Book of Abstracts

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Preface

Program of the conference "Computer Simulations in Physics and beyond" is concentrated on the analysis and discussion of research and activity in computer simulations which generally meets on the boundary of scientific branches, i.e. which are multidisciplinary research. Multidisciplinary is essential of the knowledge evolution, in our case it is connected with the knowledge outcome due to the using computer as research tool. It is clear that it is possible only by combination of knowledge from researcher with different scientific background and different competence. Development of computations demonstrates that computational algorithms and methods of simulations could not be related to some particular research area and is rather lies on the cross-border. Accordingly, program committee members reflect that rainbow of our program and their expertise in informatics, applied mathematics, statistical physics, computational physics, quantum computing, bioinformatics, quantum chemistry, etc.

Conference program are based also on the leading activity of Russian researchers in computing, physics, mathematics, and biology.

Important feature of the conference is a large number of young researchers and students, with poster and oral presentations.

Scientific program is consisting with 4 types of presentation.

1. Plenary talks. Invited plenary speakers, leading researches in the field, will give plenary talks. Talks would be of review type, with focus on the computational methods and results in the field of research. Plenary talks are scheduled for each day before lunch and lasts 40 minutes.

2. Invited talks at parallel sections. Invited 30 minutes talks are the basis for sectional work.

3. Contributed talks of 20 minutes at parallel sections. Selection for contributed talks provided by the international program committee. We plan combine program into 12 sections, with 4-5 sections running in parallel at each afternoon. We keep at least one slot for young researchers in each section.

4. Poster contribution. Each participant is eligible for at least poster presentation. Best poster prize will be awarded for the best poster by young researcher.

Topics of parallel sections
1. Simulations in Statistical Physics
2. Physics and mechanics of polymers
3. Space research: simulations and big data
4. Methods and software for simulations in research and engineering (hydrodynamics, aerodynamics, etc.)
5. Simulation of brain activity

6. Bioinformatics, methods and algorithms in genome research
7. Methods and algorithms in drug development
8. Simulations in material science
9. Simulation and analysis of social networks
10. Simulation and analysis of technical networks (roads, urban transportation, data networks, etc.)
11. Algorithms, methods, and tools with properties of scalability and enhanced parallel simulations
12. Informatics and education

From Particle Condensation to Polymer Aggregation

W. Janke, J. Zierenberg, and P. Schierz

Abstract:

A new simulation method to study temperature-driven droplet formation is discussed that allows a shape-free determination of free-energy barriers [1]. Combined with theoretical considerations for nucleation in particle systems, this leads to finite-size scaling predictions for the barrier at fixed density. Using parallelized multicanonical Monte Carlo computer simulations [2], this approach is first validated for a Lennard-Jones particle gas and then generalized to bead-spring polymers. Our results suggest an analogy of polymer aggregation with particle condensation, when the macromolecules are interpreted as extended particles. The talk concludes with a brief comment on the role of kinetic energy [3], which is commonly neglected in Monte Carlo simulations.

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Transport in drying sessile droplets

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In this talk, we review some of the recent developments in the studies of evaporation of liquid droplets of capillary size placed on a solid substrate, such as methods for suppression of the coffee ring effect and studies of hydrothermal waves. We have studied Marangoni convection induced by thermal conduction in the drop and the substrate by means of detailed numerical calculations. The convection is demonstrated to be able to result not only in a single vortex, but also in two or three vortices, depending on the ratio of substrate to fluid thermal conductivities, on the substrate thickness and the contact angle. The detailed description of the fluid flows is presented for a wide range of parameters.

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Dynamic Computation of Dielectric Effects in Self-Assembly and Active Matter

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The ability of matter to self-organize in complex dynamic structures is increasingly used to generate new, active materials. Progress in this field critically depends on the predictive capabilities of reliable and efficient computer simulation strategies. We have recently developed such methodologies for the coupling of dielectric solvers with particle-based simulations, making possible dynamic simulations that fully incorporate self-consistently calculated polarization charges. I will introduce our approach and discuss how the impact of these developments ranges from the prediction and control of colloidal and nanoscale self-assembly and aggregation to the understanding of dynamical properties of self-propelled particles that form the basic building blocks of active matter.

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The study of the effects of sea-spray drops on the marine atmospheric boundary layer by direct numerical simulation

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Detailed knowledge of the interaction of wind with surface water waves is necessary for correct parameterization of turbulent exchange at the air-sea interface in prognostic models. At sufficiently strong winds, sea-spray-generated droplets interfere with the wind-waves interaction. The results of field experiments and laboratory measurements show that mass fraction of air-borne spume water droplets increases with the wind speed and their impact on the carrier air-flow may become significant. Of special interest is the influence of sea spray on momentum and sensible and latent heat exchange between the upper ocean and atmosphere which is crucial for our understanding of conditions favorable for the development of anomalous weather phenomena such as tropical hurricanes and polar lows. So far, the effects of sea spray on the atmospheric marine boundary layer have been studied mostly by phenomenological modeling. Numerical modeling was mainly concerned with Lagrangian dynamics of spray drops in a wind flow with prescribed properties of turbulent fluctuations. The objective of the present study is to elucidate possible effects of sea spray on the momentum, heat and moisture transfer in marine boundary layer under strong wind-forcing conditions by performing direct numerical simulation (DNS) of turbulent, droplet-laden air-flow over a waved water surface. Three-dimensional, turbulent Couette air-flow is considered in DNS as a model of a constant-flux layer in the atmospheric surface layer. Two-dimensional stationary waves at the water surface are prescribed and assumed to be unaffected by the air-flow and/or droplets. Droplets are tracked in a Lagrangian framework, and their impact on the carrier flow is modeled with the use of a point-force approximation. We take into account both momentum and sensible and latent heat exchange between the drops and the surrounding air flow. The results show that drops dynamics and their impact on the carrier air-flow is controlled by many factors including drops velocity at injection, drops gravitational settling velocity, surface wave slope, bulk relative humidity and temperature of the atmospheric boundary layer as compared to the sea surface conditions.

This work is supported by RFBR (Nos. 15-35-20953, 16-55-52025, 16-05-00839, 17-05-007317) and by the Russian Science Foundation (Nos. 14-17-00667, 15-17-20009).

Advances in Theory and Practice of Tensor Decompositions Using Low Rank Matrices

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Numerical data are frequently organized as d-dimensional matrices, also called tensors. However, only small values of d are allowed if we need to keep this data in a computer memory. In the case of many dimensions, special representation formats are crucial and it looks natural to try the so called tensor decompositions. In the recent decade, the known tensor decompostions have been considerably revisited and the two of them appeared and are now recognized as the most adequate and useful tools for numerical analysis. These two are the Tensor-Train and Hierarchical-Tucker decompositions. Both are intrinsically related with low-rank matrices associated with a given tensor. In the talk, we expound the role of low-rank matrices for the construction of efficient numerical algorithms and consider possible developments of the idea of cross approximation that proved to be very fruitful for matrices and then has been successfully extended over to tensors. The nice property of the approach is that we construct the approximation using only a small portionof the data.

The idea of cross approximation is substantiated by the maximal volume concept for low-rank approximation of matrices and related with the classic problem of choosing a "good" basis from a given set or vectors. We discuss possible advantages of using "good" frames and what it may give for better work with tensors.

We also consider how these tools facilitate some new approaches to solving numerical problems in several application areas, such as drug design, thin optical coatings, coagulation and fragmentation of particles, identification of a model parameters etc.

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Monte Carlo methods for massively parallel architectures

M. Weigel

September 29, 2017

While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so *serial* code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. Monte Carlo methods based on Markov chains are intrinsically serial and hence cannot be straightforwardly parallelized. For systems with short-range interactions, it it is possible to use domain decompositions to update several degrees of freedom simultaneously. A complementary approach simulates several chains in parallel, be it at different temperatures such as in replica-exchange Monte Carlo or at the same temperature by simply pooling the statistics from independent runs. I give an overview of parallel implementations of Monte Carlo methods in statistical physics and, in particular, focus on two especially promising approaches: the first is a parallel variant of the multicanonical simulation method that uses independent walkers to speed up the convergence and shows close to perfect scaling up to 10^5 threads. The second approach is a sequential Monte Carlo method known as population annealing, that simulates a large population of configurations at the same temperature and then uses resampling and successive cooling to propagate the population. This approach is particularly suitable for parallel computing, and I present an efficient GPU implementation. A number of improvements turn this approach into a fully adaptive algorithm for the simulation of systems with complex free-energy landscapes.

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Hierarchical modeling of turbulent flows

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Since the inception of Computational Fluid Dynamics, turbulence modeling and numerical methods evolved as two separate fields of research with the perception that once a turbulence model is developed, any suitable computational approach can be used for the numerical simulations of the model. Latest advancements in wavelet-based numerical methodologies for the solution of partial differential equations, combined with the unique properties of wavelet analysis to unambiguously identify and isolate localized dynamically dominant flow structures, made it possible to develop a cardinally different framework for modeling and simulation of turbulent flows with the tight integration of the numerics and physics-based modeling. The integration is achieved by combining spatially and temporally varying wavelet thresholding with hierarchical wavelet-based turbulence modeling. The resulting approach provides automatic smooth transition from directly resolving all flow physics to capturing only the energetic/coherent structures, leading to a dynamically adaptive variable fidelity approach. The self-regulating continuous switch between different fidelity regimes is accomplished through spatiotemporal variation of the wavelet threshold and two-way feedback mechanism between the modeled dissipation and the local grid resolution. This defines a new concept of model-refinement. The ability of the proposed methodology to capture the flow-physics at the desired level of fidelity is demonstrated for the benchmark problem where the fidelity of turbulence simulation, measured by the ratio of the SGS and total dissipations, automatically adjusts to time-varying user prescribed levels. Finally, the implementation of the proposed model-refinement concept within classical LES methodology and possible feedback mechanism to incorporate a filter-width/model adaptation, preferably coupled with adaptation of the numerical resolution, are also discussed.

The out-of-equilibrium landscape of neural networks learning algorithms: from driven stochastic processes to quantum annealing.

R.Zecchina
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Abstract:

Training deep neural networks is a highly non-convex problem which however is often solved in practice by variants of Stochastic Gradient Descent.

In order to shed light on this phenomenon, we have developed a large deviation analysis based on a local entropy measure which has revealed the existence of subdominant and extremely dense regions of optimal solutions that have a number of highly desirable properties. They are wide minima with good generalization properties. The analysis allowed us to develop a number of novel stochastic algorithms and to find a fundamental connection with quantum annealing. We will show that in spite of the fact that the energy landscape is exponentially dominated by local minima that trap classical thermal annealers, quantum annealing converges efficiently to subdominant dense regions of optimal solutions. This is a concrete example of exponential quantum vs thermal speed up.

SIMULATION OF THE DIFFRACTION LIMITED GAUSSIAN AND VORTEX ILLUMINATIONS OF SUPPORTED METALLIC FILMS

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(Dated: May 31, 2017)

Nanoscale motion of film on dielectric substrate driven by energy absorption from a femtosecond laser pulse produces redistribution of mass of the film and results in formation of frozen surface structures [1-4] and shocks [5]. We consider the tight focused optical pulses of different radially distributed intensity from the Gaussian shape (when absorbed energy has a maximum in the center) to the shape corresponding to the vortex pulses (when absorbed energy has a minimum =0 in the center). Our approach combines two-temperature hydrodynamics codes together with molecular dynamics code. The molecular dynamics code is based on Voronoi decomposition of mass. The Monte-Carlo description of electron heat conductivity added to the molecular dynamics package allows us to include real values of large and thermally important conductivity of metals. Conductive heating and after that cooling of matter cause melting and later recrystallization of a film. We simulate dynamics of solids (film, substrate) together with hydrodynamics of liquid (film, substrate) separated by the first order phase transformation zones.

Our approach includes all underlying physical processes associated with laser-induced energy absorption, electron-ion energy exchange, thermal conduction, acoustic relaxation and hydrodynamic flows. Physical model is based on separation of "slow" and "fast" processes. Hybrid calculations use two-temperature hydrodynamics, scalable molecular-dynamics simulations, and a semi-analytical thin-shell model. These calculations provide accurate predictions of the final nanoscale solidified morphologies.

Simulations of femtosecond laser action on films is necessary because they are linked to a promising technologies. Among them are: processing thin-film transistors, scribing thin-film solar cells, ablative fabrication and light-induced forward transfer (LIFT)-printing of advanced plasmonic and dielectric nanophotonic metasurfaces and circuits. In comparison to subnanosecond laser pulses, the ultrashort ones are broadly used during such precise ablation, ensuring an ultimate spatial resolution.

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Electron tunneling lifetime in atomic systems, a projected Green's function method

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Atoms exposed to strong laser field can lose electrons via the process of tunneling or multi-photon ionization. Recent progress in attosecond technology allows detailed measurement of these processes. Complementary theoretical calculations of model systems are necessary to help reveal the mechanism of an electron to tunnel through a barrier. In this work, we adopt a projected Green's function (PGF) method for the calculation of the tunneling lifetime of an electron escaping from some small atoms. The method has been used in the past to calculate the tunneling lifetime of an electron in quantum wells. This method allows us to evaluate the tunneling lifetime for a specific barrier width in a very straightforward way. Results of calculated electron tunneling lifetime in model systems such as quantum dot (QD) are shown to be comparable with other theoretical studies. Based on this, we have been able to obtain the tunneling lifetime of the electron escaping from hydrogen, helium, neon, argon atoms under electric field.

Superconducting Nanowire Single-Photon Detector as a Key Element for Quantum Photonic Integrated Circuits

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Currently, many physical systems are studied for the realization of qubits including superconducting circuits, trapped ions and atoms, quantum dots, color centers in a solid and photons. Here after short introduction we focus on the last item in the list - photons. Due to the fact, that photons interact weakly with an optically transparent medium, do not interact with each other, have several degrees of freedom for encoding of quantum information as well as have a fast propagation speed, the photons are the best choice for creation a quantum networks. However, while the manipulation of individual photons did not cause any difficulties, the creation of two-, three- and more deterministic qubit gates require strong nonlinear interaction between photons. In this case, the advantages of the photons are transformed to their shortcomings and for a long time limited the use of photons as qubits.

Fortunately, Knill, Laflamme and Milburn (KLM) proposed the concept of linear optical quantum computing (LOQC), allowing you to create non-deterministic gates using photons, linear optical elements and detectors. Despite the fact that the implementation of the KLM-protocol is possible in free space, the need for a large number of optical components and their precise configuration requires the more complex solutions. Due to a number of advantages, such as scalability, small footprint, low weight, no need for optical alignment as well as a power consumption and CMOS-compatibility, quantum photonic integrated circuits (QPICs) can successfully solve this problem. The most popular material platforms for QPICs realization are silicon, gallium arsenide, and polycrystalline diamond. Each platform has its own advantages and disadvantages and is characterized by its degree of development. Nevertheless, all of these platforms have the fundamental blocks that require combining on-chip, such as single photon source, linear optical elements and single-photon detectors. In the presentation, I'm going to talk about operation principles, a history of development as well as the latest success of the most promising approach for QPICs realization, based on hybrid nanophotonic-superconductor devices. The realization of large scale QPICs, can produce a profound impact on science and technology, material engineering, as well as quantum information processing including quantum computing, simulation and metrology.

Operator-difference method for astrophysical MHD problems.

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We represent some features of the application of completely conservative Lagrangian operator-difference numerical scheme on triangular gird of variable structure to the simulation of the magnetohydrodynamical(MHD) astrophysical problems. The application of the Lagrangian grid requires its remapping during the evolution of the fluid flow. There are different ways of interpolation of the grid functions on a remapped grid. We discuss in detail the procedure of conservative remapping of grid functions during grid reconstruction procedure. The scheme described in the paper gave us possibility to simulate different astrophysical problems.

Phase transitions in evolutionary space games

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We study the dynamics of a space evolutionary game based on the prisoners' dilemma. The game features a series of sharp transitions between several regimes, characterized by abrupt changes in the densities of the components and non-trivial geometric rearrangements of the game field. We investigate critical properties of the resulting phase transitions and discuss the geometric properties of the emergent interfaces between components.

Relaxation Oscillations of the Repressilator Model

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The study of genetic oscillators is of interest, because they are simplified models of key biological processes, such as the cellular cycle and the circadian rhythm. The simplest genetic oscillator called a repressilator consists of three components A_j, $j = 1, 2, 3$. Its distinctive feature is that the component A_3 suppresses the synthesis of A_2, the component A_2 suppresses the synthesis of A_1, and the component A_1, closing the cycle, suppresses the synthesis of A_3. Further each component of the oscillator is a composition of matrix ribonucleic acid (mRNA) of concentration m_j and protein of concentration p_j. The evolution in time of these concentrations is described by the system

$$\dot{m}_j = -m_j + \frac{\alpha}{1 + p_{j+1}^{\gamma}} + \alpha_0,\ \dot{p}_j = \varepsilon(m_j - p_j), \quad j = 1, 2, 3,\ p_4 = p_1, \quad (1)$$

where $\alpha, \alpha_0, \gamma, \varepsilon$ are positive parameters.

As a rule, this model is studied under the assumptions of the smallness of ε and α_0. In this case, replacing $\varepsilon t \to t$ and discarding the parameter α_0, one obtains a singularly perturbed system, to which the well-known Tikhonov reduction principle is applied. The reduction procedure results in the following system:

$$\dot{p}_j = -p_j + \frac{\alpha}{1 + p_{j+1}^{\gamma}}, \quad j = 1, 2, 3, \quad p_4 = p_1. \quad (2)$$

For a fixed $\gamma > 2$ and for $\alpha \ll 1$ we consider the existence, asymptotics, and stability of the self-symmetric cycle (invariant with respect to the cyclic permutation of the coordinates)

$$(p_1, p_2, p_3) = (p(t), p(t + h), p(t + 2h)), \quad (3)$$

where $h > 0$ is the phase shift, and $p(t)$ is periodic with period $T = 3h$.

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Distributed time synchronization algorithms and opinion dynamics

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Abstract

We propose new deterministic and stochastic models for synchronization of clocks in nodes of distributed networks. An external accurate time server is used to ensure convergence of the node clocks to the exact time. These systems have much in common with mathematical models of opinion dynamics in large multi-agent networks. There is a direct analogy between the "time server/node clocks" pair in asynchronous networks and the "leader/follower" pair in the context of social network models. In deterministic models the internal synchronization can be achieved by applying some of special linear iterative procedures called agreement algorithms or network consensus algorithms. Stochastic models, in the presence of random noise in nodes, are more realistic but their longtime behavior is more complicated. It appears that the analysis of proposed models brings us to a chain of interesting problems related to underlying interaction graphs and matrices as well as to stochastic processes describing evolution of random errors in the network nodes.

Keywords: leader-follower consensus, switching graph topology, agreement algorithm, graph spectra

Method for detecting data synchronization errors in distributed information systems

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The article offers a generalized mathematical model of a distributed information systems (DIS). The main objects of the constructed model are:
1. Oriented connected graph ***Γ (N, G, B***) of an arbitrary topology with no cycles.

2. The set of nodes ***N (I, V, C***), each of which is characterized by the set of ***I*** - information objects that are used in this node, the set of ***V*** - version numbers of these objects in the node and ***C*** - the events of the change of the version numbers of each object.

3. The set of "green" arcs ***G (i, L, S, λ)*** that correspond to the channels for transfer of object changes, where ***i*** is the object whose changes are transmitted, ***L*** is the channel latency (i.e., the time required to transmit the change block minus the time required to transmit each individual change), ***S -*** the time of transmission of one change, ***λ*** is a random variable that determines the time that elapses since the first new version number of the object i appeared after the previous sending, until all the new versions begin to be transmitted along the green arc. That is, this random variable determines the time during which new versions that are included in one change block accumulate.

4. The set of “blue” arcs ***B (I, S, λ)*** that correspond to the channels of current information transmission, where ***I*** is the set of objects participating in the data transfer, ***S*** is the data transmission time, ***λ*** is the random event flow of the new transmitted data packet .

Subject to random event streams and transmission delays assigned to green arcs, new version numbers of objects appear in the model nodes and are copied to all nodes associated with the node of the original

appearance of the new version over time. At the same time on the blue arcs there are forwarding of the current data, at times, determined by the streams of random events. All the random event streams in the model and the random variables are considered independent of each other.
Based on this model, the problem was formulated to detect situations when a data package sent via the blue channel arrives at the receiving node earlier than the receiving node on the green arcs will deliver all versions of the object that were in the sending node at the time of sending. As a result, the message will not be correctly processed by the receiving party. This situation was called “The situation of late update”.

The following is an analytical solution to the problem of calculating the probability of a delayed update situation, in the event that object changes are transmitted immediately after they occur. Let the flow of occurrence of changes and sending of messages be the Poisson point process, and all nodes that are connected by blue arcs are also connected to the blue green arcs through which all objects that participate in the generation of current data transmitted through the blue arcs are updated. The graph of ***G*** is not It contains cycles of green arcs that update the same objects.

Under these conditions, the probability of the DIS running smoothly during the lifetime of T_0 is calculated by formula (1)

(1)
Where C is the information object, i is the index of the graph node, is the total flux density of the update events of the object C in node i, taking into account the updates coming from other nodes, j are the indices of the blue arcs originating from the node i nodes, - the density of the flow of events of the transmission of current data along the j-th arc. - the so-called vulnerability interval after updating the object C in node i during which data can be sent to node j that will cause the situation of a delayed update; finally, this number is known Greater than the number of updates to object C Data on the j-th arc - the so-called “vulnerability interval” after updating the object C in the node i during which data can be sent to the node j that will cause the situation of the late update. Finally, this

number is certainly greater than the number of updates of the object C, which can occur at node i. that is often known to the DIS designer at the designing phase of the system.

Then an analytical solution of the problem is carried out for the case when the delay between the occurrence of a new change and the sending of a block of changes along the green arc is determined by a random variable with exponential distribution while all other conditions are preserved. The solution obtained is substantially more complicated than the above, and its practical application will require approximating the exact solution by numerical methods. Hence, it is concluded that the simulation method can be more productive in solving the problem of calculating the probability of the uninterrupted operation of a distributed information systems in the general case, rather than searching for a general analytical solution.

Computer simulation was conducted in Matlab and confirmed the adequacy and efficiency of the proposed method.

COMPUTATIONAL ASPECTS OF THE WAVE DISTRIBUTION PROBLEM IN THE LOGISTIC EQUATION WITH SPATIAL DEVIATION

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Keywords: logistic equation, Fisher-Kolmogorov equation, diffusion, spatial deviation, numerical analysis

The most common form of logistic equation that accounts the dependency from time and spatial shifts was proposed by Gourley and Britton:

$$\frac{\partial u(t,x)}{\partial t} = \Delta u(t,x) + u(t,x)[1 + \alpha u(t,x) - (1-\alpha)(g * u)(t,x)],$$

where convolution $(g * u)(t,x) = \int_{-\infty}^{t}\int_{\Omega} g(t-\tau, x-y)u(\tau,y)dyd\tau$. If we take delta-function in the integral and move focusing point by time or spatial axis we may get equation with delay or equation with spatial deviation. We considered the process of density wave propagation in a logistic equation with diffusion (Fisher-Kolmogorov equation) and spatial deviation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u\big(1 - u(t, x-y)\big).$$

Here $u(t,x)$ is a solution, which is a population density of FK-problem at time $t > 0$ in some point x of a habitat; $y > 0$ is spatial deviation. A research of qualitative behavior of solutions of Fisher-Kolmogorov equation starts with the analysis of the wave equation profile, for which the conditions of appearance of oscillatory regimes are found. The second problem was the analysis of Fisher-Kolmogorov equation with periodic boundary conditions. We studied the stability loss problem of a spatially homogeneous equilibrium state and found spatially inhomogeneous oscillatory regimes branching from it. The last part of the research contains the results of a large numerical experiment for this equation in the case of an unbounded x domain. Numerical analysis was performed at the cluster of massive and parallel computations with the use of the OpenMP parallel computing technology. A numerical analysis of the wave propagation process showed that for sufficiently small values of the spatial deviation, this equation has solutions close to the solutions of the standard Fisher-Kolmogorov equation. At first the increase of the deviation parameter leads to the appearance of a damped oscillatory component in the spatial distribution of the solution. Further growth of this parameter leads to the destruction of the traveling wave. This is expressed by the fact that undamped in time and propagated slowly along space oscillations are close to the solutions of the corresponding boundary-value problem with periodic boundary conditions in the propagation wave region opposite to the direction of deviation. Finally, if the value of deviation is sufficiently large, then intense spatiotemporal oscillations are observed throughout the wave propagation region. Also we got some interesting analytical results for numerical experiments in case of periodic boundary conditions related with computential artifacts.

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Electromagnetic simulation of thread Peano antennas created by Context-free Grammar language.

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Our goal is to create thin films of hard electronic materials bonded by elastomers to enable unusual mechanics with important implications in stretchable devices. Therefore, we start by studying the electromagnetic field on fractals for thread antennas as a first step. This paper introduces a complete analysis on recursive level three (as an example) of thread Peano antennas first reported in the literature, since all possible feeding points in the curve are studied. We intend to fully assess the main features of these type of topology for any material. This model was mostly developed using Matlab and Phyton. The characterization in terms of impedance, VSWR, return loss and directivity are shown. The remaining features follow straightforward. Details on the antenna design, numerical results and applications are presented and discussed.

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APPLICATION OF GRID-CHARACTERISTIC METHOD TO SOME SEISMIC EXPLORATION PROBLEMS IN THE ARCTIC

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Abstruct. The aim of this work is simulation of wave propagation in the Arctic with the presence of different ice structures, using high-performance computing. In the given report grid-characteristic method is applied, which provides correctly describing the contact and boundary conditions.
Key words: numerical modeling, Arctic, seismic prospecting, grid-characteristic method, ice ridges, ice field.

Introduction

The question of developing the Arctic in Russia is of current importance as there are eight hydrocarbon fields, and their supplies are estimated approximately 2,7 trillion $м^3$. The considerable barrier on way of oil extraction in north seas is presence of different ice formations, particularly, ice ridges, icebergs. One of the main stages of planning geological survey works is mathematical modeling, that allows significantly bring down the cost of carrying out seismic exploration. In this very work numerical experiments on solving problems of seismic exploration in the conditions of the Arctic shelf were carried out.d then applied to calculate the fluxes in the finite volume discretization of the governing equations.

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Multiscale simulation of point defects behavior in nuclear fuels: uranium dioxide and uranium nitride

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Defects and diffusion are key concepts at description of nuclear fuels behavior at thermal and radiation impacts. In this work, we perform the complex study of point defects behavior for two nuclear fuels: uranium dioxide and uranium nitride. We use combination of several methods: *ab initio* calculations; molecular dynamics simulations with a new interatomic potential; thermodynamic model. The results of atomistic simulation and thermodynamic modeling allow to estimate diffusivity and concentrations of point defects for uranium dioxide and uranium nitride (including compositions different from the stoichiometric). The developed model allows us to evaluate several characteristics important for nuclear fuel description: (1) the diffusivities of xenon atom; (2) the change in thermal capacity; (3) the dependence of partial pressure (nitrogen pressure for UN or oxygen pressure for UO2) on composition and temperature. In addition, the role of defects diffusion in sintering and decomposition processes are discussed.

The investigation of the recrystallization process in the Zr-Nb alloys using atomistic simulations

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The Zr–Nb alloys are widely used in the development of modern structural materials. Thus, the alloys based on the hcp-zirconium with the Nb concentration about 1–2.5%, are one of the main materials for the manufacture of structural elements of the Russian nuclear reactors and the bcc-Ti-Zr–Nb alloys with the Zr fraction of 60–80% find applications in problems of biomedical materials. From the biomedical point, the advantage of such alloys consists in that, firstly, they are not very toxic for a human organism, and, secondly, have plastic properties close to the bone tissue. The mechanical and plastic properties of the alloy still need to be investigated, due to the variety of possible metastable transitions. It is known, that zirconium-niobium alloys can be transformed into a nanostructured state, which means that the characteristic grain size reduces to the value of 10 to 100 nm. Such a structure makes different phenomena possible at thermal, deformation, radiation and other exposures. Recrystallization is the process of the growth of average grain size by reducing some of the grains and growth of others. In general, the average grain size at a given temperature is influenced by the following factors: concentration of the component of the alloy, the initial grain size, heating rate, and voltage, which is alloy.

In our work the recrystallization is studied using molecular dynamics computer simulations. The used potential was developed in our laboratory [D. Smirnova, S. Starikov, An interatomic potential for simulation of Zr-Nb system // Computational Materials Science (2017)]. For the bcc-alloys of the Zr-Nb, the contents of the Nb are varied from 10 to 40%, for hcp—from 1 to 6%. It is known that the the grain migration rate is connected with the energy of the grain migration according to Arrhenius. Paying attention that the migration is driven by the curvature of the surface, it is possible to estimate the energy of gran migration. Firstly, the speed of the grain migration is calculated as a rate of the decrease of the average grain radius. Secondly, using the Arrhenius equation and the temperature dependence of the velocity of grain migration, it is possible to estimate the activation energy of grain migration. So, in our work we have obtained the energy of the grains' edge migration and the dependencies of the average grain size from time. The energy of grain migration, which we have obtained, is less by one order than in experiment. But it is common problem for all computer approaches and it is not clear, which factors cause such difference. At the same time, the process of grain growth can be divided at three stages, each of which must be described by its own equation. And the calculated energy depends on the way we define these stages. So, this may be the reason for such difference. Another important thing, which must be taken into account, is how the heating rate of the sample affects the temperature of recrystallization and the stages of the process. Nevertheless, the obtained values can be the evidence for the fact that the previous computer simulations are reliable and can be used for the further investigation of the mechanical properties of the alloy.

Computational Molecular Modeling of Aqueous Interfaces for Environmental and Materials Science Applications

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Molecular-level knowledge of the thermodynamic, structural, and transport properties of nano-confined water and aqueous interfaces with various materials is crucial for quantitative understanding and prediction of many natural and industrial processes, including mineral weathering, geological carbon sequestration, water desalination, geological nuclear waste storage, cement chemistry, fuel cell technology, etc. Computational molecular modeling is capable of significantly complementing the experimental investigations of such systems and can provide invaluable atomic-scale picture of the materials and processes involved, leading to a greatly improved understanding of the specific effects of the substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined aqueous solutions.

However, atomic-scale simulations are often quite challenging for many of such systems (clays, cementitious materials, etc.), because their crystal structure and atomic composition are usually not well defined and often characterized by a significant degree of structural and compositional disorder. ClayFF was originally developed in response to a strong need for a robust and flexible force field for classical molecular simulations of such interfaces and their interactions with organic and bio- molecules in aqueous environment [1]. This talk will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of these complex systems, focusing on the most recent MD simulation results on clay-related and cement-related materials, and on the most recent improvements of the original ClayFF parameterization for better agreement with experiments [2-4].

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Numerical Simulation of 2D-crystals Structures with Optimization Methods

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In this paper we present a new model of 2D-crystals. In this model atoms in a lattice reside on parallel lines (layers). The interatomic distances are the same within one layer but can differ for distinct layers. The stable structure corresponds to the global minimum of the energy function.

Since it is not possible to deal with an infinite structure we first find the periodic “core” of the lattice by minimizing the cumulative energy of the piece of a lattice bounded by a rectangle. Then we find the minimum of the energy of atoms belonging to the “core”. Formally the problem is stated as a global minimization problem where the objective function is energy of the piece of material computed using so-called potential functions. We used Lennard-Jones, Morse and Tersoff potentials.

The paper evaluates various optimization techniques for the problem, compares their performances and draws the conclusion about best choice of optimization methods and parameter selection for the problem under test. As a result we were able to locate minima meaningful from the physical point of view, e.g. reproducing graphene lattice.

Stabilization of driven quantum systems moving under the influence of dissipation and noise

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It is well known that a classical particle moving in a viscous medium permanently loses energy stored at the beginning of the motion. To protect the system from the loss of energy, it is necessary to include an external force, the action of which will prevent the action of the friction. For instance, when we are talking about of an optical mode (an electromagnetic field oscillator) localized in the resonator, we have in mind the losses of the energy of the wave in the walls of the resonator. In this case in order to stabilize the mode it is necessary to return back these losses by pumping.

It is clear that without taking into account the fluctuations, the mode can be made stable if one knows the rate of energy loss and replenishes it according to a certain law. In other words, to stabilize the mode, it is necessary to monitor the movement and include an additional loop providing feedback. At the same time, the influence of fluctuations of the bath must be taken into account, since dissipation and fluctuations are connected by the fluctuation-dissipation relation [1], therefore, already at the classical level in the problem of system stabilization, the effects of dissipation and noise cannot be divided.

The situation with the behavior of quantum systems is even more complicated when both dissipation and fluctuations are taken into account. In addition, in quantum systems it is necessary to take into account the fact that monitoring over the system will be accompanied by measurements that introduce additional irreducible effects on the system [2]. Note that recently, in connection with the development of devices for quantum communications, the problem of stabilizing quantum systems is becoming more and more relevant.

In the present work we are going to study a simple quantum system that contains all of the above features. We consider the dissipative dynamics of a quantum oscillator (optical mode) which is placed in a bosonic bath [3]. To control the system, we add an operator that is responsible for the action of the external force. In addition to the energy control problem discussed above, we will also discuss other objective functions that need to be preserved, for example, populations of energy levels and their variances, which can be partially preserved despite the effect of the bath.

The Hamiltonian of the system includes the terms describing the harmonic oscillator (optical mode), the bosonic oscillators (describing the bosonic bath), the interaction of the mode and the bath, and also the term responsible for the nondestructive measurement and the driving force. The method for solving the problem is the following. First of all, the Heisenberg equations of motion for the operators of the system are obtained. The equations for bosonic field operators are linear and may be solved exactly. After eliminating the bosonic operators the remaining equations are solved by approximate and numerical methods. In particular, for the solution of the reduced equation for the density matrix, the quantum Monte Carlo method is used [4,5]. To solve equation numerically we have used Fock basis. The infinite system of equations for mode variables has been truncated and solved by using of the Runge-Kutta method.

The results of numerical simulation, presented in the form of energy and correlation functions dependencies on time, allow predicting the influence of the feedback loop on the behavior of a quantum system.

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Efficient algorithm for DLA problem in multiple dimensions

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Understanding critical properties of non-equilibrium processes [**?**] is still a challenging problem of contemporary statistical physics. Of particular interest (both theoretical and practical) are the dynamical growth phenomena. The model for the two-dimensional (2D) growth (Diffusion Limited Aggregation) was introduced almost thirty years ago by Witten and Sander [**?**]. Structures grown by DLA look very similar to those found in nature and society [**?**], for example, ice crystals on window, mineral dendrites on the surfaces of limestones, colony of bacteria, nano-size crystals grown on the crystal surface, monolayer polymer films, interfaces in Hele-Shaw cell, urban growth, etc.

It possible to generalize 2D DLA model for higher dimensions. In this case the general description of the model stays the same. But from computational point of view the problem complexity grows as the number of dimensions increases. There are several issues we have to solve. First, when space dimension is greater than 2 boundary conditions for random walk simulation change since there is finite possibility for random walker to walk to infinity. Second, simulation of random walk requires generation of uniformly distributed random numbers that reside on a unit sphere. This could be time consuming and efficiency issue arises. Third, DLA algorithm should implement a data structure that will allow fast nearest-neighbour search and require moderate amount of memory.

We present some results on estimation of efficiency of proposed algorithms for DLA simulation and discuss on further improvements.

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Universal Scaling Laws for Cluster Growth and Aging During Collapse of a Polymer

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Using state of the art Monte Carlo simulations of a bead-spring model we investigate the homopolymer collapse by quenching the homopolymer from an expanded coiled state into the globular phase. The sequence of events observed during the collapse is independent of the quench depth. In particular, we focus on finding out universal scaling behaviors related to the growth or coarsening of clusters of monomers, by drawing phenomenological analogies with ordering kinetics. We distinguish the cluster coarsening stage from the initial stage of primary cluster formation. By successful application of a nonequilibrium finite-size scaling analysis we show that at all quench temperatures, during the coarsening stage, the cluster growth is roughly linear and can be characterised by a universal finite-size scaling function. In addition, we provide evidence of aging by constructing a suitable autocorrelation function and its corresponding dynamical power-law scaling with respect to the growing cluster sizes. The predicted theoretical bound for the exponent governing such scaling is strictly obeyed by the numerical data irrespective of the quench temperature. The results and methods presented here in general should find application in similar phenomena such as the collapse of a protein molecule preceding its folding.

Population annealing algorithm, its GPU implementation and its analysis

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Population annealing is a promising recent approach for Monte Carlo simulations in statistical physics, in particular for the simulation of systems with complex free-energy landscapes. It is a hybrid method, combining importance sampling through Markov chains with elements of sequential Monte Carlo in the form of population control. While it appears to provide algorithmic capabilities for the simulation of such systems that are roughly comparable to those of more established approaches such as parallel tempering, it is intrinsically much more suitable for massively parallel computing.

Here, we present a highly optimized implementation of the population annealing algorithm on GPUs and obtain speed-ups of several orders of magnitude as compared to a serial implementation on CPUs. Our code includes implementations of some advanced algorithmic features that have only recently been suggested, such as the automatic adaptation of temperature steps and a multi-histogram analysis of the data at different temperatures.

We also present a detailed study of the statistical error and bias in the calculations, and of application of the algorithm to first- and second-order phase transitions.

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A framework to monitor activities of satellite data processing in real-time

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Abstract. Space monitoring data centers use space weather models to predict conditions in near-Earth orbit. Being sure that correct data is used in the models is critical. Failures of various kinds happen in satellite data processing, so we need a mechanism to monitor all activities during the process, and thus identify the scope of failure and prevent incorrect data to be used. To solve the problem described above, we have developed a framework called Live Monitor at SINP MSU. The real-time monitoring subsystem of SDDS, an automatic satellite data processing system used at SINP MSU to collect and process data from Russian and foreign satellites, has been built based on the Live Monitor framework. All activities of each stage in data processing are logged by Live Monitor and shown in real-time on the Live Monitor's web interface. When an error occurs, a notification message will be sent to satellite operators via email and the Telegram messenger service so that they could take measures in time. The Live Monitor's API can be used to create a customized monitoring service with minimum coding.

Compact high-order difference approximations for rod lateral vibrations equation

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We present a compact high-order difference approximations for rod lateral vibrations:

$$\rho\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}[R^2\rho\frac{\partial^3 u}{\partial x \partial t^2}] + \frac{\partial^2}{\partial x^2}[ER^2\frac{\partial^2 u}{\partial x^2}] = f,$$

with various boundary conditions. Here, ρ is a density of a rod material, R is rod thickness, E is Young's modulus, f is a right-hand side (forcing). The equation is difficult for calculations because it is not resolved with respect to the highest derivative on time. We consider cases of constant and time-independent variable rod thickness and have studied stability of obtained schemes, as well as different properties such as approximation of first integral and eigenvalues of the boundary problem in various norms: Euclidean, Chebyshev, energetic norm. Numerical experiments show high (4th) order of approximation. Compact difference schemes are effective because they provide high accuracy order for various models of mathematical physics [1-4], and the implicit schemes may be realized by economical double-sweep (Thompson) method.

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Investigation of lunar dusty exosphere with future Russian lunar missions: Simulation Approach and Measurements Control

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Abstract:

One of the complicating factors of the future robotic and human lunar landing missions is the influence of the dust. Meteorites bombardment has accompanied by shock-explosive phenomena, disintegration and mix of the lunar soil in depth and on area simultaneously. As a consequence, the lunar soil has undergone melting, physical and chemical transformations.

Recently we have the some reemergence for interest of Moon investigation. The prospects in current century declare USA, China, India, and European Union. In Russia also prepare two missions: Luna-Glob and Luna-Resource. Not last part of investigation of Moon surface is reviewing the dust condition near the ground of landers. Studying the properties of lunar dust is important both for scientific purposes to investigation the lunar exosphere component and for the technical safety of lunar robotic and manned missions.

The absence of an atmosphere on the Moon's surface is leading to greater compaction and sintering. Properties of regolith and dust particles (density, temperature, composition, etc.) as well as near-surface lunar exosphere depend on solar activity, lunar local time and position of the Moon relative to the Earth's magneto tail. Upper layers of regolith are an insulator, which is charging as a result of solar UV radiation and the constant bombardment of charged particles, creates a charge distribution on the surface of the moon: positive on the illuminated side and negative on the night side. Charge distribution depends on the local lunar time, latitude and the electrical properties of the regolith (the presence of water in the regolith can influence the local distribution of charge).

On the day side of Moon near surface layer there exists possibility formation dusty plasma system. Altitude of levitation is depending from size of dust particle and Moon latitude. The distribution dust particle by size and altitude has estimated with taking into account photoelectrons, electrons and ions of solar wind, solar emission. Dust analyzer instrument PmL for future Russian lender missions intends for investigation the dynamics of dusty plasma near lunar surface. PmL consists of three parts: Impact Sensor and two Electric Field Sensors.

One of the tools, which allows to simulate the dust emission from the Moon and asteroids, its transport, deposition and its interaction with a lander, is the SPIS-DUST (Spacecraft Plasma Interaction Software) code which based on Particle-in-Cell (PiC) method.

This paper presents first results of SPIS-DUST modelling of the interaction between the lunar plasma environment, regolith and a lander. The model takes into account the geometry of the Luna-Glob lander, the electric properties of materials used on the lander surface, as well as Luna-Glob landing place. Initial conditions were chosen based on the current theoretical models of formation of dusty plasma exosphere and levitating charged dust particles.

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Nonlinear Interaction of Waves in Rotating Spherical Layers

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Flows of a viscous incompressible fluid in a spherical layer that are due to rotational oscillations of its inner boundary at two frequencies with respect to the state of rest are numerically studied. It is found that an increase in the amplitude of oscillations of the boundary at the higher frequency can result in a significant enhancement of the low-frequency mode in a flow near the outer boundary. The direction of propagation of the low-frequency wave changes from radial to meridional, whereas the high-frequency wave propagates in the radial direction in a limited inner region of the spherical layer. The role of the meridional circulation in the energy exchange between spaced waves is demonstrated.

Numerical Simulation for Meteoroid Dark Flight

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Meteoroid passage through the Earth atmosphere usually exhibits two consequent stages, namely: atmospheric entry as a bolide, and dark terminal part of the trajectory. Only exceptions are the massive dense bodies like metallic meteorites having completely bright path down to the planetary surface, and micrometeorites and space dust, losing velocity in upper atmosphere. Generally, the initial bright part of the trajectory is considered linear; however, more dense atmospheric layers promote the aerodynamic drag as a main contributing factor to meteoroid deceleration below speed of sound. The accurate estimation of dark flight trajectory is essential at determining the search area of meteorite fragments. Therefore, the numerical simulation becomes the most reliable mean to obtain dark flight trajectories.

To efficiently estimate the dark flight trajectory we consider following assumptions. First, we assume that the simulated meteoroid is subjected to fragmentation and can become an ensemble of fragments at the end of bolide stage of the trajectory. Second, due to large number of simulated fragments reaching orders of 10^3–10^4, we consider a simplified ballistic model, which represent the fragments as homogeneous balls with specified density. The dynamics for each fragment is governed by a system of differential equations accounting for drag and gravity. To increase accuracy of the simulation, the drag coefficient is computed via Henderson formula. The atmospheric properties are calculated via 1976 US Standard Atmosphere model, which is sufficient for endoatmospheric simulations. The temperature correction for air viscosity is carried out via Sutherland formula. The gravity acceleration and the shape of Earth are modeled according to WGS84 model. For better representation of fragments scatter area we consider Earth landscape via global satellite digital elevation map GTOPO30 with precision of 30 arc seconds. The fragmentation processes are described via expression for stagnation pressure threshold

$$p^*_{imp} = \sigma_0 m_0^{\alpha} m_P^{\alpha},$$

where m_0 is the initial mass of meteoroid, $\alpha = 0.25$ is a scaling factor, σ is the mean static strength of the meteoroid material. The sizes of the resulting pair of fragments are computed with stochastic model:

$$\xi \sim \mathrm{R}[0;1], \quad r_{P,1} = \xi r_P, \quad r_{P,2} = \left(1-\xi^3\right)^{1/3} r_P$$

Computational results show that terminal velocities and maximum splinter masses are in good agreement with corresponding observations and measurements. For example, the computed mass for the largest Chelyabinsk meteorite fragment is 692 kg and the piece recovered from Chebarkul Lake has mass of 654 kg.

Analysis of the Chandler wobble of the Earth

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We study the Chandler wobble (ChW) of the pole, using such methods for its extraction as singular spectrum analysis, Panteleev filtering, and least-squares collocation. The moving least-squares filter (MLSF) [1] shows, that ChW has average period of 433 days and phase jump over π in 1930-th. The ChW amplitude is not stable and strikingly decreased in 1930-th and the 2010-th. The ChW envelope model contains 83- and 42-year quasi-periodicities. Based on the Euler-Liouville equations we solved the inverse problem of chandler input excitation reconstruction [2]. The excitation envelope was found to have 20-year variations.

The analysis of the modulated signal with 433-day carrier frequency in a sliding window demonstrates the specific effect, we called the "Escargot effect". Its nature is the following: when extracted on a secular period (150 year), the ChW oscillation is purely prograde, and its spectrum pike is splitted, reflecting the 40-year modulation; but, when extracted in a sliding window at the instantaneous chandler frequency, a retrograde component with a 20-year envelope appears, reflecting the change of ellipticity parameters.

Chandler excitation envelope and amplitude of instantaneous retrograde component of ChW look to be similar. The explanation was found through consideration of the Euler-Liouville equation.

Besides global geodynamics, ChW modelling is important for polar motion prediction and its application and answering the question: are the climate changes on Earth and its rotation parameters interrelated [3]?

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The Different Types of Turbulence in Rotating Spherical Layers

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Turbulent flows of a viscous incompressible fluid in a layer between rotating concentric spheres under the action of the modulation of the velocity of one of the spheres have been studied experimentally and numerically. The form of spectra of turbulent pulsations of the azimuthal velocity depends on the sphere whose rotational velocity is modulated, as well as on the amplitude and frequency of modulation. The possibility of the formation of turbulence with spectra qualitatively similar to spectra obtained in measurements in the upper atmosphere is established: with the slope close to –3 at low frequencies and close to –5/3 at high frequencies and with the negative longitudinal velocity structure function of the third order. It has been shown that such spectra are formed in the regions of a flow that are strongly synchronized under the action of the modulation of the rotational velocity.

Acceleration and Particle Transport in Collisionless Plasma in the Process of Dipolarization and Nonstationary Turbulence

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Abstract

Magnetic substorms are key processes governing the energy accumulation and release in the Earth's magnetosphere. After the growth phase when the magnetotail current sheet can be thinned to the state of extremely stretched current configuration with the thickness about several proton gyroradii, the magnetic reconnection which causes magnetic dipolarization processes can begin. The sharp increase of the amplitude of a normal magnetic field in the Earth's magnetotail is usually followed by significant turbulence and can lead to the strong particle acceleration. In a frame of the model of magnetotail current sheet we have investigated numerically two general mechanisms of particle acceleration: (1) by the induction electric field during magnetic dipolarization, (2) by plasma turbulence. Multicomponent plasma containing protons, electrons and O^+ heavy ions were taken into account. The results demonstrate the particle acceleration by separate mechanisms (1) and (2) and by their joint action. It is shown that both acceleration mechanisms lead to the formation of powered tails in proton distribution functions, but their simultaneous effect is the most effective one in particle acceleration. The parametric study shows that particle acceleration has a resonance character, i.e. maximum of particle acceleration takes place when their temporal or spatial characteristics are close to the corresponding changing of magnetic and electric fields. For this reason the electron acceleration is weak during dipolarization processes, contrary to proton and oxygen ones.

Modelling of charge stabilized colloidal crystals

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Elasticity of charge stabilized colloidal crystals is studied numerically within the approximation of static lattice. Description of the colloidal systems is based on the non-linear differential Poisson-Boltzmann equation. Corresponding boundary value problems are solved numerically by finite element method. The force constants and elastic constants of different orders are obtained for different crystal systems both in two and three dimensions. The effective pair and many-body interactions are also studied and discussed.

Charge stabilized colloids are systems of electrically charged submicron particles immersed into a liquid electrolyte. There are a lot of examples of such systems in different fields of technology, chemistry and biology. The nature of the particles varies from simple plastic balls to complex objects like micelles and DNA molecules. In colloidal crystals, the particles are spatially ordered and located in the vertices of a crystal lattice. The charge stabilized colloidal crystals have some technological perspective, especially in photonics. They serve also as model systems of conventional molecular crystals. In addition, studying of colloidal crystals can pour some light onto the disordered systems as well, while presence of spatial ordering simplifies solution of structural problems.

While the interactions in colloidal systems can be rather sophisticated, the electrostatic and entropic interactions are only included in the present study. This allows description by the mean-field theory leading to the non-linear differential Poisson-Boltzmann equation. The properties of a colloidal system at any particular configuration are then fully described by solution of the corresponding boundary value problem for the Poisson-Boltzmann equation. The advantage and disadvantage of such approach is discussed in the present work.

The crystals studied are composed of electrically charged hard spheres or circles immersed into binary symmetrical univalent electrolyte. The appropriate boundary value problems were formulated and solved numerically. Numerical solution was carried out by the finite element method using free tetrahedral meshes of the second order Lagrange elements. Typical discretization contained several millions degrees of freedom while typical computer experiment incorporated up to several thousands of spatial configurations. Calculations were partly supported by the Supercomputing Center of Lomonosov Moscow State University [1].

Numerical procedures for determination of both the force constants and the elastic constants are described. The force constant determination is based on the perturbation of the ideal lattice by shifting a single particle from its equilibrium position. Elastic constants are obtained from the stress-strain dependencies.

The force constants and elastic constants of the first and second order were calculated for a wide range of the lattice parameter for different monatomic crystal systems including square and hexagonal lattices in two dimensions and simple cubic, f.c.c. and b.c.c. lattices in three dimensions. The monolayer crystals of spherical particles near charged planes were also considered. Stability of the crystals relative different types of deformation is discussed.

Some recently obtained results on the non-linear elastic properties of the crystals are presented. In particular, elastic constants up to the fifth order were calculated for the crystal with two-dimensional hexagonal crystal lattice. The results are compared to the graphene data.

Pronounced deviation from the Cauchy relations for the elastic constants was observed for all the crystals under study that gives evidence of essential role of the many-body effective interactions in such systems. Some effective pair potentials were calculated by solution of the appropriate boundary value problems for the Poisson-Boltzmann equation. The two-dimensional three-body effective potential was also calculated and applied to the description of the elasticity of the colloidal crystals. The problems arising in this study are briefly discussed.

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Numerical methods with discrete transparent boundary conditions for solving the time-dependent Schrödinger equation in unbounded domains

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This a joint study together with B. Ducomet (France), I. Zlotnik and A. Romanova (Russia).

The linear time-dependent Schrödinger equation is among the key equations in quantum mechanics and electronics, nuclear, atomic and molecular physics, wave physics, etc. Often it should be solved in unbounded space domains. To overcome this difficulty, among a lot of existing approaches we adopt the so-called discrete transparent boundary conditions (TBCs). Their advantages are the complete (100%) absence of spurious reflections from artificial boundaries, reliable computational stability and ability to ensure small relative errors in practice, the clear mathematical background and the corresponding rigorous conservative properties and stability theory, error estimates without mesh steps in negative powers in theory, etc.

We construct and study a collection of new efficient discretization methods. Among these methods are the Crank-Nicolson-polylinear finite element method with the discrete TBC, any order Crank-Nicolson-finite element method in space with the discrete TBC, splitting in potential finite-difference schemes of the 2^{nd} and 4^{th} orders of accuracy in space with the discrete TBCs, and high order of accuracy methods in time based on the global Richardson extrapolation in time, see [1-7].

We develop a rigorous stability theory and theoretical and practical error analysis.

A number of numerical results on computing the tunnel effect for various barriers/wells are presented.

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Boundary Conditions that Imitate Cauchy Problem for Finite-Difference Approximations of Basic Mathematical Physics Equations

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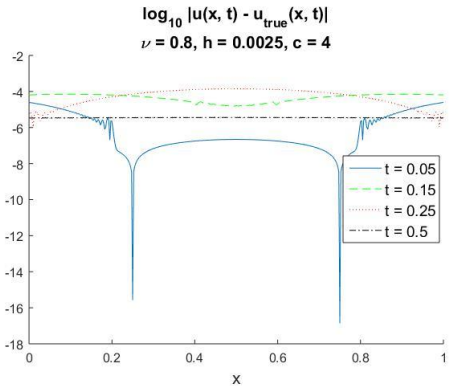
Most common physical processes can be described by evolutionary partial differential equations or systems. To calculate a solution of such problems, finite-difference schemes may be used. However, due to a finite computer memory and a computational time, solving the problem in an infinite area is impossible. At the same time, a mixed boundary problem may be solved. Usually boundary conditions describe some physical processes that occur on the area's boundary. For example, the Dirichlet boundary condition simulates solution's fixation on the boundary; the Neuman boundary condition simulates the fixation of the first normal (with respect to the boundary) derivative. Sometimes, there are no such special processes happening on the boundary. However, usual boundary conditions will reflect some waves, which in nature go away from the computational domain. The good solution of the mixed value problem should be the same as the solution for the Cauchy's problem.

The boundary conditions, which provide the solution that coincide with the Cauchy's problem solution (ICP boundary conditions) for important linear differential equations and systems with constant coefficients, exist and are nonlocal. They include integral operators like convolution. As about finite difference case we should use in the convolutions series instead of integrals. Common algorithm of building such conditions for half-space was provided in [1]. Since ICP boundary conditions are nonlocal, all solution's values in the previous time moments are required to calculate next boundary values. The Hermite – Pade approximations of the symbols of the finite-difference operators are used [2] to reduce a number of required arithmetical operations and volume of memory.

We consider few basic equations of mathematical physics: wave, diffusion and Schrödinger equations. For these equations some finite-difference approximations were considered (leap-frog, implicit Euler scheme, Crank – Nicolson, compact schemes). In every case, different ICP boundary conditions are obtained. For diffusion and Schrödinger equations, it is shown that localization of the ICP boundary conditions leads to the growth of the solution's error (difference between the exact solution and the obtained one).

As an example, let us consider one–dimensional wave equation $\partial_t^2 u = c^2 \partial_x^2 u$, where c – velocity of the wave, and approximate if with a leap-frog scheme with a space step h and a time step τ. Figure 1 shows logarithm of absolute difference between an exact solution u_{true} and the obtained one u at different slices of time ($\nu = c\tau/h$ - Courant's parameter).



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Singular solutions for vibration control problems

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We consider the control system

$$\frac{\partial^2}{\partial t^2}p\left(x,t\right)+A_x p\left(x,t\right)=g\left(x,t\right),\quad x\in G,\quad t\in\mathbb{R}_+ \tag{1}$$

subject to the initial

$$p\left(x,0\right)=v_0\left(x\right),\quad p_t\left(x,0\right)=v_1\left(x\right) \tag{2}$$

and the boundary conditions

$$B_x p|_{\partial G}=0 \tag{3}$$

Here, $p\left(x,t\right)$ and $g\left(x,t\right)$ are m-dimensional vector-valued functions defined on $G\times[0,\infty)$, G is a compact subset of $\mathbb{R}^n$ with smooth boundary ∂G, A_x is a linear elliptic operator of order 2 in G, B_x is a linear differential operator of order 1 in a neighborhood of ∂G. Suppose that $p\left(x,t\right)\in L_2\left(G\times[0,\infty),\mathbb{R}^m\right)$, g is a measurable function in t, $g\left(\cdot,t\right)\in L_2\left(G,\mathbb{R}^m\right)$, $p\left(\cdot,t\right)$, $\frac{\partial^2}{\partial t^2}p\left(\cdot,t\right)$, $v_0\left(x\right),v_1\left(x\right)\in H^2\left(G,\mathbb{R}^m\right)$.

The external force $g\left(x,t\right)$ is considered as a control function. We assume that $g\left(x,t\right)$ is a bounded:

$$\left\|g\left(\cdot,t\right)\right\|^2_{L_2(G,\mathbb{R}^m)}\leq 1 \tag{4}$$

We study the following control problem: to find the admissible control such that the coresponding solution of (1)-(3) minimize the functional

$$\int_0^\infty\left\|p\left(\cdot,t\right)\right\|^2_{L_2(G,\mathbb{R}^m)}dt\to\inf \tag{5}$$

Assume that A_x with domain $D_A=\left\{y\in H^2\left(G,\mathbb{R}^m\right),\quad Bp|_{\partial G}=0\right\}$ is a self-adjoint operator, has the discrete spectrum $\{\lambda_j\}_{j=1}^\infty$ and the orthonormal complete system of eigenfunctions $\{h_j\left(x\right)\}_{j=1}^\infty$ that are smooth in G and satisfying (3). We seek a solution of (1)-(5) in the form

$$p\left(x,t\right)=\sum_{j=1}^\infty q_j(t)h_j(x) \tag{6}$$

where $q_j\left(t\right)=\left(p,h_j\right)_{L_2(G,\mathbb{R}^m)}$, $\quad j=1,2,\ldots$, are Fourier coefficients. Expand the functions g,v_0,v_1 in the basis $\{h_j\left(x\right)\}_{j=1}^\infty$

$$g(t,x)=\sum_{j=1}^\infty u_j(t)h_j(x),\quad v_0\left(x\right)=\sum_{j=1}^\infty s_j h_j(x),\quad v_1\left(x\right)=\sum_{j=1}^\infty r_j h_j(x)$$

We get for the Fourier coefficients q_j the following system of countably many ordinary differential equations: $\ddot{q_j}(t)+\lambda_j q_j\left(t\right)=u_j(t)$, $j=1,2,\ldots$, with the boundary conditions: $q_j\left(0\right)=s_j,\quad \dot{q}\left(0\right)=r_j$. Condition (4) gives us $\sum_{j=1}^\infty u_j^2\left(t\right)\leq 1$. Substituting (6) into (5) we get

$$\int_0^\infty\left\|p\left(\cdot,t\right)\right\|^2_{L_2(G,\mathbb{R}^m)}dt=\int_0^\infty\sum_{j=1}^\infty q_j^2(t)dt$$

Thus we have an optimal control problem for the Fourier coefficients in the space l^2:

$$\int_0^\infty \sum_{j=1}^{\infty} q_j^2(t)dt \to \min \tag{7}$$

$$\ddot{q_j}(t) + \lambda_j q_j(t) = u_j(t) \tag{8}$$

$$q_j(0) = s_j, \quad \dot{q}(0) = r_j, \quad j = 1, 2, \ldots \tag{9}$$

$$\sum_{j=1}^{\infty} u_j^2(t) \leq 1 \tag{10}$$

Problem (1)-(5) with the external force in the form $g(x,t) = u(t) f(x)$ was considered in [1]. In this case the corresponding control problem for the Fourier coefficients has the same form but (8) and (10) are replaced by

$$\ddot{q_j}(t) + \lambda_j q_j(t) = C_j u(t) \tag{11}$$

$$-1 \leq u(t) \leq 1 \tag{12}$$

where $C_j \in \mathbb{R}$. In [2] for the problem (7), (9), (11)-(12) it was constructed the optimal synthesis containing singular extremals and extremals with accumulation of switchings.

In this paper for some initial conditions (2) we prove that the behavior exhibited by the solutions of (7)-(10) is similar to that of the problem with scalar control.

Note that the system (1)-(3) governs vibrations of beams, strings and other mechanical models. We consider, as an example, the problem of controlling the vibrations of the Timoshenko beam.

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Quantum Hash Functions Realization in the model of Quantum Branching Programs

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In [1, 2] we explicitly defined a notion of quantum hashing as a generalization of classical hashing and presented examples of quantum hash functions. Those functions have "unconditionally one-way" property based on Holevo Theorem [4]. More information on the role of quantum hashing for the post quantum cryptography, possible application of quantum hashing for quantum signature protocols, and technological expectations for realization of quantum signature schemes are presented in [5].

In the paper we consider quantum (δ, ϵ)-hash functions construction based on ϵ-biased sets. Such quantum (δ, ϵ)-hash function $\psi : \mathbb{F}_q \to (\mathcal{H}^2)^{\otimes s}$ hashes elements of finite field $\mathbb{F}_q$ into s-qubit quantum states. The notion of (δ, ϵ)-hash function combines together a notion of preimage (one-way) quantum δ-resistance property and the notion of quantum collision ϵ-resistance properties. These properties are quantum generalization of classical one-way resistance and collision resistance properties required for classical hash functions.

Important property for hash function is a computational effectiveness. In our research we prove that considered construction of quantum (δ, ϵ)-hash function is computed effectively in the model of Quantum Branching Programs [3]. We consider two complexity measures: a number $Width(Q)$ of qubits that QBP Q uses for computation and a number Time(Q) of computational steps of QBP Q. Such QBP Q is of $Width(Q) = O(\log \log q)$ and $Time(Q) = \log q$.

We prove that such QBP construction is optimal. That is, we prove lower bounds $\Omega(\log \log q)$ for QBP width and $\Omega(\log q)$ for QBP time for quantum (δ, ϵ)-hash function presentation.

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The Development of efficient Algorithms for multi-threaded parallel Processing in the Module Scaling digital Images

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Abstract. Scaling of images finds wide application it many tasks. The object of the research in this work is the methods for scaling digital raster images.

The main aim of this work is to develop efficient multithreaded parallel algorithm bicubic interpolation raster image to implement this algorithm as a program in C++.

The main aim of this work is to develop an effective parallel algorithm bicubic interpolation raster image to implement this algorithm as a program in C++.

Also the aim of this work is to develop applications with a graphical user interface for the operating system Window for demonstration of the algorithm and study the relationship between algorithm performance and the degree of parallelization.

In the progress of the work was designed and implemented parallel algorithm bicubic interpolation of raster images in C++.

In the process, arose the need to carry out comparative analysis to examine and to analyze the methods the nearest neighbor method, bicubic interpolation, bilinear interpolation, method of supersampling and method of directional interpolation for image scaling.

Also implemented algorithms for step and bilinear interpolation, directional interpolation and their concurrent modification in C++.

The result created an application with a graphical user interface and implemented all the required functionality. The application allows you to perform forward and reverse scaling of the image by various methods of interpolation and save the result.

During testing on a multi-core General-purpose processors confirmed the assumption about the feasibility of parallelization of the algorithm is bicubic interpolation. Use just a few threads of computation provides a significant acceleration of this and other implemented algorithms.

Developed multithreaded parallel algorithms have demonstrated their effectiveness and can be applied in practice in the processing of digital images. A method of bicubic interpolation is the most preferred from the viewpoint of smoothness of the resulting image.

Comparative evaluation of the effectiveness of the methods on the criterion of time and acceleration. It was found that for large amounts of initial data and large coefficients for the direct and inverse scaling of multithreaded parallel algorithms are more efficient than sequential algorithms.

Docker Containers Manager: A Simple Toolkit for Isolated Work with Shared Computational, Storage, and Network Resources

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Containers are isolated user-space instances run by the same OS kernel, allowing their users to enjoy many of the benefits of virtual machines with little overhead. With containers, multiple applications can be installed on the same computer without the risk of dependencies conflict, and run without additional costs for emulating hardware and different operating systems. Docker is one of the most popular container platforms for Linux. It provides numerous tools for configuring and managing containers. However, giving users full access to Docker capabilities on a server amounts to giving them unrestricted access to the server.

We present a simple set of command line interface tools called Docker Containers Manager (DCM) that allow users to create and manage Docker containers with pre-configured SSH access while keeping the users isolated from each other and restricting their access to the Docker features that could potentially disrupt the work of the server. The tools allow to deploy and debug medium-sized distributed systems for simulation in different fields on one or several local computers.

Users can access DCM server via SSH and are automatically redirected to DCM interface tool. From there, they can create new containers, view the status of the existing containers (only those started by the user are visible), stop, restart, pause, unpause, and remove them. The containers will also be accessible via SSH using the same private key(s), but on different server ports. To create a new container, a user must specify an image to be used as the container's root filesystem. Some images are provided by the DCM server administrators. After a user has configured a container to meet one's needs, the changes can be committed to a new image from which the user can create copies of the container. Users can also view the list of available images and remove their own images. Potentially these images can be migrated to publicly accessible repositories.

When creating a new container, a user can request additional publicly available ports to be mapped to the respective ports of the container, allowing for some network services to be run within the container. Server administrators can also permit certain users to use additional options when creating their containers, e.g. setting a restarting policy or lifting some security restrictions.

Lastly, server administrators can use scripts to create new users (setting up their access and storage directories to be mapped to every container) and delete users, also removing all their containers and (optionally) images.

All commands were implemented as Python scripts.

Slastnikov S., Belov A.

Applying swarm intelligence algorithms for NP-hard problems

Abstract

Article devoted to applying some swarm intelligence approaches for solving NP-hard discrete optimization problems. Shown how these approaches could be combined to get better results. Some experimental modeling results are performed and discussed. Finally, we discuss ways to parallelize presented algorithms.

The analysis of conservative and optimistic parallel discrete event simulation algorithms on small-world networks

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We study synchronization algorithms in parallel discrete event simulations (PDES). We build models for the evolution of local virtual times (LVT) in the conservative and optimistic synchronization algorithms. The question addressed in our study is how the underlying communication topology affects the synchronization. We run our models on regular and small-world topologies and compare the results. The main findings for the conservative algorithm are: i) critical exponent does depend on the fraction of the long-range links logarithmically; ii) the width of the LVT profile (i.e. the desynchronization degree) becomes finite in the limit of infinite number of processing elements. We also found that synchronization issue depends mostly on the average shortest path of the network, and clustering coefficient does not influent synchronization. The work is supported by grant 14-21-00158 of the Russian Science Foundation.

Electron wave packet dynamics for spin dependent tunneling current induced in one-dimensional nanostructure.

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Recent advances in nanotechnology have allowed us to fabricate nanoscale building blocks such as supremolecules or semiconductor quanum dots [1,2]. In due course these nano-objects would be assembled "archtectually" [3] to form nanosale circuits operating, possibly, under the principle of quantum mechanics. Since electric current in such nano-circuits is not macroscopic but consists of a few number of electrons, it must be quantum mechanical in nature, that would be characterized by interference as well as discreteness.

To study the nature of such quantum mechanical current we have recently developed a computation code for solving the time-dependent Schroedinger equation directly for a system of a few electrons bound to a quasi-one-dimensional nanoscale potential well. This system is also coupled to electrodes at borh terminals which is modelled by absorbing boundaries. In the present study we have focused on a system fabricated with three-terminals mimicking nanoscale transistors, namely, source, gate and drain. The source-drain transient current has been calculated by a flux of the probability density of the electron wave packet absorbed on the downstream side of the drain region where an absorbing potential has been placed. A remarkable dependence of the transient current on the spin configuration of the transmitted electrons has been observed. The origin of this spin dependence will be discussed on the basis of the nodal pattern of the electron wave packet.

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[3] Molecular Architectonics: http://molarch.jp/?lang=en

Development of atomistic description for Zr-Nb alloys: study of phase transitions and diffusivities

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Zirconium-Niobium alloys attract wide attention due to two different fields of their applications. Originally, hcp-based zirconium alloys are widely used for structural applications in nuclear reactors. However, recently the bcc-based Zr-Nb alloys gain an interest as potential candidates for role of material for high-productive medical implants. Here we report a new attempt to study properties of Zr-Nb alloys using atomistic simulations (including *ab initio* computations and classical molecular dynamics). We consider Zr-Nb alloys based on hcp and bcc zirconium. Niobium content here may vary from 1 to 20 at. %, depending on the structure of given alloy.

For the development of opportunities in the modeling of these alloys, we constructed a new angular-dependent many-body interatomic potential [1]. The potential functions were fitted towards the *ab initio* data. We approve that the chosen potential fitting technique (i.e. "force-matching method") is very helpful for study of metallic systems containing a variety of different phases. The constructed model was applied for investigation of properties of different phases (alpha, beta, omega) existing in Zr-Nb alloys, as well as for detection of transformations between these phases.

We also performed molecular dynamic simulations illustrating that the created interatomic potential can be applied for predictions dealing with self-diffusion in Zr and Zr-Nb alloys. As an example, we report diffusivities of Zr and Nb in hcp Zr-Nb alloys computed for the models containing up to 5 at. % of niobium. The calculated diffusivity of niobium rises with increase of its content in the alloy. The simulations also show that for a studied concentration range addition of niobium slightly enhances self-diffusion of zirconium in the alloys. The work is also devoted to description of niobium incorporation and clusterization in hcp zirconium. It is confirmed that for a single niobium atom incorporated in hcp zirconium lattice the octahedral position is the most favorable. We also estimated the energy describing niobium cluster formation in pure hcp zirconium.

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Theoretical investigations on the physical properties and fabrication mechanisms of MXenes

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MXene, as a new family of two-dimensional materials, has aroused extensive attentions in recent 6-7 years. Due to their outstanding absorbtion capacities, favorable hydrophilies and conductivities, MXenes were proposed to show widespread potential applications such as in energy storage, sewage disposal and electromagnetic shielding. In this presetation, we systematically studied the structural, mechanical and electronic properties of the carbide MXenes firstly[1]. It implied that the physical properties of the MXenes are significantly depended on the surface functional froups. Moreover, some MXene members show semiconducting characteristics. Based on above, we further investigated the possibility of using those semiconducting MXenes with moderate band gaps (1~2 eV) as the materials for semiconducting devices[2,3]. The key properties of carrier mobility and thermal conductivity were studied. The results shown that the oxygen functionalized M_2CO_2 (M=Ti, Zr, Hf) possess relatively high hole mobilities which are of the order of 10^4 $cm^2V^{-1}s^{-1}$, while Sc_2CT_2 (T=F, OH) MXenes present favorable electron mobilities. The lattice thermal conductivities of these MXenes are significantly related to the metal atom M, where the Sc-containing MXenes generally show higher thermal conductivities than others. With respect to the M_2CO_2 (M=Ti, Zr, Hf) MXenes, their thermal conductivities increase with the increasing atomic number of M, and the room temperature thermal conductivity of Hf_2CO_2 is approximated to that of pure iron. Noteworthily, we have developed a new approach to synthesis MXenes cooperated with experiment. Instead of etching the traditional MAX phases, the layered ternary carbides $M_nAl_3C_{n+2}$ and $M_nAl_4C_{n+3}$ (n equals to 3 or 4) were adopted as precusors, and we have successfully synthesized the Zr- and Hf-containing MXenes [4,5]. The schematic diagram of the synthesis of the $Zr_3C_2T_x$ MXene is shown in Figure 1.

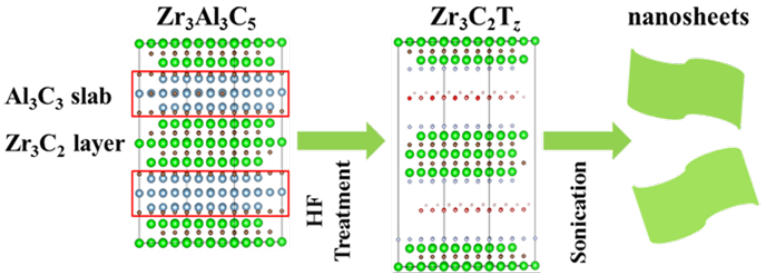

Figure 1. The schematic diagram of the synthesis of $Zr_3C_2T_x$

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On the time required to freeze water

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Abstract

The behavior of the TIP4P/ICE model of water at low temperatures will be studied in detail. The growth rate of ice will be determined for TIP4P/ICE and compared to recent experimental results. By using the seeding technique the nucleation rate for the formation of ice at several pressures will be estimated and compared to experimental results, showing good agreement. The interfacial free energy between ice and water increases with the applied pressure and this is the key to understand why the homogeneous nucleation line is not parallel to the melting curve.
By using Avrami's expression we estimate the crystallization time for supercooled water. For the TIP4P/ICE the minimum in the crystallization time is found at about 55K below the melting point, and its value is of about ten microseconds. This value is compatible with the minimum cooling rate required to avoid the formation of ice and obtaining a glass phase. The crossover from the nucleation controlled crystallization to the growth controlled crystallization will be discussed for systems of finite size. This crossover could explain the apparent discrepancy between the values of J obtained by different experimental groups for temperatures below 230K and should be considered as an alternative hypothesis to the two previously suggested: internal pressure and/or surface freezing effects. The thermodynamic properties of the fluid phase at low temperatures will be studied in detail. A maximum in the compressibility was found for the TIP4P/ICE model in supercooled water. The relaxation time is much smaller than the crystallization time at the temperature at which this maximum occurs so that this maximum is a real thermodynamic feature of the model. The possibility of a liquid liquid critical point for the TIP4P/ICE will be discussed.

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Grid-characteristic method on unstructured meshes: problems and applications.

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Forward simulation of wave processes can be applicable to a wide variety of areas: non-destructive testing, seismic measurements, low-speed collision modelling. However, in cases of heterogeneous media and complex geometry in 3D it remains to be a challenging question for today. Usage of essentially unstructured tetrahedral computational grids is the most common approach to deal with an entirely arbitrary geometry. An explicit second-order dimensional-splitting method based on hyperbolic properties of wave equations is proposed for that case. The method is applied to the simulation of ultrasound investigation in human body within the scope of linear elastic and acoustic rheology models with Maxwell viscosity. The approach is demonstrated to be robust, however, the accuracy of simulation near small grid inhomogeneities leave something to be desired.

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Abstract

In this paper, we study our research on creating effective path finding algorithm using offline and online computed tactical information. We consider the Voronoi-based navigation mesh and construct pathfinding trajectories over adjacent cells of Voronoi diagram, represented by graph. We study the diffusion process of kill/death ratio on graph in a first person shooter and its effects on online learning more safe trajectories during several rounds of playing multiplayer video game. We compared the results with offline visibility map and obtained the results that adding frag map calculated over diffusion process on path finding graph results in average 12% advantage in terms of match scores over several rounds.

Numerical simulation of the dome of an atomic reactor destruction due to the earthquakes

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One of the main dangers for people nowadays is the earthquakes. During the initiation of seismic activity, a set of elastic waves with different amplitudes and frequencies propagate from the hypocentre. Reaching the day surface, they cause vertical and horizontal movements of the ground that leads to the disruption of ground facilities. To ensure the safety of people in cities it is crucial to have technologies for precise estimation of seismic resistivity of buildings. Nowadays the mainstream is the the calculation of the natural frequencies of construction. It is believed that if the set of frequencies, in the form of a superposition of which a perturbation is representable, is far from the natural frequencies of the structure, then the seismic stability of this structure is great. Unfortunately, this method doesn't provide adequate precision.

In this work we present the other method based on the numerical solution of the elastic system of equations with destruction using grid-characteristic method on hexahedral meshes. The discrete model of destruction is used. Two different mechanisms are taking into account. When the main stress is higher than the tensile strength of material a new crack (plane) is generated with the normal along the main stress. Shear destruction is identified if deviator of stress tensor exceeds the yield stress of material. In this case the shear modulus is drastically decreased.

To illustrate this method, we simulated the influence of dynamic signal from the earthquake on the dome of an atomic reactor as full-wave 3D problem. To cover the whole calculation domain a set of 22 structured meshes was used (see Fig. 1). Characteristic diameter of this construction was 20 m, thickness of wall – 2 m, height of foundation – 2m. One shot of the earthquake was simulated (see Fig. 2). Its duration was 50 ms, wave length – much bigger than total height of construction.

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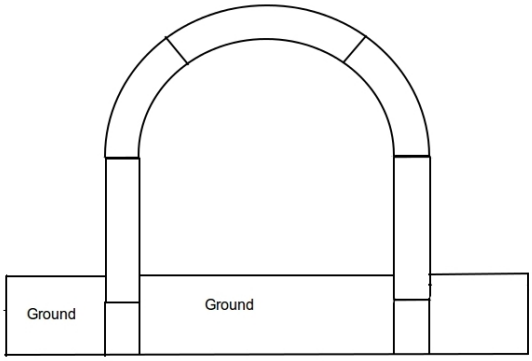

Figure 1. 2D slice of nuclear power plant model

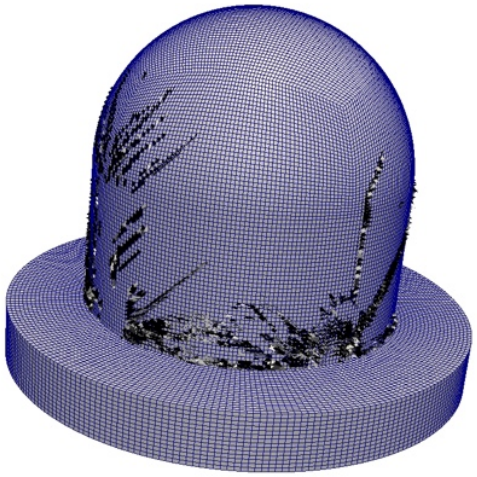

Figure 2. Zones of destruction due to high amplitude impact

ON PORTING OF APPLICATIONS TO NEW HETEROGENEOUS SYSTEMS

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This work is devoted to the development of guidelines for the porting of existing applications to GPGPU. The paper provides an overview of the current state of the parallel computation area with respect to GPGPU. Various approaches to the organization of parallel computations are considered, and their effectiveness is evaluated in relation to the application under study. Special attention is given to delicate relation between vectorization (done on the level of most internal loops of code) and parallelization (done on the external computational tasks). The proper combination of this makes it possible to get optimal speed-up. But in reality it can be too ideal point of view because of two principle limitations – memory of the GPGPU and the link between CPU and GPGPU.

We argue that due to those limitations it is impossible to work out general strategy of porting applications to any GPGPU. Anyway for particular codes and special GPU's the proposed approach makes it possible to get speed-up's up to hundreds. This becomes even more effective when combined with virtualization of GPGPU to provide the balance between the size of computing core and rate of data transfer to it.

We illustrate our approach on the examples of OpenFoam and DSMC porting to P100 GPU. It is clear, that only combination of all proposed measures makes it possible to get necessary speed-up.

As a result, a strategy has been developed for migrating the application to a heterogeneous system. The results of the work can be applied when transferring similar applications to GPGPU or modified to transfer other types of applications.

An integral model of the convective jet including the pressure effect and the forms of the vertical fluxes in the turbulent surface layer of the atmosphere

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Abstract:

The study presents a modified integral model of the convective jets that includes the effect of the pressure. The model corresponds to the steady turbulent jets that arise from the point sources of the heat and the momentum in the neutral or unsteady stratified atmosphere. The analytical solutions of this model are presented in the polynomial forms of the dependence of the vertical velocity and the buoyance on the height. The comparison between the exact solutions of this model and the analytical solutions of the integral models of the stationary jets, which are based on the vertical boundary-layer approximation, is performed.

It is shown that for the buoyant jet in the neutral stratified atmosphere the effect of the pressure force increases the amplitude of the temperature variance and decreases the amplitude of the vertical velocity by 10%. For the spontaneous jet in the unsteady stratified atmosphere the effect of the pressure force maintains the amplitude of the temperature variance and increases the amplitude of the vertical velocity by 15%.

It is found that there are dynamic invariants expressing the law of the uniform distribution of potential, available potential and kinetic energies along the axis of a jet. Essentially, the assemble of the spontaneous jets forms the profiles of the second turbulent moments of the vertical velocity and buoyance near the horizontal homogeneous heated underlying surface in the convective layer of the atmosphere and the ocean.

NONCLASSICAL NONEQUILIBRIUM TRANSPORT ON THE BASIS OF NUMERICAL SOLVING THE BOLTZMANN KINETIC EQUATION

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There are some interesting specific physical kinetic effects based on the gradients of macroscopic quantities (temperature, pressure etc), such as thermodiffusion, thermal transpiration, thermophoresis and others. These phenomena are beyond the scope of description by thermodynamic methods. But there are other effects related to problems with nonequilibrium boundary conditions. For investigation of these new problems the direct methods of solving the Boltzmann and other kinetic equations [1, 2] have been used. Such problems have been studied in [3, 4]. For different problems with nonequilibrium boundary conditions nonclassical transport in flows appears. In particular, heat can be transferred from the region with the lesser temperature to the region with the greater temperature. The result does not contradict to the well-known relations of thermodynamics which are valid for states near equilibrium. In the problems under consideration Knudsen number is of the order of unity, so the Chapman-Enskog expansion is unsuitable. Thus in a general case macroscopic relationships, e.g. the Fourier equation cannot be derived. For some problems results of the mathematical simulation have been confirmed by analytical approximations. Several solutions by the Boltzmann equation were compared with the solutions by Direct Simulation Monte Carlo method, this comparison shows good coincidence. One important result has been obtained for a heat conduction between two plates with different temperatures. The average macroscopic mass flow in this problem equals to zero. For such a problem with traditional kinetic boundary conditions with diffuse reflections of molecules the ordinary heat conduction qualitatively corresponding to the Fourier law is obtained in the whole range of Knudsen number. For a problem with nonequilibrium boundary conditions a mentioned anomalous heat conduction was observed for Knudsen number of the order of unity. New problems with nonequilbrium boundary conditions of the "membrane-like" type is also considered, the regimes with anomalous transport are demonstrated. Possible experimental tests with the use of the so-called optical lattices (see [5]) and perspectives of applications are discussed. The present results can be compared with the recent construction of Maxwell's demon (for a single-electron device), see e.g. [6].

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How the methods of natural sciences can help in the studies of ethnically mixed families?

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Statistical physics is the branch that uses different mathematical methods in solving not only physical problems. The field of application may be the interdisciplinary studies of many social phenomena. The reason is that they have a stochastic nature. The aim of the paper is to display the opportunities of using the methods of natural sciences in the social sciences. The example is suggested of the joint research in demography, sociology, statistics, and ethnography of ethnically mixed families. These are the marital couples where a husband and a wife consider themselves as belonging to different ethnicities. It was demonstrated that application of the reasons used in the kinetic theory helps us to introduce new measure that describes mutual attitudes for a specific combination of ethnicities. The idea of this measure calculation is quite simple. We simply relate the number of marriages established from the reasons of full randomness of collisions of "particles" (persons) and their connection irrespective to their type, and the phenomenology – the actual number of families for a given combination of husband's and wife's ethnicity observed form the population censuses. What we mean by "collision" is any form of personal or social interaction (meeting, conversation, participation in small groups at work, family, schooling, tourism, journey, sports, etc.). This measure may be called inter-ethnic propensity, or its inverse value as an inter-ethnic distance. One more new measure is used to describe a propensity to form ethnically mixed marriage with a spouse of any different ethnicity. Numerically it is calculated as a share of ethnically mixed families of a given ethnicity among all the families of this ethnicity. Similar to chemistry, it may be called "valency".

It was shown that in such multiethnic country like Russia both measures cannot be estimated as the good and adequate ones. The reason is a significant inhomogeneity of ethnicity distribution by territory of the country. Some of such peoples have their own national republics, some do not have such administrative-territorial organization but reside in a few number of regions. However this does not mean that the measures introduced are the wrong ones. Simply before their calculation we require to perform co-called "geographical" decomposition that explicitly takes into account the fact and the extent of territorial distribution of population of all the ethnicities in this country by regions. In terms of kinetic approach for gases it may have the analogy of various density of different particles by the volume they are placed in, that is required at consideration of their physical properties.

The paper also aims to display that using of methods from natural sciences lets us produce much more clear explanation, more simple understanding, modeling, interpretation of the processes under consideration.

Description of the models and measures mentioned, the results of the approach suggested were published in the new electronic journal Demographic Review (Demograficheskoe obozrenie, in Russian) and presented at the international conferences at the HRU Higher School of Economics and Moscow State University.

As a new problem statement in ethnography not solved yet an analogy with thermodynamics is suggested for analysis of ethnical population structure and its evolution. Some questions in this field are: Is the entropy actually growing over time as applied to the composition of population by ethnicities? May the dynamics of the population of the USA considered as the well-known "melting pot" for ethnicities be interpreted in the way similar to the second law of thermodynamics? Why this law is not valid in the general case for population ethnic structure at the level of city or country?

2D composites with rod-like fillers: Computer simulation of electrical conductivities

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By means of computer simulation, we examine electrical conductivity of two-dimensional composites with rod-like fillers [1–3]. We use a lattice approach. A host matrix (a substrate) is treated as a square lattice; rod-like fillers are represented as linear k-mers, i.e., particles occupying k adjacent adsorption sites of the lattice. The k-mers are deposited onto the lattice by the random sequential adsorption. Overlapping with predeposited k-mers, hence, a monolayer is formed. Detachment of the deposited k-mers from the surface is forbidden. We consider two different models, viz., an insulating host matrix and conducting fillers and a conducting host matrix and insulating fillers. A high electrical contrast between a host matrix and fillers is assumed. We examine both the isotropic and anisotropic systems. We transform the monolayer into a random resistor network to calculate its effective electrical conductivity. The electrical conductivity of such a monolayer in both the x and y directions for different lengths and concentrations of the k-mers is calculated [1], and its behavior in the vicinity of insulator-to-conductor phase transition is analyzed. An insulator-conductor phase transition is observed near the percolation threshold. For large values of k (k=64,128), the electrical conductivity increases rapidly with the initial increase of concentration of fillers from 0 to 0.1

Additionally, we examine the effect of defects on the behavior of electrical conductivity in such composites [2]. In our study, the defects in the host matrix are distributed randomly and these lattice sites are forbidden for the deposition of k-mers. The k-mers are deposited onto the substrate until a jammed state. The defective sites are distributed randomly on the deposited k-mers. The lattice sites filled with k-mers have a high electrical conductivity, whereas the empty sites, and the sites filled by either types of defect have a low electrical conductivity. The effect of the concentrations of defects on the electrical conductive is studied.

We also study effect of diffusional relaxation of deposited particles on electrical conductivity of the 2D composite [3]. In this study, after deposition of k-mers up to a given concentration, the random walk (translational diffusion) of deposited k-mers is allowed. When the concentration of fillers exceeds the percolation threshold, the system in its initial state is a conductor. Diffusional reorganization leads to a decrease in the electrical conductivity. The conductor–insulator phase transition occurs when the concentration of fillers is slightly above the percolation threshold.

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Anderson transitions of matter waves in laser speckle potentials

Giuliano Orso

Anderson localization, namely the absence of waves diffusion in disordered media, is a completely general phenomenon resulting from the interference of multiple scattering paths. We present recent numerical results [1,2] for Anderson localization of matter waves, describing the behavior of ultra-cold atoms in laser speckle potentials. Our computations of the critical point of the Anderson transition, the mobility edge, are based on a high order spatial discretization of the Schrodinger equation, to which we apply transfer matrix and finite size scaling techniques.

[1] G. Orso, PRL 118, 105301 (2017)
[2] M. Pasek, G. Orso and D. Delande, PRL 118, 170403 (2017)

Multioperators strategy for constructing arbitrary high-order approximations and schemes for PDE's with applications to fluid dynamics.

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The multioperators technique is outlined as a way to construct arbitrary high-order numerical analysis formulas and, in particular, arbitrary high-order approximations to PDE's. High orders are obtained via increasing numbers of basis operators with fixed stencils rather than by enlarging stencils or polynomial orders (that is, by increasing numbers of basis functions). Using a mesh with the mesh size h, the basis operators are generated by one-parameter families of compact approximations $L_h(c)$ approximating a target operator L. The resulting multioperator then looks as $L_M(c_1, c_2, \ldots . c_M) = \sum_{i=1}^{M} \gamma_i L_h(c_i)$ where $c_1, c_2, \ldots . c_M$ are the input values of parameter c.The $c_i$values uniquely define the γ_i coefficients making approximation orders like $O(h^K)$ where K is proportional to M. Considering c-values as free parameters, one can control the multioperators properties. Using multioperators with chosen numbers M and the c- values, one can construct arbitrary high-order formulas for derivatives, integrals, interpolation/extrapolation etc..

In the present talk, multioperators-based schemes for convection, convection-diffusion and fluid dynamics equations are considered. Using recent version of the basis operator composed by two-point operators, the $2M$th-order multioperators for the first derivatives in space are constructed. Presently, the schemes up to 36th-order are tested against benchmark problems. The parameter's values were chosen to minimize the phase errors of convection equations for the highest wave numbers supported by meshes. The optimized schemes are aimed in particular at highest resolution of small scales during possibly long time integration when investigating for example turbulence, aeroacoustic problems etc..

Examples of using 10-16th-order multioperators-based schemes for the Navier-Stokes are presented. They concern with flow instability and sound radiation of subsonic and slightly supersonic jets and isolated vortices. The hybrid schemes for strongly discontinuous solutions are outlined. They are tested against the Riemann problems with strong shocks and contacts.

Elastic migration based on the Born approximation

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One of the main methods of fossil fuels discovery and engineering surveying of geological structure of Earth's crust is seismic tomography. Migration imaging is one of its techniques, which solves the problem of locating interfaces in the medium under investigation. There are many methods solving this problem in the acoustic case. Obvious switchover to elastic media, where compressional and shear waves are present, could enhance migration images.

In this work we discuss a method of migration imaging for elastic quasi-homogeneous media based on computation of adjoint operator in Born approximation. For permanently polarized point source $\mathbf{f}^{\mathrm{e}}(\mathbf{r},t) = \delta(\mathbf{r}-\mathbf{r}_{\mathrm{s}})f''(t)\mathbf{f}$ and velocity survey data $\mathbf{d}$ at points S and times T migration images are determined by the equations

$$\mathrm{migr}_{\beta}(\mathbf{r}) = \frac{1}{\rho(\mathbf{r}_{\mathrm{s}})}\sum_{\alpha}\int_{S}\int_{T}\mathbf{d}(\mathbf{r}_r,t)\cdot\mathbf{D}^{\mathrm{r}}_{\alpha}\left\{\mathbf{D}^{\mathrm{s}}_{\beta}(\boldsymbol{\varphi}_{11}+\boldsymbol{\varphi}_{12})+\mathbf{D}^{\underline{s}}_{\beta}(\boldsymbol{\varphi}_{21}+\boldsymbol{\varphi}_{22})\right\}dtdS,$$

$$\boldsymbol{\varphi}_{ij} = (-1)^{i+j}\frac{f\left(t-s_{\beta}R_{s,i}-s_{\alpha}R_{r,i}\right)}{16\pi^2 c_{\beta}^2 R_{s,i}R_{r,i}}\mathbf{f},$$

$$R_{i,1}=R_i,\qquad R_{i,2}=\underline{R_i},\qquad R_i=|\mathbf{r}_i-\mathbf{r}|,\qquad \underline{R_i}=\left|\mathbf{r}_i-\underline{\mathbf{r}}\right|,\qquad \underline{\boldsymbol{r}}=(x,y,-z)^{\mathrm{T}},$$

where $\alpha,\beta\in\{\mathrm{p},\mathrm{s}\}$, $\mathbf{D}^{i}_{\mathrm{p}}=\nabla^i\nabla^i$, $\mathbf{D}^{i}_{\mathrm{s}}=-\nabla^i\times\nabla^i\times$, $\mathbf{D}^{\underline{i}}_{\beta}$ is obtained from $\mathbf{D}^{\underline{i}}_{\beta}$ by $\partial_{z_{\mathrm{s}}}\to-\partial_{z_{\mathrm{s}}}$, $s=c^{-1}$ and c_p, c_s are pressure and shear waves velocities. Migration images for model with curvilinear interfaces are shown at Figure 1. Described method is compared to a popular method based on Kirchhoff integral formula too.

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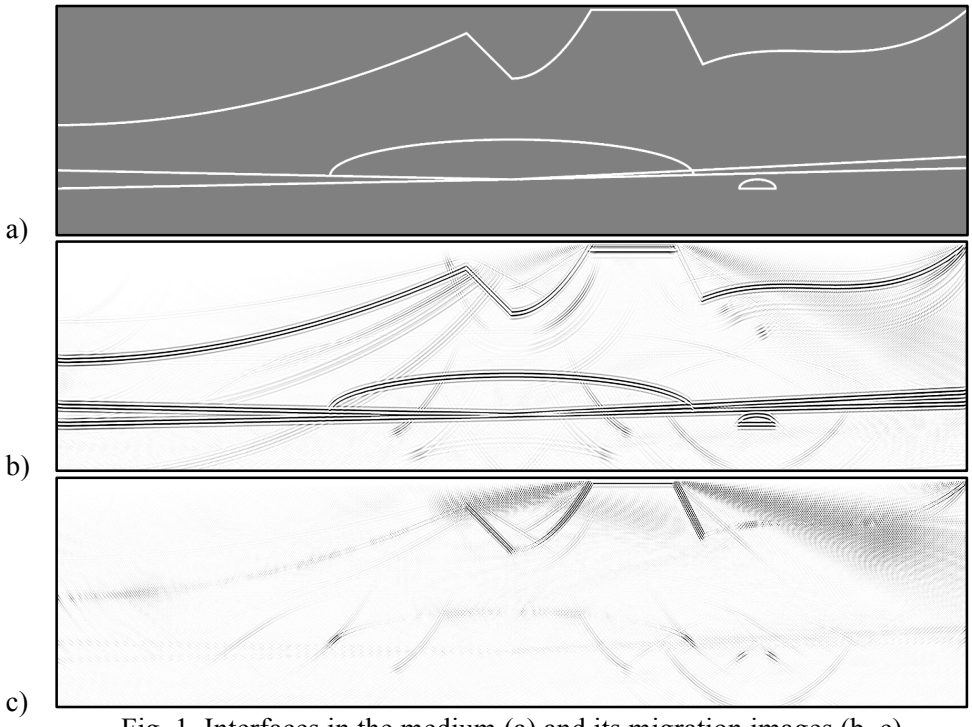

Fig. 1. Interfaces in the medium (a) and its migration images (b, c)

Enhancement in specific heat by nano-crystallization: softening of phonon frequencies mechanism

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Abstract

The temperature dependent specific heat $C_p(T)$ of nanocrystalline *Cu (8 nm)* and *Pd (6 nm)* is theoretically analyzed and compared with specific heat of their corresponding bulk materials in the temperature range from *150* to *300 K*. It is revealed that the C_p values of nanocrystalline *Cu (Pd)* are about *10% (40%)* higher than that of their corresponding bulk form, the softening of phonon frequencies at interfaces in nanocrystalline materials is argumented as the main mechanism responsible for enhancement in C_p in present work. Lattice (phonon) specific heat is obtained following an overlap repulsive potential using Debye model. In nanocrystalline materials having large interface volume ratio, the phonon frequencies and Debye temperature are comparatively less at the interfaces than at the core of nanocrystal. The contributions to specific heat due to atoms present at interfaces (C_{ph}^{IF}) and those present at the core of nanocrystal (C_{ph}^{NC}) are estimated separately by estimating the characteristic Debye temperature (θ_D) from elastic force constant (κ). The temperature derivative of the internal energy yields the electronic contribution to specific heat (C_{el}). The present investigation based on the softening of phonon frequencies mechanism is successful to explain the enhancement in specific heat by nano-crystallization.

Keywords: Nano-crystalline materials; specific heat; phonons.

Properties of the Tent map for decimal fractions with fixed precision

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Abstract. A one-dimensional discrete Tent map is a well-known example of a map whose fixed points are all unstable on a segment [0,1]. This map leads to the positivity of the Lyapunov exponent for the corresponding recurrent sequence.
Therefore in a situation of general position, this sequence must demonstrate the properties of deterministic chaos. However if the first term of the recurrence sequence is taken as a decimal fraction with a fixed number "k" of significant digits after the decimal point and all calculations are carried out accurately, then the situation turns out to be completely different. In this case first the Tent map does not lead to an increase in significant digits in the terms of the sequence, and secondly demonstrates the existence of a finite number of eventually periodic orbits, which are attractors for all other decimal numbers with the number of significant digits not exceeding "k".

In this paper we consider the simplest, not containing parameters, Tent map

$$T(x) = 2 \cdot \min\{x, 1-x\} = 1 - 2 \cdot |x - 1/2|, \qquad (1)$$

and the recurrent sequence

$$x_{n+1} = T(x_n). \qquad (2)$$

Various modifications of this map containing additional parameters can be found both in papers dealing with environmental processes [1,2], and in cryptography [3,4] and in modeling open systems [5,6].

In this paper, the following is shown. Definitions. The set I_k (k = 1,2, ...) is a collection of numbers of the form $0.\alpha_1\alpha_2\alpha_3\ldots,\alpha_k = \sum_{i=1}^{k} \alpha_i \cdot 10^{-i} \in I_k$, where α_i are integers from 0 to 9, and $\alpha_k \neq 0$. The number of elements of this set is $NI_k = 9 \cdot 10^{k-1}$. $I_{k1} \cap I_{k2} = \varnothing$ *if* $k1 \neq k2$. If $J_k = 0 \cup \bigcup_{q=1}^{k} I_q$, then the number of elements of the set J_k is a value $NJ_k = 10^k$.

We call a cycle $S_k(m_k)$ a set of m_k elements $\in I_k$ for which the following property holds: for any $x \in S_k(m_k)$ an image $T(x) \in S_k(m_k)$. The length of the cycle (a number m_k) is determined by the number k by the formula $m_k = 2 \cdot 5^{k-1}$. Statement. For each set I_k there is a unique cycle $S_k(m_k)$.
The union of all cycles contained in a set J_k is the set of numbers $G_k(M_k)$ occurring in all cycles $G_k(M_k) = 0 \cup \bigcup_{q=1}^{k} S_q(m_q)$. The number of elements in the collection of cycles is $M_k = 1 + \sum_{q=1}^{k} m_q = \frac{1}{2}(5^k + 1)$ (odd number). The ratio of the number of these elements to the total number of elements is $\mathrm{M_k/NJ_k} = (2^{-k} + 10^{-k}) \cdot 2^{-1} < 2^{-k}$.
Definition. The sequence of numbers defined by the recurrence relation (2) is called an *orbit* of the map (1), induced by the quantity x_0. We call the orbit as eventually periodic orbit, if the orbit has the structure $x_0, x_1, x_2, \ldots, x_m, x_{m+1}, x_{m+2}, \ldots, x_{m+n}$, and $x_{m+n} = x_m$.

Statement. The set $G_k(M_k)$ consists of eventually periodic orbits and is an attractor for any $x_0 \in J_k$. All the statements are true only when using exact calculations (symbolic calculations) without round-off, which is possible in the package Mathematica.

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DFT simulations of Sb(111) surface states.

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Antimony is a Pierls semimetal. I.e. electronic and atomic structure is a consequence of Pierls transition. Atomic structure can be described in terms of Pierls distortion of a simple cubic structure of praphase. As a result a lattice period of Sb in [111] direction exceeds twice one of the praphase. Doubling of period leads to creation of covalent bods between double atomic plains while the double plains are connected by Van der Waals forces. Dispersion of bulk electrons reveals a small gap in a vicinity of Γ point. Surface states spectrum is a resulted from surface crystal lattice symmetry [1]. Non degenerated Dirac massless cone of surface states in a vicinity Γ point with a Dirac point at 270 mev below the Fermi level is due to strong spin orbit coupling.

In this work we present the results of our simulations of Sb(111) crystal structure and surface states in a frame of DFT approximation. The simulations were performed for Sb(111) cleaved both by Van der Waals and covalent bonds. Crystal structure of Sb(111) cleaved by Van der Waals bonds can be described in terms of bulk like structure with a small distortion of atomic interplane distance (about 1%) in the vicinity of the surface. In contrast, structure of the crystal cleaved by covalent bonds reveals break of Pierls distortion in a top 8 atomic layers. Dirac cone is robust to a way of cleavage while a local break of a Pierls transition in a vicinity to the surface leads to deformation of electron spectrum of a bulk electrons. As a result electron subbands appears of in an energy gap close to the Fermi level. Dirac cone of surface states was found to be robust on adsorption of Pb at the surface. The results of simulations were confirmed in ARPES, STM, STS experiments.

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New approach for structure reconstruction with machine learning methods in XFEL and Cryo-EM experiments.

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Structure reconstruction is one of important goals of modern science. Knowledge of atomic structure lead to significant achievements in various science fields. Rapid evolution in machine learning provide new instruments for data analysis in computer vision, classification, and other fields.

The rapid development of neural networks allowed to create new algorithms and data analysis schemes that are highly competitive with the best existing algorithms that have developed over the decades. In this work we present review of current state of art machine learning techniques for experimental data processing and 3d structure reconstruction of nanoscale particles and macromolecules. The methods are designed for X-ray Free Electron Lasers (XFEL) and Cryogenic Microscopy (CryoEM) experiments. We show our machine learning techniques to be effective for experimental data filtering and sorting and be promising for particle orientation determination. We examine various algorithms including Neural Networks, Decision Trees, Support Vector Machines and show their applicability and optimal sets of parameters for different stages of analysis. Our work is a joint effort of teams from Kurchatov Institute Supercomputer, CryoEM laboratory and DESY.

Evaluation of dislocation mobility and plastic properties of molybdenum using molecular dynamics.

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Being a widely spread construction material, alloyed and pure molybdenum is usually affected by continuous external stresses. Therefore it has to be studied in terms of plasticity and creep which is helpful for safety issues. Plastic properties of metals are considered to be governed by variety of processes including twining, martensite transitions and dislocation movement. In case of body-centered cubic metals, the contribution of twinning and martensite transitions to plastic properties can be neglected and plasticity can be studied in terms of motion of dislocations.

Since dislocations in real materials usually form a complex forest, it is challenging to study the behaviour of a single dislocation in an experiment. The use of molecular dynamics, which has already shown good results in simulation of atomic-level processes, allow one to consider the movement of a single dislocation. In this work the dislocation movement was studied using the method of molecular dynamics with ADP interatomic potential.

To perform dislocation mobility estimation, the calculation cell with a single dislocation was created. The results of calculations showed the screw dislocation to be less mobile than edge one which is in a agreement with the common conception. It means that plastic properties of molybdenum is controlled by the motion of screw dislocations. In addition, two regimes of dislocation motion are shown to exist: thermo-activated and viscous regimes. The main differences between these two regimes are the forms of velocity-stress and velocity-temperature dependencies. Moreover, the movement in the thermo-activated regime is characterised by kink-pair nucleation and migration. In contrast, the behaviour of kinks do not govern the motion in the viscous regime.

Using theoretical models of a dislocation movement, we estimated the enthalpy of a kink-pair nucleation and the friction coefficients of the dislocation motion in the viscous regime. In addition, making a comparison to experimental data we estimated the density of dislocations in the molybdenum single crystal. Finally, the obtained dislocation mobility functions allowed us to make the estimation of yield stress of molybdenum using the method of dislocation dynamics.

Optimal vaccine allocation in two SIR centers with migration fluxes

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Abstract

The aim of this work is to investigate the optimal vaccine sharing between two SIR (susceptible-infected-removed) centers in the presence of migration fluxes of susceptibles and infected individuals between the centers. Optimality of the vaccine allocation means the minimization of the total number of lost working days during the whole period of epidemic outbreak $[0,t_f]$, which can be described by the functional $Q = \int_0^{t_f} I(t)\mathrm{d}t$ where $I(t)$ stands for the number of infectives at time t. We explain behaviour of optimal allocation which depends on the model parameters and the fraction of available vaccine V.

Diffusion mechanisms in systems ionic liquid - aromatic hydrocarbons by molecular dynamics simulation

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Ionic liquids (ILs) have been extensively studied as replacements to sulfolane in the separation of aromatics from alkanes. The employment of ionic liquids (Ils) could reduce energy requirements and operating costs of the aromatic extraction from oil and its a result of their nonvolatile character. However, the ILs studied so far have shown mass-based aromatic distribution ratios lower than the sulfolane values, which would increase the solvent-to-feed ratio in the extractor. The performance of hydrophobic ionic liquids on extraction of aromatic compounds such as benzene, toluene, anisole, phenol and c-hexane derivatives from aqueous solution was investigated experimentally.

The presented research studied the effect of aromatic hydrocarbons on structure and diffusion in ILs. The MD method was applied using a modified DL_POLY_4.05 with a time step of 2 fs. The long-range electrostatic interaction was taken into account by the Ewald method. In the calculations, the cations, anions, and atoms forming the molecules of the added substance (hydrocarbons : benzene, toluene, phenol , anisole and c-hexane) ware treated as solid charged model systems with a fixed geometry. The methyl in the dmim+ and toluene ware treated as a pseudoatom with the total charge. All the studies were conducted for systems composed of 192 dmim+ cations, 192 chlorine anions Cl^-, and one solute molecule at T = 400 K. The unit cell volume was calculated from the experimental values of the ionic liquid density at $T = 400$ K. The calculations used periodic boundary conditions. The electrostatic interaction at short distances was described using point charges on each atom. The interaction between dmim+ and Cl– molecules in the ionic liquid was described using the Buckingham potential for interactions at short distances. The Berendsen thermostat was used to stabilize the system in the $N\,V\,T$ - ensemble.

Analysis of the data allowed to establish:

(1) The salvation effect in systems ionic-liquid (dmim+/Cl-) - non-polar solute molecules (benzene, c-hexane) has qualitatively similar to the behavior of the hydrophobic hydration of aromatic solute molecules in liquids like water. The results of the computer experiment for the average total energy of the intermolecular interaction $\langle E\text{tot}\rangle$ for the dmim+/Cl– non-polar solutions at $T = 400$ K show that the intermolecular interaction $\langle E\text{tot}\rangle$ does not depend on the physical characteristics of the structural and non-polar substances dissolved. Therefore, as a possible selection criteria for the data analysis is not appropriate to consider the thermodynamic and structural characteristics of the system. In this case, need to do analysis of its dynamic properties. Based on the data obtained from MSD and VAF the different diffusion mechanisms [1] of nonpolar solute molecules in IL ware determined.

(2) The salvation effect in systems ionic-liquid (dmim+/Cl-) - polar solute molecules (toluene, phenol, anisole) has qualitatively similar to the behavior of the hydrophobic hydration in liquids like water too [2] . The results of the computer experiment for the average total energy of the intermolecular interaction $\langle E\text{tot}\rangle$ for the dmim+/Cl–polar hydrocarbons at $T = 400$ K show that the intermolecular interaction $\langle E\text{tot}\rangle$ depend on polarity and the physical characteristics of the structural and polar substances dissolved. Based on the data obtained from MSD and VAF the different diffusion mechanisms [3] of polar hydrocarbons solute molecules in IL ware determined.

(3) Dissolution of hydrocarbons molecules whose size is much higher than the maximum length of the hydrogen bond leads to a radical restructuring of the network of hydrogen bonds in the system up to the loss of its percolation properties.

The results showed that IL had good ability in the extraction. Molecular structure of aromatic compounds was found to have a great influence on the extraction. Due to the increase of the hydrophobicity of solute, the partition coefficient of aromatic compounds was increased.

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Modeling of charge-stabilized colloidal crystals with bcc crystal lattice

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Elastic properties of the charge-stabilized colloidal crystals with body-centered cubic crystal lattice are studied numerically. The study is based on the Poisson-Boltzmann non-linear differential equation [1].

The system under study is an array of spatially ordered electrically charged spherical particles immersed into the electrolyte solution. Such systems have some technological applications, in particular, in photonic crystal manufacture. They can also serve like models for disordered colloids and more complicated systems of micelles or polyelectrolytes including DNA molecules.

Colloidal crystals are treated as a medium with initial stress governed by the Poisson-Boltzmann (PB) nonlinear differential equation [1]. The properties of the system are fully described by solution of the PB equation and no prescribed inter-particle potentials are needed. Owing to the non-zero initial stress, elastic properties of charge-stabilized colloidal crystals have some specificity as compared with conventional crystals [2], in particular, the first-order elastic constants of these crystals are not equal to zero. Numerical procedure to determine the first and second order elastic constants and its program implementation are described.

Elastic properties of the colloidal crystal are fully described by solution of the boundary value problem for the Poisson-Boltzmann equation. The boundary value problem is formulated for the crystal in an arbitrary spatial configuration. Both the constant surface charge density (cc) and constant potential (cp) models of charged particles are included. Parametrization of the model by the value of deformation and the lattice parameter enables building a unified procedure for the numerical solution of the boundary value problem which is suitable for any configuration. Numerical solution of the PB equation is carried out by the finite element method using the irregular meshes of tetrahedral elements. Typical triangulation contains several millions degrees of freedom while typical computer experiment incorporates up to several thousands of spatial configurations. Calculations were partly supported by the Supercomputing Center of Lomonosov Moscow State University [2].

Elastic constants of the first and second order were obtained for different values of the lattice parameter. Stability of the crystals and the role of the many-body effective interactions are discussed.

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Simulation System for Making Political and Macroeconomical Decisions and Its Development

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Abstract. Object of this research are macroeconomical indicators, which are important to descript economical situation in a country. Purpose of this work is to identify these indicators and to analyze how the state can affect these figures with available instruments. Here was constructed a model where the targets can be calculated from raw data – tools in the field of economical policy.

Software code that implements all relations among the indicators and allows to analyze with high accuracy, sufficiently successful economic policies and with the help of some tools, you can achieve better results. This model can be used to forecast macroeconomic scenarios. The corresponding values of the objective (outcome) variables are set as a consequence of the configuration data of the previous period, subject to external influences and depend on the instrumental variables.

The results may be useful in economical predictions. The results were successfully checked on real scenarios of Russian, European and Chinese economics. Moreover, the results can be applied in the field of education. This program is available to use as “economical game”, in which you can virtually implement various macroeconomical scenarios and draw conclusions about their success.

Lattice study of effective gluon mass at various boundary conditions

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

Monte Carlo Simulation of Random-Anisotropy Amorphous Magnets

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Amorphous alloys based on rare-earth metals are of great interest due to their unique magnetic properties. In this work we report on the Monte Carlo simulation of magnetic properties of binary amorphous alloys of the Re-Tb system which are not studied so far.

Using the Monte Carlo method in the frame of the Heisenberg model, the computer simulation of magnetic properties of pure amorphous Tb and Re-Tb amorphous alloys was performed. The model Hamiltonian contained two terms responsible for nearest-neighbour exchange interaction between the Tb ions with the mean value J_0 and for random single-ion anisotropy D. For pure amorphous Tb the dependence of the temperature of the spin-glass-like transition T_f on the D/J_0 ratio was calculated. Thus, the magnetic phase diagram for an amorphous magnet with random anisotropy in the $D/J_0 - T$ coordinates was constructed.

In the models of the Re-Tb amorphous alloys, the spin-glass-like phase transition was also observed. With increasing concentration of Tb atoms, the transition temperature linearly increases, which is in a good agreement with the experimental results. The spin-glass transition is observed only above the percolation threshold in this system, i.e. at x>13 at. % Tb.

Magnetic structure of Re-Tb amorphous alloys was studied on the microscopic level with the use of spin-spin correlation functions and angle spin correlation functions.

The magnetization relaxation after switching off the external magnetic field at different values of D/J_0 was also studied. For amorphous Tb and Re-Tb amorphous alloys the magnetization relaxation goes on in two stages. In the first stage, the magnetization decreases abruptly by a definite magnitude ΔM_Z. At this stage the magnetic moments reorient to the directions determined by the random anisotropy axes. At the second stage the magnetization decreases very slowly according to the logarithmic law. At this stage the magnetic moments of Tb atoms rotate by small angles due to competition of exchange interaction and random anisotropy.

Algorithms for solvents of unilateral matrix polynomials over prime finite fields

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Unilateral (monic) matrix polynomial of n-th order is an expression of the form

$$\mathcal{F}(X) = X^d + \mathbf{F}_{d-1} \cdot X^{d-1} + \cdots + \mathbf{F}_2 \cdot X^2 + \mathbf{F}_1 \cdot X + \mathbf{F}_0,$$

where $\mathbf{F}_i, i = 0, ..., d-1$ («coefficients») and X («variable») are $n \times n$ matrices.

In this work the entries of all matrixes are from the arbitrary fixed prime finite field $\mathbb{F}_p$.

The solvent of $\mathcal{F}(X)$ is an $n \times n$ matrix $\mathbf{S}$, such that $\mathcal{F}(\mathbf{S}) = \mathbf{0}$, where $\mathbf{0}$ is zero n-th order matrix.

The work proposes and compares several algorithms for finding solvents. All these algorithms use approach of dividing the set of all (universe) $n \times n$ matrices into several sets, and the solvents among each set the algorithms search separately.

The *first* algorithm divides all $n \times n$ matrixes over $\mathbb{F}_p$ into the three sets: the set of diagonalizable matrixes, the set of non-diagonalizable matrixes, having Jordan Normal form and the set of matrixes not having Jordan Normal Form.

The *second* algorithm divides the set of all $n \times n$ matrixes over $\mathbb{F}_p$ into the set of singular matrix and sets $\Omega_2, ..., \Omega_p$, where each Ω_i contains matrices X such that $X^i = X$ for minimal such i.

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Modeling of Fiber Orientation in a Twin-Screw Extrusion Process

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This study is to predict the fiber orientation in a co-rotating, intermeshing twin-screw extrusion process through numerical simulations based on mathematical models describing the polymer as well as fiber motions. The continuity and momentum equations are employed to describe the coupling of pressure and velocity in the flow field. The fiber orientation is governed by the tensor equation depicting the fiber behaviors of rotation and translation in space. The constant-temperature polymer melt is assumed to be fully filled in the flow path between the barrel and two co-rotating screws, and air-melt interface is not present in the simulated flow field. A dynamic grid-updating scheme is proposed to discretize the studied transit flow problem characterized by a strongly varying flow domain inside the barrel due to a periodical rotational motion of two co-rotating intermeshing screws. A body-fitted grid is separately generated for every time instance in the unsteady simulation. In this study, fibers are allowed to translate and rotate but without any breakage. The flow field is first obtained from a finite volume approach to solve the coupled governing equations, whereas a particle tracing scheme is adopted to compute the flow history of fibers traveling across the screw. Then the tensor equation is solved for fibers residing at different locations. This study can help to disclose the quantitative correlations between the processing parameters and fiber behaviors together with the understanding of fiber mechanics in an extrusion process.

Numerical simulation of solitary waves on deep water with constant vorticity

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In theoretical studies of water waves it is common to consider the fluid motion as purely irrotational. However, wave dynamics can be strongly affected by interaction with shear currents. In nature shear is generated near the water surface due to the action of surface wind stress, or near the bed of the water basin. An important special case is that of a linear shear flow, i.e. a flow with a uniform vorticity distribution. In such a system only potential part of velocity field is time-dependent, and usual techniques developed for potential waves can be applied to study its dynamics. It is known that long waves propagating against the current are weakly dispersive, and according to weakly nonlinear theory on deep water their evolution is described by Benjamin-Ono equation, which has soliton solutions. We investigate characteristics of solitary deep water waves on a flow with constant vorticity by numerical simulation within the framework of fully nonlinear equations of motion (Euler equations) using the method of surface-tracking conformal coordinates. The main aim of our work is to ensure that solutions observed are stable. To this end, we model soliton formation as a result of disintegration of an initial pulse-like disturbance. Evidence is obtained that solitary waves with height above a certain threshold are unstable.

Analytical structure of transition matrix in the Wang-Landau algorithm

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We investigate accuracy and convergence of Wang-Landau (WL) algorithm [1,2], calculating the density of states via the random walk. We build transition matrix in the energy space (TMES) [3]. We argue that criteria of the histogram flatness can be understood analyzing the properties of the TMES. TMES goes loser to the true value with the proper algorithm of the simulations and the density of states (DOS) became closer to the true values. The convergence of the density of states can be controlled by the difference of largest eigenvalue of the matrix from the unity. We calculate TMES for the case of 1d Ising model. The entries of the TMES is the probabilities of the transition between energy levels in Wang-Landau algorithm.

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Numerical modeling of thermal regime in inland water bodies with field measurement data

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Vertical temperature distribution is one of the main characteristics of natural geophysical objects. It has a great impact on biology and ecology of inland water bodies such as lakes and water reservoirs, significantly affects eutrophication, and is characterized by strong seasonal and short-term variability.

There are different models, one- and multi-dimensional, which are used for computation of the hydrological parameters, such as thermal regimes of inland water bodies. Models based on one-dimensional heat equation have less requirements for computing resources than multi-dimensional models, and demonstrate satisfactory agreement with experimental evidence [1]. On the other hand, these models require validation in accordance with the parameters of given water body, and field measurement data are used for this purpose.

Modification of the program complex LAKE, proposed in [1], and its validation in accordance with the parameters of mid-sized lowland water bodies with an example of Gorky water reservoir are reviewed in this research.

Modification is as follows:

1) Input temperature profile is defined with temperature difference between surface and bottom and thickness of mixed layer in previous version, whereas input profile is arbitrary defined as two-dimensional array of points from file in modified version. This modification allows to reproduce thermocline stratification typical for the present case.

2) Parameterization of dependence between wind speed and turbulent stress on air-water boundary is introduced. It is obtained with empirical data on wind-wave coupling of given water object.

3) Parameters of meteorological conditions are collected with combined method: information is taken from data of hydrometeorological station and files of meteorological reanalysis NCEP/NCAR.

Field measurement data is used for verification of modified model. These data were obtained from the observations during expeditions in the period 2014-2017. Measurement of the vertical temperature profiles were carried out with STD-probe, and transparency of the water was controlled with Secchi disk. Value of this parameter allows to obtain information about coefficient of solar radiation extinction in water body which is used in program complex. Coefficient of turbulence enhancement by wave breaking is adjusted empirically.

Numerical simulation with the modified model gives results which are in good agreement with the real seasonal variations of thermal regime in Gorky water reservoir. Standard deviation does not exceed 1℃ for all performed realizations. However, regimes with strong mixing are reproduced more accurate, than regimes with strong heat and weak mixing. It can be explained by not quite adequate simulation of mixing for the case of weak wind or by incorrect meteorological data, particularly the value of downward solar radiation.

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INVARIANT NUMERICAL CHARACTERISTICS OF DIFFUSION CHAOS IN THE PROBLEM OF BELOUSOV REACTION SIMULATING

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Keywords: Belousov reaction, diffusion chaos, numerical analysis

We consider the problem of mathematical modeling of oxidation-reduction oscillating chemical reactions, based on the mechanism of Belousov reaction. The process of main components interaction in the Belousov reaction can be interpreted by the predator-prey model phenomenologically similar to it. Thereby, we consider a parabolic boundary value problem consisting of three Volterra equations

$$\dot{x} = D_1\Delta x + r_1[1 + a(1 - z) - x]x, \qquad \left.\frac{\partial x}{\partial \nu}\right|_{\partial\Omega} = 0,$$

$$\dot{y} = D_2\Delta y + r_2[x - y]y, \qquad \left.\frac{\partial y}{\partial \nu}\right|_{\partial\Omega} = 0,$$

$$\dot{z} = D_3\Delta z + r_3[\alpha x + (1 - \alpha)y - z]z, \qquad \left.\frac{\partial z}{\partial \nu}\right|_{\partial\Omega} = 0,$$

which represents a mathematical model of this reaction. Here $x(t,s)$, $y(t,s)$, $z(t,s)$ stand for the concentration density of $HBrO_2$, Ce^{4+}, and Br^-, $s \in \Omega \subset \mathbb{R}^2$, $t > 0$; parameters $r_1, r_2, r_3, a, D_1, D_2, D_3$ are positive; $\alpha \in (0,1)$; Δ – Laplace operator; ν – direction of outer normal to the border $\partial\Omega$ of bounded flat area Ω with measure equals to unity.

Numerical analysis showed that as the diffusion coefficient d decreases the oscillating modes of the distributed model become more complicated. Coexisting chaotic regimes of different nature arise including chaotic oscillations with relaxation properties and self-organization modes. The solutions of the first type are similar in their properties to the homogeneous stable relaxation cycle of the system (deep minima and high δ-like bursts of the average by space value $x(t,s)$). In self-organization modes the minima of the average by space value $x(t,s)$ are separated from zero, and the bursts are not so large as in other solutions.

The calculations described in this paper were carried out using parallel technologies on a computational cluster with a massively parallel architecture.

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Modern random number generators using AVX512 instruction set

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Abstract:
The special purpose of this work is to accelerate random number generators with the use of AVX512 technology. AVX512 consists of 32 512-bit registers and set of instructions. Such instructions allow to process 16 unsigned integers simultaneously. The use of vectorization improves the performance of all the generators. The most modern and reliable generators were chosen: MT19937 [1], MRG32K3A [2], LFSR113 [3], GM19, GM31, GM61 [4, 5], and GM29, GM55, GQ58.1, GQ58.3, GQ58.4 [6, 7], PHILOX4X32_10[9]. The library contains realizations written in ANSI C, realizations based on SSE command set, realizations based on AVX2 command set and realizations based on AVX512F command set and arises from RNGAVXLIB [8]. The AVX512 implementations produce exactly the same pseudorandom sequences as the original algorithms do. The library also contains the ability to jump ahead inside the RNG sequence and to initialize independent random number streams with block splitting method for each of the RNGs. AVX512 implementations are being up to 55 times faster than the ANSI C implementations.
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BIFURCATION OF SPATIALLY NONUNIFORM REGIMES IN ONE BOUNDARY-VALUE PROBLEM WITH DEFLECTION

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Let us consider nonlinear parabolic boundary-value problem:

$$u' = d\ddot{u} - \gamma u + F(u) \tag{1}$$

with boundary conditions

$$u'(0,t) = 0,$$
$$u'(1,t) = \alpha u(0,t)$$

Parameters $\alpha, \gamma \in \mathbb{R}$, $d > 0$, smooth function $F(u)$ has an infinitesimal order more than the first.

Equally with parabolic boundary-value problem (1), let us consider the following system of differential equations:

$$\dot{u_j} = p^2\left(u_{j-1} - 2u_j + u_{j+1}\right) - \gamma u_j - u_j^3, \qquad j = \overline{1,p}, \tag{2}$$

which model this problem. In this case boundary conditions substitute for

$$u_0 = u_1,$$
$$u_{p+1} = u_p + \frac{\alpha}{p}u_1.$$

The problem of oscillatory loss of stability for spatially nonuniform regimes of system (2) is interesting.

Our task of research was to find critical values of parameter α, when in system (2) there appears Andronov-Hopf bifurcation.

The research was carried out by means of special software. All calculations were performed on a large number of independent streams of GPU. So the program uses the technology of parallel calculations NVIDIA CUDA.

As a result of numerical research there were found spatially nonunifom regimes, which branch by reason of Andronov-Hopf bifurcation.

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Keywords: Andronov-Hopf bifurcation, nonlinear parabolic boundary-value problem, spatially nonuniform regime.

THE OSCILLATIONS OF OBLATE DROP BETWEEN HETEROGENEOUS PLATES UNDER UNIFORM ELECTRIC FIELD.

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The forced oscillations of the incompressible fluid drop under the action of the uniform electric field are considered. In equilibrium, the drop has the form of a cylinder bounded axially by the parallel solid planes and the contact angle is right. The drop is surrounded by an incompressible fluid of different density. The external electric field acts as an external force that causes motion of the contact line. In order to describe this contact line motion, the modified Hocking boundary condition [1] is applied: the velocity of the contact line is proportional to the deviation of the contact angle and the speed of the fast relaxation processes, whose frequency is proportional to twice the frequency of the electric field. The case of heterogeneous plates is investigated. The Hocking parameter depends on the polar angle in this case. The main purpose of this paper is to develop a method for studying the forced oscillations of the drop on heterogeneous substrates and determining the contact angle. The function describing the change in the coefficient of the interaction between the plate and the fluid (the contact line) is expanded in a series of the Laplace operator eigenfunctions. The resulting system of inhomogeneous equations for unknown amplitudes was solved numerically.

It is shown that an increase in constant Hocking effect of the electric field becomes more important than the mechanical dissipative effects in the motion of the contact line. This leads to an increase in the amplitude of the oscillation and a resonance. For small values of the Hocking parameter λ_0, i.e. with a strong interaction energy between the contact line and plate, the oscillations amplitude is small. In opposite case, the amplitude of the surface forced oscillations is large and tends to infinity in the limit $\lambda_0 \to \infty$. There are not "antiresonant" frequencies, i.e. such external frequencies, for which the contact line does not move and the contact angle does not change.

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Exponential Heat Capacity in Natural Nickel Nanolattice: A Quantum Size Effect

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Abstract: Quantum size effect-induced heat capacity of metal nanoparticles at low temperatures was predicted 79 years ago to be exponential. The exponentially decaying heat capacity at low temperature ($T \rightarrow 0$) of metal nanoparticles for equal level spacing (δ) due to quantum size effect (QSE) has not yet been observed experimentally except their reduction or enhancement, compared to their bulk counterparts. In defiance, we demonstrate here observation of exponentially decaying heat capacity, below 45.2 K, associated with quantum jumps, exceptionally in 4 nm naturally assembled hexagonal closed packed (hcp) lattice of nickel nanoparticles; high magnetic fields have negligible effect on these features. Magnetic susceptibilities in contrast reveal evolution of quantum size effects with decrease in particle size. They exhibit sharp rise below about 30 K and vestiges of saturations below 5 K. On the basis of computer simulation, the former is explained by Curie-like characteristics of odd electrons while the latter tend towards the orthogonal even-like case. These characteristics, ascribed to the ensembles of Ni nanoparticles, will give a new direction in understanding this crucial thermodynamic phenomenon.

Analysis of the optimistic algorithm in the method of parallel simulation of discrete events

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We investigate synchronisation aspects of an optimistic algorithm for parallel discrete event simulations (PDES). We present a model for the time evolution in optimistic PDES. This model evaluates the local virtual time profile of the processing elements using the Small-World topology. We expect to see the scalability effect. We present results of the simulation of the model and emphasise predictive features of our approach.

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Sensitivity of the hitting probability to the finite size of the random walk

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We investigate numerically the hitting probablity of the random walk in the plane. We simulate the random walk with the finite size of the steps and compare the computed hitting probablity the exact result for the diffusing particle hitting the circle. We found that deviation of the hitting probability depend on the size of the step with the non-trivial limit. We present results computed by the several algorithms, and discuss the comparison.

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Ab initio simulation of phonon and electronic properties of $BaGa_2GeS_6$ crystal with disordering in Ga-Ge sublattice.

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New nonlinear crystal $BaGa_2GeS_6$ has been synthesized recently in powder [1] and in single-crystalline forms [2]. It has prominent nonlinear characteristics in IR region of spectrum (2-10 μm) which are of the same order as that for the crystals used in practice, e.g., $AgGaS_2$, while $BaGa_2GeS_6$ is much more stable chemically. $BaGa_2GeS_6$ crystallizes in trigonal *R*3 space group. The main peculiarity of the crystal structure is a disordering in gallium-germanium sublattice as both of atoms share the same crystal site with general 9b position. Thus, the simulation of phonon properties is of a special interest as disordering has to be taken into account. The vibrational spectra of the crystal under study are not presented in a literature as far as we know. In this work, an *ab initio* calculation is presented of phonon and electronic properties of $BaGa_2GeS_6$ crystal.

The calculations were performed in the DFT approximation using the ABINIT package, the LDA non-conserving pseudopotential and the approach of generation of alchemical pseudopotentials for gallium-germanium crystal site. The crystal geometry was optimized as a first step of calculations. The optimized lattice parameters are close to experimental ones within 1.2 %. The dispersion as well as partial densities of electronic states for the $BaGa_2GeS_6$ were calculated. The phonon frequencies and their symmetries for optical vibrational modes were found and are in good agreement with the experimental data obtained by means of Raman and IR-reflection spectroscopies [3]. TO-LO splittings, phonon dispersion and density of vibrational states were calculated.

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Ab initio study of vibrational spectra of multifferoic $CuCrO_2$.

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$CuCrO_2$ with delafossite-type structure is interesting object from the points of view of both fundamental physics and practical applications. It crystallizes in trigonal R-3m space group and has a layered structure. The only magnetic Cr^{3+} ion of $CuCrO_2$ forms planes with triangular lattice what leads to high frustration of magnetic interactions [1]. The presence of spontaneous and magnetic-field induced electric polarization [2] enabled to recognize $CuCrO_2$ as a new multiferroic material. Due to the presence of defects $CuCrO_2$ has a p-type conductivity which could be enlarged by special methods of synthesis. Its "transparent conductivity" could be utilized in optoelectronical applications, e.g., in solar cells [3]. In a recent paper [4], the magnon-phonon interaction was reported in $CuCrO_2$. For analyzing such interactions comprehensive information on phonon properties is in need. Raman spectra of $CuCrO_2$ were studied in [5]. Except two expected Raman modes an additional spectrum was registered tentatively assigned to the density of phonon states. In this work, the results of *ab initio* calculations of phonon spectra are presented.

Calculation of phonon properties of $CuCrO_2$ in the center of Brillouin-zone was performed using the DFT-LCAO approximation in the CRYSTAL14 code using the pob-TVZP basis sets for all atoms and the B3LYP hybrid pseudopotential. The magnetic moment of Cr^{3+} was locked to ferromagnetic state. The calculated frequencies for Raman-active modes, namely, 449.5 cm^{-1} (E_g-mode) and 741 cm^{-1} (A_{1g}), are in satisfactory coincidence with the experimental data [5]. The frequencies, eigenfunctions, and TO-LO splittings of infrared-active phonons were calculated: two A_{2u}-modes have energies 410.7 and 793.2 cm^{-1} and two E_u-modes – 122.6 and 496.6 cm^{-1}. Calculations of phonon dispersion across Brillouin zone were performed in a superlattice 2×2×2. The calculated dispersion revealed structural instability at the T-point which can be interpreted as structural tendency to the primitive cell doubling. While the simulated frequencies of Raman modes are close to the experimental ones, phonon DOS obtained do not match with the extra lines observed in Raman experiments. Other possible reason for the appearance of the extra lines in Raman spectra could be dynamical folding of the Brillouin zone, second-order Raman scattering, or activity of IR-modes in Raman spectra due to the violation of selection rules.

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Algorythms for research critical parameters of Prisoner's Dilemma.

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In this work we describe algorythms for investigating critical properties of
Prisoner's Dilemma model. They include consistent algorythm of the model, how it was parallelized,
Hoshen-Kopelman algorythm, boundary calculation algorythm and computation of statistics

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Hybrid method for modeling slow gas mixture flows in devices with micro- and macro- space scales

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Modern rapid development of MEMS and NEMS requires novel numerical methods which can handle different space scales from microns to meters at the same time. This usually requires integration of different techniques for each scale. However, nowadays a lot of works demonstrate the lack of proper numerical tools, concentrating on proper description of the phenomena at only one scale and using rough and simplified methods or simplified engineering models for description at the other scale.

The method presented here is the incorporation of two different numerical techniques. MacCormack model of the linearized Boltzmann equation is used to simulate the gas flow at microscale. At macroscale the system of Navier-Stokes equations for multicomponent gas mixture is solved using finite volume method. Key feature of presented algorithm is that Navier-Stokes equations are adopted for low Mach number limit which leads to significant performance improvement in case of slow gas flows. Another moment that requires special treatment is the proper incorporation of components flow rates obtained from microscale into boundary conditions for macroscale problem.

Presented algorithm is used to simulate the performance of a novel gas separation device, which utilizes membrane with applied temperature and pressure differences as its main part. Obtained results are then compared with experimental data, proving validity of the presented method.

Regional model based on adapted WAVEWATCH III and WRF models for the prediction of surface wind waves on the reservoir and wind

A Kuznetsova, G Baydakov, D Sergeev, Yu Troitskaya

A regional model for the prediction of surface wind waves on the Gorky Reservoir and of the wind over the water area is proposed. The wind was calculated in the WRF model with and without Large Eddy Simulation (LES) block. The use of LES in the WRF model with the unchanged cell size of the topographic grid has led to the formation of numerical errors, which are planned to be eliminated in the subsequent numerical experiments by reducing the cell size. It is expected that with a smaller value of the cell size, the wind speed calculation results with WRF + LES will help to create highly accurate forecasts. The WRF model wind calculation results were used as wind forcing of the WW3 model. A comparison of the mean wave parameters with the measured in the experiment at the Gorky Reservoir was made. In general, the results are satisfactory and meet the needs of operational modeling of wind and waves, but there is an underestimation of the calculated data. Further improvement of calculations is planned due to, first, the elaboration of the used topography. Secondly, among the assumptions made in the calculations, the deep water approximation assumption is made. Taking into account the real bathymetry of the Gorky Reservoir, as well as the inclusion of WW3 source terms associated with the transition to shallow water, can make a positive impact on the results. Thirdly, the data assimilation from the additional sources like private weather stations along the perimeter of the pond will be performed.

Dynamics of Spatial Evolutionary Game

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The work is supported by grant 14-21-00158 of the Russian Science Foundation.

We study the dynamics of a spatial evolutionary game based on cellular automata and use the prisoners' dilemma as rule for interaction. The game features a series of sharp transitions between several regimes, controlled by the interaction parameter between players, and non-trivial geometric rearrangements of the game field. We investigate critical properties of the resulting phase transitions and discuss the geometric properties of emergent structures of players.

Modeling of monolayer charge-stabilized colloidal crystals

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Elastic properties of the monolayer charge stabilized colloidal crystals are studied numerically. The study is based on the Poisson-Boltzmann non-linear differential equation [1].

The system under study is a layer of spatially ordered electrically charged spherical particles that are allocated between two charged planes and immersed in the electrolyte solution. The system is treated as a two-dimensional crystal with the hexagonal crystal lattice relative to the deformations in directions parallel to the planes. The elastic constants of the crystal are found from the stress-strain dependences. Unlike conventional crystals, the charge-stabilized colloidal crystals are the mediums with initial stress for which the first-order elastic constants are not equal to zero. Numerical procedure to determine the first and second order elastic constants and its program implementation are described.

Within the framework of the adopted model, the properties of the colloidal crystal are fully described by solution of the boundary value problem for the Poisson-Boltzmann equation. The boundary value problem is formulated for the crystal in an arbitrary spatial configuration, both initial and deformed. Parametrization of the model by the value of deformation and the lattice parameter makes it possible to build a unified procedure for the numerical solution of the boundary value problem that is suitable for any configuration. Solution is carried out by the finite element method using the irregular meshes of tetrahedral elements. Typical discretization contains several millions degrees of freedom while typical computer experiment incorporats up to several thousands of spatial configurations. Calculations were partly supported by the Supercomputing Center of Lomonosov Moscow State University [2].

Elastic constants of the first and second order were obtained for different values of the lattice parameter. Dependence of the elastic properties from the model's parameters as well as stability of the crystals and the role of the many-body effective interactions are discussed.

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Molecular-dynamic simulation of atomic process under filament formation in memristive structure based on silicon oxide

Developers of memory elements for computers are actively working towards the creation of a fundamentally new type of nonvolatile memory based on the so-called memristive effect - the phenomenon of abrupt change in the conductivity of nanometer film structures when the voltage applied to them changes (both in magnitude and direction) [1]. The relevance of this task increases in connection with the possibility of using memristors to create new types of computing devices based on neuromorphic networks [2]. The memristive effect was observed in structures where nanometer films of various types were used as the working element: organic, metal-oxide, glass. The actual task also is to create memristor structures based on amorphous silica (AS), since the technology of working with this material has been successfully implemented in the microelectronic industry. The observed memristive effect in structures based on films of this material 5-100 nm thick is associated with the formation of thin (from 1 to 10 nm) conductive filaments under the action of strong electric field. When switching polarity, the conductivity of the filaments changes to several orders of magnitude, which is due to the processes of restructuring the local filament atomic structure. Currently, there has been a fairly sustainble notion of the main role of oxygen vacancies and oxygen ions in these processes, both for metal oxides [3] and for amorphous silica [4]. In the AS, an increase in the concentration of vacancies provides an increase in the conductivity by the hopping mechanism or due to the formation of continuous filaments of "pure" silicon. The concentration of vacancies can reach abnormally high values, up to tens of percent. In comparatively few attempts to model the motion of vacancies in an electric field, the Monte Carlo method was used [4]. In this case, the migration energy values, obtained mainly by the *ab initio* method for crystalline [4] or amorphous structures [4], were used using only a very small number of atoms that make up model clusters.

The purpose of this paper is to use the molecular dynamics method using the LAMMPS program to estimate the filament structure and migration energies of the vacancy in the AS, depending on its stoichiometry, average vacancy concentration. The results obtained will be used in the future at modeling the processes of filament formation and their evolution in the switching processes. An essential feature of AS is the ionicity of its bonds, which does not allow the correct use of traditional interaction potentials. Therefore, in the calculations we used a potential of the type REAX.ffiled [5], which takes into account the peculiarities of the bond chemistry under atomic rearrangements. The calculation was carried out as follows. In the AS cluster, different stoichiometry was created by replacing the ions (atoms) of oxygen with silicon ions (atoms). Further, the central region of the cluster with dimensions X * Y * Z, modeling the filament, was saturated with oxygen vacancies with different concentrations. Then, the energy of migration of oxygen vacancies in different configurations of the atomic grid surrounding it was estimated.

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Generative Adversarial Networks in particle physics simulations

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Abstract

Simulation is an important part of physics analysis in particle and nuclear physics. Experimentalists need tools for simulation, but current detailed detector simulations, based on Monte Carlo techniques, such as Geant4, require a large amount of computing resources that will not scale to meet the growing demands resulting from large quantities of data, expected during HL-LHC runs. Deep learning is a completely new approach. We work on a Deep Learning-based framework to enable not only high-fidelity fast simulation of particle showers in calorimeters, but also providing some related quantities such as particle type or energy. Our approach is generic in the sense that it allows for simulating any kind of detector and particle. We will present the first three-dimensional images of energy showers in a high granularity calorimeter, obtained using Generative Adversarial Networks.

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COMPUTER MODELING OF TECHNOGENIC THERMAL POLLUTION ZONES IN LARGE WATER OBJECTS

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The density stratification effects caused by inhomogeneities of temperature and mineralization fields can play an important role in the formation of both hydrological and hydrochemical regimes of surface water bodies. However, they can not be described in the framework of hydrodynamic models using the shallow water approximation. Such effects can be accurately described only using the hydrodynamic models in three-dimensional formulation.

In the present work, using the example of the Permskaya Thermal Power Plant (Permskaya TPP or Permskaya GRES), which is one of the largest thermal power plants in Europe, we investigate the thermal pollution zones created due to discharge of heated water from TPPs. The study is performed for different technological and hydrometeorological conditions. Since the vertical temperature distribution in such wastewater reservoirs is highly inhomogeneous, the computations should be performed in the framework of 3D model. However, the execution of such computations for large water bodies meets considerable difficulties due to the limitated computational resources. Because of that we introduce and implement a combined scheme, which includes the calculations based on 1D, 2D and 3D models. According to this scheme, 1D model is constructed for the entire water body, 2D model for the domain of 30 km length including the Permskaya TPP and 3D model for the domain of 10 km which includes the intake and discharge channels of the TPP. A comparative analysis of the results of 3D computations with the existing data of field measurements has shown that the proposed scheme of computations is very efficient for simulation of temperature fields and estimation of their characteristics for different scenarios including those which are the most unfavorable from the ecological and/or technological viewpoints.

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Asymptotics of N-dimensional tori in the generalized Korteweg – de Vries equation

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Let us consider the boundary problem

$$u_t + u_{xxx} + (\alpha u + \beta u^2)u_x = au + bu^2 + cu^3,\ u(t, x+T) = u(t,x), \quad (1)$$

where $u(t,x) \in W_2^3$ for all $t > 0$; parameters α, β, c, T are constants, the parameter a is small enough:

$$a = \varepsilon a_0,\ 0 < \varepsilon \ll 1. \quad (2)$$

Let N is a fix natural number. We are interested in the construction of the N-dimension torus asymptotics in a sufficiently small neighbourhood of zero. Fix positive $k_1, \ldots, k_N$. We find the solution of (1) in the form of the range

$$u = \eta(t,\varepsilon) + \sum_{j=1}^{N} \left(\xi_j(t,\varepsilon)\exp(ik_jx + ik_j^3t) + c\overline{c}\right) + \ldots, \quad (3)$$

where the symbol $c\overline{c}$ means the term which is complex conjugated to the previous one. The terms are trigonometric polynomials from t and x. Here functions $\eta = \eta(t,\varepsilon)$, $\xi_j = \xi_j(t,\varepsilon)$ and their derivatives are small enough. The last ones are represented by η, ξ_j and ε from the conditions for the resolvability of the corresponding problems in the class of trigonometric polynomials:

$$\begin{cases} \dot{\eta} = \alpha_1\varepsilon\eta + \alpha_2\eta^2 + \sum\limits_{j=1}^{N} \alpha_{3j}|\xi_j|^2 + \alpha_4\eta^3 + \eta\sum\limits_{j=1}^{N}\alpha_{5j}|\xi_j|^2, \\ \dot{\xi_j} = \beta_{1j}\varepsilon\xi_j + \beta_{2j}\eta\xi_j + \xi_j\Big(\sum\limits_{s=1}^{N}\beta_{3js}|\xi_s|^2 + \beta_{4j}\eta^2\Big),\ j = 1, \ldots, N. \end{cases} \quad (4)$$

It is proved the statement linking the rough stable modes (4) and the solution of the boundary value problem (1). This statement works for sufficiently small values of ε. So when the condition is not fulfilled, a numerical experiment is needed to ascertain whether the boundary problem (1) has coexisting multifrequency modes or not. A numerical experiment to identify these regimes was carried out.

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Simulation of hydrogen and oxygen atoms interaction with the point defects on the hydrogenated diamond surface

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Synthetic diamond crystals are an important material for many high-tech areas. Some properties of diamond are of particular interest, namely: high thermal conductivity, high refractive index, transparency in a wide range of wavelengths, chemical inertness, and high hardness. Creating a high-quality surface, up to an atomically smooth one, is an important condition for the manufacture of reliably functioning components of synthetic diamond. Another important target is to provide a surface relief structure with desired geometrical characteristics.

Currently, reactive ion etching in a plasma environment of different gas composition is an effective method of smoothing the diamond surface. A promising technique of preparing a diamond surface is its reactive ion plasma etching in gas mixtures containing hydrogen and oxygen atoms [1-3]. This type of impact is inevitably accompanied by a significant number of surface defects. However, the mechanisms of chemical interaction between the hydrogen and oxygen atoms and H- and O-containing molecules and fragments with the point and line defects on the diamond surface remain largely underinvestigated.

We present the results of quantum-chemical simulation of the hydrogen and oxygen atoms interaction with a number of point defects on the reconstructed hydrogenated diamond surface C(100)-(2×1): a monovacancy, divacancy and adatom. We applied the approach developed earlier in [4-6].

We used the C_mH_k clusters as model objects to simulate the reconstructed C(100)-(2×1) diamond surface. Simulation of mono- and divacancies, adatoms, and steps was carried out by removal or adding of one or more atoms in the central parts of the clusters. We calculated the cluster energy, atomic bond orders, population of the atomic orbitals, molecular and localized orbitals. We provide a comparison between the processes of H and O atoms interaction with an ordered and defect cluster surface. We investigated the interactions of hydrogen and oxygen atoms and H- and O-containing fragments with different types of surface defects [4]. Our calculations indicate a possibility of smoothing out the diamond surface when the hydrocarbon radicals are adsorbed from the gas mixture. This result is consistent with the experimental data [1]. It is shown that the most likely single etching acts among the considered processes is the formation of CO molecules from adatoms and oxygen from the gas phase. We assumed that "empty" dimer rows are formed as a result of etching vacancy defects on the surface. Perhaps further etching of "empty" dimer rows leads to the formation of steps on the surface. The most effective process of restoring an ordered surface is the attachment of CH_2 fragments to divacancy defects. The results can be used to analyze the physical and chemical processes on the diamond surface during reactive ion etching using hydrogen- and oxygen-based plasma.

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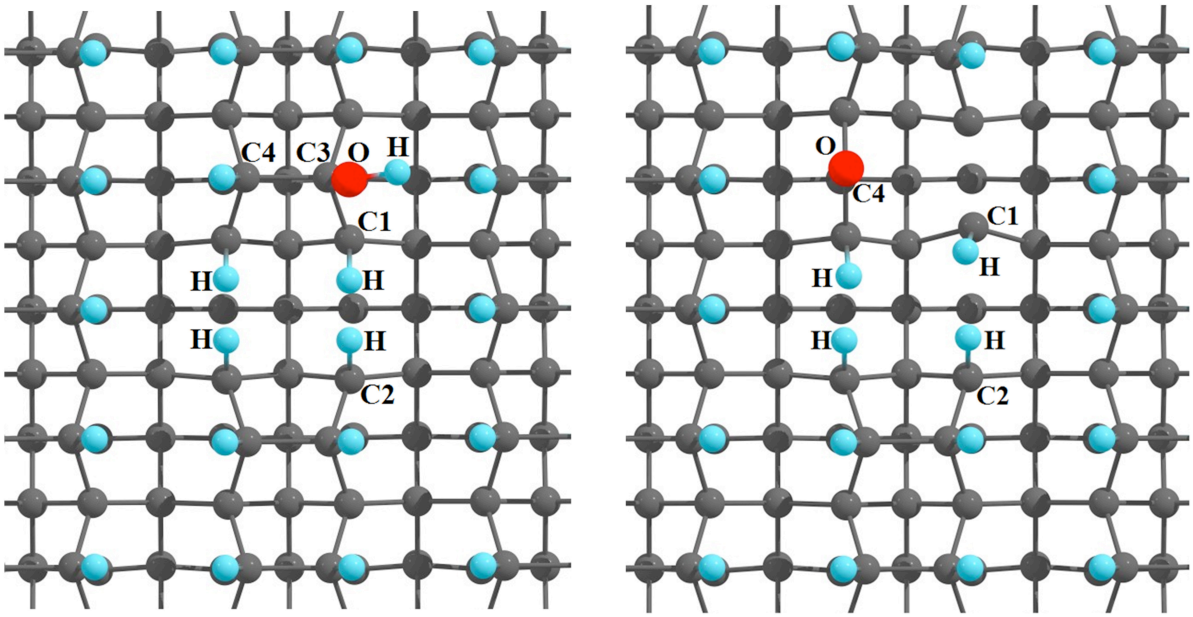

Figure 1. Result of OH fragment chemisorption near the divacancy (a); complex defect consisting of the divacancy and the monovacancy in the same dimer row (b).

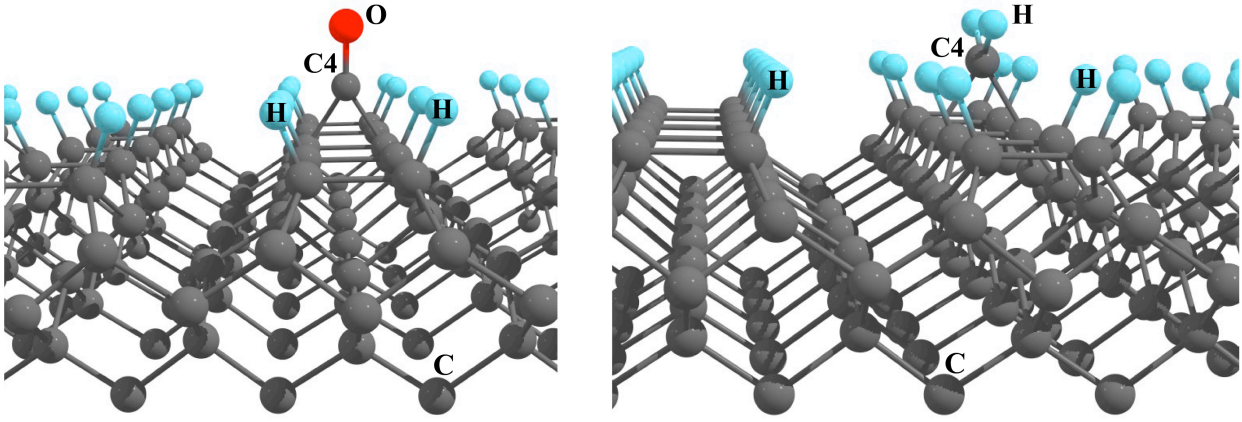

Figure 2. Result of chemisorption onto the adatom: a) O atom; b) H atoms.

BUCKLING BEAM DRIVEN OSCILLATIONS

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Oscillations of an elastic beam with longitudinal compression were considered. The beam consists of two steel strips connected on free ends and fixed on opposite ones. Compression is achieved by a strained string. Excitation of oscillations is performed by exposure of alternating magnetic field on a magnet placed on the loose end. The law of motion with a change in the frequency of the harmonic action was registered.

As a result of the full-scale experiment a large set of data was obtained. This set contains ordered periodic oscillations as well as disordered oscillations specific to dynamical systems with chaotic behavior.

To study the invariant numerical characteristics of the attractor of the corresponding dynamical system correlation integral and correlation dimensionality as well as β-statentropy were calculated. Large numerical experiment showed that calculation of β-statentropy is preferable to the calculation of the correlation index.

Based on the developed algorithms the dependence of β-statentropy on the frequency of the external action is constructed. The constructed dependence can serve as an effective tool for measuring the adequacy of the mathematical model of forced oscillations of buckling beam driven oscillations.

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The model of turbulent transfer and dynamics of small-scale turbulence in the stratified fluid.

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This paper is mainly devoted to the kinetic approach for describing small-scale turbulence in the upper layer of the ocean. This approach, connected with the use of the probability distribution function of the values of the hydrophysical fields characterizing the current, was developed by the authors earlier [Ostrovsky,Troitskaya,1986]. However,in recently interest in the study of turbulent processes in upper ocean mixing has increased. This is associated with the key role of the upper mixed layer in transferring momentum, heat and mass through the of the oceanic surface layer . This turbulence processes are currently being investigated on the basis of numerical technique -Large Eddy Simulations (LES) or Direct Numerical Simulation (DNS). However, the main regularities of this turbulent processes under consideration can also be investigated in the framework of simpler, so-called Reynolds equations averaged over an ensemble of stationary two-dimensional Navier-Stokes equations (RANS). The unknown turbulent Reynolds stresses are expressed in terms of the gradients of the average velocity field using the turbulent viscosity coefficients, parametrized in accordance with the determining role of various physical phenomena in the mixing process. Recently, the group led by SS Zilitinkevich [Zilitinkevich et al.,2007] has made changes to the standard RANS scheme These changes primarily concerned the exchange between the kinetic and potential energies of turbulent fluctuations and the construction of a hierarchy of turbulent closure models of various complexity levels with allowance for an additional parameter-the turbulent time scale under various turbulence regimes. Many conclusions obtained in the work of SS Zelitinkevich's group coincide with the results obtained in the framework of the kinetic approximation those described in this work.

When using the probability distribution function, a closure problem occurs. It is most simply solved in two limiting cases. The first of these is the case of a quasihomogeneous, isotropic small-scale turbulence, when the characteristic time scale of the energy-carrying vortices is small in comparison with the periods of the average processes. The dominant term in the kinetic equation is the term describing the influence of pressure pulsations and equivalent to the collision integral in the kinetic theory of gases. Therefore, this approximation can be called "strongly collisional". In another limiting case, which previously have not been considered, the random field changes little in the period of the flow. In this situation, when the average components of the fields a lot more pulsating, and the last is fashionable to neglect with the closure of kinetic equation. This approximation can be called "collisionless" by analogy with plasma physics, where it is called the collisionless approximation, which neglects the pulsatile components The applicability as "strongly collisional" and "collisionless" approximation is provided in a number of typical hydro situations. Here are these two approaches applied to the study of the interaction of small-scale turbulence by shear flows and internal waves in the ocean, internal waves and fine structure of currents, as well as to build a model of generation of wind vonpeta this approximation can be called "strongly collisional".Expressions for turbulent fluxes of momentum,mass,energy and other hydrodynamic characteristics in a stratified medium are derived using a kinetic"strongly collisional" approach. The form of the derivations is simply defined by the assumption that the distribution function is near to Gaussian one. The evolution of turbulence in stratified fluid is investigated. It is revealed that the possibility of maintaining the level of turbulence in weak shear flows is explained taking into account the effect of mutual transformation of the potential and kinetic energy of turbulent pulsations. The self_similar turbulent density jump evolution has been studied in the scope of a turbulence closure modernized theory which takes into account the anisotropy and mutual transformation of the turbulent fluctuation kinetic and potential energy for a stably stratified fluid. The numerical calculation, performed using the equations for the average density and kinetic and potential energies of turbulent fluctuations, indicates that the vertical profiles of the buoyancy frequency, turbulence scale, and kinetic and potential energies drastically change when the turbulence anisotropy is strong.

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ON ONE PECULIARITY OF THE MODEL DESCRIBING THE INTERACTION OF THE ELECTRON BEAM WITH THE SEMICONDUCTOR SURFACE

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The problem of heat distribution in semiconductor materials irradiated with sharply focused electron beams in the absence of heat exchange between the target and the external medium has been considered by mathematical modeling methods. In the quantitative description of energy losses by probe electrons, a model based on a separate description of the contributions to the energy of absorbed and backscattered electrons is used (N.N. Mikheev and M.A. Stepovich, "Distribution of Energy Losses in Interaction of an Electron Probe with Material", Industrial Laboratory, Vol. 62, No. 4, Pp.221-226, 1996.). Using the features of this approach, the nonmonotonic dependence of the temperature of the maximum heating of the target ΔT on the energy of the primary electrons E_0 is explained. Calculations show the dependence of the maximum heating of the samples ΔT on the energy of the primary electrons E_0. The results of the calculations show that the contribution of electrons absorbed in the target to the total energy losses of the probe electrons in the target is decisive for the probe energy of less than about 2...3 keV, and then the curve 2 decreases monotonically. We note that for heavy semiconductors (for example for CdTe), the energy loss of the absorbed electrons becomes practically zero at an energy of about 8 keV. For light samples (for example for Si) and samples with average ordinal numbers (for example for GaAs), the energy losses absorbed by the target absorbed and back scattered (reflected) electrons become commensurate with the electron energy of the probe about 8 keV, and at higher energies the contribution of backscattered electrons predominates. This can be explained by the deeper penetration and large scattering in the target of the probe electrons and, as a consequence, the lower probability of the exit from the target of electrons experiencing small-angle scattering in the volume of the semiconductor. The presence of a rather sharp increase in the contribution of reflected electrons to the total curve leads to the formation of a "step" in the figures of the dependence of the maximum temperature on the energy of the primary electrons. We also note that backscattered electrons least influence the value of the maximum heating for light samples and, in part, samples with average ordinal numbers; this effect is observed most in heavy semiconductor targets.

ON THE POSSIBILITY OF USING THE GALERKIN PROJECTION METHOD TO SIMULATE THE TWO-DIMENSIONAL DIFFUSION OF EXCITONS GENERATED BY AN ELECTRON BEAM IN A SEMICONDUCTOR MATERIAL

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This paper presents the results of using the Galerkin projection method for modelling a two-dimensional diffusion of excitons, electron beam excited in a semiconductor material (Polyakov A.N., Noltemeyer M., Hempel T., Christen J., Stepovich M.A. Experimental Cathodoluminescence Studies of Exciton Transport in Gallium Nitride // Bulletin of the Russian Academy of Sciences. Physics. 2012, vol. 76, no. 9, pp. 970-973.). The problem is solved in a cylindrical coordinate system. The required concentration of excitons found in the form of partial sum double of Fourier series on system of modified Laguerre functions. Received the ordinal error estimation residuals corresponding to the approximate solution of the time-dependent diffusion. During the simulation parameters were used for the gallium nitride.

Modeling of Fiber Orientation in a Twin-Screw Extrusion Process

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This study is to predict the fiber orientation in a co-rotating, intermeshing twin-screw extrusion process through numerical simulations based on mathematical models describing the polymer as well as fiber motions. The continuity and momentum equations are employed to describe the coupling of pressure and velocity in the flow field. The fiber orientation is governed by the tensor equation depicting the fiber behaviors of rotation and translation in space. The constant-temperature polymer melt is assumed to be fully filled in the flow path between the barrel and two co-rotating screws, and air-melt interface is not present in the simulated flow field. A dynamic grid-updating scheme is proposed to discretize the studied transit flow problem characterized by a strongly varying flow domain inside the barrel due to a periodical rotational motion of two co-rotating intermeshing screws. A body-fitted grid is separately generated for every time instance in the unsteady simulation. In this study, fibers are allowed to translate and rotate but without any breakage. The flow field is first obtained from a finite volume approach to solve the coupled governing equations, whereas a particle tracing scheme is adopted to compute the flow history of fibers traveling across the screw. Then the tensor equation is solved for fibers residing at different locations. This study can help to disclose the quantitative correlations between the processing parameters and fiber behaviors together with the understanding of fiber mechanics in an extrusion process.

Identification of current carrying part of a random resistor network: electrical approaches *vs* graph theory algorithms

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For many decades, the physical properties of inhomogeneous media have attracted a lot of attention in the scientific community. This interest is supported by numerous applications such as the production and use of nanocomposites. Theoretical prediction of the effective properties of such composites is very important for the analysis of material performance and for the design of new materials. Particular interest is paid to the electrical properties of binary materials. The theories and models relating to the electrical conductivity of mixtures of conducting and insulating species continue to attract great interest from researchers. One of the possible ways to theoretical study of binary mixtures is consideration them as random resistor networks (RRN). When a potential difference is applied between two points of such the network or between two bus bars attached to the opposite borders of the network, the set of current carrying bonds is called the backbone. The remaining bonds are called dangling ends or dead ends. The backbone can be also defined as the union of all the self-avoiding walks. These two definitions provide two different approaches for identification of backbones. On the one hand, one can use Ohm's law or Kirchhoff's rules to calculate potentials and currents in the RRN [1,2]. On the other hand, one can apply search algorithms on graphs [3,4]. Each of these approaches have both advantages and drawbacks.

Direct calculations of electrical potentials and currents are based on floating-point arithmetic and, hence, produce round-off errors. Some ghost currents may arise due to these round-off errors which impedes the backbone extraction. Moreover, these calculations deal with huge systems of linear algebraic equations (SLAE) and require a lot of computer memory. Only relative small or sparse systems can be treated in these approaches because number of equations to be solved is proportional to linear size of the system to the power of 2.

Graph theory algorithms are sometimes difficult to understand and to realize. Some of them can produce stack overflow because of recursion. In fact, application of these algorithms also is restricted to the RRN of moderate size.

We have implemented several different algorithms for backbone identification. The algorithms were applied to backbone identification for different system sizes and concentrations of conducting bonds. Our analysis suggests that a universal algorithm suitable for any possible problem is absent. Most likely, each particular task needs specific algorithm.

The algorithms which allow parallelization look very promising [5].

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Science and ethics meet: a mathematical view on one kind of violation of publication ethics

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During last decade, a problem of malpractice and misconduct in scholarly publications attracts more and more attention from the academic community [1,2]. The problem has many manifestations, including, but not limited to, duplicate publications and plagiarism [1], predatory journals [3], and close related to them author, diploma, and degree mills [4,5]. Incorrect list of co-authors (i.e., gift, guest, ghost authors) is one of possible kinds of malpractice [6]. Gift and guest authors are persons who did not make a significant intellectual contribution to a published research but included into the co-authors list because of different reasons. During last couple of years, "author contribution statement" became a mandatory section of article in many journals. This fact evidences that improper co-author lists are often suspected. Unfortunately, explicit "author contribution statement" is hardly able to stop Mr. Fraud. Academic community badly needs a tool to detect and prevent malpractice. Scientific methods are successfully used for plagiarism detection and analysis of publications in predatory journals [7], nevertheless, possibilities to use scientific methods for "gift author" detection is not clear yet [8]. Application of network analysis [9,10,11,12,13,14,15] to co-author networks looks very promising as a potential tool for improper author lists detection.

We present some new attempts applying network analysis to indicate improper co-author lists. Our research is based on an assumption that there may exist some stable groups or persons which permanently include so-called "gift authors" into co-author lists. If this assumption is correct then such the artificially enlarged co-author networks presumptively have some anomalies in their properties. https://www.dissernet.org/ evidences that malpractice and misconduct in Physics and Mathematics is minimal in compare with other sciences, humanities, and arts. This fact allows using properties of co-author networks in physical science as a reference sample.

We restricted our consideration only to articles indicated in doctoral thesis as main publications. Open access full texts can be found at the official portal of the Higher Attestation Commission of the Ministry of Education and Science of Russian Federation http://vak.ed.gov.ru/dis-list.

The information allows building co-author networks and networks as applicant–supervisor–opponent. Average clustering coefficient, graph density, and average degree have been calculated for particular clusters. We suppose that such the quantities may be used for identification of suspicious co-author networks which presumably are artificially built and may contain gift and/or guest authors. Research is in progress.

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Modeling and simulation of a programmable quantum processing device

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We propose a model of a programmable quantum processing device realizable with existing nanophotonic technologies and which can be viewed as a basis for new high performance hardware architectures. We present protocols and their physical implementation on the controlled photon transfer for executing basic single-qubit and multi-qubit gates. The possible operation of this quantum computer scheme is analyzed.

The physical architecture is formalized by a mathematical model of the Quantum Processing Unit.

A Quantum Processing Unit (QPU) is a device consisting of 4 modules controlled by a classical device. They include:

- An s-qubit *Quantum Memory* module, that allows to store quantum states. The contents of the memory is described by the current state $|\psi\rangle \in H^{2^s}$. The quantum memory module is capable of exchanging qubits with quantum transistor and quantum communication channel.
- A *Quantum Transistor* is a 3-qubit device capable of performing quantum transformations. There are three types of operations described in a physical architecture: QET, PHASE and CQET. Generally, we can consider an array of quantum transistors working in parallel, but here for simplicity we leave just one module.
- *Init* is an initialization module that can create a quantum state given its classical description and save it to the quantum memory. Without loss of generality we can consider a single-qubit initialization in state $|0\rangle$, since any other state can be obtained via universal set of operations.
- *Measure* is a measurement module that implements a photon detecting procedure and gives a classical bit out of qubit being measured.

In the proposed model, we use three whispering gallery mode cavities coupled in a linear chain. Each cavity contains artificial or natural atom that can be quantum dot, nitrogen vacancy center or rare earth ion. The excitation transfer between left and right cavity can be blocked via the atom in the middle cavity that leads to controlled excitation transfer operation.

The proposed model is obviously a hardware-specific modification of the quantum circuit model of computation achievable within existing technologies, and it is universal as well, since the available set of operations provides a universal basis for quantum computations.

A quantum algorithm in this model can be described by a (t, s) *quantum program*, which is the sequence of t instructions of several types (described below) over s-qubit quantum memory. These parameters correspond to the key complexity measures: t is the time of computation and s is the required space.

In order to make a QPU programmable via the classical controller, we've developed a Quantum Programming Framework running (QPF) over JAVA virtual machine. This framework has two main parts - the dispatcher and the service. The service adapts the high-level user commands to the low level for further implementation. The dispatcher was created to support the different types of connections between the classical computer and the QPU - it can be either a physical device or a QPU simulator which is also a part of QPF. Due to the absence of the physical device our framework runs over QPU simulating system that implements the mathematical model given above.

The QPU simulating system also implements a noise model. The memory contains $s = s_i + s_n$ qubits: s_i "information" qubits and s_n "noise" qubits describing random impulses. In addition to computational operations we introduce transformations describing decoherence models that are applied to the QPU current state. The intensity of noise can be set by external parameters of the QPU simulating system.

The work is performed according to the Russian Government Program of Competitive Growth of Kazan Federal University. Work was in part supported by the Russian Foundation for Basic Research (under the grant 17-07-01606).

FRACTAL TOMOGRAPHY AND ITS APPLICATION IN 3D VISION

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The method of fractal tomography - the method of artistic static and dynamic 3D vision is offered. It based on the projection onto transparent screens of 3D multifractal slices (Fig. 1), and is developed by the author. This method is the subsequent development in the system of earlier glasses-free 3D visualization technologies, such as holographic and raster (lenticular).

The proposed method uses the division of a 3D fractal object into slices for several transparent screens displayed in the depth of the object. Images of slices are projected simultaneously (synchronously in the dynamics of the video), each slice is projected onto the screen, at a distance from the viewer corresponding to the depth of the cut. When the multilayer screen with multiple slices is viewed frontally, the viewer sees a three-dimensional fractal world, varying in depth and with lateral shifts of the viewer relative to the screen, without additional means (glasses), the viewer receives the resulting images corresponding to the 3D vision.

The experiment used 3D multifractal, consisting of 4 fractal functions (FFi, i=1,…4), visualizing a 3D fractal world with objects similar to trees:

$$\begin{cases} FF1=\_Rotate(X=0.75;\ Y=0;\ Z=0.375) \\ FF2=\_RotateC(X=22.875;\ Y=-48.375;\ Z==190.125) \\ FF3=\_FlipXYc(c=1) \\ FF4=AmazingSurf(Scale=1.2203125;\ MinR=0.125;\ Fold=1.15;\ X=5.421875;\ Y=1.9296875; \\ \quad Z=-14.4296875;\ ScaleVary=0;\ Sphere\_or\_Cylinder=0) \end{cases} \quad (1)$$

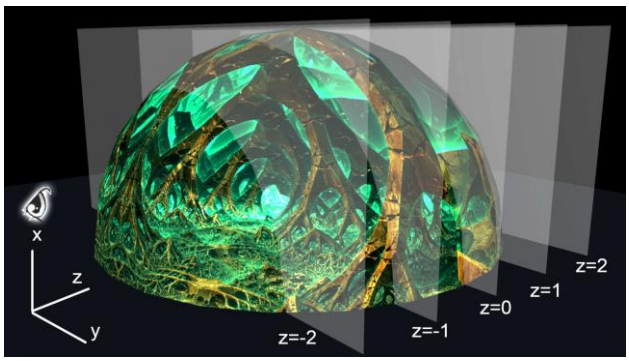

Fig.1. Calculation of sections (slices) of 3D multifractal

Fig. 2. View of a real mobile demo installation, with dynamic 3D visualization, containing three screens from the perspective of the viewer

A mobile demonstration unit of the computed fractal tomography was developed, demonstrating a 3D glasses-free vision of both static and dynamic multifractals (Fig. 2). A video report on the scientific experiments can be viewed from the link [1].

Sourse

1. https://cloud.mail.ru/public/FSeo/ePzfykQQe

TRANSITIONAL CIRCUITRY FOR STUDYING THE PROPERTIES OF DNA

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A method for studying the properties of DNA using specialized transitional biochemistry is considered.

In DNA research, it seems to be a circuit built on the principles of logic and memory of intelligent circuits of an optimal computer in transient biocircuitry.

Elements of transition biochemistry are the atom and the bonds between atoms. Algorithms for representing parts of DNA have been developed in the form of mathematical models of elements necessary for the subsequent analysis of the functional and parameters of a part of DNA.

Mathematical modeling of physical processes in the biochemistry is carried out in a special program, where the properties of the studied mathematical model of a part of DNA are determined, such as the performance of logic functions and memory functions, levels of operating signals, noise immunity, speed, power consumption.

Experiments were carried out for various dimensions of parts of DNA, showing the presence of logical functions and memory properties. In Fig. 1 shows a structural model of parts of DNA that have a memory function. When the atomic triggers are combined, an atomic serial memory register is obtained, to store the information vectors. In Fig. 2 presents the results of modeling physical processes in the model of a part of DNA demonstrating the memorization of information (functional F1) in one side of the "benzene" ring.

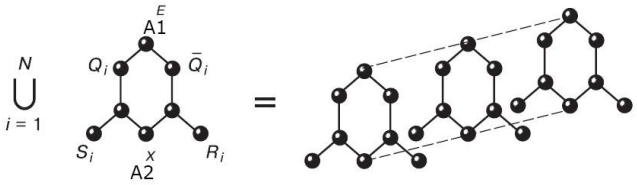

Fig. 1. Model of a part of DNA with memory properties

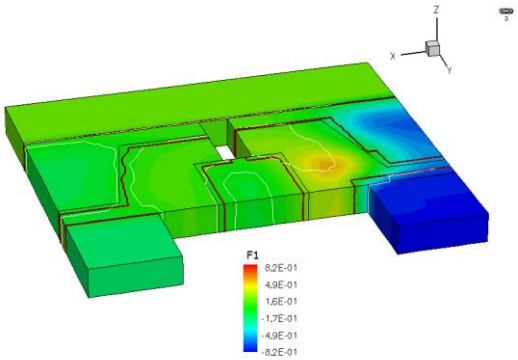

Fig.2. The results of modeling physical processes in the DNA part model for determining the memory functional F1

Transitional circuitry [1,2] is universal, both for biocircuits and for optimal circuits of solid-state nanoelectronics. The novelty of the method is confirmed by the receipt of patent for invention [3].

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Staggered grid residual distribution scheme for Lagrangian hydrodynamics

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Keywords: Lagrangian hydrodynamics; residual distribution scheme; finite elements.

ABSTRACT

This work is focused on the Residual Distribution (RD) interpretation of the Dobrev et al. scheme [2] for the numerical solution of the Euler equations in Lagrangian form. The first ingredient of the original scheme is the staggered grid formulation which uses continuous node-based finite element approximations for the kinematic variables and cell-centered discontinuous finite elements for the thermodynamic parameters. The second ingredient of the Dobrev et al. scheme is an artificial viscosity technique applied in order to make possible the computation of strong discontinuities. The aim of this paper is to provide an efficient mass matrix diagonalization method in order to avoid the inversion of the global sparse mass matrix while keeping all the accuracy properties and to construct a parameter-free stabilization of the scheme to get rid of the artificial viscosity. In addition, we study the conservation and entropy properties of the constructed RD scheme. The robustness and accuracy of the proposed RD scheme is demonstrated on several challenging one-dimensional and two-dimensional test problems such as the Sedov problem, see Figure 1.

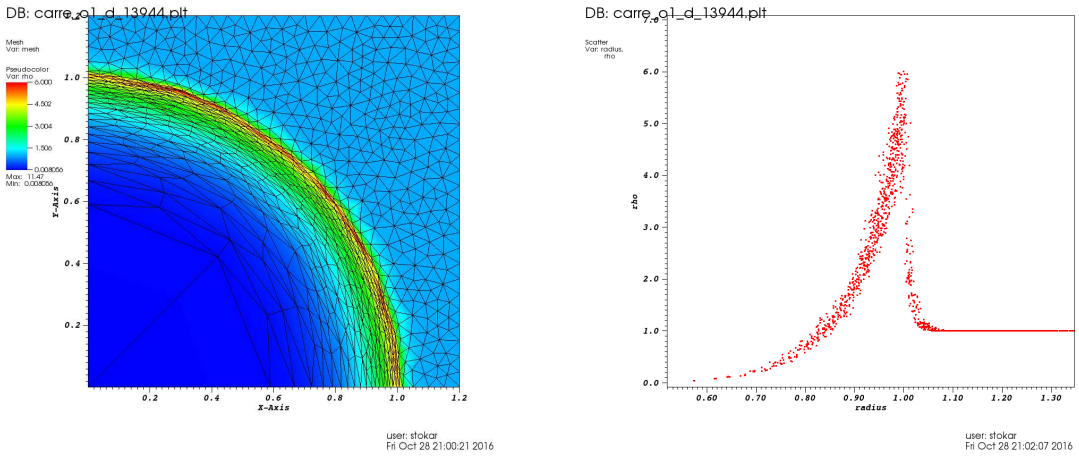

Figure 1: Sedov problem: density

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Compact high-order difference approximations for rod lateral vibrations equation

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We present a compact high-order difference approximations for rod lateral vibrations:

$$\rho\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}[R^2\rho\frac{\partial^3 u}{\partial x \partial t^2}] + \frac{\partial^2}{\partial x^2}[ER^2\frac{\partial^2 u}{\partial x^2}] = f,$$

with various boundary conditions. Here, ρ is a density of a rod material, R is rod thickness, E is Young's modulus, f is a right-hand side (forcing). The equation is difficult for calculations because it is not resolved with respect to the highest derivative on time. We consider cases of constant and time-independent variable rod thickness and have studied stability of obtained schemes, as well as different properties such as approximation of first integral and eigenvalues of the boundary problem in various norms: Euclidean, Chebyshev, energetic norm. Numerical experiments show high (4th) order of approximation. Compact difference schemes are effective because they provide high accuracy order for various models of mathematical physics [1-4], and the implicit schemes may be realized by economical double-sweep (Thompson) method.

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Quantum Hashing and Small-biased Sets

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Fingerprinting was one of the first techniques for constructing effective randomized algorithms (which are more effective than any deterministic algorithm) [1, 2]. In quantum case, fingerprinting is a procedure that maps classical data to a quantum state that identifies the original data (with high probability). One of the first applications of the quantum fingerprinting method is due to Ambainis and Freivalds [3]: for a specific language they have constructed a quantum finite automaton with an exponentially smaller size than any classical randomized automaton. An explicit definition of the quantum fingerprinting was introduced by Buhrman et al. in [4] for constructing effective quantum communication protocol for equality testing.

We define a notion of quantum hash function which is quantum one-way function and quantumly collision resistant function. We show that one-way property and collision resistance property are correlated for a quantum hash function. The more the function is one-way the less it is collision resistant and vice versa. We show that such a correlation can be balanced.

We present an approach for quantum hash function constructions by establishing a connection with small biased sets [5] and quantum hash function constructions: we prove that small sized ε-biased sets allow to generate balanced quantum hash functions. Such a connection adds to the long list of small-biased sets' applications. In particular it was observed in [5, 6] that the ε-bias property is closely related to the error-correcting properties of linear codes. Note that the quantum fingerprinting function from [4] is based on a binary error-correcting code and so it solves the problem of constructing quantum hash functions for the binary case.

For the general case, ε-bias does not correspond to Hamming distance. Thus, in contrary to the binary case, an arbitrary linear error correcting code cannot be used directly for quantum hash functions.

Next, recall that any ε-biased set gives rise to a Cayley expander graph [7]. We show how such graphs generate balanced quantum hash functions. Every expander graph can be converted to a bipartite expander graph. The generalization of these bipartite expander graphs is the notion of extractor graphs. Such point of view gives a method for constructing quantum hash functions based on extractors.

This construction of quantum hash functions is applied to define the notion of keyed quantum hash functions. The latter is used for constructing quantum hash-based message authentication codes (QMAC). The security proof of QMAC is based on using strong extractors against quantum storage developed by Ta-Shma [8].

The work is performed according to the Russian Government Program of Competitive Growth of Kazan Federal University. The work was in part supported by the Russian Foundation for Basic Research (grant 17-07-01606).

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Magnus expansion of evolution operator in the problem of flux qubit optimal control

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We propose a new approach to study the quantum dynamics of superconducting qubit based on Josephson junctions (flux qubit). We discuss the problem of optimal control the qubit states by a short pulses (flaxon) which is carried only a magnetic flux quantum [1, 2]. Such kinds of operations are required for the implementation of the fast quantum logic at frequencies ~ 10 GHz at the switching times ~ 10ps. This issue sets a number of requirements such as working conditions in the THz band, high repeatability, and therefore theoretical, numerical optimization of the control signal (shape parameters) are necessary.

The Hamiltonian of the superconducting flux qubit [1] can be represented as

$$H(t)=\frac{\hbar}{2}\left(\Delta\sigma_z+\varepsilon(t)\sigma_x\right), \tag{1}$$

where $\hbar\Delta$ is the distance between qubit levels; $\varepsilon(t)$ is the control function (proportional to the magnetic flux); σ_x,σ_z are Pauli matrices. We will be interesting in the switching process of the qubit from one basic state to another under the action of two type single quantum pulse: $\varepsilon(t)=\varepsilon_m\theta(t)\theta(t-\tau)$ (where ε_m is the amplitude pulse and $\theta(t)$ is Heaviside function) and $\varepsilon(t)=\varepsilon_m\exp\left(-(t-t_0)^2/2\tau^2\right)$ (here τ is the typical pulse duration and it is supposed to be $t_0>>\tau$ for a gaussian pulse). The time dependence of the two-component wave function of a qubit is determined by: $\psi(t)=U(t)\psi(0)$, where the propagator (evolution operator) $U(t)\equiv U(t,0)$ ($U(0)=\mathrm{I}, U^+=U^{-1}$) is the solution of the equation

$$i\hbar\frac{\partial U(t)}{\partial t}=H(t)U(t). \tag{2}$$

The solution of the Eq. (2) can be written in the form: $U(t)=\hat{\mathrm{T}}\exp\left(-i\int_0^t dt_1 H(t_1)\right)$, where $\hat{\mathrm{T}}$ is chronological ordering operator. Usually the solution of Eq. (2) is found by perturbation theory or by a numerical solution of the system of equations obtained when the operator is parameterized in a certain basis.

In this paper we develop a technique for calculation of the operator Eq. (2) based on the construction of approximate representation of the evolution operator – Magnus expansion. The essence of the method is the following. At the first, the evolution operator can be represented in the form of: $U(t)=e^{A(t)}$, where the anti-Hermitian operator which may be written in the form $A=-i\hat{T}$ ($\hat{T}^+=\hat{T}=T_x\sigma_x+T_y\sigma_y+T_z\sigma_z$). According to [3], the operator $A(t)$ is expanded in the series, where the terms are proportional to the corresponding degrees of the Hamiltonian operator: $A=A_1+A_2+A_3+\ldots$. Secondly, for the two-component wave function the evolution operator U can be written in the form:

$$U=\cos T\begin{pmatrix}1&0\\0&1\end{pmatrix}-\frac{i\sin T}{T}\begin{pmatrix}T_z&T_x+iT_y\\T_x-iT_y&-T_z\end{pmatrix}, \tag{3}$$

where time-depended functions $T_x(t)$, $T_y(t)$ $T_z(t)$ and $T(t)$ which are defined by pulses shape.

Thus, the qubit evolution procedure is reduced to constructing the matrix U according to the Eq. (3) and further by calculating the wave function by using a simple rotation in the "pseudospin" space of the qubit as: $\psi(t)=U(t)\psi(0)$. We demonstrate that the developed technique allows us to select analytically and numerically the optimal form of a single quantum pulse (amplitude ε_m and duration τ) that is important for implementing the rapid single flux quantum logic.

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