, b]$, and a function $g(\tau)$ $(\tau \in T)$ satisfies the condition $g(b) = 1$, $g(a) = 0$. The simplest example $g(\tau)$ may be the function $g(\tau) = \dfrac{\tau - a}{b - a}$. Here are linear interpolation formulas:

$$L_1(F; x) = F(x_0) +$$

$$+\frac{1}{n+1}\sum_{k=0}^{n}\int_T \frac{a_k(\tau)x^{(k)}(\tau) - b_k(\tau)x_0^{(k)}(\tau)}{a_k(\tau)x_1^{(k)}(\tau) - b_k(\tau)x_0^{(k)}(\tau)} \times d_\tau F\left[x_0(\cdot) + g(\tau)\left(x_1(\cdot) - x_0(\cdot)\right)\right],$$

$$L_1(F; x) = F(x_0) + \frac{F(x_1) - F(x_0)}{(n+1)(m+1)} S_{n,m}(x) + \int_0^1 \delta F[g(\cdot, \tau); h(\cdot)]d\tau,$$

where $x_0(t)$, $x_1(t)$ are the nodes of interpolation, t_i are fixed points of the segment T,

$$h(t) = x(t) - x_0(t) - \frac{x_1(t) - x_0(t)}{(n+1)(m+1)} S_{n,m}(x),$$

$$S_{n,m}(x) = \sum_{k,i=0}^{n,m} \frac{a_{ki}x^{(k)}(t_i) - b_{ki}x_0^{(k)}(t_i)}{a_{ki}x_1^{(k)}(t_i) - b_{ki}x_0^{(k)}(t_i)},$$

$g(\tau)$, $g(t, \tau)$, $a_k(\tau)$, $b_k(\tau)$ and a_{ki}, b_{ki} are given functions and numbers, m is fixed integer, Gateaux differential $\delta F[x; h] = \dfrac{\partial f}{\partial x}h(t) + \dfrac{\partial f}{\partial x'}h'(t) + \cdots + \dfrac{\partial f}{\partial x^{(n)}}h^{(n)}(t)$. A number of other interpolation formulas is given in [1].

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Complexes of localized states in ac-driven nonlinear Schrödinger equation and in double sine-Gordon equation[1]

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Complexes of localized states are numerically analyzed in two dynamical systems: externally-driven nonlinear Schrödinger equation (NLS) and disturbed double sine-Gordon equation (2SG). Numerical approach is based on numerical continuation of solutions of respective ordinary differential equations and linearized eigenvalue problems [1, 2, 3]. Multi-soliton complexes of ac-driven, damped NLS are investigated in the case of weak damping. Shown that two-soliton complexes in the undamped, small driving case can be stably travel with constant velocity. Properties of multi-fluxon solutions of 2SG are studied in dependence on parameter of the second harmonic contribution. Interconnection between coexisting constant, fluxon and multi-fluxon solutions is analysed.

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Propagation of information along the open spin-1/2 chains

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The quantum communication lines becomes one of the attractive areas of quantum information. There are many publications devoted to the problem of the state transfer along the spin-1/2 chain from the sender S to the receiver R under the different conditions: homogeneous chain [1], inhomogeneous chain [2,3] homogeneous chain in the inhomogeneous magnetic field [4]. Comparison of different methods of state transfer is represented in [5]. In general, this is a complicated procedure requiring the very accurate adjustment of the chain parameters. Here we propose to consider the transfer the information about state of sender S instead of the state transfer itself. By the information we mean the independent parameters in a density matrix describing the state of the sender S. If all these parameters may be uniquely reconstructed from the analysis of the state of the receiver R, then the information is completely transfered from S to R. Our algorithm is based on an evident remark that the information encoded into the state of the subsystem S of a quantum system initially (at t = 0) becomes distributed over the whole quantum system at $t > 0$ due to quantum interactions. Consequently, this information, in general, can be extracted, either completely or partially, from any subsystem of a quantum system. We suggest a method of extraction of information, which is based on the polarization measurements on the receiver R. After the state of the receiver R is defined, we have to solve a system of linear algebraic equations to define the original parameters of the sender S. If the above linear system is uniquely solvable, then the parameters of S may be uniquely determined and consequently the information is completely transfered. Otherwise the information is either partially transfered or does not transfered at all. We consider the spin-1/2 chains of three and four nodes and show that the complete information may be transfered almost at any instant (except for the finite number of instants), unlike the perfect (or high probability) state transfer. The later is possible only at fixed instants. This justifies the advantage of the quantum information transfer in comparison with the quantum state transfer. The basic results are published in [6].

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Моделирование случайных блужданий на обобщенном множестве Кантора[1]

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Предложен метод построения случайного блуждания на обобщенном множестве Кантора [1] с помощью случайных бинарных последовательностей конечной длины, изменением каждого элемента которых управляет конечная цепь Маркова с двумя состояниями. В простейшей схеме (в предположении о независимости элементов последовательности) с однородными цепями были получены выражения для математического ожидания и автокорреляционной функции случайного процесса. Также были рассмотрены схемы с неоднородными цепями и с "контекстно-зависимыми" последовательностями, где будущее значение каждого элемента определяется не только его текущим значением, но и текущими значениями окружающих его элементов. Показано, что рассмотренный метод тесно связан с методом IFS (iterated function system) [2] и позволяет конструировать случайные блуждания на более сложных фрактальных структурах, например, на треугольном множестве Серпинского.

Предложенный весьма простой и вместе с тем эффективный метод может быть использован в исследованиях процессов переноса на фрактальных структурах и феноменов т.н. "странной кинетики" [3].

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Unilamellar vesicles structure analysis using parallel Asynchronous Differential Evolution[1]

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The Separated Form Factors model (SFF) [1, 2] has been extended for analysis of structure of polydispersed population of unilamellar DMPC vesicles in 40% sucrose from the small angle synchrotron scattering (SAXS) data. The average radius and polydispersity of vesicles as well as parameters of internal structure of bilayer, have been determined by fitting to SAXS spectra.

The fitting problem requires the multidimensional (7–8 parameters) global minimization which is organized by means of the Asynchronous Differential Evolution (ADE) method [4, 5]. This approach is appropriate to solve multidimensional global minimization problems and allows effective parallel computer realization.

We show that parameters of vesicular system obtained in the frame of our SFF–ADE approach, are in reasonable agreement with previous estimations on the basis of small angle neutron scattering analysis [1, 2, 3]. Also we present results of methodical calculations demonstrating efficiency of our MPI-based parallel computer code.

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Higher-order accurate numerical solution of Burgers' equation

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This talk presents higher-order accurate finite-difference schemes for numerical solution of Burgers' equation which arises frequently in mathematical modelling used to solve problems in fluid dynamics. The accuracy of the proposed schemes is demonstrated by some test problems. The numerical results are found in good agreement with exact solutions. The schemes are very simple, so these are very easy to implement.

Approximation of polynomials on compact in R^3 polynomials of the best approximation in the L_2 lowest level in the system of symbolic mathematic MAPLE

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The report sets out the mathematical foundations of approximation polynomials on compact in R^3 polynomials of best approximation in the lower level of L_2. Developed and implemented a polynomial approximation algorithm for the perturbed ellipsoid lower degree polynomials. The algorithm is implemented as a program in the Maple symbolic mathematics: Mikheev S.A., Tsvetkov V.P., Zhuravlev V.V., Tsvetkov I. V. Approximation by polynomials of lower degree polynomials // certificate of state registration of computer software 2013610527, registered in the register of programs 09 January 2013 year.

Critical points and points of a bifurcation of the rotating magnetized Newtonian polytropic with $0.9 \leqslant n \leqslant 1.6$ index

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In this report, the presence of critical points and bifurcation points of rotating Newtonian polytropes with an index of $0.9 \leqslant n \leqslant 1.6$ has been shown for the first time. The symbolic-numerical calculation error in metric L_2 has reached the size of 10^{-5}order. The approximate analytical solution of the problem to the above mentioned accuracy has been set forth. The critical value of polytropic curve index $n = n_k = 1.54665$ has been calculated which is the highest one among the critical points and bifurcation points. Value n_k corresponds to the infinitely slow polytropic curve rotation. Furthermore, in

this paper, there have been predicted the presence of the period jump at the bifurcation point T_b and estimated the relative value of this jump $\Delta \mathrm{T}_b/\mathrm{T}_b \sim (\mathrm{B}_{0in}/(\sqrt{\mathrm{G}\rho_0}\mathrm{a}_1))^{4/3}$ (B_{0in}- characteristic value of an internalmagnetic field of a polytropes, G- gravitational constant, ρ_0- central density, a_1 - equatorial radius of a configuration).

Robust fitting for the estimation of hidden parameters in the experimental distributions on the plane

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The registration of two event characteristics, for example, e (energy) and t (time), gives a two-dimensional experimental distribution $A(e,t)$, where sometimes it is difficult, however, to extract the desired component, which could be adequate to a model $f(e,t,P)$, where P is the vector of parameters of interest.

A striking example of this situation is the determination of the scintillator irradiation time using a temporal autocorrelation spectrometer of delayed coincidences. In this case the $A(e,t)$ contains too many parts, conflicting with the model $f(e,t,P)$, and this greatly complicates the application of the standard data fitting technique.

We have used the robust fitting, which automatically suppresses the impact of elements of $A(e,t)$, inadequate to the model of f, by using an adaptive weight function.

A brief idea of this method can be described as follows. Let us, at least approximately, build the data $a(e,t)$ on the basis of $A(e,t)$, which can be divided into the 2 parts: $a_1(e,t)$ and $a_2(e,t)$, the first of which can serve for constructing the estimates of parameters P.

The least squares estimator is the minimization of the expression

$$F = \sum_{e,t} w(e,t)[a(e,t) - f(e,t,P)]^2 \qquad (5)$$

If we go to the generalized weights $w(e,t,P_0)$, using a priori information about the distribution $a_1(e,t)$ and, in particular, about the parameters P_0 (in iterative processes the estimates of the previous iterations), for example, by the formulas

$$w(e,t,P_0) = \begin{cases} 1/\|\sigma(e,t)\|^2 & \text{if } h(e,t) < c; \\ (1+\beta)/(\|\sigma(e,t)\|^2(h(e,t)/c)^2 + \beta)) & \text{else} \end{cases}$$

where σ is the statistical error of the data, $h(e,t) = a(e,t) - f(e,t,P_0)$, and c and β are the predefined constants, then minimization of (5) will give us a stable unbiased estimate of the vector P.

Anti-Frobenius algebras and quadratic Poisson brackets[1]

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In [1] Odesskii, Rubtsov and Sokolov considered a special class of linear and quadratic Poisson brackets related to ODE systems with matrix variables. Using these brackets, they generalized m-dimensional Manakov top $u_t = u^2v - uv^2$, where u and v are $m \times m$-matrices in independent variables, to the case of arbitrary set of $m \times m$-matrices $x_1, \ldots, x_N$. Quadratic Poisson brackets in question are of the form

$$\left\{x^{j_1}_{i_1,\alpha}, x^{j_2}_{i_2,\beta}\right\} = r^{\gamma\varepsilon}_{\alpha\beta} x^{j_2}_{i_1,\gamma} x^{j_1}_{i_2,\varepsilon},$$

where $x^j_{i,\alpha}$ are entries of the matrix x_α and

$$r^{\gamma\varepsilon}_{\alpha\beta} = -r^{\varepsilon\gamma}_{\beta\alpha},$$

$$r^{\lambda\sigma}_{\alpha\beta} r^{\mu\nu}_{\sigma\tau} + r^{\mu\sigma}_{\beta\tau} r^{\nu\lambda}_{\sigma\alpha} + r^{\nu\sigma}_{\tau\alpha} r^{\lambda\mu}_{\sigma\beta} = 0.$$

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These relations mean that tensor r is a constant solution of the associative Yang-Baxter equation. Such solutions up to equivalence are in one-to-one correspondence with exact representations of *anti-Frobenius algebras* up to isomorphism.

Let M be the proper divisor of N. We consider $N(N-M)$-dimensional anti-Frobenius algebras

$$\mathcal{A}_{N,M} = \{A \in \mathrm{Mat}_N \mid \sum_{i \equiv r \pmod M} a_{ij} = 0 \quad \forall\, r = 1, \ldots, M,\ \forall\, j = 1, \ldots, N\}$$

equipped with non-degenerate anti-symmetric bilinear form

$$(x, y) = \mathrm{tr}\,([x, y] \cdot \mathrm{diag}(\lambda_1, \ldots, \lambda_N))$$

for arbitrary pairwise distinct parameters λ_i. The special case $M = 1$ is equivalent to the construction from [1].

Using computer algebra system Sage [2], we obtained the formula for components of tensor r corresponding to $\mathcal{A}_{N,M}$. They are too huge to be presented here. With this formula one can construct corresponding quadratic Poisson brackets and non-abelian systems of ODEs using the approach of [1]. It turned out that only the case $M = 1$ considered in [1] leads to a new integrable system of ODEs.

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Reaction diffusion systems, autowaves, and their physics

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The physical mechanisms supporting propagation of nonlinear concentration autowaves of the activator in the active media with chemical reactions and diffusion are analyzed [1]. One often wrongly believes that movement of concentration autowave is supported by diffusion flux of the activator, which flows forward on a course of movement of the leading wave front and initiates the process of autocatalytic synthesis of the activator before the front: its concentration increases here rapidly, reorganizing the spatial profile of the autowave, which is shown as a spatial shift of the leading front in the direction of the diffusion flux. But such "explanation" faces paradox: it does not explain existence both the standing autowaves, which generate diffusion flux, and the autowaves moving against diffusion flux direction. To resolve this paradox, concepts of spatial production/destruction zones are introduced (into them the activator is synthesized/decayed), and integral powers of these zones are defined. In the case of one-dimensional reaction diffusion medium the general equations are deduced, which display that velocity and a direction of propagation of the leading front of an autowave are defined by imbalance of the production/destruction zones, instead of value and a direction of the diffusion flux generated by this front. Using equations mentioned, classical Zeldovich – Frank-Kamenetsky's formula for the velocity of autowave in the bistable reaction diffusion medium with cubic polynomial kinetic function is deduced in a new way.

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Nilpotents in the Clifford algebra of Euclidean 3-space and their intensional sense

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Within the framework of Space Algebra, the Clifford algebra Cl_3 generated by the three-dimensional Euclidean space E_3 over real numbers, a structure of nilpotents of index 2 is investigated [1, 2]. The general view of these elements is derived *ab init*, and their algebraic and geometric properties are revealed. The equivalence of action of the groups of phase transformations (U_1) and rotations (SO_3) on the nilpotents of index 2 is discovered: the phase transformations of the nilpotent, which are realized by its multiplications on the complex exponents, lead to its spatial rotations in E_3, and vice versa. It is proved that nilpotents of index 2 are the unique elements of Cl_3, for which the equivalence of action of the groups U_1 and SO_3 takes place; thus, this property of nilpotents is a characteristic one. The results obtained elucidate the geometry of vacuum solutions to the Maxwell equations without sources, which describe plane harmonic electromagnetic waves, the photons, with two types of helicity, and lead to the non-formal hypothesis that real physical space is at least a six-dimensional one: in the minimal case its basis consists of six linearly independent elements – three vectors and three bivectors generated by these base vectors.

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Modeling of phase dynamics of two parallel Josephson junctions stacks[1]

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The superconducting layers in the high-T_c anisotropic superconducting materials, as $Bi_2Sr_2CaCu_2O_8$ form a stack of coupled Josephson junctions [1]. It is interesting to consider for some applications the circuits which consist of two stacks of coupled N_1 and N_2 JJ in parallel connection. In the simplest case $N_1 = N_2 = 1$ this is the well-known superconducting quantum interference device (DC-SQUID) [2]. This device is used as a magnetometer to detect incredibly small magnetic fields [3].

We obtain the system of nonlinear differential equations, which describes phase dynamics of two parallel stacks of JJ in the framework of the CCJJ+DC model [4, 5]. Using the fourth order Runge – Kutta method we solve this system of equations and calculate the total current voltage characteristics (CVC). All currents and CVC for each stack are described in detail. We compare the CVC for the two parallel JJ stacks with two parallel single JJ.

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Second order finite volume scheme for Maxwell's equations with discontinuous dielectric permittivity on structured meshes

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A second order finite volume scheme on structured meshes is presented for numerical solution of Maxwell's equations with discontinuous dielectric permittivity. The scheme is based on approaches of Van Leer [1], Lax Wendroff[2], and Lebedev [3] and employs a special technique for gradient calculation near dielectric permittivity discontinuities. Unlike the previous approach [4] the scheme employs structured meshes. Scheme was tested for problems with linear and curvilinear discontinuities. Test results support second order of approximation in space and time.

Proposed scheme was successfully applied to modeling photonic crystal devices [5]. For photonic waveguide with a bend reflection and transmission coefficients were obtained for different bend configurations. A number of configurations and frequencies with zero reflection coefficients were identified.

The use of structured meshes makes the scheme a viable alternative to the finite difference time domain method [6] and leads to easy parallelization using OpenMP or MPI.

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