

Book of Abstracts

**International Conference on Computer
Simulation in Physics and beyond
September 6-10, 2015, Moscow, Russia**

Papers are published under their authors' responsibility

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Preface

Computer simulations are fast growing approach for doing research in sciences. It is auxiliary to experimental and analytical research. The main goal of the conference is in the development of methods and algorithms which take into account trends in the hardware development, and which may help to intensive research. Conference should play role of the venue were senior scientists and students may have opportunity to speak each other and exchange ideas and views on the developments in the area of high-performance computing in most sciences.

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 reflects that rainbow of our program and their expertize 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 are consists 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:

- Simulations in Statistical Physics
- Physics and mechanics of polymers
- Methods and software for simulations in research and engineering
- Bioinformatics, methods and algorithms in genome research
- Simulations in material science
- Simulation and analysis of social networks
- Simulation and analysis of technical networks (urban transportation, data networks, etc.)
- Algorithms, methods, and tools with properties of scalability and enhanced parallel simulations
- Informatics and education
- Quantum computing

Plenary Speaker Thesis

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Impacts of Current Hardware and Software Developments on Simulation Sciences **Norbert Attig**

For more than a decade single compute core performance is no longer doubling every 18-24 months. Physical limitations due to successive chip miniaturisation are visible and it becomes increasingly difficult to dissipate the heat being generated by tiny high-clocked and densely packed compute cores. To circumvent these limitations massive parallelism has been introduced: more and more processors – each of them equipped with an increasing number of moderately clocked compute cores – are assembled in big systems to reach highest performance. Moreover, accelerators like general-purpose graphical processing units (GP-GPUs), field programmable gate arrays (FPGAs) or Intel's Many Integrated Core (MIC) architectures are increasingly used to further boost the application performance.

These developments have had a serious impact on applications, an effect which has a history of several decades. Application codes can only benefit from the new architectures if they are optimized with respect to massive parallelism and the incorporation of accelerators. Application scientists and experts in high-performance computing (HPC) therefore have to make common efforts to master this challenge. Additionally, a much closer collaboration between hardware architects and computational scientists has to be established to make them mutually aware of hardware and software issues and to enable robust solutions to be developed jointly.

In the presentation current hardware and software developments will be introduced. By means of several activities of the Jülich Supercomputing Centre it will be demonstrated how a computer centre can support and guide its users towards new technology, how new technology can be influenced by user demands, how hardware developments trigger new software developments and finally, how the successful exploitation of these technical advances leads to new scientific insights.

Keywords: Hardware and Software, High-Performance Computing, Simulation Sciences

Plenary Speaker Thesis

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Academic research groups: evaluation of their quality, quality of their evaluation ***Bertrand Berche***

Using empirical data from the British system of evaluation of the academic research (RAE, REF), we have developed a few years ago a very simple model which apparently accounts for the quality of academic research groups as a function of their size. The process of assessing research being time consuming, and consequently expensive, policy makers have proposed alternative to peer-reviewing. Recently, we have compared predictions from a scientometrics based evaluation with a peer reviewing system. The talk will summarize the work done in this context.

Keywords: Research evaluation, scientometrics, sociophysics

Keynote Speaker Thesis

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Solution of Financial Mathematics Real-Time Problems by Virtual Supercomputer *Alexander Bogdanov*

One of the typical spheres of “complex applications”, i.e. computational tasks that deal with large amounts of significantly irregular information when the rate of input data subject to processing in a reasonably limited time varies by several orders is financial mathematics. Finally, the end user to make a decision should have information in a comprehensible form. Such applications are characterized by the following factors.

- Tremendous number of end users (brokers)
- Large variety of heterogeneous sources of information
- Unpredictable moments of sudden data volume “explosion”
- Necessity to keep in mind as long prehistory as possible to make the prognoses more precise
- Limited time to make decisions, in practice in a real time manner

The most effective way to solve the mentioned problems is usage of cloud computing technologies with the following conditioning.

- Processing algorithms should be parallelized
- Proper load balancing should be provided
- Each end user provided by virtual supercomputer in a cloud

We suggest the natural paradigm of algorithm parallelization providing real-time operation and displaying most effectiveness in clouds by use of virtual supercomputer. We suggest the mechanism for load balancing in “complex applications” equalizing disbalances by order of magnitude.

Keywords: financial mathematics, Virtual Supercomputer, real time, cloud, natural paradigm of algorithm parallelization

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Logically simple algorithms — the way to success of exaflops calculation

Boris Chetverushkin

In the presentation is devaluated to the problems of using high performance computers with extreammassive parallelism. Only logically simple algorithms gives the opportunity for their effective using. One of the way of constructing such kind of the algorithms is to use of connection between kinetic and hydrodynamic description of continuum media. It is demonstrated the results of simulation of some 3D magnetogasdynamics problem; using for approximation the mesh with more then 10^9 nodes.

Keynote Speaker Thesis

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Numerical simulation of small-scale mixing processes in the upper ocean and atmospheric boundary layer

Oleg Druzhinin, Troitskaya Yu. I, Zilitinkevich S.S.

The processes of turbulent mixing and momentum and heat exchange occur in the upper ocean at depths up to several dozens of meters and in the atmospheric boundary layer within interval of millimeters to dozens of meters and can not be resolved by known large-scale climate models. Thus small scale processes need to be parameterized with respect to large scale fields. This parameterization involves the so-called bulk coefficients which relate turbulent fluxes with large-scale fields gradients. The bulk coefficients are dependent on the properties of the small-scale mixing processes which are affected by the upper-ocean stratification and characteristics of surface and internal waves. These dependencies are not well understood at present and need to be clarified. We employ Direct Numerical Simulation (DNS) a research tool which resolves all relevant flow scales, does not require closure assumptions typical of Large-Eddy and Reynolds Averaged Navier-Stokes simulations (LES and RANS). Thus DNS provides a solid ground for correct parameterization of small-scale mixing processes and also can be used for improving LES and RANS closure models. In particular, we discuss the problems of the interaction between small-scale turbulence and internal waves in the upper ocean as well as the effect of the surface waves on the atmospheric boundary layer over water surface.

Keywords: Small-scale mixing, atmospheric boundary layer, upper ocean, numerical simulation

Plenary Speaker Thesis

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Discontinuous Percolation

Hans Herrmann

Abrupt changes in Nature and society can often be traced to the sudden appearance of a finite spanning cluster. While normally percolation exhibits a continuous phase transition, under special conditions the transition can also become of first order. I will illustrate the mechanisms behind the sudden appearance of a macroscopic percolating cluster. Very instructive is the history of the product rule also called “explosive percolation”. The scaling of bridge bonds allows to exactly solve the spanning cluster model having a first order transition at $p_c=1$. Suppressing the largest cluster by forcing a Gaussian size distribution renders an abrupt transition at $p_c<1$. An interesting relation to the watersheds of random landscapes and SLE can then be established. Finally one can find exactly the transition from a second to a first order phase percolation transition by establishing a relation to the q -state Potts model using Gliozzi’s algorithm. This model appears as a limiting case in the pollution of dielectric plates by metallic dust.

Keynote Speaker Thesis

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Protein aggregation might not be related to protein misfolding

Chin-Kun Hu

Ideas and methods of statistical physics have been shown to be useful for understanding some interesting problems in physical systems [1]. After the development of molecular biology, it is of interest to know whether one can use ideas and methods of statistical physics to understand some interesting biological problems from the molecular level. In this talk, I will address the problem of protein aggregation, which is related to many human diseases. Simple models have been found to be useful for understanding the behavior of protein aggregation [2,3,4]. It has been proposed that protein aggregation is due to protein misfolding [5]. However, Figures 1(a) and 2(a) of [3] show that peptide chains aggregate with the conformation of the first excited state of the one chain system rather than the ground state conformation, and Fig. 2(a) is a stable conformation. Figures 2, Fig. 4, Table1, and Table 2 of [4] show that most stable conformation of one chain system is different from the most stable conformation of two-chains system. In such cases, protein aggregation is not due to protein mis-folding [6]. It is of interest to study or review similar problems in other systems.

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Surface 3D nanostructuring by tightly focused laser pulse: Lagrangian codes and molecular dynamics

Nail Inogamov, V. V. Zhakhovsky, and V.A. Khokhlov

There are many important applications where an ultrashort tightly focused laser pulse irradiates Ti deposited onto a dielectric substrate. This is important for nanoplasmonics, laser printing, and microelectrooptics. The technique allows to form the nanoantennas [1] of a submicron size, or to form the periodic matrix arrays [2] of nanoholes, or crowns, or bumps for metaoptics applications, or to cause nanoblistering of the irradiated Ti for laser bio-printing and laser induced forward transfer (LIFT) technologies [3]. We present the detailed picture of laser peeling and 3D structure formation of the thin and thick (relative to a depth of a heat affected zone in the bulk targets) Ti on substrate. The underlying physics was not well understood previously. Our approach is based on a physical model which takes into consideration the modern calculations of the two-temperature equation of state [4] and the two-temperature transport coefficients together with coupling parameter [4]. This is very significant because absorption of an ultrashort pulse (duration 10 fs - 1 ps) excites electron subsystem of metal or dielectric and transfers substance into the two-temperature state with hot electrons (typical electron temperatures 1-5 eV) and much colder ions. It is shown that formation of submicron 3D structures is consequence of the electron-ion energy transfer, melting, delamination of a Ti from a substrate under combined action of electron and ion pressures, capillary deceleration of the delaminated liquid metal or semiconductor, and ultrafast freezing of molten material. We find that the freezing is going in highly non-equilibrium regime with strongly overcooled liquid phase. In this case the Stefan approximation is non-applicable because velocity of the solidification front is driven not by the temperature gradient and the cooling rate but this velocity is limited by the diffusion rate of atoms in the molten material. To solve the problem we have developed the two-temperature Lagrangian code including all this reach physics in. Another powerful tool used to solve the problem is based on the density functional theory for condensed matter in the two-temperature states, on the developing of the embedded atom potentials, and running of the high-performance molecular dynamics code on a modern multi-processor computers.

Work was supported by Russian Science Foundation (project No. 14-19-01599).

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Computer Simulation Studies of Polymer Adsorption and Aggregation

Wolfhard Janke

The talk gives an overview on our recent computer simulation studies of polymer adsorption and aggregation using generic coarse-grained models. The simulations are performed with Monte Carlo methods in generalized ensembles (multicanonical and parallel tempering) and analyzed from a canonical and microcanonical view. The adsorption properties are discussed for polymer chains interacting with a flat patterned surface or being confined in a spherical cage. Special emphasis will be given to the scaling properties of conformational transitions in dependence of the polymer's bending stiffness. Bending stiffness also plays a key role for semiflexible polymer aggregation. Our recent results show that this is the distinguishing parameter that controls whether amorphous aggregates or twisted bundle-like motifs are formed.

Keywords: Computer simulations, Generalized ensembles, multicanonical simulations, polymer adsorption, polymer aggregation

Plenary Speaker Thesis

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Beyond Moore's Law? Seeking Quantum Speedup Through Spin Glasses Helmut G. Katzgraber

There has been considerable progress in the design and construction of quantum annealing devices. However, a conclusive detection of quantum speedup remains elusive. Based on insights from the study of spin glasses combined with large-scale Monte Carlo simulations and data mining techniques, in this talk I present ideas on how to construct tunable hard benchmark problems that work around the intrinsic noise and technical constraints of current quantum optimization machines. Our results show that a careful design of the hardware architecture and benchmark problems is key when building quantum annealers.

Keywords: spin glasses, quantum annealing, Monte Carlo simulations, data mining

Plenary Speaker Thesis

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Maths Meets Myths - Quantitative Investigations of Ancient Narratives **Ralph Kenna**

In recent years, the Statistical Physics Group at the Applied Maths Research Centre (Coventry, UK) has been developing a new, network-science approach to the analysis of ancient texts. Our first investigations in this field focussed on comparative mythology and our first publication [Pádraig Mac Carron & RK, Universal properties of mythological networks, EPL 99 (2012) 28002], generated enormous interest and impact worldwide (15,000 downloads so far, a record for the journal). Since then, we have become aware of excellent work taking place around the world involving quantitative investigations of ancient narratives including mythology, folktales, annals and epics. Here I will (a) contextualise the broader relationship between science (especially statistical physics) and the social sciences & humanities; (b) review some existing quantitative approaches to the analysis of ancient narrative data and (c) give details of our own investigations and the reactions of humanities scholars.

Keywords: Networks, Complexity, Mythology, Epics, Humanities

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Study of Superconductivities in Polycyclic Aromatic Hydrocarbon

Hai-Qing Lin, G. H. Zhong, Z. B. Huang, X. W. Yan, C. Zhang, X. J. Chen

In this talk, I report our progress in studies of polycyclic aromatic hydrocarbon (PAH) superconductors. They might provide route to high T_c superconductors and give hints on novel pairing mechanisms. We carry out extensive numerical and experimental investigations on PAH starting from single benzene ring to phenanthrene ($C_{14}H_{10}$, three benzene rings), dibenzopentacene picene ($C_{22}H_{14}$, five benzene rings), coronene ($C_{24}H_{12}$, six benzene rings), and $C_{30}H_{18}$, seven benzene rings). Their structures, magnetic and superconducting properties as functions of doping and pressure are examined. Our results demonstrate that (1) there exists a unique superconducting phase in all PAH; (2) the spin polarized ground state is realized for charged molecules in the physical parameter regions; and (3) electron correlation is playing an important role in these compounds.

Plenary Speaker Thesis

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Puzzle of supersolid: history and current state

Yurii Lozovik

Possibility of supersolid, the phase with coexisting superfluidity and crystal order in macroscopic and mesoscopic systems is discussed for different physical realizations and correlation regimes. The theory and computer simulation results are analysed.

Plenary Speaker Thesis

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Spanning Trees, Continents, and the Quantum/Classical Divide on D-Wave 2 machines

Mark Novotny, J.S. Hall, L. Hobl, K. Michielsen

Experiences with and results from using D-Wave 2 computers will be presented. Adiabatic Quantum Computers (AQC) with thousands of qubits would be a disruptive technology, allowing calculations that classical computers could not ever perform in any reasonable timeframe. A brief introduction to AQCs in general, and a brief description of the D-Wave 2 machine will be presented. In general, ideal AQCs can conceptually be viewed as SIMD (Single Instruction Multiple Data) machines that run $2N$ simulations in parallel, with N the number of qubits. The D-Wave description will include specifications comparing and contrasting the former 500-qubit Vesuvius processor with the 1000-qubit Washington processor. Results from running on both Vesuvius and Washington processors will be presented. We have performed computations with D-Wave machines for random spanning trees on both processors. Every random spanning tree on the D-Wave Chimera graph encompasses every qubit, but uses only a subset of the couplers between qubits. We performed simulations of random spanning trees drawn from the uniform ensemble of all spanning trees, and this ensemble utilizes all Chimera couplers between qubits. A subset of some of our other calculations on D-Wave machines will also be presented. Our current main goal is to perform test calculations on D-Wave machines to discern strengths and weaknesses, and to determine how it operates as and how it differs from an ideal AQC.

Keynote Speaker Thesis

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Computational problems in Arctic Research

Igor Petrov

We can highlight some of the major classes of problems at the Arctic area, which can be solved by numerical simulations on high-performance computing systems:

- Simulation of the interaction of different ice formations (icebergs, hummocks, and drifting ice floes) with fixed ice-resistant platforms;
- Simulation of the interaction of icebreakers and ice-class vessels with ice formations;
- Modeling of the impact of the ice formations on the ground pipelines;
- Neutralization of dangerous for fixed and mobile offshore industrial structures from ice formations;
- Calculation of the strength of the ground pipelines;
- Transportation of hydrocarbons by pipeline;
- The problem of migration of large ice formations;
- Modeling of the formation of ice hummocks on ice-resistant stationary platform;
- Calculation the stability of fixed platforms;
- Calculation dynamic processes in the water and air of the Arctic with the processing of data and its use to predict the dynamics of ice conditions;
- Simulation of the formation of large icebergs, hummocks, large ice platforms;
- Calculation of ridging in the dynamics of sea ice;
- Direct and inverse problems of seismic prospecting in the Arctic;
- Direct and inverse problems of electromagnetic prospecting of the Arctic.

The system of equations for modeling of these processes is the system of equations which describes continuum mechanics, in particular, solid state physics, acoustics, and fluid dynamics. For the numerical solution of the relevant problems it is necessary to develop or adopt adequate modern computational methods and algorithms for high-performance computers. The study was funded by Ministry of Education and Science of the Russian Federation under grant agreement No. 14.575.21.0084 on October 20, 2014 (the unique identifier PNI: RFMEFI57514X0084) in the Moscow Institute of Physics and Technology (State University).

Keywords: numerical simulations, high-performance computing systems, computing modeling

Keynote Speaker Thesis

Arkady M. Satanin

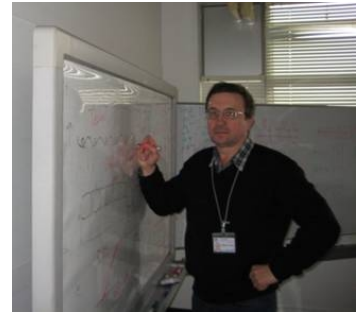
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Generation of entangled microwave photons in superconducting circuits

The superposition principle is the basis of quantum theory. When this principle is applied to composite systems a new concept of entanglement is appeared. It was introduced by Schrödinger in quantum theory in the last century and at present time this principle became a central topic in discussion as main resource of quantum information and quantum computational problems. Entanglement is a property shared by two or more correlated systems. Quantum correlations are also responsible for a number of interesting effects in mesoscopic systems. These correlations may be realized in superconducting waveguides and circuits with embedded Josephson junctions and such kind of circuits are considered as promising candidates for future quantum information processing.

In the present work we consider a coplanar waveguide (or resonator) with embedded Josephson junctions. The waveguides of chosen architecture may be used both as electromagnetic pumping and control of an inserted Josephson junction. The Josephson junction is supposed to be coupled directly with electromagnetic waves in the line with arbitrarily large strength. For a weak driving pulse a single Josephson junction operated as a linear oscillator and demonstrated the linear response for an excitation. At the same time a strong driving pulses can cause the transition of Josephson oscillator in nonlinear regime of excitation. In this case in the first approximation only the Kerr type nonlinearity can be taken in account. It is shown that even in this case in the spectrum of excitation along with main resonance (1:1) the fractional resonance (1:3) also may appear. It means that the Josephson oscillator is trapped to nonlinear fractional resonance for long time and it can radiate three microwave photons for each incoming absorbed photon. Physically three photon processes is the manifestation of well known parametric down-conversion in the system under the consideration. It was shown directly by using a canonical transformation of the Josephson junction Hamiltonian. We note that if the Hamiltonian of system is an odd function of the phase drop on the Josephson junction the two photon processes take place. We have investigated the condition of reemitting photons by nonlinear systems in the regime when only a few levels (the finite Hilbert subspace) of system may be activated. This will be possible due to anharmonicity of a single oscillator or when the Josephson oscillators will be coupled into a cluster (for instance as in the case of a 3J qubit). In particular, for a single oscillator the generation of three correlated Fock-photons (non-separable states) it becomes possible only when the more than three lowest states are involved in the resonance. To characterize the generated Fock-states we have used different correlation functions including of the Schmidt decomposition procedure for the scattering amplitude of photons.

In summary we will discuss the application of correlated microwave photons for distribution of entanglement in quantum communication networks.

Plenary Speaker Thesis

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Classical and quantum anisotropic Heisenberg antiferromagnets

Walter Selke

Classical and quantum Heisenberg antiferromagnets in a magnetic field with uniaxial exchange, XXZ, and, possibly competing, single-ion anisotropy are studied. The models display a variety of interesting features, including spin-flop and biconical ("supersolid") phases, as well as bi- and tetracritical points. In particular, chains, square and cubic lattices are considered. Most results are obtained using Monte Carlo simulations, e.g., stochastic series expansions.

Keywords: anisotropic Heisenberg antiferromagnets, Monte Carlo simulations, multicritical points

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On modern problems and methods for data analysis in human genomics

Vladimir Shchur and R. Durbin

The costs of DNA sequencing have decreased dramatically during the last few years. Now we generate a huge amount of genomic data, for example in the near future millions of complete human genome sequences. On the one hand this growth opens new possibilities for study and understanding of fundamental genetic principles, population structure, disease mechanisms etc. On the other hand, these large databases need new fast and efficient analysis tools. We will discuss problems at the borders of computer science, genetics and statistics that arise in handling these genomic data, and some modern methods and approaches for solving them.

Keywords: human genomics, genome analysis, large data

Plenary Speaker Thesis

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Lattice Boltzmann simulations of flowing matter across scales: classical, quantum and relativistic *Sauro Succi*

Over the last near three decades, the Lattice Boltzmann (LB) method has gained increasing interest as an efficient computational scheme for the numerical simulation of complex flows across a broad range of scales, from fully-developed turbulence in real-life geometries, to multiphase and microflows, all the way down to biopolymer translocation in nanopores. Lately, the method has also shown promising potential for the simulation of quantum-relativistic flows, such as quark-gluon plasmas and electron transport in graphene. After a brief introduction to the main ideas behind the LB method, we shall illustrate a few selected applications, along with future prospects for future multiscale applications, including recent coupling to electronic structure simulations.

Keywords: Computer simulation, Lattice Boltzmann, Multiscale modeling

Keynote Speaker Thesis

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Fragmentation of fractal random structures

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Breakup phenomena are ubiquitous in nature and technology. They span a vast range of time and length scales, including polymer degradation as well as collision induced fragmentation of asteroids. In geology, fragmentation results in the distribution of grain sizes observed in soils; fluids break up into droplets and fluid structures such as eddies undergo fragmentation. On the subatomic scale, excited atomic nuclei break up into fragments. Practical applications, such as mineral processing, ask for optimizations according to technological requirements and efficiency considerations. More generally, a wide range of structures from transport systems to social connections are described by complex networks, whose degree of resilience against fragmentation is a recent subject of intense scrutiny.

We analyze the fragmentation behavior of random clusters on the lattice under a process where bonds between neighboring sites are successively broken. Modeling such structures by configurations of a generalized Potts or random-cluster model allows us to discuss a wide range of systems with fractal properties including trees as well as dense clusters. We present exact results for the densities of fragmenting edges and the distribution of fragment sizes for critical clusters in two dimensions. Dynamical fragmentation with a size cutoff leads to broad distributions of fragment sizes. The resulting power laws are shown to encode characteristic fingerprints of the fragmented objects.

Keywords: critical phenomena, fragmentation, non-equilibrium processes

Plenary Speaker Thesis

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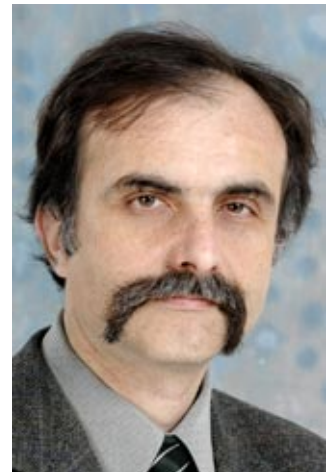
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The grand challenge of quantum computing: bridging the capacity gap

The fabrication and control of macroscopic artificial quantum structures, such as qubits, qubit arrays, quantum annealers and, recently, quantum metamaterials, have witnessed significant progress over the last 15 years. This was a surprisingly quick evolution from theoretical musings to what can now be called quantum engineering. Today, we stand at the point where existing theoretical and computational tools become inadequate for predicting, analyzing, and simulating the behavior of such structures, in which quantum superposition and entanglement play the key role.

The long-known fundamental impossibility of simulating large enough quantum systems by classical means manifests itself already at the level of systems containing as few as several hundreds of qubits. Such a system is still too small to be used as an efficient quantum simulator of comparable systems, but already too large for us to tell with certainty, using the existing classical tools, whether it behaves as a quantum system should. Furthermore, the complexity of already existing quantum processor prototypes confronts us with an engineering problem designing a reliable quantum device and testing its reliability.

Taking the optimistic view that quantum computing is not fundamentally restricted by, for example, the size of a system capable of demonstrating quantum behavior, it would be possible to create quantum computing devices that will allow us to design and fabricate ever bigger and better quantum computers, as well as other macroscopic quantum devices, of a character and use of which we cannot even imagine at the moment. Alternatively, we may find fundamental limits to the applicability of quantum mechanics. Nevertheless, this can happen only if the gap between our current ability to characterize large quantum systems and the capacities of the smallest workable quantum computers is bridged.

Bridging this capacity gap is thus the immediate grand challenge for the field: a challenge that must be met if we hope to make further progress in quantum computing and quantum engineering or if we hope to discover fundamentally new physics, or both.

One possible approach to this task is to consider a system of qubits as a special case of a quantum many-body system and to generalize theoretical methods that have proven to work very well in numerous applications in condensed matter physics and quantum statistical mechanics.

Effective conductivity of tessellations in the plane

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The numerical method is suggested for obtaining effective conductivity of two-dimensional tessellations. For periodic structures the finite difference method with relaxation is used for solving Laplace equation with the corresponding matching conditions between components of a composite, and with corresponding periodic boundary conditions. The method allows one to obtain effective conductivity with high accuracy both when the perturbation theory is applicable and when the component conductivities significantly differ. The method has been applied to two-colored and three-colored periodic tessellations in the plane and has been compared with available analytical results.

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Numerical analysis in the problem of capacity of systems of densely placed bodies

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Analysis of capacity (conduction) of system of many bodies was started in the works by Maxwell and Rayleigh [1, 2]. Subsequently, significant attention has been paid to the capacity (conduction) of systems of closely spaced bodies, especially after Keller reported [3] that the solutions of Maxwell's and Rayleigh are not valid near the singularity (when bodies "almost touch"). For a long time rigor results in the field were known only for periodic systems of bodies. Recently, rigor analysis was done for the random closely spaced bodies [4, 5]. It has been proven that for closely spaced bodies solution of the boundary value problems for the Laplace equation may be functions which can be found by solving a finite-dimensional problem. This finite-dimensional problem is associated with Delaney-Voronoi network for the system of bodies. This is the core of the so-called network approximation method for continuous problems. The fundamental role in the network approximation method plays strong energy localization effect (shielding Tamm effect [6]). It was found that the network approximation exists not for any system of closely placed bodies, but only for bodies for which the shielding Tamm effect takes place (existence or non-existence of the shielding Tamm effect it determined by the shape of the bodies).

Observation of energy localization effect in systems of closely spaced bodies is difficult, both because of the necessary carry out measurements in very thin gaps between bodies and due to the lack of tools for experimental observation of such physical quantity as energy. The use of computers has allowed to solve this problem and get images of the energy distribution between pairs of bodies and in systems of bodies (for small number of bodies). That is, numerical calculations, which may be done with high accuracy for Laplace equation, were used as a replacement for hard-realizable experiments.

There will be presented new results concerning the fall of the capacity (conductivity) of systems of closely spaced bodies in the presence of defects in the matrix between the neighbor bodies. In this problem, numerical computations are the only possible substitute for experiments. There will be presented comparison of the numerical values and values obtained by the simplified method of [3] for finite (small) values of distance between the bodies and sizes of defects.

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Dynamical systems for modeling the evolution of the magnetic field of stars

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The cycles of solar magnetic activity are connected with a solar dynamo that operates in the convective zone. Solar dynamo mechanism is based on the combined action of the differential rotation and the alpha-effect. Application of these concepts allows us to get an oscillating solution as a wave of the toroidal field propagating from middle latitudes to the equator. We investigated the dynamo model with the meridional circulation by the low-mode approach. This approach is based on an assumption that the solar magnetic field can be described by non-linear dynamical systems with a relatively small number of parameters. Such non-linear dynamical systems are based on the equations of dynamo models. With this method dynamical systems have been built for single and double layer media and contains the meridional flow and thickness of the convection zone of the star. It was shown the possibility of coexistence of quasi-biennial and 22-year cycle and existence of the triple cycle (quasi-biennial, 22- and grand minima). We obtained the different regimes (oscillations, vacillations, dynamo-bursts) depending on the value of the dynamo-number, the meridional circulation, and thickness of the convection zone. We discuss the features of these regimes and compare them with the observed features of evolution of the solar and geo magnetic fields. We built butterfly-diagrams for the helicity, the toroidal and poloidal magnetic field for different regimes.

Non-equilibrium critical vortex dynamics of disordered 2D XY-model

Aging and memory effects are nontrivial features in the non-equilibrium behavior of systems with slow dynamics. At slow evolution from a non-equilibrium initial state, the aging of a system is manifested in slowing down relaxation processes with the time passing from the preparation of a sample (its "age") and is accompanied by the violation of the fluctuation-dissipation theorem. A significant interest has been recently focused on non-equilibrium processes in magnetic materials.

Non-equilibrium critical behavior of structurally disordered planar magnets described by the two-dimensional XY-model has been studied by Monte-Carlo methods. For systems evolving from a high-temperature non-equilibrium initial state, the influence of defects of the structure on aging effects, as well as the violation of the fluctuation-dissipation theorem for quenching temperatures in the low-temperature phase, has been analyzed. Power law temperature dependences of the limiting values of the fluctuation-dissipation ratio have been revealed for the first time.

Non-equilibrium memory effects has been investigated from fluctuation-dissipation ratio. It was found that non-equilibrium critical coarsening of vortex subsystem lead to presence of quasi-long-range order. Critical slowing down effects of coarsening growth in disordered system caused by vortex pinning on impurities. The temperature dependences of the spin stiffness for disordered systems were calculated. Using this dependences it were determined temperature ranges of applicability of the spin-wave approximation and temperatures of Beresinskii-Kosterlitz-Taules transition of disordered 2D XY-model with various spin concentration.

This work was supported by Russian Science Foundation (project no. 14-12-00562). The simulations were supported by the Supercomputing Center of Lomonosov Moscow State University and Joint Supercomputer Center of the Russian Academy of Sciences.

The spatially inhomogeneous structures in the solution of Fisher–Kolmogorov equation with delay

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Keywords: attractor, bifurcation, Fisher-Kolmogorov equation, Ginzburg-Landau equation

We considered the problem of density wave propagation in a logistic equation with delay and diffusion (Fisher-Kolmogorov equation with delay). It was constructed a Ginzburg-Landau equation in order to study the qualitative behavior of the solution near the equilibrium state. The numerical analysis of wave propagation shows that for a sufficiently small delay this equation has a solution similar to the solution of a classical Fisher-Kolmogorov equation. The delay increasing leads to existence of the oscillatory component in spatial distribution of solutions. A further increase of delay leads to the destruction of the traveling wave. That is expressed in the fact that undamped spatio-temporal fluctuations exist in a neighborhood of the initial perturbation. These fluctuations are close to the solution of the corresponding boundary value problem with periodic boundary conditions. Finally, when the delay is sufficiently large we observe intensive spatio-temporal fluctuations in the whole area of wave propagation.

On behavior of stochastic synchronization models

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Abstract

There exist many popular physical systems describing different synchronization phenomena (coupled oscillators, Kuramoto model, etc.). Stochastic synchronization models considered in the present talk are mainly motivated by computer science applications. Their dynamics is different from dynamics of the above mentioned physical systems and is based on special synchronization-like interactions between components. We discuss behavior of stochastic synchronization models in different limit situations: when the number of components is large and/or when the time is large.

**RESONANCE PHENOMENA IN EXTENDED MATHIEU EQUATION:
THEORY AND SIMULATION**

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Phenomenon and mechanisms of an energy transfer between degrees of freedom of a dusty plasma system are of great interest in the field of dusty plasma [1,2]. One of such mechanisms [1] is based on parametric resonance. Such phenomena can be described by the extended Mathieu equation [1,3]: $\ddot{x} + 2\lambda\dot{x} + \omega_0^2(1 + h \cos \omega_p t)x = \eta(t)$, where λ is a friction coefficient, h is an amplitude of modulation, ω_0 is an eigen frequency of system and ω_p is a frequency of parameter, $\eta(t)$ is a stochastic force with zero mean value.

Classical Mathieu equation is studied for $h \ll 1$, $\lambda = 0$ and $\varepsilon = \omega_p - 2\omega_0/n \ll \omega_0$ on the level of the first order of accuracy [4].

Acting by an analogy with [4] and using averaging over an ensemble of distributions of $\eta(t)$, we can obtain an expression for the growth rate of the amplitude s . Since this approach can be used only for small values of parameters, while there may be significant friction force and h may be above 1, parallel computer simulation is used to obtain numerical solution for a wide range of parameter values. The resonance areas boundaries obtained analytically and the ones obtained numerically are close only for non-friction system with $h < 1$.

The approach proposed in [4] leads to serious differences with the numerical solution of the equation in the presence of friction ($\lambda \neq 0$). This is because this approach takes into account only terms of zero-order of accuracy with λ . So this approach works only with assumption that $\lambda \ll 1$ and for solution of the first order of accuracy. The authors have proposed a solution that takes into account terms of other orders of smallness. The results obtained this way are closer to the data obtained numerically. It also explains such phenomenon as the shift of the point with a minimum value of h in which the resonance occurs.

The extended Mathieu equation is studied by analytical approach and computer simulation. The solutions for higher order of accuracy are obtained. The method for numerical solution and for estimation of the resonance zone, the time of onset and the growth rate of the amplitude is proposed. The solution for the extended Mathieu equation is obtained for wide range of parameter values. The results of numerical solution are compared with analytical solutions of different order and known analytical results for Mathieu equation. The theory is improved in order to reduce inaccuracies.

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A new model kinetic collision operator

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New form of the model collision operator is derived. A one-component and many-component systems are considered. The collision operator proposed takes properly into account the relaxation of the first 13 hydrodynamic moments. A technique for reconstruction of the model collision integral based on a known expression for the linearized model operator is proposed. It is shown that, within our model, the model collision operator does not contain the complicated exponential, common for the ellipsoidal statistical models. Boltzmann's H-theorem is proved for our model.

**The Numerical Hydrodynamic Modeling of Interacting Galaxies by means
Hybrid Supercomputer on base Intel Xeon Phi accelerators**

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The collisions of galaxies play a important role into a formation of a variety of galaxies, because over the course of a Hubble time, an ordinary galaxy may suffer up to ten collisions with the other galaxies in its cluster [1]. Numerical simulation is main approach for research of these processes. The need to reproduction of various details of flow e.g. some instability processes, forces us to employ the most powerful supercomputers available.

The main ingredients of galaxies are gaseous component and collisionless component for describe of stars and dark matter. Traditionally, a collisionless component is described using N-body models. Nevertheless, this model has disadvantages because of spurious generation of entropy, thermodynamically non self-consistency of star formation and supernovae feedback, increased communication overhead and poor load balancing [2]. The “collisionless stellar hydrodynamics” approach is based on the equations for first moments of the collisionless Boltzmann equation and is adequate for the movement of particles at high kinetic energy in a cluster. In addition, for a description of “collisionless stellar hydrodynamics” and hydrodynamic models an unified numerical methods and parallel algorithms was used [2].

For the system of hyperbolic equations the combination of operator splitting approach (Fluid-in-Cells technique), Godunov method and piecewise-parabolic method on local stencil for high order solver was used. The dual energy formalism for guarantee of non-decrease entropy [3] was used. The subgrid-physics model : a star formation, a supernovae feedback, molecular hydrogen formation, cooling and heating functions, was included. By means numerical simulation on RSC PetaStream was modeled one scenario of interacting galaxies : regions of active star formation/supernovae feedback, and regions with molecular hydrogen formation.

Using of an unified approach for construction of parallel numerical method [4, 5] allowed obtaining on RSC PetaStream supercomputer speed-up factors of 134 for Intel Xeon Phi accelerator and maximum efficiency of 92% is demonstrated using 64 Intel Xeon Phi in native mode on the cluster RSC PetaStream of the Joint Supercomputer Center of the Russian Academy of Sciences.

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Kelvin-Helmholtz instability development in presence of the magnetic field shear and the density profile

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The development of the Kelvin-Helmholtz instability (KHI) on the magnetopause has been investigated in the frame of the ideal MHD taking into account the different scales of the magnetic shear (MS), the region where the magnetic field is changing, and the vortex sheet (VS), the region where the velocity is changing, with no restrictions imposed on the oscillations propagating angle. The linear analysis has shown that the disturbances tilted at small angles with respect to the magnetospheric magnetic may grow faster than the disturbances propagating exactly perpendicular to the magnetospheric magnetic field. The research also includes dependence of the unstable oscillations spectra on the density profile. The results obtained suggest for the density profile to play a crucial part in the instability development. The first results of the numerical simulation of the KHI development with different MS and VS scales are presented. The vortex structures for the different ratio of the MS width to the VS thickness are compared.

Implicit scheme for the Maxwell equations solution in case of flat 3D domains

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A standard scheme for Maxwell equation solution in plasma physics is the leap-frog scheme. The advantages of the scheme are second order of accuracy, time reversibility, simplicity, however the stability condition is $ct/h < 1$, where $h = \min\{h_x, h_y, h_z\}$, c – the light speed. In case of flat ultrarelativistic beams in supercolliders the beam sizes ratio $\sigma_x:\sigma_y:\sigma_z$ may be 1:200:60000. The high ratio of vertical beam sizes provides higher luminosity, and the purpose of the experiments is to increase the maximum available luminosity. The high relativistic factor requires the domain boundaries to be close to the beam. The three-dimensional problem of ultrarelativistic beam dynamics in supercolliders is complicated, and the present effective parallel load-balanced algorithms based on the leap-frog scheme limit the beam sizes ratio to $\sim 1:50:500$. However, the stability condition in case of such flat domains (but not the accuracy condition) forces to decrease the time-step with decreasing of the minimal spatial step, and to decrease the number of times-steps in order to achieve a specified time moment.

We present a new finite-difference scheme for Maxwell's equations solution in three dimensional cases for the cases of different scales in different directions. We overcome the conditional stability by modifying the standard scheme into implicit one. The new scheme satisfies the Gauss law for the electric and magnetic fields in the finite-differences, what is important for the whole algorithm of the beam dynamics.

The approximation order and the stability of the scheme in one-dimensional and three-dimensional cases are analyzed. The study of the wave propagation in different directions demonstrated that the both schemes are non-invariant on the angle with the coordinate axes, but the differences between the two schemes results are insignificant. It is shown, that the scheme maintains the amplitude of the wave and maintains the wave propagation speed with the second order in space and time.

New Compact Equation for Numerical Simulation of 1D and 2D Freak-Waves on Deep Water

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We applied canonical transformation to water wave equation not only to remove cubic nonlinear terms but to simplify drastically fourth order terms in Hamiltonian. Unlike in [1],[2] we choose four-wave interaction coefficient in very suitable form:

$$\begin{aligned} \tilde{T}_{k_2 k_3}^{k k_1} &= \frac{(k k_1 k_2 k_3)^{\frac{1}{2}}}{2\pi} \min(k, k_1, k_2, k_3) \theta(k k_1 k_2 k_3) = \\ &= \frac{(k k_1 k_2 k_3)^{\frac{1}{2}}}{8\pi} (k + k_1 + k_2 + k_3 - |k - k_2| - |k - k_3| - |k_1 - k_2| - |k_1 - k_3|) \theta(k k_1 k_2 k_3) \end{aligned} \quad (1)$$

Equation of motion is the following:

$$\frac{\partial c(x, t)}{\partial t} + i\hat{\omega}_k c(x, t) - i\hat{P}^+ \frac{\partial}{\partial x} \left(|c(x, t)|^2 \frac{\partial c(x, t)}{\partial x} \right) = \hat{P}^+ \frac{\partial}{\partial x} \left(U(x, t) c(x, t) \right) \quad (2)$$

here $U(x, t) = \hat{k}|c(x, t)|^2$ - advection velocity, \hat{k} is the modulus wavenumber operator and \hat{P}^+ is projection operator to the upper half-plane.

The new compact equation (2) generalized for the “almost” 2-D waves i.e. waves slightly inhomogeneous in the transverse direction y . In this case frequency $\hat{\omega}$ depends on both k_x and k_y as $\hat{\omega}_{k_x, k_y}$, while nonlinear terms not depend on y , and c now depends on both x and y :

$$\frac{\partial c(x, y, t)}{\partial t} + i\hat{\omega}_{k_x, k_y} c(x, y, t) - i\hat{P}_x^+ \frac{\partial}{\partial x} \left(|c(x, y, t)|^2 \frac{\partial c(x, y, t)}{\partial x} \right) = \hat{P}_x^+ \frac{\partial}{\partial x} (U(x, y, t) c(x, y, t)) \quad (3)$$

Due to specific structure of nonlinearity the equation (3) can be effectively solved on the computer.

We have performed numerical simulations of sea surface waving in the framework of equations (2, 3). Initial condition in numerical experiments was chosen as slightly perturbed monochromatic wave. After some time we observed the freak wave formation.

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Desiccation of sessile particle-laden droplets: beyond ‘coffee-ring effect’

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The review is devoted to our recent results in simulation of the processes during desiccation of the sessile droplets [1–6]. Our special attention is focused on two particular cases when evaporation is inhibited by a mask [1] or by an obstacle [2] and when a droplet contains both dissolved substances and suspended particles [4].

Desiccation of the sessile droplets attracts a great attention of the researchers due to a wide range of application from nanotechnology to medical tests. When the concentration of the solute is high enough to ensure good adhesion and strong anchoring (pinning) of the triple line, a drop is desiccating with constant base.

Simple models were proposed to describe temporal dynamics of both the shape of the drop and the volume fraction of the colloidal particles inside the drop [3–6]. The concentration dependence of the viscosity is taken into account [4–6]. It is shown that the final shapes of the drops depend on both the initial volume fraction of the colloidal particles and the capillary number. Drying processes of sessile droplets of blood serum (i.e. colloids with the salt admixture) on a solid hydrophilic horizontal substrate are studied [4]. The simulation of spatial distribution of the components in the droplet of biological fluid drying on a substrate is performed using advection–diffusion equation. The proposed model explains the redistribution of components in a sessile drop of biological fluid when it dries. Competition between advection and diffusion leads to large particles (protein) accumulating at the edge of the drop, while solutes (salts) are distributed more uniformly across the diameter of the sample [4]. In our model, we simulate an experiment. A thin colloidal sessile droplet is allowed to dry out on a horizontal hydrophilic surface. A mask just above the droplet predominantly allows evaporation from the droplet free surface directly beneath the holes in the mask. We consider one special case, when the holes in the mask are arranged so that the system has rotational symmetry of order m . Advection, diffusion, and sedimentation are taken into account. The simulation demonstrates that the colloidal particles accumulate below the holes as the solvent evaporates. Diffusion can reduce this accumulation [1]. Drying processes of colloidal film on a solid substrate under a solid disk are studied [2]. A model is proposed to describe temporal dynamics of both the shape of the film and the volume fraction of the colloidal spherical particles inside the film. Initially, the system is single-phase (liquid), then in the area, where the volume fraction of the colloidal particles reaches critical value, solid phase forms. This area holds the shape, prevents the hydrodynamic flows and evaporation from its free surface. In liquid area viscosity and diffusivity depend on the volume fraction of the particles. The rate of solvent mass loss per unite surface area per unite time from the film by evaporation under a disk was obtained numerically from the Laplace's equation for the vapor concentration in the area over the film. During the first desiccation stage the volume of the film under the disk is liquid; the rest of the film becomes solid. When the whole volume of the film becomes solid dried film has a dip below the disk [2].

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Data-intensive multispectral remote sensing of the nighttime Earth for environmental monitoring and emergency response

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Most of the remote sensing applications rely on the daytime visible and infrared images of the Earth surface. Increase in the number of satellites, their spatial resolution as well as the number of the simultaneously observed spectral bands ensure a steady growth of the data volumes and computational complexity in the remote sensing sciences.

Recent advance in the nighttime remote sensing is related to the enhanced sensitivity of the onboard instruments and to the unique opportunity to observe "pure" emitters in visible infrared spectra without contamination from solar heat and reflected light. A candidate set of the night-time emitters observable from the low-orbiting and geostationary satellites include steady state and temporal changes in the city and traffic electric lights, fishing boats, high-temperature industrial objects such as steel mills, oil cracking refineries and power plants, forest and agricultural fires, gas flares, volcanic eruptions and similar catastrophic events. Current satellite instruments can detect at night 10 times more of such objects compared to daytime.

We will present a new data-intensive workflow of the nighttime remote sensing algorithms for map-reduce processing of visible and infrared images from the multispectral radiometers flown by the modern NOAA/NASA Suomi NPP and the USGS Landsat 8 satellites. Similar radiometers are installed on the new generation of the US geostationary GOES-R satellite to be launched in 2016.

The new set of algorithms allows us to detect with confidence and track the abrupt changes and long-term trends in the energy of city lights, number of fishing boats, as well as the size, geometry, temperature of gas flares and to estimate monthly and early flared gas volumes by site or by country.

For real-time analysis of the nighttime multispectral satellite images with global coverage we need gigabit network, petabyte data storage and parallel compute cluster with more than 20 nodes. To meet the processing requirements, we have used the supercomputer at the Kurchatov Institute in Moscow.

Natural Oil Reservoirs: Computer Simulation of the Sedimentary Architecture

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Sedimentary structures under certain circumstances may serve as hydrocarbon traps. A proper oil-site drilling strategy requires adequate geometric and structural models of these geological objects. Modeling sedimentary architecture in hydrocarbon reservoirs is traditionally approached through purely geostatistical methods or structure imitating object-based methods. Such models are flexible and easy to condition to data from wells, seismic profiles, and outcrop analogs, however the geometry and arrangement of sedimentary bodies often lack realism. More realistic prediction of sediment distribution can be provided by the mathematical simulation of the physical processes, responsible for forming the reservoir structure. Applying process-based approach we aim at reproducing the hierarchy of heterogenous occurrences in sedimentation complexes of the fluvial genesis. Using a mathematical model of the floodplain evolution we developed software to simulate the formation of sedimentary bodies with facial heterogeneities. The model describes the processes of river-bed and -banks erosion, sediment-load transfer and deposition. It also includes the process of oxbow lakes formation characterized by argillaceous deposits. Numerical experiments demonstrate the ability of the model and software to reproduce the geometry of the typical elements of the fluvial sedimentation complexes – large crescent-shaped in plan and wedge-shaped in cross section bodies composed of sand with clay layers

NUMERICAL MODELING OF COMPLEX GEOPHYSICAL FLOWS IN SHALLOW WATER APPROXIMATIONK. V. Karelsky¹, A. S. Petrosyan^{1,2}¹ Space Research Institute of the Russian Academy of Sciences² Moscow Institute of Physics and Technology (State University)

Shallow water approximation is used widely to study the large-scale processes in Earth and planetary atmospheres, in oceans. The main difficulty in numerical simulation of nonhomogenous shallow water equations consists in their nonlinearity and their non-divergence property determined by nonhomogeneity of the right-hand side of the momentum conservation equations due to bed complexity. The presence of a non-divergent term induces highly nonlinear effects caused by stepwise change of hydrodynamic quantities in the areas of its sharp change in addition to nonlinear phenomena due to hyperbolic structure of shallow water equations. The other problem consists in compatibility of solutions of traditional depth-averaged equations with depth-averaged solutions of initial Euler equations due to significant role of shallow flows dependences on vertical coordinate. Numerical methods have been developed and effectively used in studies of shallow water flows on complex boundary when an external force effects are insignificant.

In present work we propose to use the Riemann-solver which is adapted to the flow parameters for calculating shallow water flows over an arbitrary bed in the presence of external force. The proposed method belongs to the family of methods based on the solution of the dam-break problem. The method consists in reducing of the problem to successive solutions of classical shallow water equations on the flat plane using Godunov method with allowance for the vertical nonhomogeneity effect in calculating the fluxes through the boundaries of cells adjoining to stepwise boundaries. The vertical nonhomogeneity leads to the Riemann problem solution on a step based on the quasi-two-layer shallow water model. Quasi-two-layer model is extended here for a generalized time-dependent bed which represents an external force. The term time-dependent bed means that at each time moment bed can have different values. We are solving the shallow-water equations for one layer, introducing the fictitious lower layer only as an auxiliary structure in setting up the appropriate Riemann problems for the upper layer. Besides quasi-two-layer approach leads to appearance of additional terms in one-layer finite-difference representation of balance equations. These terms provide the mechanical work made by nonhomogeneous bed interacting with flow.

The main difficulty in modeling of fluid flows over a complex bed consists in that both partly and complete flooded domains may take place. Partly flooded domains present a real challenge for most finite-difference schemes and require special efforts need to be made to capture such domains. Algorithm suggested in our work avoids this difficulty in a natural way. We extend algorithms to the case of multiply-connected domains including partly flooded and dry regions. Partly flooded domains may appear in flows when fluid depth is related to the value of bed gradient when approximated by steps. In this case the step wall is partly wetting and the algorithm suggested in present work considers exactly mechanical work done only by this part of the step. Mechanical work done by nonhomogeneous bed means that the work is done in the process of interaction of non-stationary flow with nonhomogeneous bed, with the step and with part of the step. Numerical simulations are performed based on the proposed algorithm of various physical phenomena, such as a breakdown of the rectangular fluid column over an inclined plane, large-scale motion of fluid in the gravity field in the presence of Coriolis force over an mounted obstacle on underlying surface. Computations are made for two dimensional dam-break problem on slope precisely conform to laboratory experiments. Interaction of the Tsunami wave with the shore line including an obstacle has been simulated to demonstrate the effectiveness of the developed algorithm in domains including partly flooded and dry regions.

Computer simulation of Arctic problems by grid-characteristic method

Favorskaya Alena Vladimirovna, Petrov Dmitry Igorevich, Khokhlov Nikolay Igorevich

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Oil exploration in the Arctic has its own features. For example, the signals from the source propagate through the sea and the ice and they influence to the measured or calculated seismic response.

We simulate wave propagation in media with linear-elastic and acoustic layers. The complete system of equations describing the state of a linearly elastic body and a system of equations describing the acoustic field are solving. The use of the grid-characteristic method provides correctly describing of wave processes and to obtain all types of seismic waves. Correct the contact and boundary conditions, including the contact condition of between acoustic and linear-elastic layers are used.

We consider several problems, in particular

1. Numerical simulation of seismic prospecting in the Arctic shelf.
2. Study the effect of ice, the interposition of receivers and sources in problems of seismic exploration in the Arctic shelf by a detailed analysis of wave patterns and seismograms.
3. Study the effect of icebergs on the seismograms obtained during seismic prospecting in the Arctic.

The study was funded by Ministry of Education and Science of the Russian Federation under grant agreement No. 14.575.21.0084 on October 20, 2014 (the unique identifier PNI: RFMEFI57514X0084) in the Moscow Institute of Physics and Technology (State University).

Application of atomistic simulation for modeling of gas hydratesG.S. Smirnov^{1,2}, V.V. Stegailov^{1,2}¹ *Joint Institute for High Temperatures RAS, Izhorskaya street 13, building 2, Moscow, 125412, Russia*² *Moscow Institute of Physics and Technology (State University), Institutskii per. 9, Dolgoprudny, Moscow region, 141700, Russia*

The continuing rapid development of theoretical and computational methods of atomistic simulations during past decades provides a basis of analysis and prediction tools for chemistry, material science, condensed matter physics, molecular biology and nanotechnology. Nowadays molecular dynamics (MD) method that describes motion of individual atoms by the Newton's equations is a research tool of highest importance. The computational speed and the efficiency of parallelization are the main factors that pose limitations on the length and time scales accessible for MD models (the achievable extremes for classical MD are trillions of atoms and milliseconds, a typical MD step being 1 fs).

We can distinguish critical avenues in the development of high performance MD models. Quantum MD models demonstrate much higher requirements to the data communication speed and hence to the interconnect properties. The deployment of hybrid architectures for electronic structure calculations and quantum MD is not mature enough. Classical MD models are less demanding with respect to data communication. The main limitation in classical MD is the computational complexity of interatomic potentials that is determined by the performance of supercomputer nodes. Therefore hybrid architectures of nodes are considered as a major perspective. In this work we compare different hardware for the software packages widely used for atomistic modeling.

We use molecular dynamics to study properties of methane and hydrogen hydrates. Gas hydrates are crystalline water-based inclusion compounds in which guest molecules are trapped inside cavities of the hydrogen-bonded water network. Several clathrates and filled-ice structures are known. Structure type primarily depends on guest size, temperature and pressure. Gas hydrates allow compact storage of hydrocarbons since one volume of hydrate may contain 180 volumes of gas. Recently, they have attracted interest due to the possibility of being used for hydrogen storage. The pure hydrogen hydrates form at very high pressure, however, the addition of a promoter molecule, for example, tetrahydrofuran or methane, significantly reduce the formation pressure. Practical usage of hydrogen hydrates requires knowledge of their thermodynamic and kinetic properties, mechanisms of formation and decay in a wide range of pressures and temperatures.

In this work, we perform coexistence simulations of methane hydrates for pressures up to 5000 bar for different water models. We calculate the kinetic stability boundary of the superheated metastable sI structure and analyze the effects of the heating rate, system size and cage occupancy [1]. We also report molecular dynamics simulation of several possible structures for the new hydrogen hydrate clathrate. We show the strength of molecular simulation as a supplement tool for the analysis of experimental data [2].

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Influence of hydrophobic properties of dissolved substance to the local structure of the ionic liquid dmim⁺/Cl⁻ at 400K

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Ionic liquids (IL) are a new class of solvents that find their application in various sectors of the chemical industry, which in the future may become alternative substances to replace volatile organic solvents in hazardous chemical plants. Spectroscopic and neutron research confirm the existence of hydrogen bonds between cations and anions of ionic liquids. Most specific interaction between the ions and cations leads to the formation of hydrogen bonds between ions and cations, which hardly sensitive to adding polar or non-polar substances. Experimentally shown that the addition of non-polar compounds to ionic liquids leads to anomalous temperature dependence of the solubility of nonpolar substances in ionic solutions at different concentrations. In this case, decrease the solubility of nonpolar substances in IL with increasing temperature. The dependence of the anomalous behavior of the solubility of nonpolar substances in IL correlates with the size of molecules soluble substances.

Determine the impact of the structure and size of molecules nonpolar substance on the process of local structure and dynamic properties of ILs allows the use of molecular modeling, which allows to analyze the interaction of solvent molecules (dimethylimidazolium chloride (dmim⁺/Cl⁻) and solute (argon, methane benzene) at the micro level. This, in turn, helps to explain the behavior of macro-characteristics of the liquid systems.

Given that one of the classic lines of research in physical chemistry is the study of movement and interaction in solution at infinite dilution and their properties depending on the size dissolved in the IL solute molecules (argon, methane benzene). The method of molecular dynamics (MD) was used to investigate the effect of non-polar molecules to form the local structure of dmim⁺/Cl⁻ at T = 400K. It is found that that the amount of non-polar molecules, what dissolved in dmim⁺/Cl⁻ and affect the nature of its size in a solvent. Increasing the size of nonpolar molecules leads to the rupture of hydrogen bonds between the components of ionic liquids and the loss of grid percolation properties of hydrogen bonds in the studied systems. Obtained, in the case of infinite dilution in the absence of interaction between the nonpolar solute molecules there are various mechanisms restructuring local structure of IL.

Computer Simulation of Charge Stabilized Colloidal Crystals

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The 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 simplest plastic balls to complex objects like DNA molecules and viruses. In colloidal crystals, the particles form spatially ordered structures so that their centres are 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. The present work is devoted to numerical study of elasticity of charge stabilized colloidal crystals.

Interactions in colloidal systems can be rather sophisticated [1]. Within the model approach of the present work, colloidal crystals are treated as a special medium with initial stress governing by only electrostatic and entropic interactions. The crystals studied are composed of electrically charged hard spheres or circles immersed into binary symmetrical univalent electrolyte (1:1 electrolyte).

The properties of the crystals are described in the framework of mean-field theory leading to the non-linear differential Poisson-Boltzmann equation [1]. In contrast to the linearized theories, the Poisson-Boltzmann equation incorporates the non-linearity of charge distribution with respect to the electric potential, so that the non-linear effects are fully included. The dimensionless Poisson-Boltzmann equation for 1:1 electrolyte has a very simple form:

$$\nabla^2 \varphi = \sinh \varphi. \quad (1)$$

Electric charge on the surfaces of particles obeys either constant potential or constant charge density condition. Within the framework of the model, the properties of a colloidal crystal at any particular configuration are fully described by solution of the corresponding boundary value problem for the Poisson-Boltzmann equation. After the solution is obtained, the energy and stress tensor as well as the forces on the particles and osmotic pressure can be easily calculated. The boundary value problem for any particular spatial configuration of colloids was solved numerically. Numerical solution was carried out by finite element method using free tetrahedral meshes of the second order Lagrange elements. Typical discretization contained several millions degrees of freedom. Calculations were partly supported by the Supercomputing Center of Lomonosov Moscow State University [2].

Elastic properties of charge stabilized colloidal crystals in the present work are studied within the approximation of static lattice. Numerical procedures for determination of both the force and 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 directly obtained from the stress-strain dependencies. As it was mentioned above, the charge stabilized colloidal crystals are the systems with initial stress, so that, in contrast to the conventional crystals, the first order elastic constants are not equal to zero.

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. Elastic constants obtained from the stress-strain dependencies and calculated from the force constants are in a good agreement with each other. Stability of the crystals relative different types of deformation is discussed.

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 problems of pair and three-body effective interactions in charge stabilized colloids are discussed.

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Mathematical modeling of emission in small-size cathode

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We consider mathematical modeling of heat transfer and melting through emission in a small-size truncated conical semiconductor cathode.

Our model consists of heat equation (with right-hand side related to Joule heat), equation for the current density inside the cathode and equation relating the current density to the electric potential, and conditions on the free boundaries (boundaries between the solid and liquid phases) which are called Stephan and Gibbs-Tomson conditions.

Our model must take into account some specific features of real cathode such as small size (height of the cathode is about 10 – 15 μm) and very high current density which is a reason of possible melting. The latter implies a free boundary problem.

Though all equations are linear, the whole problem becomes nonlinear because of the presence of free boundaries whose location is unknown and their finding is also a part of problem. We use the following technique: we consider this problem as the limiting (in the weak sense) problem for the other problem known as the phase-field system:

$$\frac{\partial \theta}{\partial t} + \frac{1}{2} \frac{\partial \varphi}{\partial t} = k \Delta \theta, \quad \varepsilon^2 \frac{\partial \varphi}{\partial t} = \varepsilon^2 \Delta \varphi + \varphi - \varphi^3 + \varepsilon \kappa \theta.$$

Here $\varepsilon \rightarrow 0$ is a small parameter and in the limit we obtain the model described above.

Though our model assumes a situation where the cathode has a domain occupied by the liquid phase, it cannot be used in situations where the liquid phase domain appears in the initially solid cathode. So we propose our own method for incorporating the nuclei, which is an external method with respect to the phase field system. We incorporate a nucleus as an unstable state in a small volume of the old phase, or we can say that we artificially create an unstable "mushy region" in a small volume of the old phase. Of course, this raises the problem under what conditions a "mushy region" can be created.

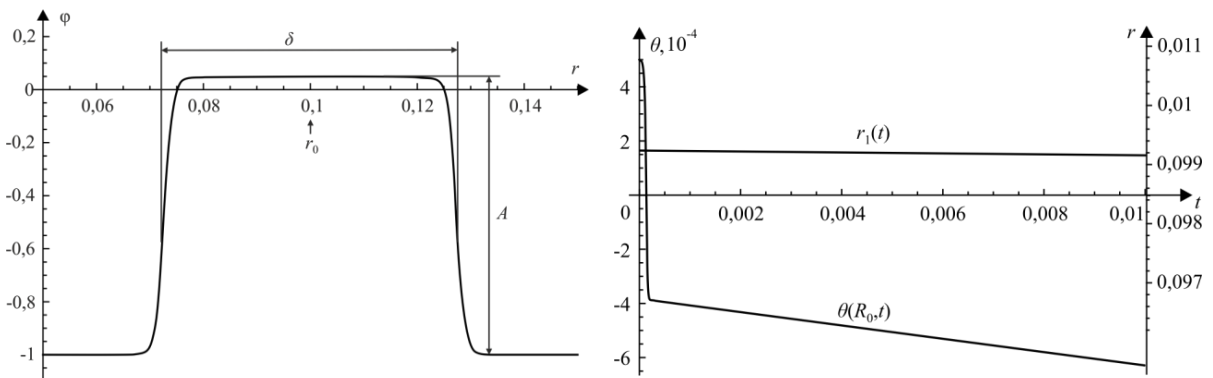
As the nuclei we consider the family of functions which are sums of simple waves for $t = 0$:

$$\varphi = A - (A+1) / \left(1 + \exp\left(-\frac{r - (r_0 + \delta/2)}{\beta \varepsilon \sqrt{2}}\right) \right) - (A+1) / \left(1 + \exp\left(\frac{r - (r_0 - \delta/2)}{\beta \varepsilon \sqrt{2}}\right) \right).$$

Typical nucleus is shown in the figure below.

Now we present our algorithm for the nucleus incorporation. We calculate the temperature till the time moment at which it begins to exceed the melting temperature. At this moment, the computation stops (the process modeling is stopped), and then it starts again with the calculated temperature taken as the initial condition for θ and with φ given by the nucleus equation. We also take into account the possible increase in the Nottingham effect after liquid phase formation.

The plot below shows position of the left free boundary of liquid phase domain and temperature in the top surface of cathode in dimensionless units as $\theta = 0$ is the melting temperature. We can see that after the liquid phase formation, the temperature begins to decrease and the left boundary moves to the right. After some time, the liquid phase must disappear, and the temperature will increase again. This brings the system to the periodical mode of sequential melting-solidification. But because of our restricted calculation resources, we cannot model the whole situation.



Plots of the liquid phase nucleus and time-dependence of the temperature and the free boundary position.

Computer Simulation of Thin Stripper Target Behaviour Under Bombardment of Intense Pulsed Ions

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I. INTRODUCTION

The problems of stripper target behavior in the nonstationary intense particle beams are considered. In the report I try to describe the experimental behavior of foil in the conditions of Brookhaven National Laboratory (BNL) linac.

II. HISTORICAL SKETCH OF STUDYING THE BEHAVIOR OF CARBON TARGETS UNDER ION BOMBARDMENT

The different approaches to quantitative estimations of the lifetime of carbon stripper targets are described in the historical scale.

III. INFLUENCE OF RADIATION DAMAGE ON THE FOIL LIFETIME

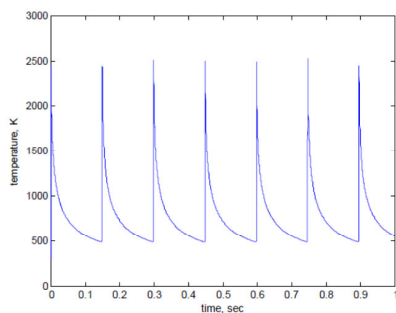
The influence of radiation damage on stripper foil lifetime is related with the point radiation defect accumulation giving rise to deformation of crystal lattice and mechanical destruction of foil.

IV. EVAPORATION OF A TARGET BY AN INTENSE PULSING BEAM

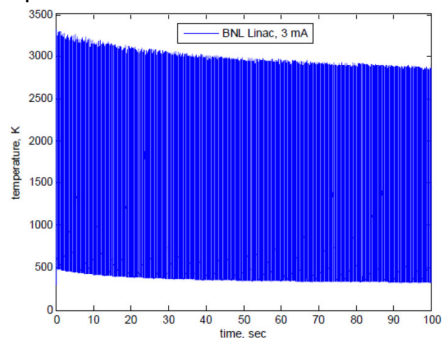
Consideration of temperature field of foil under bombardment by nonstationary intense particle beams giving rise to its evaporation produces the couple of differential equations related the temperature and the thickness of foil which has been solved by means of numerical computer simulation.

V. RESULTS OF CALCULATION AND DISCUSSION

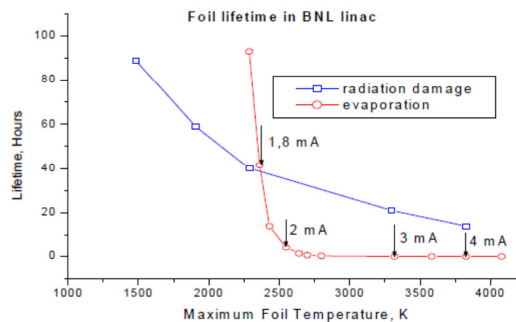
Lifetimes of stripper targets under intensive nonstationary beams can be described by two failure mechanisms: radiation damage accumulation and evaporation of a target. At the maximal temperatures less than 2500K the radiation damage dominates; at temperatures above 2500K the mechanism of evaporation of a foil prevails.



A temperature field of a BNL linac target in the first second of work at a pulse current 2 mA .



Deformation of a temperature field in a target of BNL linac, caused by the reduction of thickness of a foil due to its evaporation.



Calculated dependences of lifetime of BNL linac foil due to processes of radiation damage and evaporation.

Simulation of catalytic properties of thermal barrier coatings for space vehicles in dissociated air

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Heterogeneous processes play a key role in controlling the heat flux to the surface of reusable space vehicles during their entry into the atmosphere. Elucidation of the mechanisms of these processes and determination of their basic kinetic characteristics are important for developing effective thermal protection systems.

The relevance of studies of the properties of thermal barrier coatings has been enhanced by the advent of new materials for promising reusable hypersonic aircraft, which need effective thermal protection at surface temperatures of ~2000 K. In addition, all the more challenging become the issues of reducing the heat load on the surface of spacecraft and probes designed to descend into the Martian atmosphere and then to return to Earth.

In this paper elementary stage rate coefficients of a complete set of a heterogeneous catalytic recombination in dissociated air on surfaces of thermal-protective ceramic tile coverings β -cristobalite and α -Al₂O₃ are defined by means of quantum mechanics calculations within the limits of cluster models. The processes of a shock (IR) and associative recombination (LH) of adatom of oxygen and nitrogen were considered.

The obtained values of the rate constants were used to calculate the values of the heterogeneous recombination probability on surface covers, and recombination heat flows for a diffusion layer near the surface under study at surface temperatures of 200–2000 K and pressures of 1000–7000 Pa.

Analysis of the results showed that the contributions from the two model mechanism cannot be rigorously separated in the entire temperature range, except for low temperatures (up to 800 K), where the ER mechanism dominates and high temperatures above 1000 K), where the LH mechanism provides up to 70% of the recombination probability.

The approaches grounded on usage of methods of quantum mechanics, allow to fathom better the gear of heterogeneous catalytic processes and to define rate coefficients of the elementary processes without engaging of experimental data.

Computer simulation of GaAs/GaAs(001) epitaxial growth considering V/III flux ratio

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The kinetic Monte Carlo method is used to investigate V/III flux ratio effect on the submonolayer growth processes during molecular beam epitaxy of GaAs on the GaAs(001) substrate. The crystal is represented as a two-dimensional lattice having the physically adequate zinc blende structure of GaAs. The starting surface is prepared in the $\beta 2(2 \times 4)$ reconstruction of GaAs(001) with two top layer As dimers per unit cell. We take into account the alteration of activation energy of each included microscopic process depending on the location and top-layer environment of a particle.

We observe that at temperature (T) of 580°C and growth rate (ν) of 0.1 monolayer (ML) per second the island density (N) is saturated after deposition of 0.06 ML GaAs in the range of $V(\text{As}_2)/\text{III}$ flux ratio $J_{\text{As}/\text{Ga}}$ from 3 to 40. The simulation yields $N = 2 \cdot 10^{12} \text{ cm}^{-2}$ at these technological parameters. Islands preferentially form in the trenches and favor elongation along the $[1\bar{1}0]$ direction (Fig. 1). These results give good agreement with experiments [1,2].

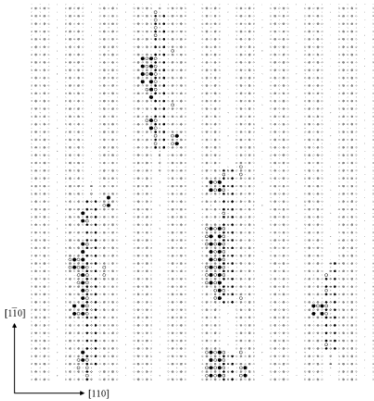


Fig. 1. Island morphology in a simulation area of $160 \text{ \AA} \times 200 \text{ \AA}$ after deposition of 0.06 ML GaAs at $T = 580^\circ\text{C}$, $\nu = 0.1 \text{ ML/s}$, $J_{\text{As}/\text{Ga}} = 10$

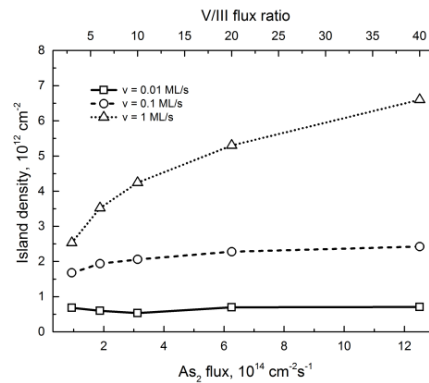


Fig. 2. Island density as a function of V/III flux ratio after deposition of 0.06 ML GaAs at different growth rates ($T = 580^\circ\text{C}$)

We reveal the V/III flux ratio dependence of the island density. It rises nearly two times with the increase of $J_{\text{As}/\text{Ga}}$ from 3 to 40 at 550°C ($\nu = 0.1 \text{ ML/s}$) and nearly three times at a growth rate of 1 ML/s ($T = 580^\circ\text{C}$) (Fig. 2). The calculated fraction of arsenic atoms in the growing film made it clear that As_2 desorption is low under these conditions whereas at lower growth rates and higher temperatures arsenic atomic fraction is less. Moreover, at a rate of 0.01 ML/s larger flux ratios are needed to provide stoichiometric GaAs growth since arsenic atomic fraction exceeds 0.5 at $J_{\text{As}/\text{Ga}} \geq 10$. Otherwise, surplus Ga adatoms form uncovered strings in the trenches.

The fraction of arsenic atoms rises with the increase of V/III flux ratio, but after deposition of 0.2 ML GaAs and more it exceeds 0.5 over the wide range of $J_{\text{As}/\text{Ga}}$ from 3 to 40 and doesn't change significantly. Thereby, V/III flux ratio influences the island characteristics but doesn't break compound stoichiometry. It enables enhanced control of GaAs epitaxial film morphology.

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**Structure and electronic spectra of silicon nanoclusters passivated by hydrogen and oxygen:
evolutionary algorithm and first-principles study**

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Nanoclusters and nanoparticles belong to the most intensively studied objects of solid state physics. This keen interest is stimulated by their potential applications in many fields, such as nanoelectronics, nano-optics, solar energetics and biomedicine. It is known that the properties of nanoobjects are greatly different from the properties of bulk solids with the same chemical composition. This difference even being experimentally observed is not easy for understanding. First-principles calculations, which are so informative in crystal research, meet here considerable difficulties caused by an unknown atomic structure of clusters. From the mathematical point of view, the problem of structure prediction is reduced to searching the spatial arrangement of atoms giving the global minimum of the total cluster energy. Because of a huge number of possible atomic configurations, focusing the search on areas, where the total energy is fairly low, is highly important, as it makes practicable the first-principles calculation of cluster structure.

Solving this problem, the evolutionary algorithm implemented in the USPEX code has shown its superiority over other methods of structure optimization. In this presentation we apply this method in combination with density functional calculations to study the structure and electronic spectra of silicon nanoclusters passivated by hydrogen ($\text{Si}_{10}\text{H}_{2m}$, $m = 0, \dots, 11$) and oxygen ($\text{Si}_{10}\text{O}_{2m}$, $m = 0, \dots, 14$). A significant number of investigated objects and their wide diversity give rich information about the advantages and sensitive points of such computational method. In particular, we note that the fast convergence of evolutionary search is not universal, but strongly depends on the energy distribution of metastable isomer structures and their energy separation from the ground state structure. It was found that hydrogen and oxygen atoms have distinct positions in silicon nanoclusters and dissimilarly affect their structure. Hydrogen atoms are situated on the cluster surface, where they passivate the dangling bonds of Si atoms. With hydrogen addition the cluster structure becomes sparser and approaches the structure of polymers. The positions of oxygen atoms follow more complicated trends. At low concentration they go presumably to the cluster core forming there small regions of quartz-like structure. When oxygen concentration exceeds the SiO_2 composition, new added O-atoms occupy the cluster surface that makes a cluster more reactive. Using our first-principles results, we also considered the thermodynamics of $\text{Si}_{10}\text{H}_{2m}$ and $\text{Si}_{10}\text{O}_{2m}$ cluster ensembles and selected the most stable cluster compositions (so called "magic" clusters). To understand these structure trends, we use electron bond analysis and considered the electronic spectrum of clusters, involving their quasiparticle spectrum calculated by the precise GW method. Despite such first-principles simulation requires large computation, it provides valuable information about the processes of cluster formation.

**Numerical studies of fundamental principles of ion transport in electrochemical systems
based on autocatalytic redox–mediator mechanism**

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A new autocatalytic EC'' mechanism of electrochemical reactions has been proposed recently [1]. Similar to the well-known electrochemical catalytic mechanism EC', the conversion of electrochemically inactive reagent is carried out due to its chemical reaction with one of the solute components of the mediating redox couple, but in the EC'' case the reagent is transformed into a component of this couple in the course of the reaction. As a result, accumulation of the homogeneous catalyst, i.e. of the mediating redox couple takes place, so that such a process has got autocatalytic features. A particular example of such EC'' mechanism is provided by the electroreduction of halogen oxoanions XO_3^- (for $X = Cl, Br$ or I), which in some cases passes by means of a combination of the electrochemical and chemical steps, namely a reversible transformation between the components of the redox couple:



while the oxoanion is reduced via comproportionation reaction:



For passage of a current, j , under steady state conditions the system of Eqs. (3) with boundary conditions (4) describes the concentration profiles inside the diffusion layer for such a reaction at the uniformly accessible electrode surface:

$$D_A d^2A/dz^2 = v, \quad D_B d^2B/dz^2 = 5v, \quad D_C d^2C/dz^2 = -3v, \quad v = k A(z) B(z) \quad \text{for } 0 < z < z_d \quad (3)$$

$$A(z) = A^0, \quad B(z) = 0, \quad C(z) = C^0 \quad \text{for } z = z_d; \quad dA/dz = 0, \quad D_B dB/dz = -j/F, \quad D_C dC/dz = j/2F \quad \text{for } z = 0 \quad (4)$$

Eqs. (3) may be partially integrated, resulting in analytical relations between each pair of concentrations. Then, this system of equations and boundary conditions may be reduced to the equations for dimensionless concentrations:

$$d^2b(x)/dx^2 = a(x)b(x), \quad a(x) = 1 - J[x_{dk} - x - b(x)]/x_{dk}, \quad c(x) = 0.1[x_{dk} - x - 6b(x)] \quad \text{for } 0 < x < x_{dk} \quad (5)$$

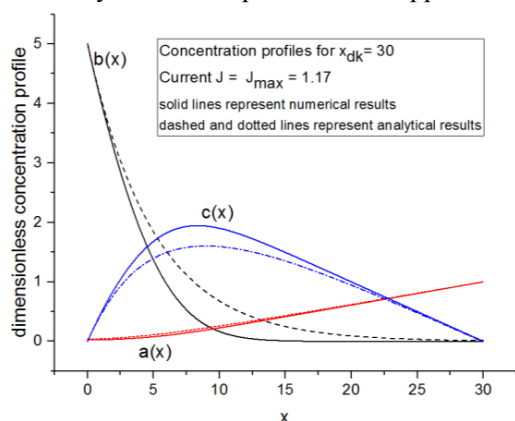
where $x \equiv z/z_k$, $x_{dk} \equiv z_d/z_k$, $z_k \equiv (D_A/5kA^0)^{1/2}$, kinetic layer thickness, J , dimensionless current density.

Eqs. (5) are combined with conditions at two boundaries: $b(x_{dk}) = 0$, $db/dx = -1$ for $x = 0$.

Its solution was found by choosing a trial value: $b(0) = b_0$, to perform the numerical integration of Eqs. (5) with the use of the Runge-Kutta routine. Thus found $b(x_{dk})$ value served to determine the next b_0 value, in order to approach $b(x_{dk})$ stepwise to 0. This test and trial procedure provided the concentration profiles for any combination of the x_{dk} and J values. The solutions must also satisfy to the condition that no concentration is negative within the whole x interval. The maximal current density, J^{\max} , was found for each x_{dk} value from the condition that one of the concentrations becomes equal to 0 in a point (Fig. 1).

These numerical results were compared with approximate analytical formulas, which had been derived in [1]. Excellent agreement was found for relatively weak current densities. Numerical and analytic results for the $J^{\max}(x_{dk})$ dependence are very close to each other even for the range of very strong currents (Fig. 1). On the other hand, marked difference has been discovered in the latter case for the concentration profiles (Fig. 2).

Thus, one may conclude that the numerical approach carried out in this study represents a very prospective method both for verification of approximate analytical results (where they may be obtained) and for theoretical predictions for regimes where analytical technique cannot be applied.



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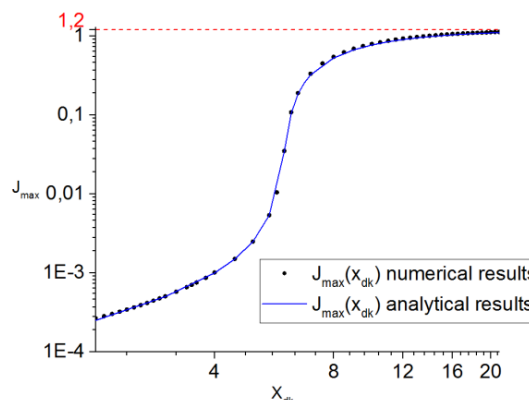


Fig. 1 (on the right) The maximal current density, J^{\max} , as function of x_{dk} .

Fig. 2 (on the left) Profiles of dimensionless concentrations for of XO_3^- , X^- and X_2 species (denoted as $a(x)$, $b(x)$, $c(x)$, correspondingly).

The use of fuzzy modelling for predicting the values of the classic potential barrier of the reaction phenyl radical with hydrocarbons

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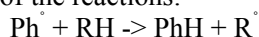
Experimentally reactivity of organic compounds in radical reactions is determined by the activation energy (E) or the value of the classical potential barrier (E_e) according to the formula

$$E_e = E - 0.5(hL\nu_i - RT)$$

where ν_i are vibrational frequencies for stretching bonds, R is the gas constant (J/mol·K), h is the Planck's constant, L is the Avogadro number and T is the reaction temperature (K).

In [1,2] was proposed empirical models of elementary bimolecular radical reactions of abstraction, which allows to build non-linear correlations between the classical potential barrier radical bimolecular reaction and thermochemical properties of reactants.

We consider experimental sample of the reactions:



The experimental sample of 97 reactions of the phenyl radical with various hydrocarbons is obtained from the database on rate constants of liquid phase radical reactions [3], which 12 were the control sample. The dissociation energy of the C-H bonds are taken from [4]. For this sample $D_f = 474$ kJ/mol [4] and $\alpha = 0.945$ are constant. Therefore, the dependence takes the form:

$$E_e = \varphi(D_{ei}, br_e)$$

To approximate the values of the classical potential barrier the Mamdani's fuzzy inference method was used based on the using the matching degree to which they belong to each of the fuzzy rule via membership functions, equal the real number α_i , characterizing the degree of membership of input A'_1, A'_2, \dots, A'_n to fuzzy sets $A_{i1}, A_{i2}, \dots, A_{in}$ in the background of the i -th rule

$$\alpha_i = \min_{j=1}^n \left[\max_{x_j} (A'_j(x_j) \wedge A_{ij}(x_j)) \right]$$

where X_j is the domain of the variables ($x_1 = D_{ei}$ и $x_2 = br_e$).

On the example of reactions between substituted phenyl radicals and hydrocarbons an attempt was made to identify the dependence of classical potential barrier of radical reactions by the fuzzy knowledge base built on basis of quantitative and qualitative parameters.

Using a fuzzy knowledge base built by experts, and Mamdani's fuzzy inference method using membership functions

$$\mu^G(x) = \frac{1}{1 + \left(\frac{x-b}{c}\right)^2}$$

produces a good approximation of the values of the classical potential barrier for phenyl radical reactions with hydrocarbons.

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Some generalized models of random sequential adsorption of linear k -mers on a square lattice: jamming and percolation

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The review is devoted to our recent findings regarding the percolation and jamming of the linear k -mers (particles occupying k adjacent sites) on a square lattice [1–5].

Deposition of large particles such as colloids, polymers or nanotubes on substrates can be considered and studied as the random sequential adsorption (RSA). In ideal RSA model, objects randomly deposit on a substrate; this process is irreversible, and the newly placed objects cannot overlap or pass through the previously deposited ones. The adsorbed objects may be identical or present a mixture of objects of different sizes and shapes. With a large enough concentration of the deposited objects, they can form a spanning path between the opposite sides of the substrate and this concentration corresponds to the percolation threshold. If the deposition of the objects goes infinitely long, a jamming state is reached. At the jamming state, there are still voids between the previously placed object on the substrate, but their size and shape are not sufficient to deposit even one additional object.

Great efforts have been devoted to studies regarding percolation and jamming for the RSA deposition of elongated particles, particularly linear k -mers.

Very often, the real surfaces are chemically heterogeneous and contain defects; moreover, the substrates may be prepatterned. The structure of the elongated particles, e.g., carbon nanotubes, adsorbed on the substrate may also be highly heterogeneous, e.g. due to their chemical functionalization. Different variants of the more general RSA models, taking account of the heterogeneity of substrates, interactions between the deposited particles and the possibility of surface diffusion have been proposed. These models are more realistic in their description of the experimental results for colloid particle adsorption on substrates characterized by a wide spectrum of binding energies. The jamming and percolation of k -mers on disordered (or heterogeneous) substrates with defects, or k -mers with defects, have also attracted great attention. Moreover, anisotropy can be introduced by postulating unequal probabilities for deposition of elongated objects along different directions.

In more general RSA model the anisotropy of deposition can reflect the influence of the external fields, flows or anisotropy of the substrate. The adsorption of the elongated particles in the presence of the external fields produces the anisotropic layers. Another generalized RSA model of cooperative sequential adsorption accounts of the presence of very strong near-neighbor (NN) lateral repulsive interactions and dependence of the adsorption probabilities on the local environment. In the simplest case, the constraint assumes that all NN locations are empty. For this model the percolation is observed only at some interval $k_{\min} \leq k \leq k_{\max}$, where the values k_{\min} and k_{\max} depend upon the fraction of forbidden contacts d .

For ideal RSA and completely disordered system, a conjecture has been offered that percolation is impossible when k exceeds approximately 10^4 .

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Heavily parallelized codes for the energy minimization and Monte Carlo simulation of polymer knots

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Polymer rings, also called catenanes in the chemical literature, constitute a frequently occurring motif in nature and in artificial soft matter materials. Very often in DNA and sometimes in proteins, these rings form very complicated knots. Knots are also relevant in polymer materials, for instance by increasing their breakability or altering their elastic behavior. The study of the mechanical and thermal properties of polymer knots poses several challenges and is a highly interdisciplinary problem. To obtain a satisfactory statistics, several hundreds of billions of knot conformations must be sampled during a Monte Carlo simulation. This requires the development of fast algorithms that are able to take into account the topological properties of the knot. On the other side, the energy landscape of a polymer knot is very complex. Sophisticated algorithms of energy minimization are necessary in order to explore this landscape.

In this talk the results of a recent study of the statistical mechanics of very long polymer knots will be presented. This case demands in a compelling way the application of heavily parallelized codes. In the investigation, the Wang-Landau multicanonical Monte Carlo algorithm has been used. The polymers are mainly, but not only, defined on a lattice. Some of the problems arising in Monte Carlo numerical simulations and in exploring the energy landscape of very long polymer knots will be discussed together with their solution. The results obtained in understanding the mechanical and thermal properties of these interesting physical systems will be shown.

Graphite melting: atomistic kinetics resolves longstanding controversyNikita Orekhov^{1,2*}, Vladimir Stegailov^{1,2,3}

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Graphite is one of the most wide-spread carbon allotropes. Unique thermophysical properties of graphite result in its important role in science and engineering. However, the experimental data on graphite melting temperature still remain controversial despite the long history of investigation. The experimental results of several works cover the wide span from 3800 to 5000 K that is an essentially larger uncertainty than the errors of individual experiments. The analysis of many experiments suggested a dependence of the measurement results on heating rate; however this fact has not been explained satisfactorily.

Here we report the results of molecular dynamics (MD) calculations on the kinetics of two competing processes in graphite: the heterogeneous melting at the solid-liquid boundary and the homogeneous melting due to the spontaneous formation of liquid phase nuclei. Our MD results show an unexpectedly weak kinetics of the melting front propagation in graphite that is several orders slower than that in metals and a high stability of crystal under superheating up to 4800-5000 K (i.e. slow rate of liquid nucleation via homogeneous mechanism).

The heating of the sample in an experiment can be characterized by the heating rate $\dot{T}(t) = \text{const}$. In the case of ultrashort pulse experiments the heating rate can be more than 10^9 K/s. The surprisingly slow melting kinetics of graphite melting revealed from MD simulations allows us to make a hypothesis that at a sufficiently high heating rate the temperatures well above T_m can be reached before the moment of formation of the liquid phase amount enough for the melting detection ($T = T_m^d$).

The analysis carried out in this work shows that the homogeneous nucleation mechanism limits the sample temperatures at 4900-5000 K even at $\dot{T} \sim 10^{12}$ K/s. This upper estimate coincides with the graphene melting temperatures and with the highest experimental values of graphite melting temperature. However, at $T < 4500-4600$ K the homogeneous nucleation rate is negligible that, taking into account the slow nature of heterogeneous melting, allows essential crystal superheatings at the timescale of milliseconds.

The results obtained can be considered as an essential argument in favor of the hypothesis that at $\dot{T} > 10^5-10^6$ K/s the de facto detected in pulse heating experiments “graphite melting temperatures” T_m^d corresponds to the temperatures when the decay of the superheated metastable solid graphite takes place. And therefore these temperatures are not strictly speaking the graphite melting temperatures in the thermodynamic sense T_m .

Open-shell molecule: Problems of computer simulation and the reality of spin contamination of the molecule ground state

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Open-shell molecules belong to atomic systems with a considerable electron correlation. Close-to-degeneracy electron states strongly influence the spin symmetry consideration due to which complicated schemes related to configurational interaction (CI) are needed to provide appropriate computer simulations of the species. The paper presents one of possible ways to tackle the problem by using CI bi-determinant Hartree-Fock approximation. A particular attention is given to spin-contamination of the states that is a distinguishing characteristic of the electron correlation at any level of the theory. Basing on results obtained for graphene molecules and addressing the available experimental data allow for suggesting that the spin contamination of the ground state of open-shell molecules is a physical reality.

Quantifying the differences between the auction and the negotiated market: the role of the structure of interactions

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It is commonly admitted among economists, that a market with a centralized structure (like an auction market) is more efficient than a decentralized one. The reason for this, being the fact that in the former, all the actors dispose of the same information while the negotiations remain private in the decentralized one. There is a large number of works comparing both types of market and recent studies start paying attention to the structure of the interactions [1-2].

The *Boulogne-Sur-Mer Fish Market*, the most important one of France in terms of quantity, is an excellent case study to investigate this problem. This old market, which had operated in a decentralized way for long time, was led by UE regulations to adopt a centralized structure. However, this new way of functioning did not convince the economic actors and it was finally admitted, in 2006, to allow the two forms of market (auction and bilateral negotiation submarkets) to coexist in the same place. Detailed data concerning the daily transactions is available, allowing for a comparison of the behavior both sub-markets under similar economic, seasonal, climatic and social, conditions.

In this work we are interested in the structure of the social interactions that take place among the actors of both submarkets. These interactions can be described by the means of a complex network where the nodes are of two different kinds, (representing buyers and sellers), and the links, that stand for the interactions, only connect nodes of different kinds. The network so obtained is *bipartite*. This network has weighted links when one takes into account the interactions of the whole period.

We study this problem applying the tools and concepts commonly used to study ecological mutualist systems [3]. In these systems the interactions between actors of two different guilds brings a mutual benefit to both, like in *plant-pollinator*, or *plant-seed-dispersers* networks. We investigate if some similar mechanism structures the negotiated market where the actors come to know each other after a repeated number of visits and transactions.

Our results show that the structures of the social interactions developed in both submarkets are different. In particular, we define an index that accounts for the “fidelity” of the interaction between the different couples of actors in both markets. The probability distribution of this fidelity index looks scale free in the negotiated market while it shows a sharper decrease in the auction one, suggesting that there is a threshold for the fidelity of the agents in the latter.

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Multilayer network model of mutualistic ecosystems: network structure and biodiversity.

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Considerable attention is currently being paid to the study of ecological systems, as they often provide valuable services to mankind. A sustainable management of ecosystems as well as a proper assessment of the impact of human activity on them can only be achieved with a good understanding of their properties. *Mutualistic* ecosystems, involve two groups of species that are clearly differentiated, usually animals and plants, who help each other in fulfilling essential biological functions, as in the case of *pollination networks*, where a set of plants is pollinated by the insects that feed from the nectar of their flowers.

Usually they are described by a bipartite network where only vertices of two different kinds (animals and plants) are connected by links that represent the mutualistic interactions. Observed networks show a particular structure called *nestedness*, which implies that the system is composed of *generalists* (species that interact with most species of the other guild) and *specialists* (i.e. species that interact with very few species of the other guild) that mainly interact with generalists.

The origin and the consequences of the nested structure of mutualistic ecosystems as well as the pertinent characterization of such ordering are a matter of strong debate in the ecological community. The relationship between the structure of mutualistic ecosystems and the dynamics that led to this structure is still an open problem. In the seminal paper of May [1], the ecosystem is described by a dynamical linear model, with a random interaction matrix. His results show that a large ecosystem with high connectivity (the connectivity being associated to the complexity of the system) is unstable. Since then, special attention has been paid to the structure of the interaction matrix. Bastolla

et. al [2] study a population dynamics model that includes plant-animal mutualistic interactions and animal-animal and plant-plant competing interactions, in mean field approach, except for the weak mutualism regime, where a more realistic mutualistic term is included. They conclude that the nestedness minimizes competition, allowing for an increase of biodiversity. As the parametrization of the studied models is quite arbitrary, it becomes crucial to assess how the obtained results behave face to the variation of these parameters.

In this work we investigate the influence of the network structure on the biodiversity of a mutualistic ecosystem. We study a non-linear population dynamics model and we take the structure of interactions explicitly into account both, in mutualistic and competition terms.

The ecosystem may be treated as a two layers of competing agents, one for plants and another for animals, coupled by the mutualistic interactions. The projection of the bipartite matrix on the animals' or plants' subspaces give the number of counterparts shared by any two given species of the same guild and may be used to model the corresponding competition term.

We study the steady states obtained for real matrices as a function of the intensity of the interactions and we analyse how these states vary with the nestedness of the system while controlling or not for degree distributions. Our results show the existence of a trade-off between the different interactions, so that the largest biodiversity is achieved with a non-trivial combination of mutualism and competition.

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Virtual network as excitable medium

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We simulate the spread of an activity in a virtual group.

Dissemination of ideas and opinions in virtual networks, *e.g.*, in social networks, the Internet, academic networks, the blogosphere, etc. is of special interest. The researchers utilize different models to simulate the dissemination of information in networks. We perform simulations using the model of excitable medium [1] and the epidemic models [2]. We suppose that the structure of the virtual group corresponds to a scale free network [3].

Moreover, to simulate the spread of certain ideas in a professional virtual group, we considered the propagation of excitation in an inhomogeneous excitable medium of high connectivity [4]. We assumed that the network elements form a complete graph. Parameters of the elements are normally distributed. The simulation showed that interest in the idea can fade or fluctuate depending on the settings in the virtual group. The presence of a permanent excited element with relatively high activity leads to chaos, *i.e.* the fraction of members of the community actively interested in an idea varies irregularly.

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**Optimization problems for WSNs: trade-off between synchronization errors
and energy consumption**

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Abstract

We discuss a class of optimization problems related with stochastic models of wireless sensor networks (WSNs). The goal is to minimize a cost functional which accumulates synchronization errors and energy consumption over a given time interval.

We show that optimal solutions for such models can contain singular arcs. We discuss possible algorithms of numerical solutions of these optimal control problems.

Open marketplace for simulation software on the basis of a web platform

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The work examines the current trends in designing of systems for convenient and secure remote job submission to various computer resources, including supercomputers, computer clusters, cloud resources, data storages and databases, and grid infrastructures by authorized users, as well as remote job monitoring and obtaining the results. Currently, high-performance computing and storage resources are capable of solving independently the majority of practical simulation problems in the field of science and technology. Therefore, the focus in the development of a new generation of middleware shifts from the global grid systems to building convenient and efficient web platforms for remote access to individual computing resources.

The sets of features of the web platforms can vary significantly. The following are the basic features of web platforms: web platforms for job submission provide remote submission, monitoring, and obtaining the job results; web platforms for job submission and software installation provide, in addition to the preceding features, remote installation and configuring of application packages; web hubs provide features from the two preceding items plus providing the features of professional social networks, for example, allowing to exchange the experience in the use of the platform tools, interaction with the developers, forming the rating of individual application packages/tools.

Further line of development of the web toolkit, suggested in this work, is related not only with the quantitative increase in the number of web-based platforms for remote access and the expansion of scientific, engineering, and manufacturing areas in which they are used, but also with the improvement of the technology of remote deployment of new application software on resources interacting with the web platforms.

This approach will help to overcome an important problem associated with the use of the Software as a Service (SaaS) model in scientific areas, namely, limited set of application packages offered by SaaS providers. Often, these providers focus on mass servicing of single-type customers and scientific activity is beyond the scope of their interests. Currently, the provision of services for providers of application software in the context of scientific-oriented web platforms is not developed enough. Although some implementations (for example, e-Science Central; <http://www.esciencecentral.co.uk>) have services for remote application software deployment, they are still insufficient to ensure the creation of a web platform capable of performing the whole range of tasks characteristic for a free open market. The web platforms of application software market should have all the above mentioned features plus provision of information and computing web services for interaction between the providers and consumers of simulation application packages based on market principles (analogue of such app stores as AppStore, Google Play etc.)

The technology of creating such web platforms market of application software is based both on the original solutions and on the synthesis and adaptation of the solutions used in research hubs (e.g., nanoHUB; nanohub.org), cloud and grid systems, as well as in on-line app stores. However, unlike the on-line app stores, the platform will not only provide information services for searching the tools needed by users, but also provide the feasibility of direct using of the necessary tools. Thus, the future web platforms will provide a single entry point both for web service providers and for their customers.

Method of assessment of textual emotiveness with use of psycholinguistic markers on base of morphological features for analysis of social processes in networks and blogs

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Abstract: A new quantitative approach in identifying the emotionally colored texts that reflect the excited state of its authors is proposed. This approach uses special psycholinguistic markers of text based on morphological characters ratios of russian language. To apply such markers the morphological parser in combination with ensemble of SVM classifiers is developed. Each SVM classifier corresponds to certain morphological feature. The results are later aggregated to determine correct form of each word. Testing results of selected topics texts are presented. The study was conducted using texts from different sources such as news, regular blogs, microblogs, social network posts. It showed that results of developed approach can be a useful extension of Big Data methods of traditional sentiment analysis and it can be applicable in developing methods of personality computing.

Syntactic parsing sentences in Russian language based on selected set of parameters and neural networks

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The model of russian language parser based on a combination of neural networks along with extraction of set of parameters which allows to establish relations with the minimal syntactic ambiguity is presented. The parse tree of sentence is constructed in the format of Russian National Corpus (RNC). RNC texts containing morphological and syntactic markup are used for training neural network models as part of procedure. Estimates of accuracy of the developed parser procedure in comparison with the other russian language parser systems have been performed.

A probabilistic-entropy approach of finding thematically similar documents with creating context-semantic graph for investigating evolution of society opinion

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Abstract

An algorithm of finding documents on a given topic based on a selected reference collection of documents along with creating context-semantic graph for visualizing themes in search results is presented. The algorithm is based on integration of set of probabilistic, entropic, and semantic markers for extractions of weighted key words and combinations of words, which describe the given topic. Test results demonstrate an average precision of 99% and the recall of 84% on expert selection of documents. Also developed special approach to constructing graph on base of algorithms extract key phrases with weights. It gives the possibility to demonstrate a structure of subtopics in large collections of documents in compact graph form.

A comparison of learning abilities of spiking networks with different spike timing-dependent plasticity forms

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Abstract:

Investigation of different factors' influence on the learning process through spike timing-dependent plasticity (STDP) was performed. It is shown that result of learning is sensitive to the form of input signal and spike pairing scheme used in STDP. The following factors were analyzed: the choice of spike pairing scheme, shapes of postsynaptic currents, and the choice of input type signal for learning. All experiments were performed using the NEST simulator. The analysis of performance of several STDP rules along with several neuron models (leaky integrate-and-fire, static, Izhikevich and Hodgkin-Huxley) was carried out. The best combinations of input signal and spike pairing scheme of STDP, which are useful for practical problems, were extracted.

Ising model on plane: numerical solution

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Abstract

The critical two-dimensional Ising model is studied with four types boundary conditions: free, fixed ferromagnetic, fixed antiferromagnetic, and fixed double antiferromagnetic. Using bond propagation algorithms with surface fields, we obtain the free energy, internal energy, and specific heat numerically on square lattices with a square shape and various combinations of the four types of boundary conditions. The calculations are carried out on the square lattices with size $N \times N$ and $30 < N < 1000$. The numerical data are analyzed with finite-size scaling. The bulk, edge, and corner terms are extracted very accurately. The exact results are conjectured for the corner logarithmic term in the free energy, the edge logarithmic term in the internal energy, and the corner logarithmic term in the specific heat. The corner logarithmic terms in the free energy agree with the conformal field theory very well.

Monte Carlo-based bond switching method for generation of the SiC/SiO₂ interface

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Efficient approach for generation of amorphous structures without coordination defects can be achieved by using the Monte Carlo method of Wooten, Winer, and Weaire WWW [1]. This method is based on Monte Carlo (MC) approach for generation of random networks by bond switching. New configurations are generated by switching pairs of bonds: two bonds are broken, and new two bonds are created. After randomly selected bond switching, the structure was relaxed using the developed empirical potential for Si-O-C system. The probability of bond switching is determined by Metropolis factor [$\exp(-\Delta E/kT)$, $\Delta E > 0$; 1, $\Delta E < 0$], where ΔE is the change of system energy as the result of bond switching, T – parameter of modelling.

Energies and structures in local minimum was found by the second-generation reactive empirical bond order potential (REBO2) [2,3] with presented parameters for Si-O-C system. Diffusion atomic oxygen from oxidized bond into not oxidized bond was added to model SiC/SiO₂ interface. The probability of diffusion atomic oxygen is determined by Metropolis factor. Note that bond switching in this case can be applied not only to oxidized bond, but also to not oxidized bond with oxygen in environment.

The interface energy is a key property of an interface and it determines interface stability. Based on the developed potential set for Si-O-C system we investigated interface energies of several SiC/SiO₂ model structures. The interface energy can be calculated by subtracting the bulk energy of the amorphous oxide and crystalline Si and SiC from the total energy. It was found that exist parameter of modelling T in which interface energy approach show that modelling interface SiC/SiO₂ structures more stable then interface of beginning crystal SiC/ β -cristobalite structures.

This algorithm can be applied to model thermodynamic roughening of the SiC/SiO₂ interface obtained in technological processes of oxidation SiC, which cannot be calculated by molecular dynamics because of time of technological processes.

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Theoretical investigation of stable formation conditions for $\text{Fe}_x\text{Ni}_{1-x}$ alloy films on paramagnetic substrate.

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This work is devoted to theoretical investigation of the adsorption of permalloy-like thin films on the different non-magnetic materials, such as Ag and W. For theoretical description we applied the method of multi-parameter test functions the parameters of which are determined by the numerical minimization procedure of the interfacial energy functional in the subsurface region. In this paper we apply the method of calculation of the energy characteristics of the non-activated adsorption ferromagnetic films based on the method of spin-density functional taking into account temperature effects and inhomogeneous distribution of magnetization [1].

We calculated formation condition of stable $\text{Fe}_x\text{Ni}_{1-x}$ alloy films, depending on the component concentration x of the film. The equilibrium vacuum gap D_{\min} and the equilibrium film thickness h_{\min} are determined from the minimum of the total interfacial energy [2]. The energy and magnetic characteristics of $\text{Fe}_x\text{Ni}_{1-x}$ films on close-packed W and Ag surfaces are calculated in dependence on concentration x for different temperatures.

T, K	Θ	X, %
0	0,8	40
100	0.7	0-40
	0.8	40-80
	0.9	100
300	0.8	80-100
	0.9	60-80
	1	40
400	0.9	80-100
	1	80

Table 1. Conditions for formation of stable $\text{Fe}_x\text{Ni}_{1-x}$ film on Ag(111) substrate.

An analysis of results of investigation suggested that $\text{Fe}_x\text{Ni}_{1-x}$ films cannot form on close-packed W, Ag at low values of Θ and the realization of an energetically more advantageous island adsorption is predicted.

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MONTE CARLO SIMULATION OF MAGNETIC MULTILAYERED STRUCTURES WITH GIANT MAGNETORESISTANCE EFFECTS

D.E. Romanovskiy, V.V. Prudnikov, P.V. Prudnikov

Abstract:

Description of giant magnetoresistance effects in magnetic multilayered structures with the use of the anisotropic Heisenberg model for determination of magnetic properties of thin ferromagnetic films forming these structures is given. Monte Carlo simulations of magnetic properties for structures, which are constructed from two ferromagnetic films divided by nonmagnetic film, are carried out. The temperature and magnetic field dependencies are considered for ferromagnetic and antiferromagnetic configurations of these structures. The calculation of the magnetoresistance coefficient is carried out for different thicknesses of the ferromagnetic films. It was shown, that the obtained temperature dependence for the magnetoresistance coefficient is agreed very well with experimental results, measured for the magnetic multilayered structures similar to structures, which are considered in our investigations.

The universal behavior of dense clusters of magnetic nanoparticlesN.A. Usov^{1,2}, O.N. Serebryakova¹, S.V. Ermakov² and R.V. Shershnev²¹*Pushkov Institute of Terrestrial Magnetism, Ionosphere and Radio Wave Propagation RAS
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The influence of magnetostatic interactions on the properties of assemblies of magnetic nanoparticles is an important problem that has to be studied in detail to optimize the performance of assemblies in a number of biomedical applications, such as magnetic nanoparticle hyperthermia or targeted drug delivery [1,2]. In the present report a detailed numerical simulation is carried out to study the quasistatic hysteresis loops of dense quasispherical clusters of interacting magnetic nanoparticles. Both the clusters of magnetically soft and magnetically hard nanoparticles are considered. The clusters are characterized by an average particle diameter D , the cluster radius R_c , the particle saturation magnetization M_s , and the uniaxial anisotropy constant K . The number of particles in the cluster varies between $N_p = 30 - 120$. A specific algorithm is developed to create nearly spherical clusters of single-domain nanoparticles with randomly distributed particle centers. The particles easy anisotropy axes are randomly oriented. It is suggested that the particles are covered by a thin non magnetic layers to protect them from oxidation. Therefore, the exchange interaction between closest nanoparticles is absent. The Landau-Lifshitz-Gilbert equation is solved as a function of external magnetic field to simulate the quasistatic hysteresis loops of interacting nanoparticles. It is shown that a rare assembly of random clusters of nanoparticles can be characterized by two dimensionless parameters: 1) the intensity of mutual magnetostatic interaction, K/M_s^2 , and the average particle concentration within the cluster, $\eta = VN_p/V_c$. Here V is the nanoparticle volume, and V_c is the volume of the cluster, respectively. For magnetically soft nanoparticles, $K/M_s^2 \ll 1$, the universal hysteresis loops of the assembly are constructed. In the variables $(M/M_s, H/M_s)$ these hysteresis loops depend only on the particle filling factor η , which varies in the range $0 < \eta < 0.5$. The hysteresis loops of magnetically hard nanoparticles in the variables $(M/M_s, H/H_a)$, where $H_a = 2K/M_s$ is the anisotropy field, are close to the standard Stoner-Wohlfarth hysteresis loop.

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Integrating GPGPU computations with CPU coroutines in C++

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Despite various efforts on standardization, both open and proprietary, there is currently no universally available programming interface to access compute capabilities of heterogeneous systems. The two main competitors — NVIDIA CUDA and OpenCL — are being pushed by NVIDIA and AMD respectively, and none is universally and uniformly supported.

C++ is a proven language for high-performance computing, but it lags in standardization of recently rediscovered solution to elegant asynchronous processing, namely, coroutines. Coroutines have proven to be the primary means of reverting tangled and piecewise asynchronous code back to serial and readable form. While there are several concurrent proposals that involve resumable functions, coroutines for C++ already have efficient library-based solutions.

Both CUDA and OpenCL are capable of invoking callbacks as notifications for events. This allows us to integrate calls to GPGPU computation kernels and memory copies with existing ways of waiting for network I/O and general callbacks using asio and coroutines based on boost.context libraries. With these we can achieve good code readability of heterogeneously asynchronous code.

Our experience shows that for most tasks overhead of coroutines against pure callback-based code following reactor pattern is insignificant, but even straightforward integration of foreign APIs involves additional overhead of system calls of unpredictable latency.

We've tested CUDA in different context modes that determine the way CPU waits for GPUs. OpenCL was also tested as implemented by NVIDIA and AMD for their hardware. We produced experimental results for the common scenario of exchanging data with an accelerator for the smallest possible amount of work to better expose latencies.

For NVIDIA CUDA the overhead is about $50\mu s$ for the cases where no kernel synchronization is used, which is twice the running time without using our approach. While huge for this test case, computations that are worth offloading to the GPU take orders of magnitude more time, so in real applications it won't contribute noticeably. If you're using blocking synchronization, which is the case for low power devices, the overhead is half as much in absolute numbers and only 30% in relative.

The OpenCL implementation from NVIDIA is strangely a lot slower when coroutines are utilized, showing extra latencies of about $500\mu s$. Even then, this should be acceptable for long-running kernels. OpenCL for AMD GPUs is comparable with CUDA blocking case, being slightly worse at average of $95\mu s$ with extra $20\mu s$ of overhead for coroutine use.

This shows that existing libraries and APIs already allow unifying of asynchronous programming in heterogeneous environments with acceptable overheads and good readability.

Keywords: C++, CUDA, OpenCL, coroutines.

Efficiency of ARM processors for classical molecular dynamics calculations

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Supercomputing of the exascale era is inevitably limited by power efficiency. Nowadays different CPU architectures are considered as possible choices for these purposes. Recently the development of ARM processors has come to the point when their floating point performance can be seriously considered for a range of scientific applications. In this talk we present the analysis of the floating point performance of the latest ARM cores and their efficiency for the algorithms of classical molecular dynamics.

Improving the efficiency of solving discrete optimization problems (by the example of VRP)

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Abstract

Article is devoted constructing efficient metaheuristics algorithms for discrete optimization problems. Particularly, we consider vehicle routing problem applying original ant colony optimization method to solve it. Besides, some parts of algorithm are separated for parallel computing. Some experimental results are performed to compare the efficiency of these methods.

The DataForge framework for data acquisition and analysis

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INR RAS

Abstract

Recently, the software solutions became a major problem in particle physics. Most software packages for it were developed in 1990's or even 1980's, solving some specific problems for specific theoretical or experimental tasks. While mathematical solutions themselves do not strongly change over time and could not be improved very much, the software engineering made a great progress since that time. Nowadays particle physicists waste a lot of effort due to inefficient software frameworks and lack of automation.

The DataForge introduces some trends from modern software development into scientific software for particle physics research and physics in general:

1. Data analysis as a metadata processing. Everything aside from data itself is treated as a metadata. The analysis process is constructed depending on this metadata automatically.
2. Context encapsulation. Environment variables replaced by independent context variables. This allows easily making any analysis process parallel.
3. Cross-platform implementation. The framework is written in Java language and could be easily installed on any operating system supporting JVM.
4. Modular design. The plugin system allows using only the modules needed for precise task and nothing extra.

The prototype for DataForge framework is being successfully tested at "Troitsk nu-mass" experiment in search for neutrino mass.

Adaptation of the Hartree-Fock method in GAMESS (US) to Intel Xeon Phi architectureVladimir A. Mironov¹, Alexander A. Moskovsky^{1,2}¹ Lomonosov Moscow State University, Department of Chemistry, Moscow, Russian Federation² ZAO "RSC Technologies", Moscow, Russian Federation

Hartree-Fock (HF) approach is one of the basic *ab initio* methods in quantum chemistry. The idea of this method is iterative solution of Hartree-Fock-Roothaan equation. Each iteration comprises two major steps – construction and subsequent diagonalization of the Fock matrix. In direct HF method the computational cost of the Fock matrix construction is dominated by the calculation of six-dimensional integrals corresponding to the Coulomb repulsion of electrons (electron repulsion integrals, ERI). This step has theoretical $O(N^4)$ computational complexity, where N is a number of basis functions used to characterize the system. However, many of these integrals are small enough and may be neglected thereby reducing the overall complexity of this step to $O(N^{2+3})$, especially for large and sparse systems. In that case Fock matrix diagonalization ($O(N^3)$) dominates performance of the Hartree-Fock method. However, in most practically important cases the speed of Hartree-Fock method depends solely on the speed of Fock matrix construction and is usually of supercomputer scale. We therefore targeted the Fock matrix two-electron contribution code to demonstrate the applicability of the Intel MIC platform to classical quantum chemistry problems.

In this study we implemented a massively parallel version of the direct Hartree-Fock method in GAMESS (US). GAMESS (US) is one of the oldest and most popular open-source quantum chemical software packages. While used by thousands of research groups in hundreds of compute centers nowadays, many computationally intensive parts of GAMESS (US) code have been written in 70-ies and 80-ies without any consideration for the modern manycore and vectorized type of CPUs. Therefore migrating of GAMESS (US) code to novel types of CPU architectures is of great importance. Current work demonstrates the applicability of Xeon Phi coprocessors for the quantum chemistry problems. We obtained a good scalability of the current implementation on Xeon Phi cores, as well as with multiple Xeon Phi chips running in native mode (OpenMP+MPI parallelization). Future work includes more thorough performance characterization and additional vectorization of ERI calculation.

This work is supported by Intel Parallel Compute Center program.

Quantum Hashing via ε -Universal Hashing Constructions

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Quantum computing is inherently a very mathematical subject, and discussions of how quantum computers can be more efficient than classical computers in breaking encryption algorithms have started since Peter Shor invented his famous quantum algorithm. The reaction of a cryptography community was a “Post-quantum cryptography”, which refers to the research of problems (usually public-key cryptosystems) that are not efficiently breakable using quantum computers. Currently post-quantum cryptography includes different approaches, in particular, hash-based signature schemes such as Lamport signature and Merkle signature scheme. Hashing itself is an important basic concept of computer science. The concept known as “universal hashing” was invented by Carter and Wegman in 1979.

In our research we define a quantum hashing as a quantum generalization of the classical hashing. We define the concept of a quantum hash generator and offer design, which allows one to build a large number of different quantum hash functions. The construction is based on composition of a classical ε -universal hash family and a given family of functions – quantum hash generator.

The relationship between ε -universal hash families and error-correcting codes give possibilities to build a large amount of different quantum hash functions. In particular, we present quantum hash function based on Reed-Solomon code, and we prove, that this construction is optimal in the number of qubits needed.

Using the relationship between ε -universal hash families and Freivalds’ fingerprinting schemas we present an explicit quantum hash function and prove that this construction is optimal with respect to the number of qubits.

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Free-molecular Gas Flow Through the High-frequency Oscillating Membrane

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Membrane technologies are essential in many areas, mainly for the filtration and purification of liquids and gases, separating mixtures and as functional components of modern micro- and nano-electromechanical systems (MEMS, NEMS). Modern production techniques allow to obtain membranes with a wide range of characteristics. One type of membranes – track membranes are produced by irradiation of polymeric films of high-energy particles (accelerated heavy ions or fission fragments). In that way the through holes ("tracks") are formed in the film. The resulting pores are linear and have small variation in diameter – less than 5%, their diameter can be 10 – 100 nm. Thus, the main distinguishing features of the track membranes – small thickness and high uniformity of the pore size.

In this paper the possibility of using a high frequency oscillating track membranes as diffusion membranes for gas separation was studied. High frequency forced oscillation of the membrane was considered because of assumption that the membrane conductivity for a given gas can be controlled by varying the frequency and amplitude of oscillation. The problem about free-molecular gas flow through a oscillating in its plane membrane was stated and the possibility of separation of gases using such a device was investigated.

The gas flow through moving membrane was studied. Membrane was simulated by rigid body with straight cylindrical channels. Channels length was L (thickness of membrane), channels radius was R , channels axis was perpendicular to the membrane surface (see Figure 1). Membrane was placed between two tanks (1) and (2) with constant pressures P_1 , P_2 and temperatures T_1 , T_2 ($T_1 = T_2 = T_w$, where T_w – temperature of membrane material).

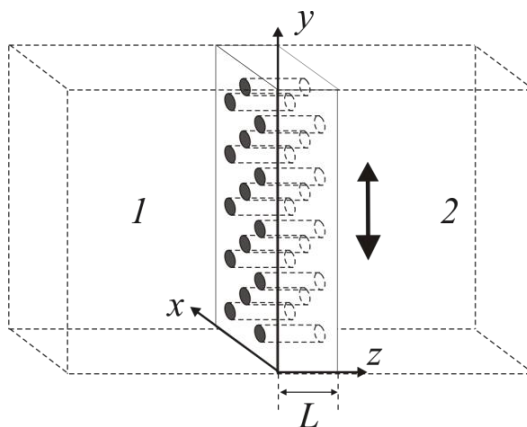


Figure 1. Problem scheme: 1, 2 – tanks, separated by track membrane, oscillation direction shown by arrow (y-axis).

Problem was solved numerically by event-driven molecular dynamics method. Passing probability was obtained in dependence on dimensionless parameters. It was shown that varying the frequency and amplitude of oscillation can lead to difference of membrane conductivity for gases with different molecular mass. This means that one can control the conductivity of the membrane for a given gas by changing the parameters of its forced oscillations.

Work was supported by Russian Foundation of Basic Research (RFBR), grant 14-01-00310 a. Computation was done on SKIF-MSU "CHEBYSHEV" supercomputer.

Ageing and memory effects in non-equilibrium critical behavior of 3D diluted Ising model with low-temperature initial state

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The macroscopic systems show abnormally slow dynamics near second phase transition critical point T_c . In the vicinity of T_c the relaxation time diverges as $t_{rel} \sim |T - T_c|^{-z\nu}$ with $T \rightarrow T_c$, where z - dynamic critical exponent and ν - correlation length exponent. Therefore statistical system quenched to exact critical point does not achieve equilibrium state during full relaxation process. Near T_c a system demonstrates several interesting effects such as ageing and memory phenomena, and violation of the fluctuation-dissipation theorem (FDT) [1, 2]. The ageing is shown at the times $t \ll t_{rel}$ only and appears in two times dependency of the correlation and the response functions. There are 2 significant times exists: observation time t and waiting time t_w . The last one is the time between preparation of a system and the moment of beginning calculate an observable like autocorrelation function, also known as *system age*. During none-equilibrium time evolution the ageing shows up in slowing down of system relaxation with waiting time increasing and demonstrates different none-ergodic effects such as the memory about initial and any middle states while $t, t_w \ll t_{rel}$ and violation of FDT [3].

There are two initial states of a system exists in order to investigate its influence on critical behaviour. The first is *high temperature* initial state when a system was prepared with $T_0 > T_c$ before being quenched and the magnetization equals to zero $m_0 = 0$. The another is *low temperature* initial state with $T_0 < T_c$ and $m_0 \neq 0$. After preparation the system are placed to the thermostat with $T = T_c$ and time evolution starts. At the time t_w we have begun the measuring of two-time autocorrelation and response functions during regime $1 \ll t, t_w \ll t_{rel}$. At the moment the none-equilibrium relaxation for different statistical systems are better investigated for the case of high temperature initial state (look at review [2]). In the work [4] it was carried out numerical Monte-Carlo investigation of disorder influence on three dimensional Ising model relaxation prepared in high temperature initial state. The ageing was observed and the asymptotic fluctuation-dissipation ratio X^∞ were calculated for systems with different spin concentrations. At the same time the relaxation from low temperature initial state is much less studied now.

We have performed the numerical investigation of the influence of disorder on dynamical non-equilibrium evolution of 3D site-diluted Ising model from low-temperature initial state with the magnetization $m_0 = 1$. It is shown that two-time dependencies of the autocorrelation and integrated response functions for systems with spin concentrations $p = 1.0; 0.95; 0.8; 0.6$ and 0.5 demonstrate ageing properties with anomalous slowing-down relaxation and violation of the fluctuation-dissipation ratio. It was revealed that during non-equilibrium critical dynamics in long-time regime $t - t_w \gg t_w \gg 1$ the autocorrelation functions for diluted systems are extremely slow due to pinning of domain walls on impurity sites. The autocorrelation function power-law delay becomes the same as for time dependence of the magnetization in the critical point and is characterized by exponent $(-\beta/z\nu)$. We have found that the asymptotic fluctuation-dissipation ratio $X^\infty = 0$ for diluted systems with spin concentration $p < 1$ while the pure system is characterized by $X^\infty = 0.784(7)$. Also we have investigated memory effects in disordered systems with cyclic their quenched to $T < T_c$ during ageing regime of critical relaxation.

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3D simulation and analytical model of chemical heating during silicon wet etching in microchannels

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Abstract.

We present simulation results of modeling silicon wet etching in microchannels. This process is applied in microsystem technology to produce self-aligned microstructures in Silicon-On-Glass (SOG) wafers used in semiconductor, optoelectronic, microfluidic devices, MEMS and other microsystems. The models developed in this work are used for designing a novel chemical heater, which can be applied in many types of devices, from microreactors to integrated microfluidic systems for biochemical analysis. Here we investigate the problem of chemical heating of a SOG chip during a highly exothermic reaction of silicon etching in potassium hydroxide (KOH) solution in a microchannel of 100-micron diameter inside a 1x1 cm SOG chip. Two modeling approaches have been developed, implemented and validated against experimental data.

First, we developed a detailed 3D model based on Navier-Stokes equations, heat and mass transfer balance equations of a laminar flow of viscous incompressible fluid in microchannel coupled to the heat transfer equation in the solid chip. Simulation results predicted temperature distributions for different KOH flow rates and silicon etching areas. Simulations show that microchannels of a small diameter do not heat the chip due to the insufficient chemical heating of the cold fluid. But large area of the etching surface (large diameter and/or length of the microchannels) lead to local overheating that may have negative effects on the device performance and durability. Simulation results were compared to experimental data for two types of microstructures: one straight channel of 100-micron diameter and array of parallel connected channels etched in silicon wafer before bonding with glass. The model correctly predicted the temperature of the chip, and therefore can be used to simulate and optimize complex microstructures.

Second, a simplified analytical model was developed as an alternative method for quick assessment of process parameters. An equation of thermal balance was solved, which included heating by chemical reactions inside the microchannel and energy loss by free convection of air around the chip at room temperature. This problem was solved analytically under the assumption of infinite thermal conductivity of chip material. An equilibrium chip temperature was obtained as a function of etching area, thus allowing fast engineering estimations at the initial stage of a device designing process. Future work includes analysis of the analytical model validity, by running additional experiments and detailed 3D/2D simulations.

Computer calculations of energy and magnetic characteristics of substitutional adsorption of the monolayer iron film in depend of surface face orientation.

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In this work, we use the variational spin-density functional method for theoretical description and computer calculation of energy and magnetic characteristics of activated adsorption of Fe ions on the Ag and Au nonmagnetic substrates at low Miller index orientations of its surface face with taking into consideration the inhomogeneous distribution of magnetization in surficial region.

The experimental investigations of ultrathin magnetic films show that the magnetic properties of system Fe/Ag are characterized by two-dimensional Ising model type, and Fe/Au by two-dimensional XY model type. Therefore, in this work we use for description of temperature dependence for the relative magnetization $m(T)$ the Onsager's exact solution for Ising type systems and the results of renormalization-group finite-size consideration for XY type systems.

We calculated the values of the structural parameters, spatial distribution of magnetization (Fig.1) and adsorption energies (Fig.2) for Fe/Ag and Fe/Au systems as a function of the parameter of coverage for different temperatures.

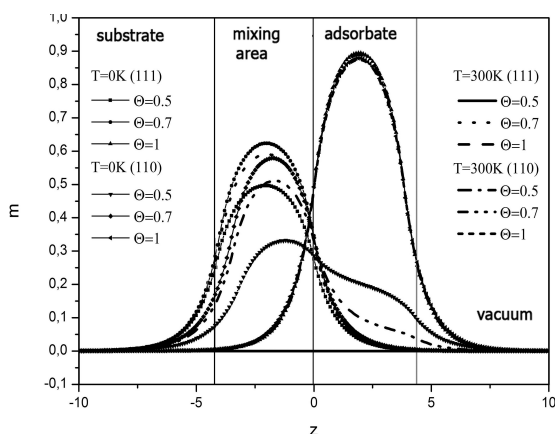


Fig.1: The spatial distribution of magnetization for the system Fe/Ag for the faces (111) and (110).

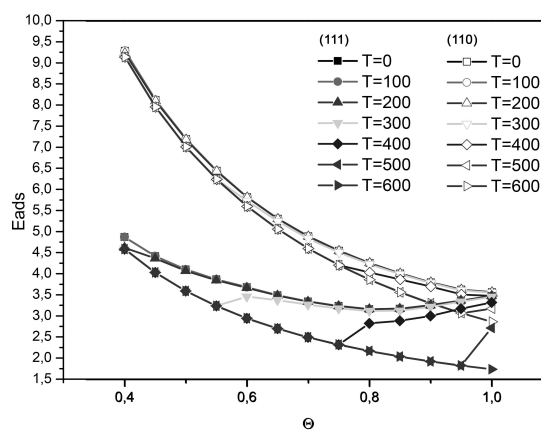


Fig.2: The dependence of the adsorption energy E_{ads} (eV/at) on the coating parameter Θ for system Fe/Ag(111) and Fe/Ag(110).

Results of calculation show that the temperature and ferromagnetic ordering lead to material effect on surface reconstruction and characteristics of adsorption at depending on the coverage parameter Θ . So, for adsorption Fe on Ag it is revealed that substitutional processes are energetically more favorable for case with small values of coverage parameter Θ when "sandwich"-structures or close to these are generated. However, with growth Θ and approaching to $\Theta=1$ the interaction of magnetic ions and appearance of spontaneous magnetization lead to formation of monolayer film on a surface without involvement of substrate atoms.

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Monte-Carlo simulation of ultrathin magnetic films critical behavior

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The Monte-Carlo study deals with ultrathin magnetic films critical behavior. Critical temperatures are calculated for films with different thickness. Striped spin configurations are demonstrated for system with strong dipolar interaction. The effective antiferromagnetic character of dipolar interaction is observed in bilayer structure. Memory effects in non-equilibrium critical relaxation of magnetization and autocorrelation function are investigated.

The study of ultrathin magnetic films critical properties is of great interest because of possibilities to use them in different application like memory devices, magnetic field sensors, etc. This research deals with Monte-Carlo simulation of ultrathin magnetic films critical behavior. Magnetic film is constructed as a three-dimensional spin lattice with Heisenberg Hamiltonian, which includes short-range exchange interaction, uniaxial anisotropy and long-range dipolar interaction.

Phase transitions are observed in systems with two different strengths of dipolar interaction. Critical temperatures are calculated for these systems with regard to the film thickness. The system with strong dipolar interaction is simulated. Such a system demonstrates striped spin configuration at moderately low temperatures with spins oriented parallel to the film surface in stripes. The effective antiferromagnetic character of dipolar interaction is demonstrated by simulation of bilayer film with certain thickness of sublayers. Dipolar interaction results in antiparallel orientations of every two spins belonging to different adjacent layers. That spin configuration may be changed by magnetic field application. The research includes simulations with parallel and perpendicular to the film surface magnetic fields.

The research includes the study of memory effects in ultrathin magnetic films. That effects are observed by magnetization and autocorrelation function calculating. The simulation is conducted at critical temperature and at some time interval the change of temperature occurs. The memory effects study is based on the non-equilibrium autocorrelation function and magnetization behavior depending on cooling or heating cycling procedure. The system starts from different initial states: from high-temperature state with $m_0 \ll 1$ and low-temperature state with $m_0 = 1$.

This work was supported by Russian Science Foundation (project no. 14-12-00562). The simulations were supported by the Supercomputing Center of Lomonosov Moscow State University and Joint Supercomputer Center of the Russian Academy of Sciences.

MODELING OF STRATIFIED FLOWS IN THE PROBLEM OF THE MORPHOLOGICAL BEHAVIOR OF A SANDPIT

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Growth of capital and road construction in Russia promotes development of the market of nonmetallic materials. Its growth rates correspond to the growth of the construction market. Nonmetallic building materials industry has the following characteristics: a large number of sandpits spread their performance - from tens of thousands to several million cubic meters of mineral resources; - rigid connection of mining operations, mining at the sandpit. Most of the sandpits located along the river systems because the actual behavior is to build a bottom pits for successful planning, implementation and use of new mining sites of non-metallic materials with regard to hydrological and hydrochemical characteristics of the river reservoir. In this case, for a description of such processes using traditional two-dimensional hydrodynamic models, in the approximation of the shallow water equations, it is not correct, because the horizontal and vertical dimensions of sandpits are comparable. Thus, to solve these problems within the framework of the shallow water equations is only possible to estimate the change in velocity of the main stream and a very approximate estimate of the intensity of sandpit blur. For correct modeling of the described problems need to build three-dimensional models of currents and sediment transport in rivers.

The studies in this paper define the characteristics of the vortex appearing in the bottom region depend on the size of the pit and the main flow speed. The influence of sandpit size and flow velocity on river free surface drop is studied. The time evolution of a career in the water object is shown. The analysis of the effect of liquid stratification caused by the discharge of waste water containing heavy impurities by large industrial enterprises is carried out. The estimation of the possibility of impurities accumulation in the career is performed.

This work was supported by RFBR and Perm Region Government (grant 13-01-96040) and by President of Russian Federation (grant 4310.2014.1 for the support of young PhD scientists and grant 4022.2014.1 for the support of Leading Scientific Schools).

Settling of a liquid drop in a porous medium saturated by another liquid

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The work deals with numerical simulations of sedimentation of a liquid drop in a porous medium saturated by another liquid. It is known that in the framework of the conventional Darcy model a planar displacement front in a porous medium is unstable if the displacing fluid has lower viscosity than the displaced one. The instability is associated with development of penetrating fingers of the less viscous fluid. The process is virtually unimpeded by viscous momentum transfer, which is negligible in porous media. This explains the short-wave nature of the instability. In practice, the displaced fluid often forms compact inclusions surrounded by the displacing fluid. In this case, we should consider displacement fronts on both forward and back sides of the inclusion. The drop is initially spherical and the interface thickness between liquids is supposed to be small (much less than the drop radius). The dynamics of this system is described using the Darcy model.

We developed software for modeling two-phase fluid dynamics in a porous medium and performed numerical simulation of a liquid drop motion under gravity. Dynamics of the interface between the phases is described using two approaches. The first one is based on the assumption of thin interface. In this case, numerical modeling of the liquid droplet motion is performed using the level set method. The basic idea of the method is the introducing distance function - an auxiliary function, which has the different signs in different phases, and zero value of this function corresponds to the interface location. At the same time, the interface is treated as the transition layer with sharply varying parameters. As a result, a two-phase system is described as a single medium with parameters (density, viscosity) depending on the distance function.

The second approach uses Buckley–Leverett model of multiphase fluid in porous medium. Each phase corresponds to the function of volume fraction that determines the quantity of this phase in selected point. Filtration of phases is described by Darcy model and the conservation laws of mass of liquids. At initial time moment, the interface between phases is supposed to be thin then, during calculation, it become thicker due to mixing of the phases.

The modeling of multiphase flows requires high accuracy treatment near the interface where parameters of medium sharply change. To satisfy this requirement we implement adaptive mesh refinement algorithm that allows maintaining fine enough mesh near interface during all time of calculations. This algorithm supports parallel computations based on Message-Passing Interface and dynamic load balancing procedure for distributing the workloads across multiple computing resources. Thus, the mesh is automatically changed to minimize diffusion of the grid near the interface. In addition, at each time step, the correction of the position of the interface is performed so that the thickness of the transition layer is kept constant. As a result, variations of the drop mass in the calculations do not exceed 1%.

We solve the problem in axisymmetric approach and introduce the stream function. Poisson equation for the stream function is solved implicitly by Generalized Minimal Residual method. The time derivatives are approximated by second-order scheme. Discretization of the spatial derivatives is carried out by finite volume method based on the integral form of the conservation equations.

Numerical modeling of the droplet dynamics subjected to gravity has shown that the instability develops at the forefront of moving droplets regardless of the ratio of fluids viscosities. The comparison of results obtained in the framework of Darcy and Buckley–Leverett models has been carried out.

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Vibrational convection of ternary mixture in a closed cavity in zero gravity conditions

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Convective phenomena in multicomponent mixtures play an important role in many natural and industrial processes. In particular, the composition of hydrocarbon deposits depends on diffusion and thermodiffusion processes (in the presence of geothermal gradient). Thermodiffusion is used for separation of isotopes in liquid and gas mixtures, in colloids, nanofluids or macromolecules separation processes. The study of convection in multicomponent systems is a poorly studied area. This is due to the fact that in multicomponent mixtures mass transfer of any component can be induced not only by the concentration gradient of this component, but also by cross-diffusion and thermodiffusion, which greatly complicates the study of such mixtures behavior. In zero gravity conditions even weak vibrations occurring on board of spacecrafts may lead to considerable effects. The present work is devoted to the investigation of vibration influence on the onset and nonlinear regimes of ternary mixture convection in a closed cavity with solid boundaries in zero gravity conditions. The interest to this problem is associated with the experiments on transport phenomena in ternary mixtures conducted on board of the International Space Station.

Calculations were carried out for the horizontally-elongated rectangular cavities with different ratios of the side lengths. The lateral boundaries are considered to be adiabatic, and the horizontal boundaries are kept at constant different temperatures. We consider the translational linearly polarized vibrations of finite amplitude and frequency. The axis of vibrations is perpendicular to the temperature gradient. The initial conditions correspond to the uniform vertical temperature and concentration gradients. Simulation is conducted for two mixtures, one of which has both solutes with a positive separation ratio, and the other – with negative separation ratio. In the absence of vibrations and gravity the instability in a ternary mixture does not occur. In this case only thermodiffusion separation of components is observed in the system: the molecules of components with a positive separation ratio move to the colder wall of the cavity, while the molecules of components with a negative separation ratio - to the warmer area. The problem was solved by finite difference method in the framework of full unsteady approach. The data on the time evolution of instantaneous and average fields and characteristics of convective flows and concentration fields are obtained (average fields were obtained by averaging the instantaneous fields corresponding to different time moments over the vibration period). A comparison of the numerical results with the existing data on the vibrational convection in the horizontal layers of binary [1, 2] and ternary [3] mixtures was carried out.

The work was supported by Russian Science Foundation (grant No. 14-01-00090)

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INVESTIGATION OF PHASE TRANSITION OF THE MODEL MAGNETIC HARD/SOFT BILAYER BY THE MONTE CARLO METHOD

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The figure of merit for a permanent magnet material is the maximum energy product $(BH)_{max}$ that is twice the maximum magnetostatic energy available from a magnet of optimal shape. The product tends to increase both with increasing coercive field H_c and saturation magnetization M_s . The maximum corresponds to an ideal rectangular hysteresis loop. Driven by this limitation, research has focused on developing new high-anisotropy materials with high M_s and Curie temperature T_c . Kneller and Hawig [1] proposed an alternative approach to enhance the TM content (and therefore increase M_s) by making a nanocomposite of exchange-coupled hard and soft magnetic phases. Such magnets are referred to as «exchange-spring» or «exchange-hardened» magnets and provide a pathway to increased $(BH)_{max}$.

We researched the magnetic properties of the model consisting of the hard and soft magnetic layers. The hard layer is distinct in an anisotropy high value (easy-axis anisotropy) while the soft layer lacks anisotropy. Exchange interactions between nearest neighbors within the hard and soft layers are ferromagnetic and defined by J_h and J_s parameters, correspondingly. An interlayer interaction at the boundary of hard and soft layers J_m for the model studied has a positive sign and takes on an intermediate value between J_h and J_s . The Hamiltonian of the system is written as:

$$H = -\frac{1}{2} \sum_{i,j} J(S_i^x S_j^x + S_i^y S_j^y) - \sum_i K(S_i^x)^2,$$

where the first sum allows for the exchange interaction of each magnetic atom with nearest neighbors inside layers with exchanges $J = J_h$ and $J = J_s$ in hard and soft layers, correspondingly, and an interlayer interaction with $J = J_m$ parameter, the second sum is a contribution of the anisotropy into a system energy, $K = K_h$ and $K = K_s$ are anisotropy constants of hard and soft layers, respectively, $S_i^{x,y}$ are projections spin localized on a site i .

Calculations are performed by the standard Metropolis algorithm of the Monte-Carlo method for the systems with linear sizes $L \times L \times L$, where $L=8 \div 40$. And the thickness of hard and soft layers is $L/2$. During the experiment the magnetization M , heat capacity C and susceptibility χ have been calculated. The temperature dependence of these thermodynamic parameters has been identified two features: the first one at T_1 and the second at T_2 ($T_2 > T_1$). On diagrams for the temperature dependence of the magnetization, these features are revealed as two sharp drops of M , and for the heat capacity and the susceptibility, are evident as double maxima. When increasing the spins in the system for hard/soft bilayer, falls on the magnetization-temperature dependence becomes sharper and maxima of the susceptibility and heat capacity take the more acute form. We believe that this behavior is due to the fact that in the magnetic hard/soft bilayer model, two “phase” transitions take place at different temperatures.

It stands to reason that in order for more realistic description of a hard/soft bilayer behavior one should take into account a mixing in boundary atomic layers, the surface roughness triggering the heterogeneous distribution of the magnetization and the smearing of a phase transition, etc. However, even such non-ideal simple model displays the effects characteristic for small systems.

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PERSONAL ASSISTANT WITH COMPONENTS OF ARTIFICIAL INTELLECT

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ABSTRACT

The article is concerned the actual problem of creation of the personal assistant with components of artificial intelligence and some aspects of its using.

This project can find its application in creation and exploitation of computing, managing and production systems of different purpose, where user needs to have tools for intelligent dialogue with a computer system and resource for knowledge accumulation.

In comparison with other ways of communication with computer systems, in this case the complexity of retrieval requests is reducing. Since the questions are formulated on natural language, the selection of searching results becomes more adequate. Teaching and knowledge accumulation, which include experience and user's references become more effective too. Beside this, the active dialogue between system and user can carried on system's initiative.

Transformation of IT infrastructure of science centre and data intensive processing

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Nowadays, there are well-seen tendency of *IT transformation* at the University campuses and scientific centres [1]. The transformation vector is on the way to the *data intensive processing*. The goal of the transformation is to bring possibility of processing and managing the big data *just on the table* of each researcher working at the University and Centre campus.

We see the possible way to reach that goal through the *centralization* of the IT management. The centralization is of both the hardware and software *management* keeping distributed hardware untouched. We present some details of our realization of the platform for the *computational physics* [2]. We discuss how that approach can be used in the IT transformation of science centre to the data intensive processing.

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NUMERICAL INVESTIGATION DIRECTIONAL SOLIDIFICATION OF BINARY ALLOYS UNDER THE ACTION OF ROTATIONAL VIBRATIONS

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Numerical simulation of the influence of high-frequency rotational vibrations on the flows and heat and mass transfer at vertical Bridgman crystal growth from alloys was conducted. We carried out numerical simulation of flows and heat-and-mass transfer at direct crystallization subject to rotational vibrations of finite amplitude and frequency, on the base of full non-stationary non-averaged equations and boundary conditions. Mesh refinement of front crystallization was used to better resolved convection flow. The numerical solution of the given problem is conducted applying finite volume method. The study takes into account the processes of inhomogeneous heat-exchange on the lateral wall, the deformation of crystallization front, two-phase zone between the melt and crystal, and dependence of solidus and liquidus temperatures on admixture concentration. Data on time-evolution of velocity, temperature and admixture concentration fields in the melt during crystallization process; and data on admixture distribution in the grown crystal with and without vibrations were obtained. The vibrations were shown to lead to considerable decrease of radial admixture segregation and increase of homogeneity of admixture distribution in the grown crystal; the formation of the paraxial depression isn't observed.

The work was made under financial support of the Russian Foundation for Basic Research (Grant 13-01-96021).

**THE OSCILLATIONS OF CYLINDRICAL DROP
UNDER INFLUENCE OF NONUNIFORM ALTERNATING ELECTRIC FIELD.**

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We study the forced oscillations and parametric drop incompressible fluid under the influence of an alternating electric field. In equilibrium, the drop has the form of a cylinder bounded axially parallel solid planes and contact angle is right. The drop is surrounded by incompressible fluid with other density. The external nonuniform electric field acts as an external force that causes the moving contact line. The electric field is periodic in time with a certain frequency. To describe the motion of the contact line is used to modify boundary condition [1]: 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 data about deviation of frequency and surface characteristics depending on Hocking constant, frequency and amplitude of an external nonuniform electric field and the geometric parameters of the system are obtained. 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. The effective boundary condition leads to dissipation of free oscillation in the absence of an electric field: there amplitude is always limited. There are also «anti-resonant» frequencies under the alternating electric field as with usual mechanical vibrations.

This work was supported by the Russian Science Foundation (project 14-21-00090).

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**INFLUENCE OF CONTACT LINE MOTION ON TRANSLATION VIBRATIONS OF A
CYLINDRICAL BUBBLE**

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The eigen and forced translation oscillations of a cylindrical gas bubble surrounded by an incompressible fluid with free deformable interface. The bubble has a cylindrical shape in equilibrium and is bounded axially by two parallel solid surfaces. Dynamics of contact lines is taken into account by an effective boundary condition [1]: velocity of the contact line is assumed to be proportional to deviation of the contact angle from the equilibrium value. The equilibrium contact angle is right. Radial oscillations of the bubble were investigated in [2].

Depending on the eigen frequency and damping rates of the parameters of the problem are investigated. Eigen frequency decreases with decreasing container radius and increase with the geometrical parameter. We found that the oscillation frequency can vanish from a certain value of Hocking constant (capillary parameter) for the main translation mode of eigen oscillations. Frequency decreases with increasing radius of the outer free surface of the liquid and increases as the geometrical parameter. Also note that the frequencies of translational modes are independent of the gas pressure inside the bubble.

Well-marked resonance effects are found in the study of forced oscillations. Thus, one can choose the droplet radius-to-height ratio such that the characteristic frequency of any mode is equal to zero, and, ultimately, to determine the capillary parameter.

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New security infrastructure model for distributed computing systems

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Distributed computing systems (DCSs) are widely used by the researchers to solve different computational problems in various fields of natural science. DCS's are especially popular in the computer simulation in physics. Perhaps one of the most significant examples of DCS is a data simulation and data processing at the LHC, which is held to the discovery of the Higgs boson. One of the most important parts of the DCS is a security infrastructure that provides: authentication and authorization, data integrity, encryption and so on. Information security is particularly important in such areas of science and technology as medicine, biological research, engineering development. On the one hand, researchers need to be sure that the results of data processing and simulation are protected from unauthorized access, on the other hand, owners of the computational resources that make up the DCS want to have guarantees that only the authorized users will be able to submit computational requests to the system.

The security infrastructure for the DCS is to provide users with a comfortable and secure access to the remote resources. Currently in most DCSs security is based on the public key infrastructure (PKI) in conjunction with proxy certificates. Proxy certificate is a special short time living certificate (for security reasons) used for the purpose of providing restricted rights delegation within a PKI based authentication system. In DCSs proxies are used to grant the rights between users and services to access to computing resources.

This approach along with the incontestable benefits of strong security has also some disadvantages. First of all it is about the usability issues. In practice an end user of a DCS may come across a formidable obstacle trying to get remote access to the components of the DCS. The fact is that obtaining and management of the X.509 certificates and proxies requires deep understanding of the basic concepts of the PKI that not all users have. The second problem with proxies is a short lifetime, while one can not predict how much time would take request processing. There are special services to support prolongation of proxy lifetime, and all this make the security infrastructure even more complicated and difficult to interact with.

We propose an alternative approach to building of the security infrastructure for the DCSs. The main idea is in using login/password for user authentication (including multi-factor authentication for strong security were needed) while well tested PKI infrastructure is used for service-to-service interaction only. The authorization is implemented by using just in time approving of the rights via a special trusted authorization service. Consequently there is no need to use proxy certificates. In the proposed model each request should be signed by the individual certificate which is not limited in time. These request certificates are registered by the authorization service in the special database and states of these certificates are tracked on real time. Having received the user's request every computational service checks against the authorization service if the request's certificate is valid and is not yet used, and executes the request only if the signature is correct. So requests signing ensures impossibility of their changing during passing and processing.

Thus both high level of security along with seamless and easy access to the computational resources for the users are achieved thanks to intentional complication of the security infrastructure by adding a special authorization service. At the moment a prototype of the proposed security infrastructure has been developed. It includes one authorization service and three other services that interact with users and with each other. The prototype is used to demonstrate the capabilities of the model and for heavy load tests.

One of the possible weak points of the proposed model is the requirement to have on-line access to the authorization service for all other services of the DCS. But the simulation using our prototype shows that such an infrastructure is quite stable and works fine at least for the systems with 20 user requests per second.

The proposed approach improves user's operational performance and greatly enhances the competitive advantage for research organizations using DCSs. Scientists and engineers, as well as teachers and students can accelerate the practical results through the use of a simplified remote access to computational resources for data processing and modeling of processes in various fields of science and technology.

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Elastic constants of charge stabilized colloidal crystal with body-centered cubic lattice

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Elastic constants of charge stabilized colloidal crystals of charged spherical particles with monatomic body-centered cubic (bcc) lattice are studied numerically. Elastic constants are derived from the stress-strain relations obtained by means of computer experiments.

The properties of colloidal systems are considered within the theory based on the non-linear differential Poisson-Boltzmann equation [1]. Electrostatic potential in any particular configuration of the crystal, both initial and deformed, is completely determined by solution of the corresponding boundary value problem for the Poisson-Boltzmann equation. Domain of the problem for initial configuration is reduced to the Wigner-Seitz cell of the bcc lattice. Domain for a strained configuration is generated from the initial domain by means of linear transformation corresponding to a given strain. The model has three parameters: lattice parameter a , radius of the particles R and surface charge density σ on the particles.

Stress-strain relations for a colloidal crystal with a bcc lattice can be written as follows [2]:

$$T_{ij} = -p\delta_{ij} + B_{ijkl}\varepsilon_{kl} + \dots, \quad (1)$$

where T_{ij} is an osmotic stress tensor, ε_{kl} is a tensor of infinitesimal deformation, and B_{ijkl} is a tensor of elastic constants of the second order, i. e. elastic moduli, and p is an osmotic pressure in the equilibrium initial configuration. In contrast to conventional crystals, the charge stabilized colloidal crystals are the systems with initial stress, which is reduced to the isotropic pressure p in the case of a bcc lattice. There are only three different elastic moduli, B_{1111} , B_{1122} and B_{1212} , for the bcc lattice. It was shown that only two types of deformation, stretching ε_{11} and shearing ε_{12} , are sufficient for complete determination of these moduli from (1). Both pressure p and stress T_{ij} under different strain ε_{kl} are calculated according to the method described in [3].

Relations (1) for stretch and shear strains were obtained from computer experiments. The corresponding boundary value problem for the Poisson-Boltzmann equation for each instant configuration was solved numerically by a finite-element method. Free tetrahedral meshes of the second order Lagrange elements were used. Pressure p and elastic moduli B_{1111} , B_{1122} and B_{1212} were obtained from experimental dependencies (1) by means of polynomial fitting. The equilibrium pressure and elastic moduli were obtained for a broad range of the lattice parameter.

An alternative set of elastic moduli C_{ijkl} enables verification of the Cauchy relations for the elastic constants [2]. The C_{ijkl} moduli are related to the B_{ijkl} ones as follows: $C_{1111} = B_{1111} + p$, $C_{1122} = B_{1122} - p$, $C_{1212} = B_{1212} + p$. Definite deviation from the Cauchy was observed for all the values of the lattice parameter that means the many-body effective interactions play some role in the charge stabilized colloidal systems.

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A Model of Quantum Communication Device for Quantum Hashing

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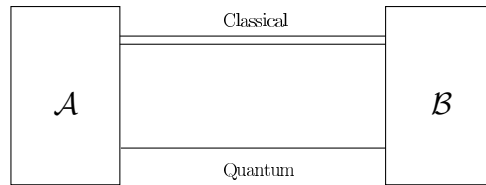
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Nowadays the area of quantum computing technology is in active experimental phase, but a large-scale fully functional quantum computer has a long way to come. So in order to develop the area of quantum programming we need to rely on the computer simulation of the quantum devices.

In this research we propose a model for one such device, which we have called a Quantum Communication Device. It can be seen as a part of a quantum communications, the latter has been already demonstrated experimentally. The main purpose of developing quantum communications is to implement quantum cryptographic protocols that outperform their classical counterparts. Among them is the well-known Quantum Digital Signature Protocol.

In [1] we have proposed a quantum hashing technique that can be used in this protocol, and we believe it can have many other cryptographic applications. The model we propose here can speed up quantum hashing and thus is a good candidate for quantum cryptographic applications.

For the Quantum Communication Device we propose the following architecture:



Here \mathcal{A} and \mathcal{B} are classical computers aided with quantum processors on multiatomic ensembles with integrated quantum memory [2], connected by a classical and a quantum channel. As we have shown in [2] such a processor can speed up complex controlled operations, which are crucial to quantum hashing.

The basic operations of the quantum processor are given by the underlying physical model and include the following list:

- loading a state from quantum memory to the processing node;
- a reverse operation of saving a state into the quantum memory;
- measuring a state;
- quantum excitation transfer between two processing nodes;
- quantum excitation transfer controlled by the third processing node;
- an operation of the phase shift for two processing nodes;
- sending a state to a quantum channel;
- saving a received state into the quantum memory.

As we have shown earlier this set of operations is universal in the Hilbert subspace that corresponds to the pairwise logical encoding of the qubits $|0_L\rangle = |0\rangle|1\rangle$, $|1_L\rangle = |1\rangle|0\rangle$. That is why, these operations form a basis for our quantum programming library and can be used to describe any quantum algorithm and communication protocol.

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Coherence of noisy oscillators with delayed feedback inducing multistability

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Delayed feedback was found to be a highly efficient tool for controlling the coherence of noisy oscillators. Even weak feedback with sufficiently long delay time can diminish or enhance the phase diffusion constant, quantitative measure of coherence, by one order of magnitude and even more. The theory of the delay feedback control of the phase diffusion has been developed in Refs. [1,2,3].

However, for long delay times and vanishing noise, the multistability of the mean frequency can occur. In the presence of multistability, noise results in intermittent switchings between states with different mean frequencies and, thus, the phase diffusion is contributed not only by fluctuations around the mean linear growth of the phase but also by the alternation of "local" mean growth rates. For weak noise---which is a physically relevant situation---it turned-out to be possible to find natural variables in terms of which the switching between two stable phase growth rates becomes a perfect telegraph process. Numerical simulation reveals that the phase diffusion become giant where the mean residence times in two states are similar.

In this work we construct the analytical theory of the effect of delayed feedback on the phase diffusion in the presence of multistability. In agreement with the results of numerical simulation we analytically derive that the phase diffusion constant has giant peaks close to the point where the residence time in two states are equal. Remarkably, while the width of the peaks linearly decreases with the noise strength, their height growth exponentially as noise strength decreases.

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A Web Tools for Research in Nonlinear Optics

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We present a web tools, namely the web platform WebNLOptics, for nonlinear optics research support. The platform provides users with an access to database of optical properties of crystal materials and computational modules installed on remote resources which implement algorithms required for development of scientific models and devices in nonlinear optics.

Nonlinear optic is a rapidly evolving area of modern physical research and engineering with many important applications such as fiber-optic communications, nonlinear spectroscopy, diagnostic of non-stationary and inhomogeneous processes in plasma and gas phases, laser biomedicine etc. These problems require a generation of ultra-short laser pulses with frequencies from vacuum ultraviolet to terahertz region of the spectrum. Different properties of nonlinear crystals can be important for nonlinear frequency conversion processes such as chromatic dispersion and birefringence, magnitude of the effective nonlinear coefficient etc. Thus the choice of the suitable crystal material is far from trivial and involve many aspects. Therefore successful development of optical devices requires complicated modeling of physical processes that occur in components of device and comprehensive database of optical properties of used materials. Currently, however, there are no a single web based tool (web platform) which allows access to data and computational resources required for research and engineering tasks in nonlinear optics.

This work presents a project of the web platform for computer modeling of nonlinear optics phenomena. We discuss general scheme of the platform WebNLOptics and interaction model between platform modules. The platform is build as a set of interacting RESTful web services (SaaS approach). Users can interact with the platform through web browser or command line interface. Such a resource has no analogues in the field of nonlinear optics and will be created for the first time therefore allowing researchers to access high-performance computing resources that will significantly reduce the cost of the research and development process.

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Keywords: Web platform, SaaS, REST, nonlinear optics, distributed computing, laser technology, frequency conversion.

Boiling of oil fields by lava intrusions

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The "Permian extinction" is one of the largest catastrophes in the life history of the Earth. Although it is known to be contemporary with the formation of the Ural mountains, some details of the process of extinction remains uncertain. The extinction is believed to be associated with the massive release of methane into the atmosphere. The hypothesis that this release was associated with the destabilisation of methane hydrate deposits by the volcanic activity becomes inconsistent with modern assessments of the amount of the hydrocarbons existing in the form of gas-hydrates, which are much more modest than earlier estimates. Destabilisation of methane hydrates was insufficient for release of that amount of methane. Simultaneously, one can notice another source of methane, which can release the estimated amount of methane. This source is oil fields in the region of the Ural mountains and adjoin part of the basin of the Volga river. Indeed, the oil fields in this area are featured by an extremely poor light fraction compared to the oils in other regions. The only possible explanation of this deficiency of the light fraction can be that it was evaporated during boiling of the oil fields by lava intrusions.

In this work we model the process of the boiling of an oil field by the temperature raise dispersing from a lava intrusion crossing the oil field and release of the gaseous fraction from this field. Our ultimate task is to find relation between input parameters of the problem and final composition of the oil (or quantitative characteristics of the release of light fractions). The challenging issue here is the thermodynamic description of the boiling process at elevated pressure. The empiric data from the industrial oil cracking are not sufficient here as this technological process is performed at atmospheric or nearly atmospheric pressure.

The following approximations and assumptions allows us to calculate the thermodynamic equilibrium between the vapour phase and the liquid oil at the boiling temperature (which depends of the current composition of oil): (i) the components are indexed by the number n of C-atoms in the molecule and the difference in thermodynamic characteristics of the interaction of these molecules with the liquid phase between various hydrocarbons is neglected, (ii) the oil composition is described by the distribution of the number of atoms n in the liquid phase, (iii) the gaseous phase is considered as a perfect gas, (iv) as the molar fraction of each component in oil is small, one can consider the relation between the vapour pressure of this component above the liquid oil and its concentration in oil adopting the theory of solubility of gases in liquids for infinitely dilute solutions---specifically, the scaled particle theory. Within the framework of the described physical model, one can derive the equation system for the change of oil composition with temperature increase and the parameters of this system. Numerical integration of this system yields the data on the oil composition after propagation of the temperature raise front from a lava intrusion.

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High accuracy relativistic magnetohydrodynamics with OpenACC and MPI

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We present the parallelized and GPU-accelerated version of the general relativistic magnetohydrodynamics numerical code. The original code is well-known as reliable open-source program which has proved its efficiency in solving equations of general relativistic magnetohydrodynamics in a curved space-time of rotating black hole. Its results agree well with astrophysical observations [1–4]. We demonstrate that using modern GPUs allows to speed up the calculations in about 10 times. We discuss weak scaling and strong scaling efficiency of the multi-GPU calculations.

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Impact of gas diffusion on bubbly flow pattern

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Abstract

Interphase mass transfer is a phenomenon of key importance in two-phase flow of gas bubbles in liquid containing dissolved gas. In particular, liquid degassing in pipes due to pressure drop could alter flow pattern and reduce mass flow rate, which is in some applications unacceptable and should be prevented. On the other hand, intensification of gas transfer at the bubble boundaries is important for airlift chemical reactors, oxidization and purification systems.

Downward pipe and bubble column flows are studied by means of numerical simulations. Mathematical model is based on the Euler-Euler approach for two-phase medium description. Modified Navier-Stokes equations with additional source terms including mass transport between phases as well as buoyancy and interphase forces are used to describe motion of each phase. Interphase interaction terms include drag force, lift force, wall lubrication force, and bubble turbulent dispersion force. Additional modification for multiphase forces includes empirical approximations for high volume fraction of dispersed phase.

The Menter $k-\omega$ -SST model is used to account for turbulence effects with additional source terms describing generation and dissipation of turbulence due to work of interphase forces. Effect of dispersion which is a characteristic feature of turbulence is clearly manifested in two-phase bubbly flows. Such effect is modeled as a source term in momentum conservation equation.

Interphase mass transfer is modeled by diffusion of the dissolved gas in the frame of the thin film approach for bubbles. Since such an approach is valid only for low speed cases, it has been extended to the case of significant interphase velocity nonequilibrium and turbulence¹. The gas evolution process is considered as isothermal one due to low latent heat of dissolution.

The developed numerical code is based on proposed model and finite volume method along with unstructured grids. Implicit unsteady numerical scheme which utilizes TVD approach for second order interpolation schemes for spatial coordinates provides numerical solution of the model equations. Phase coupled SIMPLE algorithm is used to resolve pressure-velocity coupling.

Numerical experiments were carried out to investigate impact of gas diffusion on the flow in vertical pipes and bubble columns with different types of bubble injections. A proposed model was validated by comparison of the predictions with experimental data.

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Preselecting resources to improve scientific workflows scheduling efficiency in cloud environments

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Recently emerged paradigm of cloud computing quickly became popular. It enables users to execute their computational tasks with an on-demand resource renting in a cost-effective way without the need to have and to maintain their own costly computational hardware. User satisfaction and even the question to use a cloud itself highly depend upon its efficiency, where one of the most important roles is played by the quality of scheduling.

Scheduling for IaaS clouds is an NP-hard problem to map a workflow of data-dependent tasks on cloud resources under time or money constraints. Contemporary approaches [1] are more focused on effective task distribution across resources than on effective resource selection itself. However, resource selection and therefore its cost are fundamental for cloud usage.

The approach presented here is to separate resource optimization and task distribution both conceptually and algorithmically. It involves an independent selection and iterative optimization of a subset of resources that is used as an input for task distribution algorithm on every iteration. The distribution of tasks from conventional task scheduler is used only to evaluate the quality of resource selection, and is discarded afterwards. Any existing algorithm for workflow scheduling (both cloud-aware and not) can be used to distribute tasks.

The usage of this approach leads to better results than heuristics-based scheduling algorithms, because it can improve their original output with additional iterations over resource selection stage. The presented approach also performs better than contemporary evolutionary algorithms used for cloud scheduling, because of reduced search space and independence from workflow size.

The proposed approach was implemented based on genetic algorithm for resource optimization stage and was used for experimental study. The parameters for study were taken according to real-world scientific workflows [2] and popular IaaS clouds from Amazon, Microsoft and Google. The experiment shows significant cost reduction for executing users' workflows in a cloud environment with the presented approach.

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Virtual Time Profile Modeling in Parallel Discrete Event Simulation

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Evolution of the profile of local virtual time (LVT) in Parallel Discrete Event Simulation (PDES) is revised. Model of LVT evolution in optimistic algorithm of PDES is investigated in details. Results support early idea that model belongs to the universality class of directed percolation.

Software Toolkit for Interactive Simulations of Reaction-Diffusion Problems on HPC Clusters

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We present a software for simulations of evolution equation systems of reaction-diffusion type involving first-order time derivative and up to second-order space derivatives with user-defined nonlinearities. Possible domains are sets of aligned rectangular blocks in one, two or three dimensions with Dirichlet, Neumann or periodic boundary conditions on their bounds.

User can create a project, launch it and check the results either manually or using web front-end (see <http://tracerwebui.mathmod.net> for testing purposes) that interacts with computing core.

Project is defined using a simple high-level domain-specific language including equations in Wolfram Mathematica syntax, domain geometry and boundary conditions. Results are obtained as static or animated plots since one of the independent variables represents time.

On the following stage of preprocessing the project geometry and state are translated into binary form and user-defined functions are translated into the C language and compiled into shared object suitable for computation core. The domain is decomposed if necessary according to selected computing hardware.

Computations are performed on a HPC cluster with possibly heterogeneous architecture, so that even detailed problem solutions can be obtained almost interactively.

Computing core is based on the method of lines, reducing the problem to a large system of ordinary differential equations. Spatial derivatives are approximated by finite differences on a regular grid. Despite stiffness, ODE systems are processed so far by explicit solvers (Euler, Runge-Kutta 4 or Dorman-Prince 4(5)) due to implementation issues. Since ODEs are coupled only with their immediate neighbors the solver utilizes both coarse-grain parallelism of distributing large blocks of spatial grid between different nodes or devices and fine-grain parallelism on every SIMD-like device.

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RNGAVXLIB: Program library for random number generation, AVX realization

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We present the random number generator (RNG) library RNGAVXLIB, which contains fast AVX realizations of a number of modern random number generators, and also the abilities to jump ahead inside a RNG sequence and to initialize up to 10^{19} independent random number streams with block splitting method.

The following generators are supported: MT19937 [2], MRG32K3A [3], LFSR113 [4], GM19, GM31, GM61, GM29 [1], GM55, GQ58.1, GQ58.3, GQ58.4 [1,5]. Fast AVX implementations produce exactly the same output sequence as the original algorithms. Usage of AVX vectorization allows to substantially improving performance of the generators. The new realizations are up to 2 times faster than the realizations implemented in the previous version of the library (RNGSSELIB [1]), and up to 40 times faster compared to the original algorithms written in ANSI C.

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Detailed numerical simulation of shock-body interaction in 3D multicomponent flow

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Keywords: fluid dynamics, shock-body interaction, multicomponent flow, numerical simulation, RKDG method, GPU computing, DiamondTorre algorithm

Interaction between a shock wave and an inhomogeneity in fluid has complicated behavior, including vortex and turbulence generating, mixing, shock wave scattering and reflection. In the present paper we deal with the numerical simulation of the considered process. The Euler equations of unsteady inviscid compressible three-dimensional flow are used into the four-equation model of multicomponent flow. These equations are discretized using the RKDG numerical method [1]. It is implemented with the help of the DiamondTorre algorithm, so the effective GPGPU solver is obtained having outstanding computing properties [2]. With its use we carry out several sets of numerical experiments of shock-bubble interaction problem [3]. The bubble deformation and mixture formation is observed, shown in figure 1.

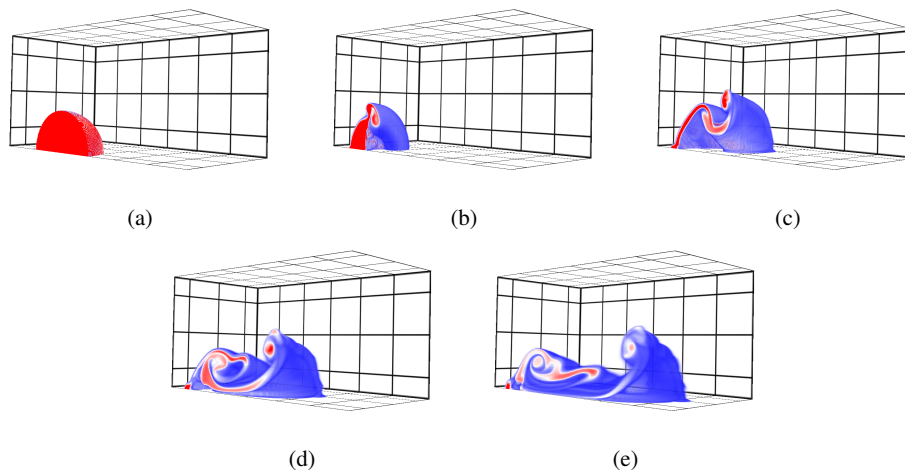


Figure 1: Rendering of a fluid component inside a bubble at different time moments: (a) $t = 0.0$, (b) $t = 1.0$, (c) $t = 2.0$ (d) $t = 3.0$, (e) $t = 4.0$; grid size is $600 \times 300 \times 300$

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Autowaves of spiking activity synchronization in a model neuronal network with relaxational synaptic plasticity

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There exists a short-term (~100 ms), repetitive, spontaneous synchronization of network spiking activity in planar neuronal networks grown *in vitro* from initially dissociated cortical or hippocampal neurons [1]. Such a phenomenon is called a population burst (PB) or network spike. It was indicated experimentally [2] that a PB might propagate in the neuronal network as a traveling wave, diverging from some occasional center.

We have generalized the results of Ref. [3], where the PBs occurred in a model neuronal network of leaky integrate-and-fire (LIF) neurons with a short-term relaxational synaptic plasticity, to the case of a spatially-dependent network topology where the probability of a connection between neurons depends on the mutual arrangement of neurons [4]. In particular, we show that a typical PB has complex spatial dynamics with a few occasional local sources of spiking synchronization, from which it propagates in the planar network as traveling waves, analogous to the divergent circular waves on the surface of water resulting from its local perturbation. This is in qualitative agreement with the results [2].

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**Numerical modelling of light transport in human ocular fundus
for photodynamic therapy planning**

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To carry out photodynamic therapy (PDT) of the human ocular fundus pathologies the accurate planning of interaction between laser light and tissues containing the photosensitizer should be performed. One of the most flexible and precise planning techniques is the numerical simulation of the therapeutic laser light distribution with prior data on the geometry and optical properties of the pathology. In the process of photodynamic therapy, it is necessary to evaluate the photosensitizer concentration in real time to achieve an optimal therapeutic effect.

In this paper, for the subretinal neovascular membrane's PDT planning using aluminum phthalocyanine as a photosensitizer the algorithm for the numerical simulation of laser light distribution in multilayer media containing photosensitizers was developed based on the classical Monte Carlo algorithm for biophotonics application [1]. The developed algorithm can be applied to different illumination geometries and allows analyzing of absorption and scattering of light on the surface and in the deep of tissue [2]. The optical properties of each layer are described by three main parameters such as absorption coefficient μ_a (cm^{-1}), scattering coefficient μ_s (cm^{-1}), and anisotropy factor that is the average cosine of the angle of light from the initial direction of light distribution. Every act of scattering occurs at an angle determined by the Henyey-Greenstein scattering phase function [3].

The formation of subretinal neovascular membrane the chorioretinal is an ingrowth of capillaries in subpigmentary or subretinal space through defects in Bruch's membrane. Due to this, the absorption coefficients of the corresponding layers increase in proportion to blood content in them and the layer with neovascularization thickens. In extreme cases, the thickening can reach hundreds of micrometers. So three scenarios were modeled, in the first one the thickness of the vascular layer was doubled, in the second scenario the retina absorption coefficient was increased and in the third case the combined effect was modelled. Three options of photosensitizer accumulation in the area of pathology were simulated - in thickened choroidea, in vessels, germinated in the subretinal space, and a combined case. The photosensitizer concentration was varied in range 10^{-5} - $5 \cdot 10^{-3}$ g/sm³.

The developed algorithm is to be used in clinical conditions for photodynamic therapy of ocular fundus pathologies with photodynamic system described in [4].

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Belov Alexander	Higher School of Economics	Russia	67
Belov Ivan	NRC "Kurchatov Institute"	Russia	72
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Boronina Marina	Institute of Computational Mathematics and Mathematical Geophysics SB RAS	Russia	40
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Chernykh Igor	Institute of Computational Mathematics and Mathematical Geophysics SB RAS	Russia	38
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Denisenko Marina	Nizhny Novgorod State University	Russia	24
Druzhinin Oleg	Institute of Applied Physics RAS	Russia	13
Dubenskaya Julia	SINP MSU	Russia	95
Durbin Richard	Wellcome Trust Sanger Institute	United Kingdom	26
Dyachenko Alexander	Landau Institute for Theoretical Physics	Russia	41
Dyshlovenko Pavel	Ulyanovsk State Technical University	Russia	49,97
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Golubenets Vyacheslav	P.G. Demidov Yaroslavl State University	Russia	105
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Hobl Lukas	Jülich Supercomputing Centre	Germany	22
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Huang Z. B.	Beijing Computational Science Research Center	China	20
Inogamov Nail	Landau Institute for Theoretical Physics	Russia	16
Ivantsov Andrey	Institute of Continuous Media Mechanics UB RAS	Russia	86,87,92
Izmailyan Nikolay	Yerevan Physics Institute	Armenia	70
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Karelsky Kirill	Space Research Institute RAS	Russia	45
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Khizriev Kamal	Amirkhanov Institute of Physics, Daghestan Scientific Center RAS	Russia	89
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Khokhlov Victor A.	Landau Institute for Theoretical Physics	Russia	16
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Konakov Stepan	St. Petersburg Polytechnic University	Russia	83
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Kovalev Valery	Lomonosov Moscow State University	Russia	26,81
Kretov Vadim	Higher School of Economics	Russia	50
Kroupnov Alexander	Lomonosov Moscow State University	Russia	52
Kryukov Alexander	SINP MSU	Russia	65,95,99
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Kulikov Igor	Institute of Computational Mathematics and Mathematical Geophysics SB RAS	Russia	38
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Levchenko Vadim	Keldysh Institute of Applied Mathematics	Russia	107
Lin Hai-Qing	Beijing Computational Science Research Center	China	20
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Mamonova Marina	Omsk State University	Russia	71,84
Manita Anatoly	Lomonosov Moscow State University; MIEM HSE	Russia	35
Manita Larisa	MIEM HSE	Russia	64
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Matsko Nikita	P.N. Lebedev Physical Institute RAS	Russia	54
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Mironov Vladimir	Lomonosov Moscow State University	Russia	42,79
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Moskovsky Alexander	ZAO "RSC Technologies"	Russia	79
MunyeV Vyacheslav	Nizhny Novgorod State University	Russia	24
Murtazaev Akai	Amirkhanov Institute of Physics, Daghestan Scientific Center RAS	Russia	89
Nagatkin Alexey	Ulyanovsk State Technical University	Russia	49
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Nizametdinov Azat	Ulyanovsk State Technical University	Russia	49
Novikov Alexander	National Research Centre "Kurchatov institute"	Russia	43
Novotny Mark A	Mississippi State University	USA	22
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Petrosyan Arakel	Space Research Institute RAS	Russia	45
Petrov Dmitry	Moscow Institute of Physics and Technology	Russia	46
Petrov Igor B.	Moscow Institute of Physics and Technology	Russia	23
Pilipenko Dmitriy	Omsk State University	Russia	71
Pimenova Anastasiya	Institute of Continuous Media Mechanics UB RAS	Russia	98,100
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Polyakov Stanislav	NovSU, Veliky Novgorod	Russia	99
Popov Ivan	Omsk State University	Russia	33
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Prikhodko Nikolay	NovSU, Veliky Novgorod	Russia	95,99
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Schmidt Alexander	loffe Institute	Russia	102
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Serenko Alexander	Novosibirsk State Technical University	Russia	38
Serenko Alexey	Moscow Institute of Physics and Technology, NRC Kurchatov Institute	Russia	69
Shcherbakov Andrew	MIEM HSE	Russia	90
Shchur Lev	Science Centre in Chernogolovka	Russia	104,106
Shchur Vladimir	Wellcome Trust Sanger Institute	United Kingdom	26
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Soldusova Anna	Omsk State University	Russia	85
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Stegailov Vladimir	MIEM HSE, JIHT RAS	Russia	47,59,76
Stogova Maria	Omsk State University	Russia	84
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Tarasevich Yuri	Astrakhan State University	Russia	42,57,63
Tchekhovskoy Alexander	UC Berkeley	USA	101
Timofeev Alexey	Joint Institute for High Temperatures RAS	Russia	36
Troitskaya Yulia I.	Institute of Applied Physics RAS	Russia	13
Tumanov Vladimir	Institute of Problems of Chemical Physics RAS	Russia	56
Usov Nikolai	Pushkov Institute of Terrestrial Magnetism, Ionosphere and Radio Wave Propagation RAS	Russia	74
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Weigel Martin	Coventry University	United Kingdom	28
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Yan X. W.	Beijing Computational Science Research Center	China	20
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Zhao Yani	University of Warsaw	Poland	58
Zhizhin Mikhail	Space Research Institute of the RAS, University of Colorado Boulder	Russia	43
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