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Relaxation and aging in jammed glasses

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Abstract:

We provide a unified description of ”aging”, the increasingly sluggish dynamics widely observed in the jammed state of disordered materials, in terms of record dynamics. Structural evolution in aging materials requires ever larger, record-sized rearrangements in an uncorrelated sequence of intermittent events (avalanches or quakes). According to record statistics, these (irreversible!) rearrangements occur at a rate ≈ 1/t. Hence, in this log-Poisson statistics, the number of events between a waiting time tw and any later time t integrates to ≈ ln(t/tw), such that any observable inherits the t/tw-dependence that is the hallmark of pure aging. Based on this description, we can explain the relaxation dynamics observed numerically and experimentally in a broad range of materials, such as low-temperature spin glasses and high-density colloids and granular piles [1,2,3]. We have proposed a phenomenological model of record dynamics that reproduces salient aspects, for example, the van-Hove distribution of displacements, intermittency and dynamic heterogeneity, over 12 decades in time using the waiting-time method [3,4]. Our studies also rules out some other explanations of aging based on trap models and continuous-time walks [5].

[l] P. Sibani and SB, https://arxiv.org/abs/1802.08845

[2] D. M. Robe, et. al., EPL 116, 38003 (2016); https://arxiv.org/abs/1802.05350.

[3] D. M. Robe and SB, https://arxiv.org/abs/1802.05350

[4] N. Becker, et. al., J. Phys.: Condens. Mat. 26, 505102 (2014), https://arxiv.org/abs/1401.6521

[5] SB et al, https://arxiv.org/abs/1803.06580.

Studies on the Rabi Model

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We report our recent studies on the quantum Rabi model (QRM). Firstly, by using a variational wave function, which facilitates to extract physics in entire parameter regime with high accuracy, we unveil a ground-state phase diagram of the QRM and argue that the main constituents are polaron and anti-polaron. Secondly, introducing an anisotropy into the QRM, in which the rotating- and counter-rotating terms are allowed to have different coupling strength, so that the model interpolates between two known limits with distinct universal properties. Through a combination of analytic and numerical approaches we compute phase diagram, scaling functions and critical exponents, and establish that the universality class at the finite anisotropy is the same as that of the isotropic limit. Our findings are relevant to a variety of systems that are able to realize strong coupling between matter and light.

Collaborators: Maoxin Liu, Stefano Chesi, Zu-Jian Ying, JQ You, Hong-Gang Luo, Xiaosun Chen

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Coarsening dynamics of the long-range Ising model

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We report Monte Carlo computer simulations of the nonequilibrium coarsening dynamics of the two-dimensional long-range Ising model. Employing a novel update scheme, our simulations perform $\sim 10^3$ times faster than the standard approach. We carefully examine previous approaches introducing a cut-off in the long-range potential in order to reduce the computational effort. Special emphasis is put on a careful analysis of finite-size effects. This enables us to establish agreement with a theoretical prediction for the time dependence of the domain growth, in contrast to previous numerical studies. Our method can easily be generalized to applications in other systems.

Optimality in self-organized molecular sorting

Marco Zamparo, Donatella Valdembri, Guido Serini,
Igor Kolokolov, Vladimir Lebedev, Luca Dall'Asta, Andrea Gamba

We introduce a simple physical picture to explain the process of molecule sorting, whereby specific proteins and lipids are concentrated and distilled into nanometric lipid vesicles in eukaryotic cells. To this purpose, we formulate a model based on the coupling of spontaneous molecular aggregation with vesicle nucleation. Its implications are studied by means of a phenomenological theory describing the diffusion of molecules towards multiple sorting centers that grow due to molecule absorption and are extracted when they reach a sufficiently large size. The predictions of the theory are compared with experimental observations and with numerical simulations of a lattice-gas realization of the model. The efficiency of the distillation process is found to be optimal for intermediate aggregation rates, where the density of sorted molecules is minimal and the process obeys simple scaling laws. Quantitative measures of endocytic sorting performed in primary endothelial cells are compatible with the hypothesis that these optimal conditions are realized in living cells.

Phase transitions in two dimensions: From the hard-disk model to active systems

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The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by reversible Markov-chain Monte Carlo methods satisfying the detailed-balance condition and by molecular dynamics. It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur even though homogeneous short-range interacting particle systems cannot develop crystalline order. Analysis of the system was made difficult by the absence of powerful simulation methods.

In recent years, we have developed a class of irreversible event-chain Monte Carlo algorithms that violate detailed balance. They realize thermodynamic equilibrium as a steady state with non-vanishing probability flows. A new factorized Metropolis filter turns them into a paradigm for general Monte Carlo calculations. I will show how the resulting Monte Carlo algorithm has allowed us to demonstrate that hard disks melt with a first-order transition from the liquid to the hexatic and a continuous transition from the hexatic to the solid. Analogous computations have also lead to our new understanding of two-dimensional melting for soft disks, that has been intensely studied in experiment.

Finally, I will discuss two-dimensional melting on a substrate (as it is realized in skyrmion systems), and for active particles, and will present a very recent application of the event-chain algorithm to Coulomb-type long-range-interacting systems.

Statistical Mechanics of Money

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By analogy with the probability distribution of energy in statistical physics, the probability distribution of money $P(m)$ among the agents in a closed economic system is expected to follow the exponential Boltzmann-Gibbs law [1]. This conjecture is confirmed by agent-based computer simulations [2]. We start from the state of perfect equality, where the total money M is equally divided among N agents, so the initial probability distribution is $P_0(m) = \delta(m - M/N)$. Then, certain amounts of money Δm are repeatedly transferred from one randomly selected agent to another in payment for products and services. If the selected agent does not have enough money to pay, we skip the transaction and go to another pair of agents. As time goes on, the initial delta-function distribution broadens and eventually converges to the equilibrium exponential distribution $P(m) = \exp(-m/T)/T$ with the money temperature $T = M/N$. This Boltzmann-Gibbs distribution represents "natural" inequality spontaneously developing due to entropy maximization in the randomized free-market model of small producers, which was extensively discussed by Karl Marx in *Das Kapital*. Empirical data on money distribution are difficult to obtain, but plenty of data are available on income distribution. Data analysis shows that income distribution in the USA [3], European Union [4], and many other countries [5] has a well-defined two-class structure. The majority of the population (about 97%) belongs to the lower class characterized by the "thermal" exponential distribution, whereas about 3% of the population are in the upper class characterized by the Pareto power-law ("superthermal") distribution, and there is no evidence for "middle class". The share of the total income going to the upper class expands dramatically during bubbles in financial markets and contracts during crashes [6]. This redistribution of income between the lower and upper classes is responsible for the overall dynamics of inequality in the last 30 years. For more information, see a popular article [7] in the special issue of the *Science* magazine on *The Science of Inequality* and the Web page `http://physics.umd.edu/~yakovenk/econophysics/`.

References

[1] A. A. Drăgulescu and V. M. Yakovenko, "Statistical mechanics of money", *The European Physical Journal B* **17**, 723 (2000), `http://dx.doi.org/10.1007/s100510070114`

[2] Justin Chen and V. M. Yakovenko, Computer simulation of money exchange models, `http://physics.umd.edu/~yakovenk/econophysics/animation.html`.

[3] V. M. Yakovenko and J. B. Rosser, "Colloquium: Statistical mechanics of money, wealth, and income", *Reviews of Modern Physics*, **81**, 1703 (2009), `http://dx.doi.org/10.1103/RevModPhys.81.1703`

[4] M. Jagielski and R. Kutner, "Modelling of income distribution in the European Union with the Fokker–Planck equation", *Physica A*, **392**, 2130 (2013), `http://dx.doi.org/10.1016/j.physa.2013.01.028`

[5] Yong Tao, Xiangjun Wu, Tao Zhou, Weibo Yan, Yanyuxiang Huang, Han Yu, Benedict Mondal, and Victor M. Yakovenko, "Exponential structure of income inequality: evidence from 67 countries", *Journal of Economic Interaction and Coordination* (2017), `http://doi.org/10.1007/s11403-017-0211-6`, `https://arxiv.org/abs/1612.01624`.

[6] A. Banerjee and V. M. Yakovenko, "Universal patterns of inequality", *New Journal of Physics*, **12**, 075032 (2010), `http://dx.doi.org/10.1088/1367-2630/12/7/075032`

[7] A. Cho, "Physicists say it's simple", *Science* **344**, 828 (2014), `http://dx.doi.org/10.1126/science.344.6186.828`

Computer Simulation in Physics and Beyond. What Is Important "Beyond"?

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Each new computing platform requires software developers to analyze algorithms over and over, each time having to answer the same two questions. Does an algorithm possess the necessary properties to meet the architectural requirements? How can an algorithm be converted so that the necessary properties can be easily reflected in parallel programs? And the situation is the same in physics, chemistry, astronomy, in all subject areas… *Changes in computer architecture do not change algorithms*, but this analysis has to be performed again and again when a program is ported from a one type of computers to another, largely repeating the work that has been done previously. Is it possible to do the analysis "once and for all," describing all of the key properties of algorithms so that all of the necessary information can be gleaned from this description any time a new architecture appears? Yes, this is exactly what the AlgoWIki approach proposes. Details will be presented in the talk.

Another closely related serious question is the choice of computer architecture for efficient solving a particular problem. The main disadvantage of the existing approaches to compare computer platforms based on the Top500, Graph500 and HPCG lists is the too limited choice of algorithms underlying the lists. The AlgoWiki project is dedicated to describing the parallel structure and key features of various algorithms from different areas so we can substantially improve comparing computing platforms and move from the three points to analysis based on hundreds of various algorithms. AlgoWiki gives almost unlimited freedom to compare various computing platforms.

Crossover between mean-field and short-range percolation

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Abstract:

We investigate the influence of the range of interactions in the two-dimensional bond percolation model, by means of Monte Carlo simulations. We locate the phase transitions for several interaction ranges, as expressed by the number z of equivalent neighbors. We also consider the $z \to \infty$ limit, i.e., the complete graph case, where percolation bonds are allowed between each pair of sites, and the model becomes mean-field-like. All investigated models with finite z are found to belong to the short-range universality class. There is no evidence of a tricritical point separating the short-range and long-range behavior, such as is known to occur for $q=3$ and $q=4$ Potts models. We determine the renormalization exponent describing a finite-range perturbation at the mean-field limit as $y_r \approx 2/3$. Its relevance confirms the continuous crossover from mean-field percolation universality to short-range percolation universality.

Interplay between charge order and superconductivity in cuprate superconductors

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One of the central issues in the recent study of cuprate superconductors is the interplay of charge order with superconductivity [1, 2]. Here [3] the interplay of charge order with superconductivity in cuprate superconductors is studied based on the kinetic-energy-driven superconducting mechanism by taking into account the intertwining between the pseudogap and superconducting gap [4, 5]. It is shown that the appearance of the Fermi pockets is closely associated with the emergence of the pseudogap [3]. However, the distribution of the spectral weight of the superconducting-state quasiparticle spectrum on the Fermi arc, or equivalently the front side of the Fermi pocket, and back side of Fermi pocket is extremely anisotropic, where the most part of the spectral weight is located around the tips of the Fermi arcs, which in this case coincide with the hot spots on the electron Fermi surface. In particular, as charge order in the normal-state [6], this electron Fermi surface instability drives charge order in the superconducting-state, with the charge-order wave vector that is well consistent with the wave vector connecting the hot spots on the straight Fermi arcs [3]. Furthermore, this charge-order state is doping dependent, with the charge-order wave vector that decreases in magnitude with the increase of doping. Although there is a coexistence of charge order and superconductivity, this charge order antagonizes superconductivity. The results from the superconducting-state dynamical charge structure factor indicate the existence of a quantitative connection between the low-energy electronic structure and collective response of the electron density. The theory also shows that the pseudogap and charge order have a root in common, they and superconductivity are a natural consequence of the strong electron correlation [3].

Keywords: charge order, Fermi arc, pseudogap, superconductivity, cuprate superconductor

References

[1] See, e.g., the review, R. Comin and A. Damascelli, Annu. Rev. Condens. Matter Phys. **7**, 369 (2016).

[2] R. Comin *et al.*, Science **343**, 390 (2014); Eduardo H. da Silva Neto *et al.*, Science **343**, 393 (2014); Y. Y. Peng *et al.*, Phys. Rev. B **94**, 184511 (2016); J. P. Hinton *et al.*, Sci. Rep. **6**, 23610 (2016).

[3] D. Gao *et al.*, Physica C **551**, 72 (2018); S. Feng *et al.*, arXiv:1807.00296.

[4] See, e.g., the review, S. Feng *et al.*, Int. J. Mod. Phys. B **29**, 1530009 (2015).

[5] S. Feng, Phys. Rev. B **68**, 184501 (2003); S. Feng *et al.*, Physica C **436**, 14 (2006); S. Feng *et al.*, Phys. Rev. B. **85**, 054509 (2012); Phys. Rev. B. **85**, 099902(E) (2012).

[6] S. Feng *et al.*, Phil. Mag. **96**, 1245 (2016); Y. Mou *et al.*, Phil. Mag. **97**, 3361 (2017).

Routing in Networks-on-Chip with Multiplicative Circulant Topology

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Constant increase in complexity of tasks to be solved and in volume of processed information makes it necessary to create complex computing devices consisting of a number of separate processor cores and various peripheral modules; to design such multiprocessor devices, architectural solutions in the field of networks-on-chip (NoCs) are used.

When designing a NOC, it is very important to optimally choose the network topology (a subsystem of processor cores and peripheral devices connection), because it basically determines how effective the NoC is. Usage of suitable topology can significantly increase productivity of the system being developed and reduce its power consumption, as well as chip resources use.

There are lots of topologies for NoC design. Among most effective and promising ones are circulant networks, which belong to regular topologies. In general, the circulant is a graph: $C(N;\ s_1, \dots, s_k)$, where N – number of nodes and s_n – generatrix whose value determines the distance between two nodes. There are lots of different types of circulants, one of which is multiplicative circulant: $C(s^k;\ 1, s, s^2, \dots, s^{k-1}) = MC(s, k)$. It is shown that even with a small network size, circulant topologies have better performance in most important network features compared to widely used mesh topologies. But the topologies, based on multiplicative circulants, have a limited number of variants, because the number of nodes must be strictly a second power of a whole number.

Because multiplicative circulants have a strict, pre-known, geometric form of the network and are characterized by the feature that the lengths of the generatrixes are the powers of one base, a specialized routing algorithm was proposed for such networks that made it possible to simplify the structure of the address part of a packet and to reduce its size. The peculiarity of the proposed algorithm is that when receiving the node number, where the packet is to be delivered, the router of current node does not calculate the whole route, but only the next step. This eliminates the need to store adjacency matrixes which consume significant memory as the number of nodes in the network increases. This is an important advantage of the proposed algorithm in the organization of data transmission in NoC, since memory is an expensive resource in terms of area and power consumption. To calculate the next step, it is enough for the router to store its own number, destination node number, and circulant features – *s* and *k*.

The test performance of the developed algorithm shows that it requires considerably less time for calculations than BFS algorithm does and is easily scalable to large-sized networks. This algorithm calculates steps using mathematical operations and has a linear complexity in contrast to the algorithm of breadth-first search from exponential dependence of the time of path searching on the size of the graph. At the same time, it is simpler than a universal adaptive algorithm for routing in conventional circulants and, accordingly, saves logical resources of the chip.

The above-mentioned algorithm was developed using HDL as part of NoC routers, and its testing in CAD Quartus II, FPGA-based prototyping, and comparison of the obtained results with other routing algorithms for circulant topologies were conducted.

Quasi-3D TCAD modeling of STI radiation-induced leakage currents in SOI MOSFET structure

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2D and 3D TCAD modeling is an effective tool for investigating the radiation hardness of various designs and technological solutions of SOI MOSFETs. Radiation degradation assessments of such important MOSFET parameters as threshold voltage (V_{th}), cut-off amplification frequency (f_{max}/f_T), transconductance (S), leakage current (I_{leak}) can be obtained using TCAD modeling.

The traditional 2D MOSFET modeling is sufficient to estimate the radiation dependencies of V_{th}, and f_{max}/f_T. However, the 3D description of the MOSFET structure should be used to determine the leakage current I_{leak}. This is due to the fact that the positive charge Q_{ot} accumulates in a thick SiO_2 layer of shallow trench isolation (STI) and a buried oxide layer (BOX) under the ionizing irradiation. Also, surface states with the N_{it} density at the oxide-silicon interface (SiO_2/Si) are induced. Moreover, the value of Q_{ot} and N_{it} depends on the intensity of irradiation. This leads to inversion of the near-surface layer along STI and BOX, and as the result to the formation of parasitic channels for the leakage current.

Thereby, 3D modeling of the complete MOSFET structure together with STI region (fully 3D) must be carried out. Synopsys Sentaurus TCAD allows carrying out for fully 3D simulation. However, the number of the difference grid elements for calculating the structure is tens of thousands, which, together with the complexity of modeling the charge capture process in the oxide and inversion of the layer in the border region, leads to very large computer time expenditures. For example, the average simulation time of the I-V characteristic for the 3D MOSFET structure with a size W/L=1.5/0.35 μm consisting of 165,000 difference grid elements was 10 hours on a computer with a quad-core Intel i7 (3400 MHz) processor and 16 GB RAM.

As an instrument of a development engineer, fully 3D modeling is unsuitable for the rapid evaluation of the device characteristics in real operating conditions and for calculating a large number of variants, primarily because of the very high expenditure of computer time. Quasi-3D model for calculation of radiation leakage currents in submicron SOI MOSFET structures is proposed. This will make it possible to reduce the computing time by a dozen times and substantially simplify the preprocessor description of the device structure in the TCAD tool.

The traditional 3D modeling of MOSFET structure in the Synopsys TCAD has replaced by the two standard subtasks by modeling the primary MOSFET and parasitic lateral STI structure. Both subtasks are solved independently, the components of the main transistor ($I_{leakMOS}$) and side parasitic transistor ($I_{leakSTI}$) leakage currents are determined, and then these components are summed to determine the total leakage current $I_{leak}=I_{leakMOS}+I_{leakBOX}+I_{leakSTI}$.

0.35 μm SOI MOSFET manufactured using 0.13 μm technology with the following structure parameters L/W=0.35/10 μm, t_{ox}=7 nm, t_{Si}=100 nm, t_{BOX}=145 nm, t_{STI}=130 nm, $N_A=8\cdot10^{17}$ cm^{-3}under the influence of ionizing radiation with a dose of up to 500 krad was simulated. Radiation models based on experimental data obtained for 0.13 μm CMOS technologies were used in modeling to determine the radiation-induced density of N_{ot} defects in SiO_2 oxide layers for BOX and STI regions and on Si/SiO_2 interfaces – N_{it}.

The results of the simulation show that in comparison with the traditional fully 3D modeling, which requires 11 hours of computer time, the computer time for the I_dV_g characteristic was reduced to 71 minutes (i.e. the computer time decreased by 9 times). Simulation for the quasi-3D model are in good agreement with the experimental data, the error in the calculations does not exceed 10%.

Development of multiprocessor system-on-chip based on soft processor cores schoolMIPS

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At present, there is a trend towards the use of systems-on-chip including a large number of processors, architectural blocks, and peripheral nodes. When designing large-scale multiprocessor systems, a balance should be observed between data transfer rate, amount of resources expended to implement the system, and ability to scale the system without cardinal changes. In such systems, it is extremely inefficient to use a bus topology or a common switch, what made that a new architecture in the form of a network-on-chip (NoC), providing high computational performance and rapid exchange of large data streams, to emerge. In addition, studies of possibilities of using processor cores of MIPS-architecture are becoming more and more urgent, since availability of educational infrastructure of soft processor core MIPSfpga and its simplified version – schoolMIPS – has started to be used in many colleges and universities to teach students computer architecture and hardware-software implementation ofr processor cores using the example of a commercial core.

This work includes a review of MIPS architecture processor cores, as well as comparative analysis of their most famous analogs, such as Nios II, OpenSPARC, RISC-V, openRISC, and MicroBlaze. Also, a comparative analysis of processor interaction subsystems was carried out, which allowed identifying advantages of the network topology consisting of routers over full switch or shared memory topology. A network of routers allows combining heterogeneous cores and blocks on a single chip and also provides simultaneous interaction of multiple blocks which greatly simplifies the topology and removes limitations on its scaling. In addition, the work carried out a review of existing implementations of communication subsystems for NoCs: Xpipes NoC base block library, QNoC with several levels of service quality, MANGO NoC with circuit-level switching for asynchronous data transmission, LRM NoC with multicast data transmission and NoC of 120 simplified microAptiv MIPS processor cores. Most developments support mesh topology and XY routing, and their main difference lies in the architecture of routers.

This work involves realization of 2 multiprocessor systems of 4 and 10 processor cores, developed on NoC topology using schoolMIPS soft-processor cores and routers with XY routing. For networks, mesh topology, providing sufficient network performance, relatively even distribution of load to the nodes, avoiding blockages, and also easy scaling, was chosen. There was implemented partitioning of switching part into input and output blocks connected by the FIFO buffer memory in the router. The arbitrator module controls interaction of the router with the connected processor core and neighboring routers. All messages, arriving at the router, are divided into packets from 1 to 8 flits; each 37 bits in length. Basic processor core schoolMIPS was improved by adding a block of RAM memory, a network interface for interaction of the core with the router, and new instructions and support for external peripherals to its architecture. Network interface is implemented as two separate modules at input and output of the processor core for receiving and transmitting data, respectively.

Maximum operating frequency of the router is 200 MHz, and the throughput reaches 2.13 Gbit / s. Measurement of network performance suggests that a network of 4 processor cores provides a speed of up to 1.87 Gbit / s, and a network of 10 processor cores – up to 1.54 Gbit / s. To implement the router 142 ALMs and 592 bits of memory were consumed; the expanded processor core schoolMIPS consumes 452 ALMs and 1692 bits of memory. The developed NOCs are not too resource-intensive, but they consume enough ALMs: NOC of 4 processor cores takes 2223 ALMs and 9136 bits of memory, and NOC of 10 processor cores – 5696 ALMs and 22840 bits of memory. The obtained results suggest that there is a possibility of NOCs development with the number of nodes up to 50 on Cyclone V SoC 5CSEMA5F31C6 FPGA (Terasic De1-SoC development board) and up to 200 nodes on Stratix IV GX EP4SGX230 (Terasic DE4 development board).

Heterogeneity of the magnetization of a thin film of a ferromagnetic semiconductor in the presence of an electric field

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The electrical manipulation of magnetism and magnetic properties has been achieved across a number of different material systems. For example, applying an electric field to a ferromagnetic material through an insulator alters its charge-carrier population.

The possibility of changing the spontaneous magnetization of a ferromagnetic semiconductor by applying an electric field was demonstrated in [1]. A thin film of a ferromagnetic semiconductor $(In_{0.97}Mn_{0.03})As$ 5 nm thick was placed on a substrate of other semiconductors.

In such a system, at a sufficiently high concentration Mn (on the order of several percent), the wave functions of the holes associated with neighboring ions begin to overlap, and a hole impurity band arises. Ferromagnetism is provided by the exchange interaction of holes with manganese ions by the Zener mechanism, i.e. indirect ferromagnetic interaction between ions is provided due to the *sd* -exchange of Vonsovsky-Ziner between holes and ions. The dependence of the density of states of a hole gas in the impurity band of energy, which overlaps noticeably with the valence band, is rather complicated. And for simplicity in the model calculation it was assumed that this dependence is the same as in a gas with some effective mass.

In this paper we consider the same theoretical model as in [2], but instead of not quite simple numerical calculations using approximate methods to derive analytical formulas for which the calculation is quite accessible in Mathematica package. This approach allows you to easily obtain possible changes in the results when changing parameters.

We introduce the density of manganese ions from the direction of the spin 5/2 and -5/2 in the easy magnetization axis $n_-^{5/2}(x), n_-^{-5/2}(x)$ and the density of holes with different projections on the easy axis $n_+^{1/2}(x), n_+^{-1/2}(x)$. The superscript here indicates the spin projection, and the bottom - at the sign of the charge. The density of the magnetic moment is determined by the hole densities

$$M(x,\Theta,E) = g\cdot\left(\frac{5}{2}\left(n_-^{5/2}(x)-n_-^{-5/2}(x)\right)+\frac{1}{2}\left(n_+^{1/2}(x)-n_+^{-1/2}(x)\right)\right),$$

$$n_-^{5/2}(x)-n_-^{-5/2}(x) = n_-\cdot\mathrm{Tanh}\left(\frac{\varepsilon_{ex}}{\Theta}\cdot\left(n_+^{1/2}(x)-n_+^{-1/2}(x)\right)\right),\quad n_+^{\pm 1/2}(z) = \frac{n_-}{2}\left(\frac{\mu^{\pm}(x)}{\varepsilon_F}\right)^{3/2},$$

which in turn are determined by the self-consistent potential $\varphi(x)$:

$$\mu^{\pm}(x) = \Phi_0 - \varphi(x) \pm \varepsilon_{ex}\cdot n_-\cdot\mathrm{Tanh}\left(\frac{\varepsilon_{ex}}{\Theta}\cdot\left(n_+^{1/2}(x)-n_+^{-1/2}(x)\right)\right),$$

$$\frac{d^2\varphi}{dx^2} = -\frac{4\pi}{\chi}\cdot\left(n_+^{1/2}(x)+n_+^{-1/2}(x)-n_-\right),\quad \left.\frac{d\varphi}{dx}\right|_{x=0} = \left.\frac{d\varphi}{dx}\right|_{x=L} = -\frac{E}{\chi}.$$

When an electric field $E\neq 0$, the Curie temperature will vary along the thickness of the film because of the spatial inhomogeneity of the hole distribution. And this leads to a change in the Curie temperature for the average magnetization.

The graphical representation of the results has a natural physical interpretation.

Computing details will be presented in the poster report of the student A. Amirova.

References

[1] H. Ohno, D. Chiba, F. Matsukura, T. Omiya, E. Abe, T. Dietl, Y. Ohno & K. Ohtani. Electric-field control of ferromagnetism. Nature Vol 408 2000, 944-946.

[2] M. A. Kozhushner, B. V. Lidskii, V.S.Posvyansii, L.I.Trakhtenberg, Effect of an electric field on the magnetic characteristics of a nanoscale ferromagnetic semiconductor. JETP, 2016, Vol. 150, No.6, p.1227-1232

Influence of Initial States and Structure Defects on Non-equilibrium Critical Behavior of 3D and 2D Ising Models

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One of the peculiarities arisen in describing the critical behavior of systems is the critical slowing down effect. It is associated with an anomalous increase in the system relaxation time t_{rel} when approaching the second-order phase transition temperature T_c. As a result, the system being at the critical point appears in no condition to reach equilibrium throughout the entire relaxation process. Therefore, at times $t << t_{rel}$, extraordinary non-equilibrium phenomena characteristic of systems with slow dynamics, such as aging, fluctuation–dissipation theorem (FDT) violation, and the effect of various initial non-equilibrium system states arise in the behavior of systems [1].

We present results of Monte Carlo description of features of non-equilibrium critical behavior in three- and two-dimensional Ising models conditioned by presence of structural quenched disorder. It was shown that limiting fluctuation–dissipation ratio (FDR) values characterizing the degree of system departure from equilibrium and FDT violation satisfy inequality $X^{\infty} < 1$ and depend on the universality class of non-equilibrium critical behavior to which they belong: one of these classes corresponds to the high-temperature, and the other to the low-temperature initial state of the system. The concept of threshold initial magnetization m_0^{th} separating these two universality classes is introduced.

It was revealed that the increase in the concentration of defects is accompanied by the strengthening of the aging effects manifested as the slowing down of correlation and relaxation processes in structurally disordered systems as compared to the pure system. Non-equilibrium initial states begin to increasingly more strongly influence peculiar features and characteristics of the system's evolution. For example, in the case of evolution from a high-temperature initial state with magnetization $m_0 << 1$, the influence of defects is manifested in quantitative changes to universal characteristics of non-equilibrium critical behavior and the limiting FDR X^{∞}. Values of these non-equilibrium characteristics in 3D Ising model demonstrate belonging to universality classes of critical behavior of weakly and strongly diluted systems [2], but non-equilibrium characteristics in 2D Ising model depend continuously on concentration of defects owing to the crossover effects in the percolation behavior [3].

For case with evolution from a low-temperature initial state with $m_0 = 1$, the autocorrelation function decreases in the long-time regime as a power-law of critical magnetization relaxation due to domain wall pinning on structural defects, while limiting FDR values determined by the domain dynamics become equal to zero. It was shown that the two-time scaling dependence of the autocorrelation function obeys relations of the ”superaging” theory suggesting enhanced influence of the system's ”age” (the time of onset of t_w measurement) determined by the power-law dependence $(t_w)^{\mu}$ with exponent $\mu > 1$ [2,4]. Values of ”superaging” exponent μ are calculated for systems with different defect concentrations.

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1. *V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp., **60**, 762 (2017).
2. *V.V. Prudnikov, P.V. Prudnikov, and P.N. Malyarenko*, JETP, **125**, 1102 (2017).
3. *V.V. Prudnikov* and *O.N. Markov*, Europhys. Lett., **29**, 245 (1995).
4. *V.V. Prudnikov, P.V. Prudnikov, E.A. Pospelov, and P.N. Malyarenko*, JETP Lett., **107**, 569 (2018).

Nonequilibrium critical dynamics of low-dimensional frustrated magnets and multilayer structures

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A significant interest has been recently focused on non-equilibrium processes in magnetic low-dimensional materials. The reduction of the dimension of magnets is accompanied by an increase in fluctuations of the spin density and the manifestation of the effects of critical slowing down and "aging" in the non-equilibrium behavior of low dimensional magnetic systems [1]. Thin films and low-dimensional demonstrates the slow critical evolution from a nonequilibrium initial state. Aging, coarsening and memory effects are nontrivial features in the non-equilibrium behavior of such systems with slow dynamics [2].

The magnetic properties of multilayer magnetic systems have been widely investigated over the past years, since they widely used in magnetic storage devices [3]. The antiferromagnetic coupling was crucial for the discovery of the giant magnetoresistance (GMR). It kickstarted the field of nanomagnetism and spintronics [4]. The using synthetic antiferromagnets in magnetic random access memory (MRAM) [5] can reduce the critical current [6] and the time for switching [7].

Magnetic order in the multilayers is complex due to a strong influence of the shape and the magnetocrystalline anisotropies of the sample. Anisotropy effects leads to dimensionality crossover in Heisenberg films [8]. This study includes the Monte-Carlo simulation of the non-equilibrium critical evolution from different initial states of low-dimensional magnetics [9] and multilayers based on anysotropic Heisenberg films [10, 11, 12].

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[1] T. Mukherjee, M. Pleimling, Ch. Binek, Phys. Rev. B, 82, 134425 (2010). https://doi.org/10.1103/PhysRevB.82.134425

[2] V.V. Prudnikov, P.V. Prudnikov, M.V. Mamonova, Phys. Usp., (2017) 60, 762-797. https://doi.org/10.3367/UFNe.2017.02.038067

[3] Y. Chen, D. Song, J. Qiu, et al., IEEE Trans. Magn., (2010) 46, 697. https://doi.org/10.1109/TMAG.2010.2041040

[4] R.A. Duine, K.-J. Lee, S.S.P. Parkin, M.D. Stiles, (2017) arxiv.org:1705.10526.

[5] D. Apalkov, B. Dieny, J.M. Slaughter, Proceedings of the IEEE, (2016) 104, 1796. https://doi.org/10.1109/JPROC.2016.2590142

[6] J. Hayakawa, S. Ikeda, Y.M. Lee, et al., Jpn. J. Appl. Phys., (2006) 45, L1057. https://doi.org/10.1143/JJAP.45.L1057

[7] A. Bergman, B. Skubic, J. Hellsvik, et al., Phys. Rev. B, (2011) 83, 224429. https://doi.org/10.1103/PhysRevB.83.224429

[8] P.V. Prudnikov, V.V. Prudnikov, M.A. Menshikova, N.I. Piskunova, J. Magn. Magn. Mater., (2015) 387, 77. https://doi.org/10.1016/j.jmmm.2015.03.075

[9] I.S. Popov, P.V. Prudnikov, A.N. Ignatenko, A.A. Katanin, Phys. Rev. B, (2017) 95, 134437 https://doi.org/10.1103/PhysRevB.95.134437

[10] V.V. Prudnikov, P.V. Prudnikov, A.N. Purtov, M.V. Mamonova, JETP Letters, (2016) 104, 776. https://doi.org/10.1134/S0021364016230132

[11] P.V. Prudnikov, V.V. Prudnikov, A.N. Purtov, M.V. Mamonova, N.I. Piskunova, J. Magn. Magn. Mater., (2018) https://doi.org/10.1016/j.jmmm.2017.11.084

[12] V.V. Prudnikov, P.V. Prudnikov, M.V. Mamonova, J. Exp. Theor. Phys., (2018).

Dynamical Scaling in Time dependence of Correlation Length in Non-equilibrium Critical Relaxation of Pure and Site-diluted 2D XY-model

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A two-dimensional systems with continuous symmetry occupy a special place among low-dimensional systems. It is known that the long-range order is broken in these systems at any finite temperature. However, the case of the 2D XY-model is characterized by realization of topological Berezinskii–Kosterlitz–Thouless (BKT) phase transition at temperature T_{BKT}. The 2D XY model is used to describe the behavior and the properties of a whole class of physical systems, in particular, ultrathin magnetic films and planar magnets with easy-plane anisotropy [1]. Despite extensive research [2], the influence of structural disorder on non-equilibrium critical phenomena in the 2D XY-model not finally resolved. The influence of structural defects on the dynamic dependencies of the correlation length $\xi(t)$ is not investigated. Dynamic dependencies of physical quantities in critical dynamics have scaling properties, where the correlation length $\xi(t)$ is of paramount importance.

Non-equilibrium critical behavior in the structurally disordered 2D XY-model is attributed to non-equilibrium processes in the vortex subsystem, spin-wave processes, and interaction of these subsystems with structural defects. These effects lead to a significant complication of the dynamic properties of the system. In particular, the aging effects in disordered 2D XY-model are transformed into subaging and superaging phenomena [3].

The present work is devoted to study of the dynamic and scaling dependence of the correlation length $\xi(t)$, second and fourth order cumulants $U_2(t)$ and $U_4(t)$, and two-time dependent autocorrelation function $C(t, t_w)$ for pure and site-diluted 2D XY-model with different spin concentrations p. We have shown that in a pure system scaling dependencies are satisfied with $\xi(t) \sim t^{1/2}$ for relaxation from low-temperature initial state and with $\xi(t) \sim (t/\ln t)^{1/2}$ for relaxation from high-temperature initial state, which correspond to the existing concepts about the dynamics of $\xi(t)$ in pure 2D XY-model [4]. However, the presence of structural disorder in system leads to a complication of the dynamic scaling dependencies of directly calculated $\xi(t)$ and cumulants $U_2(t)$ and $U_4(t)$. Dynamical scaling with $\xi(t) \sim t^{1/2}$ and $\xi(t) \sim (t/\ln t)^{1/2}$ [4] is violated, and collapse of dynamical scaling dependencies on $\xi(t)/L$ for systems with various linear sizes L is not observed in the entire low-temperature phase with $T < T_{BKT}(p)$. However, implementation of dynamical scaling dependencies on $\xi(t)/L$ takes place at $T = T_{BKT}(p)$ as in pure system. These features of the scaling dependencies were revealed for relaxation from both high-temperature and low-temperature initial states. We connect these dynamical features with the pinning of bound vortex-antivortex pairs by structural defects existing at $T < T_{BKT}(p)$.

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1. *S.E. Korshunov*, Phys. Usp., **49,** 225 (2006).
2. *V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp., **60**, 762 (2017).
3. *V.V. Prudnikov, P.V. Prudnikov, and I.S. Popov,* JETP **126**, 369 (2018).
4. *A.J. Bray, A.J. Briant, and D.K. Jervis*, Phys. Rev. Lett., **84**, 1503 (2000).

Simulation of the critical behavior of a complex spin systems by the parallel Wang-Landau method

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The computer simulation of a complex spin systems is actual area of theoretical physics research and it requires a lot of supercomputer resources (as much as there is). Last time we have wide range of algorithms to explore the critical behavior of a complex spin systems. One of them is the Wang-Landau method [1] that have few advantages relative to other Monte Carlo methods like Metropolis and cluster algorithms. There are no critical slowing down effect and wide range of applications e.g. exploring of polymer chains, protein folding, phase transitions in spin glasses. The Wang-Landau algorithm based on random walking at the energy space of spin system, and, when the energy space is large enough (especially for three-dimensional Heisenberg system), it can be observed the divergence of the algorithm and the modeling time tends to infinity, because histogram of energy levels visits will never be flat. To break those constraints the energy space can be divided on the subinterval by few replicas [2]. This approach will allow to beat divergence.

In this work we investigate the critical behavior of the three dimensional Heisenberg spin system model by serial and parallel Wang-Landau algorithm developed with use of OpenMP technology and we observe how resulting density of energy states, thermodynamical quantities and estimation time changed with the use of parallel method. Important question is about how effective this method relative to classical algorithms [3] e.g. Metropolis on three-dimensional Heisenberg model and can we use Wang-Landau method to explore properties of thin-film structures?

Most of the supercomputer systems have a lot of the computational cores and threads. Modern supercomputers often have hybrid architecture and scientists use GPUs to reduce the simulation time [4]. Therefore, we need to develop parallel methods of existing Monte Carlo algorithms to explore large and complex spin system, thin-films and multilayer structures.

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1. Wang.F., Landau D.P., Efficient, Multiple-Range Random Walk Algorithm to Calculate the Density of States // Phys. Rev. Lett. – 2001 – V. 86, P. 2050.

2. Vogel T., Li Y.W., Wust T., Landau D.P., Generic, Hierarchical Framework for Massively Parallel Wang-Landau Sampling // Phys. Rev. Lett. – 2013 – V. 110, P. 210603.

3. Barash L.Yu., Fadeeva M.A., Shchur L.N., Control of accuracy in the Wang-Landau algorithm // Phys. Rev. E. – 2017 – V. 96, P. 043307.

4. Yin G., Landau D.P., Massively parallel Wang–Landau sampling on multiple GPUs // Computer Physics Communications – 2012 – V. 183, P. 1568-1573.

Simulation of elastic properties of charge stabilized colloidal crystals

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Charge stabilized colloidal crystals are spatially ordered systems of electrically charged submicron particles immersed into a liquid electrolyte. The particles can vary from simple small plastic balls to complex objects like micelles or DNA molecules. There are a lot of examples of such systems in different fields of technology, chemistry and biology. Recently the interest in them has additionally grown in connection with the creation of self-assembling nanosystems.

While the interactions in colloidal systems can be rather complicated, the electrostatic and entropic interactions are only taken into account in the present study. This allows the use of the mean-field theory leading to the non-linear differential Poisson-Boltzmann equation. The properties of a colloidal system in any particular spatial configuration are then fully determined by the solution of the corresponding boundary value problem. Numerical solution is carried out by the finite element method.

Colloidal crystals are treated here within the approximation of static lattice. Elastic constants are found from the stress-strain and energy-strain dependencies obtained numerically. Charge stabilized colloidal crystals are media with nonzero initial stress. For that reason, description of their elastic properties is a bit more sophisticated than of the conventional crystals. Different approaches to the numerical experiments are discussed.

Elastic constants of different orders are calculated for a number of crystals with monoatomic crystal lattices. Special attention is given to the higher-order elastic constants. In particular, elastic constants up to the fifth order are calculated for the crystal with two-dimensional hexagonal crystal lattice. The results are compared to the graphene data.

The Ising spin glass: new methods for old models and old methods for new models

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The Ising spin glass in 2D exhibits rich behavior with subtle differences in the scaling for different coupling distributions. We use combinatorial optimization methods to determine exact ground states for systems with up to 10 000 × 10 000 spins. A combination of new algorithms al low us to treat samples with fully periodic boundaries and to sample uniformly from degenerate ground states for the ±J model. To establish a unified framework for studying both discrete and continuous coupling distributions in arbitrary dimensions, we introduce the binomial spin glass. In this model, the couplings are the sum of m identically distributed Bernoulli random variables. In the continuum limit $m \to \infty$, this system reduces to the Edwards-Anderson model with Gaussian couplings, while $m = 1$ corresponds to the ±J spin glass. Using this model, we derive a rigorous bound for the degeneracy of any energy level. Studying the defect energies in this model, we uncover intriguing subtleties in the behavior of the model with respect to the order in which the thermodynamic ($N \to \infty$) and continuum ($m \to \infty$) limits are taken.

[1] H. Khoshbakht and M. Weigel, Domain-wall excitations in the two-dimensional Ising spin glass, Phys. Rev. B 97, 064410 (2018).
[2] M.-S. Vaezi, G. Ortiz, M. Weigel, and Z. Nussinov, The Binomial Spin Glass, Phys. Rev. Lett., in print (2018).

Population Annealing goes Molecular Dynamics

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We adapt Population Annealing to Molecular Dynamics simulations and show the excellent accelerating performance as well as the massive potential for parallelism. For this we simulate the folding of met-enkephalin, a short peptide commonly used to test the performance of algorithms. A comparison with Parallel Tempering, the *de facto* standard for the simulation of complex systems with a rugged free-energy landscape using Molecular Dynamics, is presented. Further, the impact of choosing the temperatures of the annealing schedule via a constant energy-histogram overlap condition and the influence of the number of update-steps per temperature are checked.

Entropic population annealing algorithm and estimating the density of states of frustrated spin systems

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Estimating the density of states of systems with rugged free energy landscapes is a notoriously difficult task of the utmost importance in many areas of physics ranging from spin glasses to biopolymers. Density of states estimation has also recently become an indispensable tool for the benchmarking of quantum annealers when these function as samplers. Some of the standard approaches suffer from a spurious convergence of the estimates to metastable minima, and these cases are particularly hard to detect. We introduce a sampling technique based on population annealing enhanced with a multi-histogram analysis and report on its performance for spin glasses. We demonstrate its ability to overcome the pitfalls of other entropic samplers, resulting in some cases in orders of magnitude scaling advantages that can result in the uncovering of new physics. To do that we devise several schemes that allow us to achieve exact counts of the degeneracies of the tested instances.

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Simulation of electrical conductivity of 2D composites with rod-like fillers

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By means of computer simulation, we examined electrical conductivity of two-dimensional (2D) composites with rod-like fillers [1–4]. We investigated the effects of particles length and their alignment on electrical properties of 2D composite with high electrical contrast between a host matrix and fillers. We studied both the isotropic and anisotropic systems. We used both continuous [1,3] and lattice [3,4] approaches.

In the lattice approach [1,2,4], a host matrix (a substrate) was treated as a square lattice; rod-like fillers were represented as linear k-mers, i.e., rectangular particles 1 × k lattice faces. The k-mers were deposited onto the lattice by the random sequential adsorption. Overlapping with predeposited k-mers was forbidden, hence, a monolayer was formed. We transformed the monolayer into a random resistor network (RRN) to calculate its effective electrical conductivity.

The effect of defects on the behavior of electrical conductivity has also been simulated [2]. The defects in the lattice (impurities) and defects in the particles were considered. We examined both isotropic and anisotropic (all particles are aligned along one given direction) composites. We found that even a very small concentration of impurities has strong impact on the electrical conductivity.

For continuous problems, the model with intersections [3] and without intersections [4] rod-like particles were considered. The dependence of percolation thresholds and anisotropy of electrical conductivity versus the order parameter are discussed.

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1. Yu. Yu. Tarasevich, V. A. Goltseva, V. V. Laptev, N. I. Lebovka, Electrical conductivity of a monolayer produced by random sequential adsorption of linear k-mers onto a square lattice, Phys. Rev. E. 2016. Oct. Vol. 94, Iss. 4. P. 042112. DOI 10.1103/PhysRevE.94.042112.

2. Yu. Yu. Tarasevich, V. V. Laptev, V. A. Goltseva, N. I. Lebovka, Influence of defects on the effective electrical conductivity of a monolayer produced by random sequential adsorption of linear k-mers onto a square lattice, Physica A: Statistical Mechanics and its Applications. 2017. Vol. 477. P. 195–203. DOI 10.1016/j.physa.2017.02.084.

3. N. I. Lebovka, Yu. Yu. Tarasevich, N. V. Vygornitskii, A. V. Eserkepov, R. K. Akhunzhanov Anisotropy in electrical conductivity and transparency of films of aligned conducting rods, arXiv:1803.07354.

4. Yu. Yu. Tarasevich, N. I. Lebovka, I. V.Vodolazskaya, A. V. Eserkepov, V. A. Goltseva, V. V. Chirkova Anisotropy in electrical conductivity of two-dimensional films containing aligned rodlike particles: continuous and lattice models, arXiv: 1804.00809

Calculation of magnetic moments and lattice parameters Co-based Heusler alloys with determination of their energy favorable structure

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Cobalt-based full-Heusler compounds with composition Co_2YZ (where Y is a transition metal and Z is a main group element) are attracting attention due to their predicted half-metallic behaviour, a much desired property for spintronic devices[1-2]. Knowledge of the basic magnetic properties of these materials, especially in the form of thin films, is required both to exploit these promising materials and to understand the properties of magnetic multilayer structures based on them.

In this work we present results of structural and magnetic investigations of the Heusler compound by using VASP software package by means of the Projector Augmented Wave (PAW) method with generalized gradient approximation (GGA)[3]. From first principles the energy efficiency of the formation of various structures is investigated. The lattice parameters of Co_2FeAl(CFA), Co_2FeSi(CFS), $Co_2FeAl_{0.5}Si_{0.5}$(CFAS) Heusler alloys are calculated. The results of study magnetic properties of CFAS/Ag/CFAS multilayer structure are carried out.

Heusler compounds with the general formula Co_2YZ crystallize in the L21 and the B2 structures. At L21 structure the cubic unit cell consists of four interpenetrating fcc sublattices, two of which are occupied by Co atoms and the other two by the Y and Z atoms, respectively. At B2 structures in (0,0,0) and (1/2,1/2,1/2) sites are randomly occupied by Y and Z with an equal probability. The results of our calculations have shown that the bulk energy of CFA and CFS alloys in B2-type structure is greater than in the case of L21-type structure, this suggests that the L21-type structure is energetically more favorable. Also total magnetic moment in L21-type structure is greater than in the case of B2-type structure.

Investigation of the alloys lattice parameter dependence on the parameters of convergence made it possible to choose the optimal values of the plane waves cut-off energy Emax = 400 eV and Monkhorst Pack grid size 16x16x16. The optimized lattice constants for Co-based Heusler alloys a^{CFA} = 5.6965(9) Å, a^{CFS} = 5.6224(6)Å, a^{CFAS} = 5.5790(4) Å obtained by us are in good agreement with the experimental values.

In the case of CFAS/Ag/CFAS multilayer structure, the Ag lattice cell parameter is too small to accommodate a CFAS compound in the cube-on-cube epitaxial relationship. However, if the CFAS cube edge grows at an angle of 45° with respect to an in-plane Ag(001) direction, a good lattice match is obtained, enabling epitaxial growth. The supercell of CFAS/Ag/CFAS structure is consist of the 13 monatomic layers and vacuum layer with thickness 5Å. The layers of CFAS are placed on each side of the Ag five-layer slab. The magnetic moment of atoms is directed collinearly along the z axis.

Comparison of the values of the magnetic moment of CFAS atoms in the bulk and in the film adsorbed on Ag shows, that the Co atoms most distant from the substrate have greatest magnetic moment. For Fe atoms we obtained that magnetic moment for atoms in the bulk cell are slightly larger then magnetic moment for atoms located on substrate.

These results can be applied in numerical simulation by the Monte Carlo methods of the nonequilibrium behavior of multilayer magnetic superstructures[4].

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1. *J. Bass and W.P. J. Pratt* Magn. Magn. Mater. **200**, 274-289 (1999).
2. *V.V. Prudnikov, P.V. Prudnikov, D.E. Romanovskiy* J. Phys. D: Appl. Phys., **49,** 235002 (2016).
3. *P. G. Kresse and J. Furthmuller*, Phys. Rev. B, **54**,11169 (1996).
4.*V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp., **60**, 762 (2017).

Automated Robot's Workspace Approximation

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The workspace of a robot is defined as a set of positions that robot or its part can take. The workspace size maximization is often one of the design goals: the larger workspace the bigger area a robot can serve. A manual workspace determination can be a error-prone and time-consuming process. Thus there is a clear need for automating it.

In this work we propose an approach to cover of the working space of a robot with boxes. The interior an the boundary of the workspace are approximated with boxes with the prescribed accuracy. Two principally different ways of obtaining the coverage are considered. The first method obtains a coverage directly from robot’s kinematic equations. This approach requires minimal efforts from a user but entails a huge amount of computations for realistic robots. The second way consists in decreasing the number of parameters by reducing the system of kinematic equations to a system of inequalities. The the latter is used to construct a coverage. This approach results in more accurate approximations and requires less computational efforts. However reducing the system of equations to a system of inequalities is a non-trivial task and usually involves the human’s efforts.

We study and compare both ways of constructing the workspace approximation on model and realistic robotic systems. We show how high performance computing can significantly reduce the computational time needed to construct quality approximations.

Research and development of technologies for effective clustering of users

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Abstract

Clustering users based on information placed in social networks is a very promising task at present. The separate groups of users obtained in this way can be used in targeting advertising, searching for interlocutors by interests, searching for employees, organizing various events and searching for various partners, and much more. The quality of user clustering depends on a large number of factors, for example: the completeness and amount of information provided by the user, the quality of the initial exploratory analysis, to identify the data structure and the formation of a potentially useful vector representation of data transmitted to the input of machine learning algorithms. In this paper, existing approaches are explored and a method for effective clustering of users of social networks is developed, based on exploratory data analysis and approaches to preparing master data for machine learning.

Fractal Approach for Determining the Optimal Number of Topics.

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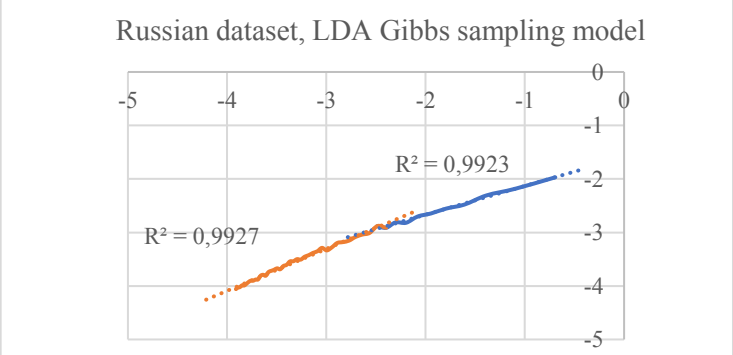
Modern information systems generate a huge number of texts such as news, blogs and comments. Analysis of big data is impossible without the construction of formalized mathematical models based on statistical physics. One of such a model is topic modelling (TM) based on Potts model [1]. This model assumes that each textual document can be considered as a one-dimensional grid and each word of a document as a node. A node can be in one of T states. Correspondingly, a collection of words (nodes) referring to one of the states can be considered a topic. The probability of a word in a document is described by the following expression: $p(w|d) = \sum_{t\in T} p(w|t)p(t|d) = \sum_{t\in T} \phi_{wt}\theta_{td}$, where $p(w|t) = \phi_{wt}$ is the distribution of words by topics, $p(t|d) = \theta_{td}$ is the distribution of documents by topics [1], T is the number of topics, W is the number of unique words. The main parameter of TM algorithm is the number of topics, which is manually defined. The study of topic model behavior as a function of topic number is extremely actual and can be realized using fractal formalism. Topic solution under fixed number of topics is a matrix ϕ_{wt} , where the number of cells is T*W, T is the number of columns of the matrix, W is the number of rows. The size of each cell is $\varepsilon=1/(WT)$. Each cell of the matrix contains the probability P_{ij} of belonging of a word w_i to a topic T_j. The probability density function has the following form [2]: $\rho_i = \frac{n_i}{WT}$, n_i is the number of cells in topic solution containing high probabilities. This value is a function of a topic number, and it varies from 1 to some number $\rho_i(\varepsilon)<1$ in the process of topic modelling. The density $\rho_i(\varepsilon)$ depends on the size of cells and degree $D(\varepsilon)$: $\rho(\varepsilon) \cong \varepsilon^{-D(\varepsilon)}$. Parameters of textual collections used in this work: 1. Dataset in Russian language: 18026 unique words, 8630 documents. 2. Dataset in English language: 50948 unique words, 15404 documents. The choice of data sets depends on the availability of the number of topics embedded in texts. In this work the following topic models were used: 1. PLSA, 2. LDA Gibbs sampling and 3. BigARTM. The figure below shows an example of TM fractal behavior of the dataset in Russian. The intersection of trend lines corresponds to a point, equal to the number of topics in the given dataset and corresponds to a point of information phase transition.



Fractal analysis of topic model behaviour allows us to show that self-similar fractal clusters exist in large textual collections. The forming of clusters occurs precisely in the transition regions. Linear regions do not lead to changes in fractals, therefore, it is sufficient to find transition regions for the study of textual collections. Accordingly, the problem of the analysing the evolution of topic models can be simplified to the problem of searching transition regions in topic models.

1. Griffiths T, Steyvers M. Finding Scientific Topics // Proceedings of the National Academy of Sciences. 2004. Vol. 101 (Suppl. 1). P. 5228–5335.
2. Koltcov S. N., A thermodynamic approach to selecting a number of clusters based on topic modeling, Technical Physics Letters, 43(6), P. 584-586.

Measuring of Cognitive Processes Indicators When Reading Educational Materials Using Brain–Computer Interface

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Effectiveness of educational process is greatly determined by indicators of students' cognitive processes when their learning activities. Using the analysis of electroencephalogram, it is possible to monitor the indicators of such processes and, as a consequence, to predict the success of educational process as a whole.

For such an analysis, alpha and beta rhythms are traditionally used. For example, using alpha-rhythm, one can track the increase of attention (especially visual one), or mental activity. Using beta-rhythms, it is possible to track the presentation of a new unexpected stimulus, mental tension, emotional arousal. However, the use of these rhythms will not always allow monitoring the effectiveness of students' educational process. In this connection, it may be of interest to use both complex indicators, characterizing several rhythms, and alternative types of rhythm, for example, theta rhythm.

To make it possible to use theta rhythm and to assess the level of understanding and interest of the text viewed, the following preliminary experiment was carried out. 10 students of technical specialties were presented (for reading) 3 texts of different subjects: physical, technical, and survey-technical ones.

When viewing each test, every subject was taken an EEG using Neuron-Spectrum apparatus, and the dominant frequency of theta rhythm in the lead FP1-FP2 (frontal region) was determined by coherent analysis of brain activity. At the end of reading, each student evaluated interestingness of the texts viewed, including commenting on the reason for such interest as well as connection of texts with research area and disciplines of studies.

The result of the experiment showed that the maximum value of the dominant frequency of theta-rhythm was observed in case of reading uninteresting texts, or texts in unfamiliar areas. Interesting, or familiar texts led to a minimum value of the dominant frequency of theta rhythm.

However, in general, the use of Neuron-Spectrum apparatus in such a situation is difficult, since it does not allow obtaining integral indicators of cognitive processes. This problem can be solved by using Emotiv Insight Brain–Computer Interface (BCI).

The work objective is to research integral indicators of cognitive processes when reading educational materials of different levels of difficulty and in different areas to evaluate teaching efficiency.

To achieve the objective, an experimental study should be conducted.

Method of conducting

a. Participants. The participants of experiment were 30 fourth-year students of NRU HSE.
b. Materials. For EEG analysis, Emotiv Insight was used. This neural interface allows assessing the following characteristics: interest, engagement, relaxation, stress, excitement, focus. Six texts in different areas were used (2 texts in humanitarian area, 2 texts in technical area, and 2 texts in mathematical area); texts in the same area were of different difficulty level. To assess comprehension of each text, some tests were developed; also, a questionnaire was developed to assess participants' preferences and interests in certain areas and disciplines.
c. Study Procedure. Experiments are conducted in the first half of the day individually for each subject in a computer class. The external conditions for all participants are the same. After conducting the briefing and explaining the meaning of experiment, the subjects filled the preference questionnaires and put on Emotiv Insight BCI. Then every subject was presented with the first text, and comprehension test (after reading) was given. Then the actions of the subject were repeated in relation to texts 2–6.

The results

For every subject, based on the results of the experiment, preferences in the scientific and technical areas, indicators of cognitive processes when reading each text, and the results of measuring reading comprehension were obtained.

Processing of the results of the experiment suggests regression, dispersion, and cluster analysis for constructing models of influence of the type of text and its difficulty on indicators of cognitive processes that make it possible to evaluate effectiveness of education.

Analysis of neural networks efficiency for determining positions of corrupted bytes

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Abstract

A lot of files and data, in general, are transferred throughout the networks. But the data may be corrupted by intrusions or package loss so, the executable files may be marked as non-executable and violate the local network policy. Thus, it's necessary to detect such files. In this paper, we present a novel method for detecting broken bytes of a file, so the corrupted files may be detected. Also, the positions of wrong bytes might be helpful in restoring the original file content. This work is devoted to study of modern neural network models applied to detect corrupted bytes of a file problem. Since recurrent neural networks (RNNs) seem to be well suited for such tasks, the main tasks of this work are to analyze the efficiency of popular state-of-the-art RNNs solving the problem mentioned above and to compare results of different models. We use data consisting of the most popular file types collected from the Internet and manually randomly added noise to that data to test our models. An experiment on this data demonstrates the advantages and disadvantages of the considered models.

Multipliers of Antiphase Solution in a System of Two Coupled Nonlinear Relaxation Oscillators

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A mathematical model of synaptic interaction between two neuron oscillators with delay in a connection chain is considered. The model is the system of non-linear differential-difference equations [1] with large parameter in right parts. Here an idea of fast threshold modulation is used.

For any natural n it is possible to choose the parameters such that the system has a periodic antiphase solution containing n asymptotically high bursts on the period. Simultaneously inphase solution with $2n$ bursts exist.

It is proved that the linearised on the antiphase solution system has unit multiplier, two multipliers which modules are close to 1, but less than 1, and all other multipliers are exponentially small. It means that antiphase solution is exponentially orbitally stable.

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References. [1] Glyzin S. D., Kolesov A. Y., Rozov N. K. On a method for mathematical modelling of chemical synapses, *Diff. Eq.*, 2013, 49:10, 1227–1244.

Numerical studies of solutions for kinetic equations with many-particle collisions

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In this work we present use of low-rank tensor decompositions for acceleration of evaluation of right-hand side of systems of kinetic equations with many-particle collisional terms. These equations can be interpreted as a generalization of classical Smoluchowski aggregation equations allowing one to consider not only binary collisions of particles but also triple particle collisions.

Straight-forward evaluation of right-hand side for such system of N equations with $k = 1, 2, \ldots, N$ requires $O(N^3)$ numerical operations and we find such complexity too high for practical investigations. However, under assumptions that the kinetic coefficients can be represented with either canonical polyadic (CP) or tensor train decomposition (TT) with rank $R \ll N$ we can propose algorithms evaluating the right-hand side with much lower complexities: $O(NR \log N)$ and $O(NR^2 \log N)$ for CP and TT respectively.

We check the accuracy of proposed approach for model Cauchy problem with constant kinetic coefficients and monodisperse initial conditions and obtain good agreement of numerical results with known explicit solution. With use of our ideas we reach high level of accuracy of numerical solutions in really modest CPU-times. We compare numerical solutions with different triple-collision rates and obtain a significant influence of accounting triple collisional effects.

The application of the Lattice Boltzmann method to the one-dimensional modeling of blood flow in elastic vessels

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The models for the blood motion in the cardiovascular system range from the 0-D lumped models, 1-D pulse propagation equations to 3D viscous flow equations [1]. In many cases the 3D approach based on the solution of the Navier-Stokes equations is too detailed while 0D lumped models are oversimplified and applicable only for the distal vasculature. In the case of the 1D models it is assumed that the radial velocity is negligible [2]. Then, integrating the Navier-Stokes equations over the radial variable the 1D nonlinear system of equations (depending only on one spatial variable, axial coordinate) for the luminal area change and the axial blood velocity is derived. The common way to solve this equations is locally conservative Galerkin (LCG) method.

I will present an alternative way to model 1D blood dynamics based on the kinetic equations, namely, using the Lattice Boltzmann approach [7]. This method describes the motion of particles on Cartesian spatial lattice (advection part), the collision of the particles in spatial nodes is modeled by assuming that the velocity distribution of the particles tends to some local equilibrium state (trend to Gaussian distribution). The Lattice Bolzmann (LB) method correctly reproduces low-Mach incompressible flows like blood motion and can be used in the modeling of the cardiovascular network. The details about 3D modeling with LB approach can be found in several papers [3]-[5].

We start with two-dimensional model D2Q9 applied to the flow in the two-dimensional elastic tube with periodic boundary conditions with pressure variations at the vessel inlet and outlet and Dirichlet boundary conditions for the moving vessel wall. Next, we sum over all spatial points perpendicular to the flow and reduce the system to the three velocity model (D1Q3) supported by the additional equation accounting for the luminal area response to the blood pressure. From this pressure-area relation we evaluate the correction coefficients for the lattice distribution densities at the each time step. This correction is necessary since it accounts for the vessel geometry (luminal) change which could not be captured by the one-dimensional LB model.

The presented method is simpler than the finite-difference methods for the nonlinear 1D blood equations [6]. The method correctly describes the change in shape of the initial pulse wave and moreover can be applied for the assessment of the forward and the backward blood pressure-velocity wave (reflected wave) superposition. The blood velocity waveforms can be obtained for the different elastic area-to-pressure responses of the vessel wall, the wall viscoelastic effects can be also potentially implemented.

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REFFERENCES

[1] C.Taylor, M. Draney, *Annu. Rev. Fluid Mech.* **36**, 197–231 (2004)
[2] S.Sherwin, V. Franke, J. Peiro, K. Parker, *J. Engng. Maths,* **47**, 217-250 (2003)
[3] H.Fang, Z. Wang, Z. Lin, M. Liu, *Phys. Rev. E,* **65**, 051925 (2002)
[4] M. Bisson, M. Bernaschi, S. Melchionna, S. Succi, E. Kaxiras, *Commun. Comput. Phys.,* **11,** 48-64 (2011)
[5] G. Pontrelli, I. Halliday, S. Melchionna, T.J.Spencer, S, Succi, *Math. Comp. Model. of Dyn. Syst*., 20, 470-490 (2013)
[6] Y. Hou, G. Kassab, *Am. J. Physio.l Heart. Circ. Physiol.* **292**, H2623–H2633, (2007)
[7] S. Succi, The Lattice Boltzmann Equation: For Complex States of Flowing Matter, OUP Oxford, 2018

NUMERICAL SIMULATIONS OF COMPLEX NONEQUILIBRIUM FLOWS IN FINITE REGIONS ON THE BASIS OF THE BOLTZMANN KINETIC EQUATION

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Direct methods for solving the Boltzmann and other kinetic equations [1] are used for studying new nonequilibrium flows in the boundary steady problems. For different problems with nonequilibrium boundary conditions (see [2, 3]) nonclassical transport in flows appears (this effect for the first time has been described in [4]). In particular, heat can be transferred from the region with the lesser temperature to the region with the greater temperature. Now we consider a problem with "membrane-like" boundary conditions. In the simplest case particles leaving the region under consideration do not collide with particles entering this region. For such a situation even equilibrium distributions for the boundary conditions can lead to nonclassical anomalous transport mentioned above due to complex interaction of the opposite directed flows. In a more complex situation a part of gas can be reflected from the membrane molecules with the diffuse condition. Numerical solutions with the use of hybrid schemes combining discrete velocity method for kinetic equations and Lattice Boltzmann Model are obtained. For this problem analytical approximations of the expansion in the inverse Knudsen number confirm these effects. Possible experimental tests are discussed. For these purposes mixed cellulose ester (MCE) membranes could be used as a material for the boundaries. As reported in [5], a pore-size of these membranes is 25 nm, so the appropriate Knudsen number is more than unity at the atmospheric pressure. This problem for a mixture of chemical reactions with the kinetic model equations [6, 7] is also solved. We have used these equations in study of nonequilibrium structures in the nonuniform relaxation problem [8] and now also apply them for investigation of complex structures of the mentioned problem.

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References

1. V.I. Kolobov, R.R. Arslanbekov, V.V. Aristov, A.A. Frolova, S.A. Zabelok. Unified solver for rarefied and continuum flows with adaptive mesh and algorithm refinement. J. Comp. Phys. 2007. Vol. 223. P. 589-608.
2. V.V. Aristov, S.A. Zabelok, M.A. Fedosov, A.A. Frolova. Problem with Nonequilibrium Boundary Conditions in the Kinetic Theory of Gases. Comp. Math. Math. Phys., 2016, Vol. 56, P. 854–863.
3. V.V. Aristov, S.A. Zabelok, A.A. Frolova. The possibility of anomalous heat transfer in flows with nonequilibrium boundary conditions. Doklady Physics, 2017, Vol. 62, No. 3, P. 149–153.
4. V.V. Aristov. A steady state, supersonic flow solution of the Boltzmann equation. Phys. Letters A. 1998. V. 250. P. 354-359.
5. V.V. Aristov, A.A. Frolova, S.A. Zabelok. Nonequilibrium kinetic processes with chemical reactions and complex structures in open systems. EPL (Europhys. Letters). 2014. Vol. 106. P. 20002-1 - 20002-6.
6. N.K. Gupta, Y.B. Gianchandani. Thermal transpiration in mixed cellulose ester membranes: Enabling miniature, motionless gas pumps. Microporous and Mesoporous Materials. 2011. Vol. 142 P. 535-541.
7. A. Rossani, G. Spiga. A note on the kinetic theory of chemically reacting gases. Physica A. 1999. Vol.272. P. 563-573.
8. M. Bisi, M. Groppi, G. Spiga. Kinetic Bhatnagar-Gross-Krook model for fast reactive mixture and its hydrodynamic limit. Phys. Review. E. 2010. Vol.81. P. 036327.

The study of the unstably-stratified marine atmospheric boundary layer by direct numerical simulation

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Prediction of the properties of the atmospheric flows over sea is important for local and regional weather forecast. This prediction typically relies on the performance of large-scale meteorological models based on bulk formulae for air velocity, temperature and humidity. The bulk formulas relate turbulent fluxes of momentum, heat and vapor to bulk air velocity, humidity and air-sea temperature difference. The most widely used parameterizations used to compute the coefficients of proportionality in the bulk formulae are formulated on the basis of the Monin-Obukhov similarity theory (MOST) for different types of air stratification (stable, neutral and unstable). In our previous studies we showed that MOST quite accurately predicts the properties of the air-flow over waved water surface under neutral and stable stratification conditions provided that stratification effects are relatively weak and flow is in a statistically stationary state. In the present work, we perform direct numerical simulation and study the air flow over a waved water surface under unstable stratification conditions where the sea surface temperature is larger than the bulk air temperature. Such situation occurs in the tropical cyclone conditions as well as in polar lows at high latitudes. Our results show that in this case, the air flow dynamics is dominated by the development of large-scale cylindrical coherent vortex structures elongated in the direction of the mean wind. These structures cause a notable deviations from the MOST predictions for the air velocity and temperature profiles.

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Two-step melting in Two Dimensions with Long-ranged and Attractive Forces

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The problem of melting in two dimensions has recently found unexpected resolution in which the essentials of the Halperin-Nelson-Young theory were confirmed. The solid and the isotropic liquid state are indeed separated by an intermediate hexatic phase, with solid-hexatic melting of the Berezinsky-Kosterlitz-Thouless type, followed by a conventional first-order hexatic-liquid transition [1]. A key challenge in these simulations are large correlation lengths which could be overcome by a new class of irreversible, rejection-free Markov-chain Monte Carlo algorithms, following the Event-chain paradigm. I will present new numerical evidence that these algorithms indeed open a new dynamical universality class, endowed with faster mixing than reversible Markov chains both for particle-type systems and for the XY model [2]. Moreover, I will present new results for the two-dimensional melting problem in the limit of long-ranged interactions, completing the phase diagram of inverted-power-law potentials, and with attractive interactions of the Lennard-Jones type [3].

[1] E. Bernard and W. Krauth, Phys. Rev. Lett. 107, 155704 (2011);
S. C. Kapfer & W. Krauth, Phys. Rev. Lett. 114, 035702 (2015).

[2] S. C. Kapfer & W. Krauth, Phys. Rev. Lett. 119, 240603 (2017);
A. Langheld and S. C. Kapfer, in preparation, 2018.

[3] F. Schmidt and S. C. Kapfer, in preparation, 2018.

MATHEMATICAL MODELING OF HEATING OF HOMOGENEOUS METAL TARGETS BY A FOCUSED ELECTRON BEAM

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Some methods for local analysis of various objects in material science are based on the excitation of an informative signal by a beam of accelerated electrons (electron microscopy, spectroscopy of characteristic losses of electron energy, X-ray spectral microanalysis, etc.). However, as shown by us earlier for semiconducting targets, when the electrons of low (100 eV-8 keV) and medium (8-50 keV) energies decelerated in the target, only a small part of energy goes to the formation of informative signals and the most part of the energy goes to heating the sample [1, 2]. We have continued such works for other objects used in physical materials science and in this paper we have considered heating of homogeneous metal targets. As in [3], the problem of heat distribution in metal targets irradiated with sharply focused electron beams in the absence of heat exchange between the target and the external medium is considered by mathematical modeling methods. For a quantitative description of energy losses by beam electrons a model based on a separate description of the contributions of absorbed in the target and backscattered electrons and applicable to a wide class of solids and a range of primary electron energies is used [4, 5]. The heat transfer equation was solved using the Green's function, and problems related to the computational stability of the solution were discussed. Quantitative estimates of the temperature rise of various metallic targets under an electronic probe are carried out. Using the features of this approach, the nonmonotonic dependence of the temperature of the maximum heating in the target on the energy of the primary electrons is explained. The results are illustrated for some homogeneous metal targets.

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[1] Rau E I, Ditsman S A, Zaitsev S V, Lermontov N V, Lukyanov A E and Kupreenko S Yu 2013 *Bulletin of the Russian Academy of Sciences: Physics* **77** 951
[2] Amrastanov A N, Kuzin A Yu, Mityukhlyaev V B, Seregina E V, Stepovich M A, Todua P A and Filippov M N 2017 *Measurement Techniques* **60** 534
[3] Stepovich M A, Amrastanov A N, Seregina E V and Filippov M N 2018 *Journal of Physics: Conf. Series* **955** 012040
[4] Mikheev N N, Petrov V I and Stepovich M A 1991 *Bulletin of the Academy of Sciences of the USSR. Physical Series* **55** 1
[5] Mikheev N N and Stepovich M A 1996 *Industrial Laboratory* **62** 221

The analysis of optimistic parallel discrete event simulation algorithm on small-world networks

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We study synchronization algorithms in parallel discrete event simulations (PDES). We build a model for the evolution of local virtual times (LVT) in the optimistic synchronization algorithm. We run our models on regular and small-world topologies and compare the results. The main parameters of the simulation are the growth rate q and the average fraction of long-range communication links p. We found the power-low dependence of the average speed of the LVT profile on the parameter q. In the model on regular lattice the calculated exponent ν is the same as in directed percolation (DP) universality class, and equals 1.67(3). The exponent ν grows with the average fraction of long-range communication links p. We also calculated another exponent of DP universality class β, which characterizes the behavior of density of local minima and maxima. The calculated exponent β differs from the one in DP universality class. For our model it is β=0.78(4), while for DP it is β_{DP}=0.276486(8). The work is supported by grant 14-21-00158 of the Russian Science Foundation.

Melting transition and phase diagram of 2d active hard disks and dumbbells

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Active materials are out-of-equilibrium systems in which the dynamics of their elements break detailed balance. Examples can be found in living systems, e.g. the collective motion of large animal groups, bacteria swarming, as well as in synthetic ones, like self-propelled grains or self-catalytic colloidal suspensions. Despite such diversity, the emergence of activity-induced collective behavior is captured by minimal models that yield accurate descriptions on their universal character. A key example is the Active Brownian Particles (ABP) model which considers spherical self-propelled particles with only excluded volume interactions. Active dumbbell model is the most simple extension of ABP for active bi-atomic rigid molecules.

Although active particles can in principle move in 3D, in most experimental set-ups they are confined to 2D. Melting in 2D is a fundamental problem that has remained elusive despite decades of intensive research. Only recently, numerical simulations * and experiments on colloidal monolayers indicate that melting of passive hard-disks takes place in two steps: as the packing fraction is increased, a first-order transition between the liquid and hexatic phases occurs, followed by a continuous Berezinskii-Kosterlitz-Thouless transition between the hexatic and the solid. Liquid and hexatic phases coexist close to the liquid phase.

We implemented a velocity-Verlet alghoritm in the open source software Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), to efficiently parallelize the numerical integration of the equation of motion for both disks and dumbbells. Simulations ran with $N = 256^2$ particles, scanning almost the entire parameter space over packing fraction and activity. We also explored inite size effects, simulating systems up to 512^2 particles.

We established the complete phase diagram of self-propelled hard disks and dumbbells in two spatial dimensions from the statistics of local order parameters. For the disks we also took advantage of a careful comparison among the equation of state of the system, measured thanks to a virial approach, spacial correlations of order parameters and distributions of local quantities (local density and local hexatic parameter) in order to examine in depth the transition scenario.
We found two different pictures for the two cases considered †,‡. The equilibrium melting scenario is maintained at small activities for the disks, with coexistence between active liquid and hexatic order, followed by a proper hexatic phase and a further transition to an active solid. As activity increases, the emergence of hexatic and solid order is shifted towards higher densities. Above a critical activity and for a certain range of packing fractions, the system undergoes MIPS and demixes into low and high density phases. For dumbbells there is a macroscopic coexistence between regions with hexatic order and regions in the liquid or gas phase over a finite interval of packing fractions. In the passive limit, this interval remains finite, similar to what has been found for the disks, but, differently from them, we didn't find discontinuous behavior upon increasing activity from the passive limit.

* E. Bernard and W. Krauth, *Phys. Rev. Lett*. **107**, 155704 (2011)
† L. F. Cugliandolo, P. Digregorio, G. Gonnella, and A. Suma, *Phys. Rev. Lett*. **119**, 268002 (2017)
‡ P. Digregorio, D. Levis, A. Suma, L. F. Cugliandolo, G. Gonnella, I. Pagonabarraga, *arXiv* (2018)

Nonlocal field theory of dipolar particles in electrolyte solutions: Debye-Hueckel theory extension

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A nonlocal statistical field theory of a dilute electrolyte solution with small additive of dipolar particles will be discussed. We will postulate that with every dipolar particle is associated an arbitrary probability distribution function (PDF) of distance between its charge centers. Using the standard Hubbard-Stratonovich transformation, we will represent the configuration integral of the system in the functional integral form. We will demonstrate that in the limit of a small permanent dipole moment, the functional in integrand exponent takes the well known form of the Poisson-Boltzmann-Langevin (PBL) functional. In the mean-field approximation we will obtain a non-linear integro-differential equation with respect to the mean-field electrostatic potential, generalizing the PBL equation for the point-like dipoles obtained first by Abrashkin et al. We will apply the obtained equation in its linearized form to derivation of the expressions for the mean-field electrostatic potential of the point-like test ion and its solvation free energy in salt-free solution, as well as in solution with salt ions. We will get a general relation for the bulk electrostatic free energy of the solution in the framework of the Random phase approximation.

Basic operators method extension for some 3D stationary astrophysical problems

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Support operator method (Samarskii's method, operator-difference method) has proven itself well in 2D numerical simulations of astrophysical problems. The idea of operator approach consists of inclusion of boundary conditions in finite difference form into the grid analogue of solving problem and formulation of the finite difference problem as operator equation. The finite difference operators are constructed in the way to fulfill corresponding relations between continuous operators (for instance, div(rot)=0, div is conjugated to -grad; div(grad) is self-conjugated etc.). The approach allows obtaining completely conservative finite difference schemes. The matrix which corresponds to the self-conjugated operator is symmetrical and can be inversed efficiently by modern iteration methods. We extended this method for three dimensional case. 3D grid analogues for continuous differential operators using a cell-node approximation were obtained. A test problem for calculation of spatial Newtonian gravitational potential was solved. The stationary heat transfer equation in spherical layer with Dirichlet boundary condition on the inner surface and third type boundary condition on the outer one was calculated. Some model results for anisotropic nonlinear heat transfer equation in neutron star outer crusts are shown.

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Similarity Theory and Linear Approximations of Turbulent Moments within the Convective Surface Layer of the Atmosphere

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Abstract:

Two limiting cases are provided by the Monin-Obukhov similarity theory for the convective surface layer of the atmosphere. The first one, so called a dynamic limit of the convective surface layer, defines a flow with zero buoyancy flux at the underlying surface and a logarithmic profile of wind within the layer. The second one, which is free-convection limit of the surface layer, defines a flow with positive buoyancy flux at the underlying surface and zero velocity of the wind.

The higher order turbulent moments can be defined by the generalize Monin-Obukhov theory for these limiting cases.

The paper is based on the assumption that a convective surface layer is divided into two sublayers: a dynamic sublayer, which is adjacent to the underlying surface, and a forced convective sublayer located higher. The turbulent moments of these sublayers can be defined independently.

This allows proposing linear approximations for the turbulent moments of the vertical velocity and the potential temperature variance within a forced convection sublayer. The free-convection limit of the Monin-Obukhov theory under no wind conditions is described by the first-order expansion terms of these approximations. The second-order expansion terms correspond to the profiles of the turbulent moments under conditions with low wind. The comparison between the proposed approximations and field data shows the correctness of the linear approximation within the forced convection sublayer.

NEW TYPE OF CENTRIFUGAL INSTABILITY IN A THIN ROTATING SPHERICAL LAYER

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Abstract: Flows of a viscous incompressible fluid in a spherical layer that are due to rotational oscillations of its inner boundary with respect to the state of rest are numerically studied. With oscillations amplitude increasing the flow becomes unstable and in addition to circulation in meridional plane of the flow toroidal structures appears near the equator plane. It is found that three kinds of instability are observed, and each kind is associated with its own range of oscillation frequencies. For large and small frequency values well known Gortler vortices in the first case and Taylor vortices in the second are observed. In both cases rotation direction in the vortices near equator plane is opposite to the direction of rotation in adjacent meridional circulation, and there is only one extreme~~s~~ of vorticity in each, upper and lower, half of meridional plane. At intermediate frequencies new spatial structures were revealed, with characteristic scale which does not exceed half of the spherical layer thickness. Direction of rotation in these structures coincides with the same for adjacent meridional circulation, and number of vorticity extremes alternates during the cycle of oscillation.

This work was supported by Russian foundation for basic research, projects nos. 16-05-00004 and 18-08-00074.

Keywords: Torsional oscillations, flow instability, Direct numerical simulation, spherical Couette flow.

Numerical simulation of the motion of a free rising air bubble

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Today the process of bubble's rising is not well described in terms of a quantitative analysis. This is not only a wealth of physical content of the problem, but also the characteristic sizes of the problem requires the using of very large computational resources. From the viewpoint of the experiment the investigation of this process requires the using of the modem, high-precision detecting devices and subsequent computer processing of the results.

There are works in which analytical models of rising bubble are proposed [1, 2]. Also, a large number of studies consider the numerical simulation of rising bubble. The most effective method for the numerical solution of this problem is the front-tracking method [5]. This method allows you to accurately describe the gas-liquid boundary and obtain an exact solution on limited computing resources.

We carried out a 3d numerical simulation of single bubble rising in the water with different diameters (1-10 mm). The regular grids with fixed nodes were used in the calculations. The free surface between the phases was determined by the CLSVOF (Coupled Level-Set VOF) method. This method is the most accurate for calculating two-phase flows on fixed grids. To account for the surface tension forces, the Continuum Surface Force Model was used. The dependence of the parameters of the trajectory on the diameter of the bubble is shown. Trajectories have a zigzag or spiral character.

The period and amplitude of the trajectories for all simulated bubble's sizes and the average speed of rising are calculated. These values are consistent with known experimental data [3,4] and with the results of numerical simulation. The problem of processing large output data was solved, by creating the original software tool with a graphical interface. This allowed to significantly reduce the time for data processing.

Bibliography

1. Magnaudet G., Magnaudet J. Path instability of a rising bubble // Physical Review Letters. - 2002. 88, №1. -P. 014502-014504.
2. Shew W.L., Pinton J.F. Dynamical Model of Bubble Path Instability // Physical Review Letters. - 2006. 97, №1. - P. 1-4.
3. R.C. Clift, J.R. Grace and M.E. Weber, Bubbles, Drops, and Particles, Academic, New York, 1978.
4. A. Tomiyama, G.P. Celata, S. Hosokawa and S. Yoshida, Terminal velocity of single bubbles in surface tension force dominant regime // Int. J. Multiphase Flow, Vol. 28. 2002. P. 1497-1519.
5. Jinsong Hua, Ping Lin, and Jan F Stene, Numerical simulation of gas bubbles rising in viscous liquids at high Reynolds number// Contemporary Mathematics, Vol. 466.2008. 190.

WAVE NUMBER SELECTION UNDER ACTION OF ACCELERATED ROTATION

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Abstract: Spherical Couette flow - flow of viscous incompressible fluid between rotating spherical boundaries is studying in wide gap with radii ratio 0.5. In this gap the first instability with outer sphere at rest results in appearance of traveling azimuthal waves with wave numbers m=3 or m=4. Selection of one from two possible m was studied numerically. While the outer sphere was held stationary, the inner sphere rotational speed was increased linearly from a subcritical flow to a supercritical one. A change in the dominant m was found to depend both on initial Reynolds number and the acceleration value. The decrease of the first as well as the increase of the second results in the same sequence of m changes: 4 → 3 → 4. It was shown that in the process of acceleration the meridional circulation and azimuthal velocity maxima are displaced from the pole toward the equatorial plane, and that meridional component of kinetic energy reaches its stationary value more rapidly than the azimuthal one.

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Keywords: wave number selection, instability, direct numerical simulation, spherical Couette flow

Title：Discrete scale invariance and Log-B periodic quantum oscillation in topological semimetals

Abstract：The quasi-particle in Dirac materials obeys the relativistic equation, and the value of fine structure constant in Dirac materials is much larger than that in the vacuum. Owing to the large value of fine structure constant, the Coulomb attraction gives rise to supercritical atomic collapse in analogy to the phenomena proposed to exist in super-heavy atoms. Moreover, the massless Dirac equation with Coulomb attraction also preserve the scale invariance, which in combination with the quantization effect, gives rise to a novel feature—the discrete scale invariance. Up to now, the discrete scale invariant quantum systems only exist in the Efimov trimers that has generated immediate interest throughout the related fields.

In this talk, I will discuss that the two-body Weyl Hamiltonian with supercritical Coulomb attraction can give rise to Efimovian quasi-bound states with discrete scale invariance. Moreover, the magnetic field introduces a new length scale. The resonant scattering between the mobile carrier and the Efimovian bound states around the Fermi energy gives rise to a novel type of log-B periodic magneto-resistance oscillations in Dirac materials, beyond the Landau level scenario.

Development of a System Generator for Marsohod Development Boards

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When working with development boards based on FPGA and system-on-chip design, it is necessary to set up the project within the framework of the tasks assigned. The automation of this task contributes not only to reduction in time for commencement of work on a project, but also to decrease in the number of potential problems and mistakes by eliminating the need to go into peculiarities of working and specifics of realization of development boards.

Many manufacturers create their own tools for making custom preconfigured projects for their boards. For example, Terasic Company with each of their development boards provides special programs (system generators) on its website. They make it possible to choose which modules should be integrated into the project. Each board requires its own generator which has to meet the requirements of software portability and be supported by different operating systems. In addition, existing system generators are limited by the existing periphery and functionality of development boards only; they cannot integrate additional modules or common add-ins into the project.

Many boards of less advanced manufacturers (such as Marsohod family, manufactured by the Russian company “Inpro Plus”), do not have system generators at all. This work is aimed at decreasing the entry threshold and reducing the time required to create projects using Marsohod boards by automation of initial configuration process, which will also make it easier to study FPGA design. The developed solution is suitable for executing projects which do not require a specific configuration and allows obtaining configuration files and preconfigured projects for development boards of Marsohod family.

Another feature of developing systems-on-chip, based on FPGA, is a lack of online development tools, such as, for example, 3D design tools provided by Autodesk. The best that exists can be referred to online compilation and modeling tools for HDL having rather limited functionality. So, developers are severely lacking some convenient tools and capabilities provided by desktop CADs, for example, “Altera Megafunctions” for adding IP functions, or “Platform Designer” for NIOS II soft-processor core configuration.

The developed system is implemented as an online service, which is one of its major advantages, since it allows uniting all system generators for different boards by a single interface. As a result, generation of configuration files becomes as easy as possible due to no need to install the application. The developed software solution has the feature to add additional modules, such as UART, on-chip RAM, etc.; moreover, it has also been added an online configurator for a simple processor core schoolMIPS, as well as the tools for generating a network-on-chip with various topologies on its base. The kernel of the system was created with Python 3 using the Flask web-framework and the Jinja2 template engine.

The configuration files were tested in CAD Quartus Prime 15+. This ensures that the created projects will be supported by various modern CAD versions for the development of projects on Marsohod boards based on CPLD / FPGA. The developed solution has a convenient and intuitive user interface, and the main work on configuration takes place on the server side. The server part is covered with functional tests, and the user interface was tested in browsers based on Chromium 50+ and in Internet Explorer 11, which guarantees support of the developed application by most modern browsers.

Quasi-Stable Solutions of the Genetic Networks Models

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The simplest genetic oscillator, known as a repressilator, consists of three elements each unidirectionally inhibiting its neighbor. More specifically, the first of them inhibits the synthesis of the second, the second inhibits the synthesis of the third, and the third, which closes the cycle, inhibits the synthesis of the first one.

The interaction of the protein concentrations and of mRNA (message RNA) concentration is surprisingly similar to the interaction of six ecological populations – three predators and three preys. This new mathematical model is represented by a system of unidirectionally coupled ordinary differential equations. The existence and stability of special periodic motions (traveling waves) for this system is studied. It is shown that, with a suitable choice of parameters and an increasing number m of equations in the system, the number of coexisting traveling waves increases indefinitely, but all of them (except for a single stable periodic solution for odd m) are quasi-stable. The quasi-stability of a cycle means that some of its multipliers are asymptotically close to the unit, while the other multipliers (except for a simple unit one) are less than unity in absolute value.

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DEVELOPMENT OF SOFTWARE MODULE FOR THE ANALYSIS OF ELECTRICAL CIRCUITS

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Abstract. Applicants often do not choose technical education because of the difficulty of this sphere or the lack of engineering knowledge and real engineering practices that so important. This issue opens up a new development space for educational software for the beginners and non-professional users. Such problem as difficulty of choosing and obtaining an engineering education is considered. This paper presents an investigation of the electrical circuits and development of a program module for the schemes analysis that could be easily embedded in educational establishments. Existing technics for analyzing electrical schemes were observed and the most effective one was chosen. The main goal was attained using the WPF technology of .NET Framework. Altogether, the research provides a simple instrument for circuit analysis that gives some helpful information about electricity and the circuitry. It automates verification of practical tasks and exercises made by students and allows to refuse the use of complex electrical stands. Furthermore, the developed application can be integrated into the educational system as a tool for teaching staff and development of popularity for technical specializations.

SIMULATION OF DELAY REACTION-DRIFT-DIFFUSION SYSTEM APPLIED TO CHARGING EFFECTS IN ELECTRON-IRRADIATED DIELECTRICS

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Abstract. The paper presents the results of mathematical modeling of reaction-convection-diffusion type system with time delay and its application to numerical simulation of charging process in dielectrics irradiated by electron bunches with average energies.
The mathematical model was expressed in the form of mixed initial-boundary value problem for generalized reaction-convection-diffusion equation in several space dimensions with permanent time delay. An advanced finite difference scheme was suggested to numerically solve the delay parabolic PDE. The modification of computational splitting scheme was based on alternating direction method of Peacman-Rachford for approximation of "diffusion" part of PDE as well as Roberts-Weiss scheme was used for approximation of "convection" part of PDE. In order to approximate the "reaction" part of PDE the "frozen coefficient" method was also applied. The procedure of approximation analysis resulted in second order accuracy for space as well as time variables. The stability analysis by means of maximum principle allowed us to specify the absolute stability of the scheme. The constructed numerical scheme was modified taking into account delay effect. The main peculiarity of delay system numerical simulation is necessity of memory-stored control for delay "window" structure (values of decision variable on each time layer including to delay period). This aspect leads to resource-intensive computational process.
The proposed algorithm was included into the general hybrid computational scheme to simulate dynamic charging process in dielectrics irradiated by electron beam. This effect can be observed at diagnostics and modification of such materials with use of scanning electron microscope techniques. The mathematical model of dielectric charging involves locally instantaneous Poisson equation and time-dependent transport equation. The latter is reaction-drift-diffusion equation in several space dimensions with time delay. Monte-Carlo simulation of electron transport in electron irradiated target was also used to estimate a source function. The special program application developed with Matlab package was designed to simulate dynamic electron beam-stimulated charging processes in dielectrics. Three modes of charging process were implemented in the program: the stationary mode, the dynamic mode of charge relaxation and the dynamic mode of charge accumulation. The relation of deposits of "drift" (convection) and "diffusion" parts in the model for dynamic modes was also discussed using analysis of value of Peclet number. The computing experiments by the example of ferroelectric crystal were performed to estimate the charge density distribution, potential distribution as well as field intensity electron beam-induced.

Keywords: reaction-convection-diffusion equation, delay parabolic PDE (partial differential equation), splitting method, electron beam irradiation, charging of dielectrics, mathematical model of charging process, simulation of charging characteristics

Gapless Spin-Liquid Ground State in the S=1/2 Kagome Antiferromagnet

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The defining problem in frustrated quantum magnetism, the ground state of the nearest-neighbor spin 1/2 antiferromagnetic Heisenberg model on the kagome lattice, has defied all theoretical and numerical methods employed to date. We apply the formalism of tensor-network states, specifically the method of projected entangled simplex states, which combines infinite system size with a correct accounting for multipartite entanglement. By studying the ground-state energy, the finite magnetic order appearing at finite tensor bond dimensions, and the effects of a next-nearest-neighbor coupling, we demonstrate that the ground state is a gapless spin liquid. We discuss the comparison with other numerical studies and the physical interpretation of this result.

1. H. J. Liao, Z. Y. Xie, J. Chen, Z. Y. Liu, H. D. Xie, R. Z. Huang, B. Normand, and T. Xiang, PRL 118, 137202 (2017)
2. Z.-Y. Xie, J. Chen, J.-F. Yu, X. Kong, B. Normand, and T. Xiang, Phys. Rev. X 4, 011025 (2014).

Quantitative thermometry of the 2D Hubbard model in optical lattices on approach to the Neel transition

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We study the two-dimensional Hubbard model at half filling using the systematic-error-free Determinant Diagrammatic Monte Carlo method. We simulate mesoscopic sized samples with varying shapes and boundary conditions, and calculate the temperature dependence of the spin-spin correlation function. Our results can form a basis of quantitative determination of temperature in recent and ongoing experimental realizations of the Hubbard model with ultracold atoms in optical lattices.

Dynamics of qubits in the field of unipolar impulses: Magnus propagator, generalized “area theorem" and motion on groups

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As is well known, that the number of sequential operations over the register of superconducting qubits is essentially limited by the decoherence time in (~ 100 μs). One of the ways to overcome this limitation can be the implementation of "rapid quantum logic" for controlling qubits, which will allow manipulating quantum states with characteristic times of ~ 10 ps [1].

We discuss here the problem of accelerating quantum computations by controlling the qubit states with short unipolar pulses with a large amplitude - fluxons. A new method for describing the qubit dynamics based on the Magnus representation for the evolution operator (propagator) of qubits is proposed. For the transitions amplitude between stationary states at the time intervals that are shorter than the decoherence time, we will solve the time Schrodinger equation for calculating the evolution operator $U(t)$ - the propagator of the system, - which determines its wave function at any time: $\psi(t) = U(t)\psi(0)$, where $\psi(0)$ is the initial state. The usual perturbation theory is not applicable for our purposes, since it is necessary to consider signals of large amplitude for obtaining appreciable changes in the level population. To calculate the propagator $U(t)$ of an n-qubit system, we use two ideas: i) The Magnus expansion [2] for the propagator in the form of an exponential from some operator $M(t)$ (the "Magnus" operator): $U(t) = \exp(-iM(t))$, for which there is a simple computational algorithm in the form of a series in powers of the Hamiltonian with any required accuracy; ii) If in some basis the Hamiltonian for n-qubits is represented by a matrix size $N \times N$, where $N = 2n$, then the оператор $M(t)$ will also have dimension $N \times N$. Consequently, by applying the well-known Cayley-Hamilton theorem, the propagator in this case can be written in the form of an expansion in powers of the matrix, and the maximum degree of the resulting polynomial is not higher $N-1$: $U(t) = u_0 I + u_1 M(t) + u_2 M^2(t) + \cdots + u_{N-1} M^{N-1}(t)$. The coefficients of the expansion u_j for all $j = 0,1,\cdots N-1$ could be explicitly expressed in terms of the eigenvalues of the matrix $M(t)$. Note that from the point of view of group theory, we are talking about the decomposition of the group exponent over the matrices of the group. The evolution of the state of the system can be represented as a motion of the qubits polarization on such a group, similar to the rotation of the Bloch vector on the SU(2) group in the case of one qubit. As an example, we will demonstrate the effectiveness of the obtained expression for describing the dynamics of one qubit under various excitation methods by unipolar pulses. From theory of two-level system we know that in the periodically modulated pulse the Rabi oscillations occur as a function of the total interaction area of the pulse. This statement is called the “area theorem”. An analog of the generalized "area theorem" is found in the case of unipolar impulses, which in a certain sense acts like the area theorem in the case of Rabi excitation.

The resulting expression for the propagator is then used to describe the influence of the pulses on a two-qubit system. First, a symmetrical configuration is considered when the qubit parameters are not different and they have the same field on the fluxon side. In this case, the matrix $M(t)$ has dimension 3×3 and belongs to the group SU(3). A three-level system of a more general type is also discussed here, which arises, for example, in the case when it is possible for one qubit to move to the higher layer under the influence of a fluxon. Analytical consideration is carried out for two qubits - a four-level system (the SU(4) group), - although the developed algorithm is applicable to any number of qubits (with allowance for computational constraints). To control the Magnus approximation, we use direct numerical simulation of the dynamics of a multi-qubit system, and as a criterion for the proximity of operations - the "degree of inconsistency" (fidelity) is used.

[1] N.V.Klenov *et al*., Beilsten J. **6**, p. 1946 (2015); N.V. Klenov *et al*., Low Temp. Phys. **43**, 789 (2017).
[2] W. Magnus, Commun. on pure and Appl. Math., 7, P. 649 (1954); P. Pechukas, J. L. Light, Journ. of Chem. Phys. **44**, 3897 (1966).

Confined and Deconfined Fractional Spin Excitations in two-dimensional Mott Insulators: A Spectral Perspective

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In this talk, I will present our recent work on spectral properties of the antiferromagnetic J1-J2 Heisenberg model, based on the extension of the electronic cluster perturbation theory to spin systems by using the mapping between spin-1/2 operators and hard-core bosons [1]. We find that deconfined spin-1/2 spinons beyond the conventional spin-1 magnons have already emerged partially even in the limit J2=0 and develop with J2, exhibiting as a continuum close to (π,0) in the Brillouin zone. In the region near J2=0.5J1, the entire spectrum is characterized by a broad continuum in which all magnons are deconfined into spinons, whose ground state is attributed to a Z2 quantum spin liquid with a help of the variational-Monte-Carlo analysis. The spinon continua are also found in the stripe phase with J2>0.6J1. In addition, I will also show the coexistence of fractional spin excitations and magnons in the spectra of the Kitaev-Γ (off-diagonal) model, which is suggested to describe the spin-orbital Mott insulator α -$RuCl_3$ [2,3].

Reference:

[1] S.L. Yu, W. Wang, Z.Y. Dong, Z.J. Yao, and J.X. Li, arXiv: 1805.07915
[2] W. Wang, Z.Y. Dong, S.L. Yu, and J.X. Li, Phys. Rev. B **96**, 115103 (2017)
[3] K.J. Ran, J.H. Wang, W. Wang, Z.Y. Dong, X. Ren, S. Bao, S.C. Li, Z. Ma, Y. Gan, Y.T. Zhang, J.T. Park, G.C. Deng, S. Danilkin, S.L. Yu, J.X. Li, and J.S. Wen Phys. Rev. Lett. **118**, 107203 (2017)

Entanglement Hamiltonian of interacting fermionic models

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Recent numerical advances in the field of strongly correlated electron systems allow the calculation of the entanglement spectrum and entropies for interacting fermionic systems. An explicit determination of the Entanglement (modular) Hamiltonian has proven to be a considerably more difficult problem, and only few results are available. We introduce a technique to directly determine the entanglement Hamiltonian of interacting fermionic models by means of auxiliary field Quantum Monte Carlo simulations. We implement our method for the one-dimensional Hubbard chain partitioned into two segments, and for the Hubbard ladder, partitioned into two chains. In both cases we study the evolution of the entanglement Hamiltonian as a function of the physical temperature.

Ref: F. Parisen Toldin, F. F. Assaad, "Entanglement Hamiltonian of interacting fermionic models", arXiv:1804.03163

How to make network communications secure in post-quantum era

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***Abstract*—We propose a new type of post-quantum system based on repetition of different error-correcting codes. The scheme can work as a public-key cryptosystem (PKC) and as digital signature at the same time. All previously known code-based PKC can work only in one of these two modes. We also investigate how this new scheme can be used for so-called light-weight cryptography what is an inherent property of communication networks in post-quantum era.**

***Index Terms*—communication network, public-key cryptosystem, digital signature, repetition of codes**

INTRODUCTION

First public-key cryptosystem (PKC) based on error-correcting codes was proposed by McEliece in [1] forty years ago, and later a dual PKC (in some sense) was suggested in [2], which is based on syndrom decoding of linear codes. After that many different families of error-correcting codes were investigated as a candidate to replace Goppa codes used in [1]. In this paper we propose a new PKC based on repetition of different error-correcting codes what is a generalization of the construction of [3]. We analyze resistance of the new PKC to attacks of [4], [5] as well as to decoding attacks. We also show how the new PKC can be used for digital signature purpose. Importance of our scheme as well as other code-based schemes is that there are no known attacks on these scheme based on a quantum computer similar to the famous Shor attack on RSA scheme [6].

CONSTRUCTION

Let us recall some basic facts about code-based cryptography .

A user A chooses a generator $k \times n$ matrix G_A of some linear (n, k)-code C_A, which has decoding algorithm Φ correcting t errors with polynomial in n complexity. The user A takes randomly two matrices: $k \times k$ nonsingular matrix S_A and $n \times n$ permutation matrix P_A and then construct *public*,i.e., known to all other users, matrix $G_{pub} = S_A G_A P_A$. Any other user (say B) to deliver a message m of length k bits to the user A sends to A via a channel vector $y = mG_{pub} + e$ of length n, where e is a vector of weight t which is *randomly* generated by B. The user A after receiving vector y calculates

$$y' = yP_A^{-1} = mG_{pub}P_A^{-1} + eP_A^{-1} = (mS)G_A + e',$$

where $e' = eP_A^{-1}$ and $wt(e') = wt(e) \leq t$ since P is a permutation.Then A applies the decoding algorithm Ψ of the (n, k)-code C_A to vector $y' = m'G + e'$, obtains the vector $m' = mS$ and finally A receives $m := m'S^{-1}$. Any other user will deal either with the problem of correcting t errors by some linear code, which looks like a random code, or with the problem to recover the code structure from its public-key matrix.

Our construction works in the following way. Consider for simplicity two linear codes V_1 and V_2 of the same dimension k but different lengths n_1 and n_2. Let G_1 and G_2 be some generator matrices of these codes. Construct $k \times n$ generator matrix $G_{1,2}$ of a new code by concatenation of matrices G_1 and G_2 (hence, $n = n_1 + n_2$).We call this construction *pseudorepetition* and denote this code as $V_1 \bigsqcup V_2$. Surely this construction can be defined for any multiplicity u of pseudorepetition, and in particular, when $V_1 = V_2 = \ldots = V_u = RM(s, m)$, one has the Sidelnikov scheme [3]. Let us note that the main obstacle for previously known structural attacks is a difficulty to find splitting the set of all coordinates on two subsets corresponding to coordinates of codes V_1 and V_2. Another advantage of the new scheme is that one code can be used for correction of many errors (probably by list decoding or by probabilistic decoding) while second code used for detecting if the first code was decoded correctly. We show how it works for pseudorepetition of RM-codes and Goppa codes.

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REFERENCES

[1] R.J. McEliece, " A public-key cryptosystem based on algebaric coding theory," In *Jet Propulsion Lab* pp.114–116, 1978.
[2] H. Niederreiter. Knapsack-type cryptosystems and algebraic coding theory. Problems of Control and Information Theory, v. 15, pp. 159-166, 1986.
[3] V.M. Sidelnikov, "Public-key cryptosystem based on binary Reed-Muller codes," Discrete Mathematics, vol. 6 (2), pp. 3–20,1994.
[4] Minder L. and Shokrollahi A. Cryptanalysis of the Sidelnikov cryptosystem. In *LNCS v. 4515*,pp. 347-360, 2007.
[5] M. A. Borodin, I. V. Chizhov, Effective attack on the McEliece cryptosystem based on ReedMuller codes, Discrete Math. Appl., vol. 4, no 3, pp. 191207, 2014.
[6] Peter W. Shor, "Polynominal time algorithms for discrete logarithms and factoring on a quantum computer," SIAM Journal on Computing, vol. 26, 5, pp. 1484–1509, Oct. 1997.

Multiuser wireless channel simulation for communication systems with nonparametric reception[*]

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In digital communications it is typical to use reception techniques based on parametric hypothesis tests such as Neyman-Person test. This approach implies that the distributions of the decision statistics are known at the receiver side and the parameters of the corresponding distributions are known or at least can be estimated accurately. However in many scenarios of practical interest those assumptions do not hold. In such cases nonparametric reception techniques that combine distribution-free statistical tests and error-correcting codes are of great interest. In particular those reception techniques are very promising for Internet of Things (IOT) and Mashine –to-Mashine (M2M) communications. Unfortunately analytical investigation of communication systems that use nonparametric reception techniques is cumbersome since very little is known on the subject so far. Thus simulation remains the main tool for investigation and validation of the solutions proposed for the systems under discussion.

Unfortunately for the case that is of most practical interest i.e. the multiuser communication scenarios the computational burden introduced by channel simulation can be very high. This paper is aimed at developing realistic model of single-user transmission via a multi-user channel with low computational complexity. In particular the case when each user uses coded Frequency Hopping OFDMA with nonparametric reception will be considered. Two models are introduced: the equivalent model in frequency domain that allows to avoid computationally expensive simulations of processes in time-domain and the reduced complexity "pessimistic" model in frequency domain. The applicability of those models is discussed and compared by simulation for several recently proposed nonparametric reception techniques. Problems of software implementation of the proposed models are addressed as well.

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Construction of computing balancing model in the Internet of Things devices system

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At this work, we have started to research development and construction of a math model for load balancing in the Internet of Things devices system. Suggested model is useful to perform experiments of modeling the parameters and behavior of the IoT devices system with different scripts of data loading. The main goals of current work are to reduce delays in the performance of tasks, to increase battery life and energy efficiency. The objectives are to describe tasks performed in IoT systems, to summarize definitions of tasks balancing methods, to develop a math model in the IoT devices system and to design various balancing methods for this model.

At first, we perform analysis and classification of tasks for the IoT devices system. Based on this classification, we assume that not each kind of tasks (and associated computations) could be reassigned to another node in system. In the end of this part we describe moveable class of tasks for IoT devices system.

At second part, we compare existing methods of computing balancing for IoT systems. We classify methods by its centralization, scaling and flexibility. Here we introduce our balancing method based on the computation offloading at heterogeneous systems with different levels of performance. This method allows moving computation to any performance level node. Similar methods already have described in the works of other authors [1][2], but they are concentrated on transfer tasks to higher performance level (e.g. cloud center).

In the end, we develop the mathematical model of the Internet of Things devices system. It is particularly based on the model proposed in work by Elizarov M. [3]. Model extended for balancing processes and node health check.

In advance, results of this work will be used for modeling and comparative analysis of balancing methods. Further, we will compare obtained results with other results, based on experiments on the virtual and physical system of devices to determine the quality of the constructed model.

References

[1] H. Flores, S. Xiang, V. Kostakos, A. Yi Ding, P. Nurmi, S. Tarkoma, P. Hui and Y. Li, "2017 IEEE International Conference on Pervasive Computing and Communications Workshops (PerCom Workshops)," in *Large-scale offloading in the Internet of Things*, Kona, HI, USA, 2017.

[2] F. Samie, V. Tsoutsouras, L. Bauer, S. Xydis, D. Soudris and J. Henkel, "2016 IEEE 3rd World Forum on Internet of Things (WF-IoT)," Reston, VA, USA, 2016.

[3] M. Elizarov, "MODELS AND ALGORITHMS OF INFORMATION INTERACTION IN THE INTERNET OF THINGS NETWORKS," Saint-Petersburg, 2017.

Overview of Educational Kit and Development of the Kit for Learning the IoT.

Abstract. The primary purpose of this paper is to overview of Education Solutions for IoT and develop of proposals for the improvement of IoT educational kits. The study draws analysis of current conditions of educational IoT sphere, a comparative analysis of educational products used for teaching of schoolchildren in the sphere of modern technologies in Russia. With that the article describes the architecture of the software and hardware platform (a learning kit) for learning IOT, and shows the developed PCB for the hardware part of the kit. Moreover, this thesis reviews methods and technical instruments employed to design software and hardware appliance.

Keywords: IoT, Educational, Electronic kit, Learning IOT.

Clustering network packets using the CLOPE algorithm

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For the modern variety of software that uses network communication protocols, the problem of ensuring reliability of work is acute. To solve such an important problem, random testing is used. This type of testing involves the generation of a large number of test data, including sets of network packets. The task of reducing the number of data stored after the research is arisen. This task can be solved by clustering the set of received packets.

To solve this problem, it is proposed to use the clustering algorithm for categorical data of CLOPE. This algorithm allows to cluster datasets without having information about source clusters, has relatively low computational complexity and ease of implementation.

The article describes the preparation and results of sets of network packets processing experiments. An approach is proposed for selecting the metaparameter of the CLOPE algorithm - the repulsion factor, which determines the resulting clustering results.

The study showed that the CLOPE algorithm can be effectively used for clustering network packets received during selective testing. The results of the research extend the toolkit for analyzing the results obtained with random testing of software.

Simplification of tensor expressions in computer algebra

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Abstract

Computer algebra are widely used in various fields of mathematics, physics and other sciences.
One of the important cases is the simplification of tensor expressions.

The work considers the reduction of tensor polynomials to the canonical form taking into account symmetry properties of permutations of indices, the symmetries associated with the renaming of the summation indices, and also the linear relations between tensors of a general form.

We give a definition of the canonical representation for polynomial (multiplicative) expressions of variables with abstract indices, which is the result of averaging the original expression by the action of some finite group (the signature stabilizer).

In practical cases, for expressions from the Riemann curvature tensors, the proposed algorithms demonstrate high efficiency.

Keywords: tensor, abstract indexed object, computer algebra, permutation group, canonical form, symmetry, multiterm linear identity

Dynamics of a Single Polymer: A Lowe-Andersen Approach

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Abstract: We investigate the dynamics of a polymer chain in a good solvent. The solvent is modeled in a mesoscopic manner, and we employ the Lowe-Andersen approach of dissipative particle dynamics to capture the role of hydrodynamics. In this regard, we compare our results for self-diffusion of the chain with available theories.

Configuration of vortex-antivortex lattices at output mirror of wide-area microchip laser.

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Pattern formation outside the equilibrium is a long-term research trend [1, 2]. The vortex lattices in high Fresnel number solid-state microchip lasers that appear a wide range of experimental parameters [3] were predicted theoretically in [4]. The subsequent numerical investigations [5] have shown the deep similarity of optical vortex lattices in lasers with spatial patterns that spontaneously occur in Faraday instability [6]. The phase of optical field is a precise indicator of electromagnetic energy circulation [7]. Exactly as in the early models of type-II superconductors placed in external magnetic field [8] the macrosopic photons wavefunction Ψ, which is visualized by electric field amplitude E, demostrates the regular lattices of field zeros with counter-rotating whirls around them [9]. The computational model for Ψ comprizes convolution integral with nonlinear kernel evaluated via Fast-Fourier transform [10] and the relaxation oscillator for gain medium coupled with wavefunction Ψ. The regular square lattices appear in a well defined region of laser gain and Fresnel numbers (fig.1). The inherent feature of these nonstationary patterns are vibrations of observed lattices which are known as optical and acoustical modes (fig.2) [3,4].

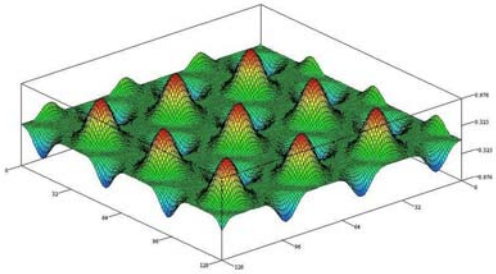

fig.1.

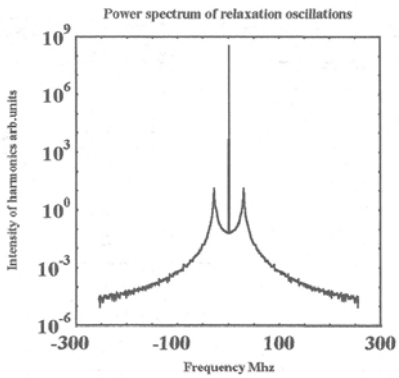

fig.2

References.

[1] M.C.Cross and P. C. Hohenberg, Rev. Mod. Phys. v. 65, 851 (1993).

[2] A.Yu.Okulov, J. Opt. Soc. Am. B, v. 3, 741 (1986).

[3] Y.F.Chen, Y.P.Lan, Phys.Rev.A, v. 64, 063807 (2001).

[4] K.Staliunas, C.O.Weiss, J. Opt. Soc. Am. B, v. 12, 1142 (1995).

[5] A.Yu.Okulov, J.Mod.Opt., v. 55, 241-259 (2008).

[6] N. Francois, H. Xia, H. Punzmann, S. Ramsden, and M. Shats, Phys/ Rev. X,v. 4, 021021 (2014) .

[7] A.Yu.Okulov, Laser Physics, v. 19, 1796-1803(2009).

[8] A.A.Abrikosov JETP, v. 5, 1174 (1957).

[9] A.Yu.Okulov, QCMC-2004, AIP Conference Proceedings, v. 734, p.366 (2004).

[10] A.Yu.Okulov, Opt.Comm., v. 99, 350-354 (1993).

Elastic strain engineering meets active learning: the case of semiconductors

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Elastic strain engineering opens new opportunities for the optimization of magnetic, electrical, and optical characteristics of nanostructured materials: fundamentally, the electronic structure of a crystal changes with the elastic strain. To map out the whole room available for the strain engineering of silicon, germanium, diamond (carbon) and other materials, an understanding of the band topology changes in the six-dimensional strain space is imperative, and exhaustively exploring the band structure by the traditional theory is rather formidable. Surrogate models based on machine learning modules can efficiently represent the dependence of the most technologically relevant electronic properties of silicon on the strain. In our work, we demonstrate that these models, relying on a limited amount of data from first-principles calculations, may reproduce the required properties with sufficient accuracy. The data amount needed for the training may be further reduced using the active learning techniques, leading to the rapid development of surrogate models for material engineering.

Application of machine-learning potentials to high-entropy alloys investigation

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High-entropy alloys represent a class of refractory materials, which have a rare combination of ductility and strength. Their ability to form a stable single-phase solid solution gives them extraordinary physical properties, gives them the ability to compete with nickel superalloys.

In order to design a new HEA, it is necessary to know phase transitions temperatures. Experimental investigations of HEA are very time-consuming: it may take a few weeks even to prepare a sample. Hence, computational investigation of HEA is of a great interest.

In this work, a new computational method of order-disorder phase transition investigation is presented. The new approach is based on the application of the machine-learning potentials as the interatomic interaction model in canonical Monte Carlo algorithm. This new method turned out being competitive with other data-driven methods.

The interatomic potentials training for the NbMoTaW system is described in this work. The results of the phase transition investigation for NbMoTaW alloy turned out being close to previous theoretical works. A new ground-state structure of the equiatomic NbMoTaW alloy system was found and described. The new method is better than the ones that were used before in accuracy and efficiency.

ESTIMATION OF LYAPUNOV EXPONENTS FOR QUASI-STABLE ATTRACTORS OF DYNAMICAL SYSTEMS WITH TIME DELAY

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Keywords: delay differential equation, Lyapunov exponents, numerical analysis, Hutchinson equation, quasi-stability

Lyapunov exponents play an important role among the invariant characteristics of dynamical systems. Analysis of the spectrum of Lyapunov exponents are widely used to study the complex dynamics in systems of ordinary differential equations and models that can be reduced to the maps. As follows from the Oseledets theorem in the finite-dimensional case the linearized on attractor system of the ordinary differential equations is always Lyapunov proper and thus the upper limit may be replaced by a normal limit, that allowing to effectively compute Lyapunov exponents. In this paper we consider the question of numerical evaluation of Lyapunov exponents for delay differential equations. The Oseledets theorem not proved in this case. We used a new algorithms with FFT, tested it on Hutchinson equation with known Lyapunov spectra and compared with results of old algorithms. The so-called quasi-stable behavior is typical for a number of gene networks models and neuronal associations that have been studied recently. The phenomenon of cycle (k-dimensional torus) quasistability in dynamical system is characterized by the fact that some of its multipliers are asymptotically close to the unit circle, and the remaining multipliers are modulo less than one (with the exception of a simple unit (k units)). In some cases, it is possible to prove the existence and give an asymptotic estimate of the studying system multipliers by using the large parameter method. However, if the large parameter methods are not applicable, it is necessary to obtain a tool for the numerical estimation of multipliers. Such a tool is provided by algorithms for Lyapunov exponents estimation. Given that the equations with delay are often applied in the models of neural and gene networks, the algorithm for Lyapunov exponents estimation for such systems will be in demand.

Singularity of optimal control in the problem of stabilizing a nonlinear inverted spherical pendulum

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Abstract

Models of inverted pendulum systems are widely used to study the dynamics of different real complex nonlinear objects. There are many papers in which computer modeling and simulation are used for controlling and stabilizing the inverted pendulum systems. Analytical results of the present talk can be useful in developing effective algorithms for computer modeling. We study an optimal synthesis in the minimization problem of the mean square deviation of a spherical inverted pendulum from the upper equilibrium position over an infinite time interval. We assume that the pendulum is attached by a hinge to a moving support point which can moves in a horizontal plane under the influence of a bounded control force. For the linearized model we found [1-2] optimal solutions in the form of logarithmic spirals that hit the origin in a finite time T. The corresponding optimal controls perform an infinite number of rotations along the circle S^1. We generalize the results obtained for the linear model to the nonlinear case.

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[1] Manita L., Ronzhina M. Optimal control of a spherical inverted pendulum // Lobachevskii Journal of Mathematics. 2017. Vol. 38, no. 5. P. 954–957.

[2] Ronzhina M.I., Manita L.A. On optimal solutions in a problem with two-dimensional bounded control // Systems Analysis: Modeling and Control. Materials of the International Conference in memory of Academician A.V. Kryazhimskiy, Moscow, May 31 – June 1, 2018. P. 90-93.

Keywords: nonlinear spherical inverted pendulum, stabilization, optimal control, singular solution

Cyclostationary models for simulation of non-stationary random processes

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No one can argue that the vast majority of processes under observation are not completely deterministic. The theory of random processes provides researchers with many basic models for their description and with rather developed techniques for their processing. As a matter of fact, the most popular and easily understood case is still a wide-sense stationary noise superimposed by the sum of sinusoids with deterministic or random parameters which remain constant at least within the observation frame. This process could be expressed in terms of its correlation function or power spectrum density as the Fourier counterpart. While the periodicity contained in the process is evident and could be extracted by a direct subtraction, the reminder of the process demonstrates time-limited statistical interdependency of any pair of its samples.

However, the stationary model would not be the best choice in the case of a process generated by more complex phenomena or changing in time environment. A possible solution here is the use of a set of locally stationary models or one yet slowly changing model as it is claimed by Kalman's and other related filtering methods. The reliable alternative to that solution could well be the global probabilistic model of the random process with the hidden periodicity which would take into account the regular change of statistical properties. Although having started in the 1950s, not so long after N. Weiner gave exhausted description of the stationary case, research into the hidden periodicities of the second order was prolific, the main results that has been obtained over few decades are generally not familiar to the significant majority of modern researchers.

The cyclostationarity, a term originally introduced by W. Bennet to describe digitally modulated pulses, generalizes the concept of the hidden periodicity including but not limited to the prominent case of periodically correlated time series and continuous signals. Not only is the cyclostationarity a natural yet not evident expansion of the stationarity, but any stationary process could be considered as a particular case of cyclosationary (CS). It is possible due to the main advantage of the CS approach which is that the characteristics of the well-known stationary models simply become the essential and additive part of the corresponding characteristics of the CS models.

The simplest yet most important and easy to understand example of wide-sense CS process. As it follows from its name, the first and second order probabilistic characteristics will be enough to express all the properties of the process. In fact, the first order or the mean function are quite the same as for the stationary case. The essential part standing the CS processes out against other types is the behavior of its two-dimensional, or dyadic, correlation function. Actually, the latter could be expanded into a Fourier series with respect to the current time in the case of strict periodicity or into generalized harmonic Fourier series in the more complex almost-periodical case whereby the frequencies are not rationally commensurable.

On the whole, originally introduced in the electrical engineering, cyclostationarity provides researchers with useful models that could be adapted to a process of any nature, i.e., physical, economic, biological, where the hidden periodicity is expected but could not be found explicitly regardless to how long the sample was observed.

On limit laws of multi-dimensional stochastic synchronization models

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Abstract

Lévy processes and related fine analytic properties of probability distributions such as *infinite divisibility or stability* play an important role in construction of stochastic models of various distributed networks (e.g., local clock synchronization, opinion dynamics). At the same time they are also interesting for a variety of physical models, e.g., for systems based of the so-called Lévy random walks (Lévy flights) or for systems formulated in the framework of free (noncommutative or quantum) probability.

Nevertheless, little is known about limit probability laws resulted from the long time behavior of such stochastic systems. In this talk we will focus on classification of limit laws which arise in models with some special network topologies.

Keywords: synchronization models, stochastic particle systems, Laplace transform

Simulation of the super-scalar processor core operation

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Abstract

Modern desktop processors are super-scalar, that is, they are able to perform several operations on several pairs of operands simultaneously. This is achieved by many ways of parallelizing calculations. The main method is the conveyor processing of machine instructions. Each processor contains from one to several cores. Each core contains one to several instruction pipelines. In fact, the pipeline is the heart of the processor. Understanding the mechanism of its work gives an understanding of the principles of computing in modern computers. A huge number of scientific and practical works are devoted to this issue, but a faster and more visual way to study the principle of conveyor processing is the launch and study of the simulation model of the processor core.

In this paper we have built and investigated such a model that allows us to trace the process of executing machine instructions by the processor core pipeline. As a basis for the modeling are taken Intel processor with microarchitecture Nehalem, although the analyzed mechanisms inherent to other modern processors. Modeling system includes the program and methodical recommendations on its use with multiple task options.

The computer model considers as an initial data a fragment of machine code on a simplified Assembler. The fragment consists of twenty instructions. Three main types of machine instructions are considered: data transfer between registers and memory cells (four variations), data processing from registers and memory cells (four variations), conditional jump to the specified address. The simulation program automatically generates a new version of the code fragment at startup or at the user's request. To study the principles of the pipeline, it is additionally proposed to specify the following parameters of the pipeline and the code: the number of store/load devices, the number of ALU (Executive devices), the percentage of memory operations. The modeling kit demonstrates the pipeline architecture consisting of two clusters: front-end and back-end and the principle of translating complex multi-cycle CISC-like instructions into simpler RISC-like micro operations (mops). In addition, it is possible to conduct a more detailed simulation of one of the three mechanisms for calculations accelerating in the processor core: multi-functional processing, out-of-order processing, speculative instructions execution after the branch prediction.

The program includes four Windows of the model, which reflects the input parameters and simulation results. As a result of the simulation program provides the following options:

- to explore the principle of translation of instructions in micro-operation ("MOPs" window),
- to study the employment cycles of the main back-end pipiline cluster when executing the given instructions (the "Pipeline" window»),
- to examine the time diagram of instructions execution from a given code fragment ("Diagram" window).

This modeling kit is useful for studying computer architecture. Understanding the features of the processor is useful for both system developers and programmers. Improving the style of writing programs will speed up their execution by the computer.

References

1. New in the Silvermont architecture of Intel Atom Z3xxx Processors: what awaits us in thin, light and inexpensive tablets for Windows 8 in 2014. The website iXBT.com [http://www.ixbt.com/portopc/atom-clover5.shtml]
2. Sergei Ozerov. Processor architecture. Pipeline, super-scalar and Out-of-Order processors. Computerra. No 37 (609). http://old.computerra.ru/2005/609/233266/
3. Oleg Nechai. Intel Core: some features of the new microarchitecture. http://old.computerra.ru/terralab/system/265305/
4. https://ru.wikipedia.org/wiki/NetBurst
5. https://en.wikipedia.org/wiki/Nehalem_(microarchitecture)

Computer Simulation for Load Balancing in EV Charging Stations Network

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Abstract

Electric vehicles (EV) are promising to become one of the most economically and environmentally viable transportation alternatives. Increasing gas prices, improvement of EV technologies and government policies supporting EV infrastructure development account for the rapid growth of electric transport. In this paper we present an approach to solve the load balancing problem in EV Charging Stations (EVCS) network, which will help network owners make most profit. Our methodology is the recommendation system that analyses EVCS customers' routes and balances the load on stations by motivating customers to charge their EVs at places with lower loads in terms of number of people at particular station. We use city simulation software to get the locations of charging stations and drivers' locations and routes. Based on that, we develop a mathematical model to calculate an optimal charging station for each customer taking into account routes of all customers. Web-based solution is developed to do the calculations and visualize the results. The solution is tested on artificial data from the simulation software to prove the efficiency of the implemented mathematical model and technical solution.

Keywords

Simulation, electric vehicle, charging station, network balancing, Internet of Things

System of Computer Simulation Modelling of Operations, Geometric Characteristics and Methods of Pulsed Optical Tomography of Nuclear Fuel Micro-Objects

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The system of computer simulation and research of fast processes of geometric industrial command setpoint testing control of micro-objects (MO) quality of nuclear fuel (drops of fluid, core samples, core samples with coating, micro fuel rods) is under consideration.

The paper refers to the area of morphological processing of projected images and its goal is to design some computer simulation models of basic operations, methods and characteristics of pulsed optical tomography:

- the approximation (image) model of three-dimensional MO and the spatial geometric characteristics of its size and shape;

- the models of operations for obtaining (generation) of pulsed discrete projected images of MO and operations of determining their number and optimal camera angles;

- the models of procedures for the numerical determination of the optimal basic features on each projected discrete image of the MO;

- the models of procedures (methods) for dynamic reconstruction of spatial geometric characteristics of MO, taking into account the basic feathers of discrete images;

- the models of defining the metrological characteristics of reconstruction methods of MO in terms of performance, accuracy and reliability.

The modeling system is organized as a hardware and software complex, built on the principle of multifunctionality, modularity, unification and openness. It consists of five subsystems: obtaining reference data; obtaining experimental data; methods of geometric control; research programs; control. The system uses C++, OpenGL and MATLAB languages.

On the base of the proposed computer models, a high-speed precision laser method of geometric contactless differential opto-electronic industrial and quality control of real-time MO flow of nuclear fuel was developed and experimentally tested. The method is based on the dynamical, few view, spatial-temporal, statistical reconstruction of size and shape of each MO and take into account the maximum and minimum overall dimensions of outlines of three mutually orthogonal two-dimensional pulsed discrete projected images of the MO.

While describing the size of each MO, the spatial geometric characteristics of MO are its overall dimensions and the average projected diameter (D) of its approximating ellipsoid of general form. Moreover, when describing the MO shape, its spatial geometric characteristic is represented as a non-sphericity coefficient (K) defined as the ratio of the maximum to minimum overall dimensions (axes) of the approximating ellipsoid.

The performance of this method is not less than 100 MO/s in the diameter range of 400 – 1500 mkm. The relative error of MO diameter control is no more than 0.25% (at the reliability of PD = 0.7 and K = 1,3 relative units), and the relative error of the non-sphericity coefficient control lie in the range of 2.3% (PK = 0.7 and K = 1.3 relative units) to 0.6% (with PK = 0.96 and K = 1.05 relative units).

Generative Models in Simulations for High Energy Physics.

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High Energy Physics experiments are aimed to shed light on open problems of the fundamental structure of the matter and the Universe. For the simplicity sake but without loss of generality, we consider an example of Large Hadron Collider (LHC) detector. A detailed simulation of the experiment includes modelling beam, the interaction of accelerated particles, production of the Standard Model and New Physics particles, prompt decays, an interaction of a particle with detectors, emulation of readout electronics and so on. All this work is the vital component for a reliable interpretation of the observed results, extracting new knowledge about the fundamental laws of the Universe.

The goal of obtaining more precise results in the current LHC experiments drives the plans to increase the instantaneous luminosity observed by the detectors significantly. Another complexity factor is the growth of the number of protons colliding at each moment in time, thus increasing the complexity of observed events. Which in turn, leads to the development of advanced approaches to triggering, reconstruction, analysis and event simulation. The latter task brings to a critical challenge: generating the significantly higher amount of Monte Carlo (MC) data, required for an analysis of the data collected at the higher luminosity, without a drastic increase in computing resources requires a significant speedup of the simulation algorithms. GEANT modelling of particles interacting with the material of the detector, in particular, the shower development in electromagnetic and hadronic calorimeters takes the most significant part of computer simulation resources.

In this research, we present the possibilities to accelerate these simulation computations by using methods of sample generation by Neural Networks. Such models are widely used for computer vision and image processing nowadays. There are two main approaches to this problem: Generative Adversarial Networks (GAN), that takes into account explicit description of the real data, and Variational Autoencoders (VAE), that uses latent variables to describe the ones. Finally, we compare both approaches for the calorimeter simulation for the LHCb experiment at LHC, discuss possible problems and advantages of these approaches.

Analysis of 3D structure resolution limits in single particle imaging with limited data

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Abstract

The ability to discover three-dimensional structure of biomolecules, like proteins and viruses, is crucial in biology and medicine. With the invention of super-bright X-ray free electron lasers (XFELs), scientists can now collect diffraction images from individual particles, but there are still challenging problems in reconstruction of high-resolution 3D structures of biomolecules from XFEL experimental data.

In real experiments the diffraction intensity from biological molecules is often weak, a small number of photon is registered at the detector, especially at high wavenumber pixels. Also experiment setup, sample preparation and injection are still challenging problems resulting in a limited number of quality diffraction patterns obtained during the experiment. Thus an important problem arises as how the amount and quality of diffraction patterns affect the result and resolution of the final 3D structure.

In the framework of the study, a single-particle experiment was simulated using the Dragonfly software [1] and it was determined how the number of diffraction images and the number of diffracted photons affects the resolution and what is the threshold values of these parameters when it is possible to make a three-dimensional reconstruction.

1. Ayyer, K., Lan, T. Y., Elser, V., & Loh, N. D. (2016). Dragonfly: an implementation of the expand–maximize–compress algorithm for single-particle imaging. *Journal of applied crystallography*, **49**(4), 1320-1335.

Probing Analog Quantum Machines with Supercomputer Simulations

Itay Hen

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The potential of analog quantum computers to defeat traditional algorithms run on standard digital computers is still a mystery.

With no examples of genuine quantum speedups nor a no-go theorem that precludes them, one of only very few avenues of research to resolve this puzzle is to study these devices via heavy numerical simulations carried out on supercomputers.

In this talk I will present results of several studies, designed to gain insight into the capabilities as well as limitations of these perplexing devices.

Effect of dispersity of particle length on the electrical conductivity of the two-dimensional systems

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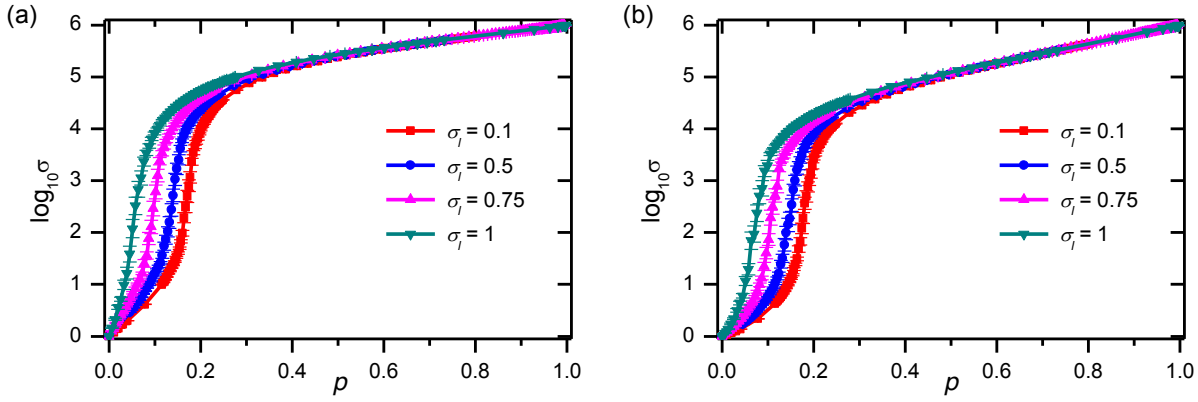
Recently, simulations of electrical conductivity of two-dimensional systems with rod-like fillers of equal length have been performed both in lattice [1–3] and in continuous [4,5] approaches. By contrast, fillers in real systems of conductive nanocomposites have different lengths follow a lognormal distribution [6]. By means of computer simulation, we examined effect of dispersity of filler length on electrical conductivity of two-dimensional (2D) composites with rod-like fillers. Continuous approach has been used. Highly conductive zero-width rod-like particles deposited uniformly with given anisotropy onto a poorly conductive substrate. Length of particles, l, varies according to the lognormal distribution. Probability density function is $f(l)=\frac{1}{l\sigma_l\sqrt{2\pi}}\exp\left(-\frac{\left(\ln l-\mu_l\right)^2}{2\sigma_l^2}\right)$. We performed simulations for the fixed value of the parameter $\mu_l=0$ and different values of the parameter $\sigma_l=0.1,0.5,0.75,1$ and for different values of the order parameter $s=N^{-1}\sum_{i=1}^{N}\cos 2\theta_i$, where θ_i is the angle between the axis of the i-th rod and the horizontal axis x, and N is the total number of rods in the system. The figure shows the results of a numerical calculation of the dependence of the logarithm of the effective electrical conductivity on the filling fraction along the direction of alignment of the rods (a) and in the perpendicular direction (b) at $s=0.5$. As the parameter σ_l was increased, the insulator—metal transition occurred at a smaller fraction of the occupation by the particles.



We acknowledge the funding from the Ministry of Education and Science of the Russian Federation, Project No. 3.959.2017/4.6.

1. Yu.Yu. Tarasevich, V.A. Goltseva, V.V. Laptev, N.I. Lebovka // Phys. Rev. E. 2016. Vol. 94, Iss. 4. P. 042112. DOI 10.1103/PhysRevE.94.042112.
2. Yu.Yu. Tarasevich, V.V. Laptev, V.A. Goltseva, N.I. Lebovka // Physica A. 2017. Vol. 477. P. 195–203. DOI 10.1016/j.physa.2017.02.084.
3. Yu.Yu. Tarasevich, V.V. Laptev, A.S. Burmistrov, N.I. Lebovka // J. Phys.: Conf. Ser.. 2018. Vol. 955. P. 012006. DOI 10.1088/1742-6596/955/1/012006.
4. N. I. Lebovka, Yu. Yu. Tarasevich, N. V. Vygornitskii, A.V. Eserkepov, R.K. Akhunzhanov // arXiv: 1803.07354.
5. Yu.Yu. Tarasevich, N.I. Lebovka, I.V. Vodolazskaya, A.V. Eserkepov, V.A. Goltseva, V.V. Chirkova // arXiv: 1804.00809.
6. L. Forró, R. Gaal, C. Grimaldi, M. Mionić, P.R. Ribič, R. Smajda, A. Magrez // AIP Advances. 2013. Vol. 3. P. 092117. DOI 10.1063/1.4821802.

Pattern formation in two-dimensional systems of rectangular particles

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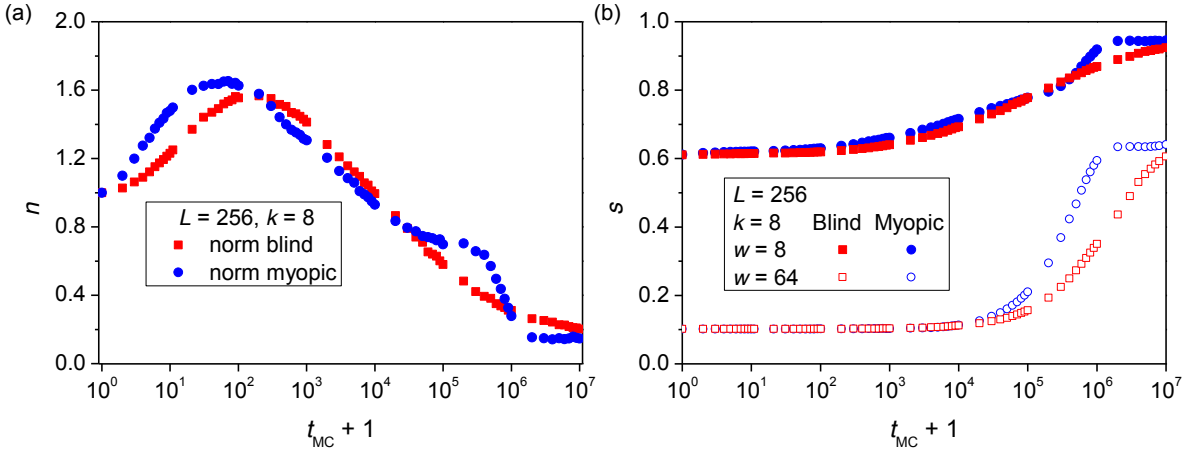
Monte Carlo simulation has been used to study reorganisation in two-dimensional systems of elongated particles. Recently, pattern formation in these systems has been reported [1–4], nevertheless, several questions are still open.

The space was assumed to be discrete, i.e., a square lattice of size $L_x \times L_y$. The simulations were performed both in square ($L_x = L_y$) and in rectangular systems ($L_x \neq L_y$). Rigid rectangular particles of size $m \times n$ lattice units were deposited onto the lattice using random sequential adsorption until a jamming state. A special attention to the case of 'needles' or k-mers, i.e., particles of size $1 \times k$, has been paid. Moreover, effect of particles shape has been studied. Two mutually perpendicular orientations of the particles were equiprobable. In the case of k-mers, the jamming state was characterised by a stack structure, i.e., the particles of the same orientation form blocks with typical size $k \times k$.

After deposition, the particles were allowed to perform a random walk. Hard-core interaction between particles was assumed, hence, any reorganisation have to be entropy-driven. Two different kinds of random walk have been studied, i.e., "blind" and "myopic" random walk rules [5]. "Blind" particle chooses the next step from among all neighbour sites. This behaviour is related to a diffusion of conventional particles, it preserves detailed balance condition [4]. "Myopic" particles are "intellectual", i.e., they choose from among all unblocked sites. This rule resembles the behaviour of particles inside active colloids. This algorithm does not preserve the detailed balance condition [4].

The normalized number of clusters, n, local order parameter, s, fraction of interspecific contacts, and mean degree of freedom of the particles have been monitored during simulations. The random walk leaded to states when particles were more free than in the initial jammed state. We calculated diffusion coefficients and found that the random walk should be considered as a subdiffusion. Examples of behavior of some quantities are presented in figure.



(a) normalized number of clusters, (b) local order parameter vs Monte Carlo steps, t_{MC}.

We acknowledge the funding from the Russian Foundation for Basic Research, Project No. 18-07-00343.

1. N. I. Lebovka, Yu. Yu. Tarasevich, V. A. Gigiberiya, N. V. Vygornitskii, Phys. Rev. E. Vol. 95, Iss. 5. P. 052130, 2017. DOI 10.1103/PhysRevE.95.052130.
2. Yu. Yu. Tarasevich, V. V. Laptev, A. S. Burmistrov, N. I. Lebovka, J. Stat. Mech. Vol. 2017, Iss. 9. P. 093203. 2017. DOI 10.1088/1742-5468/aa82bf.
3. Yu. Yu. Tarasevich, V. V. Laptev, V. V. Chirkova, N. I. Lebovka, arXiv:1803.09409.
4. S. Patra, D. Das, R. Rajesh, M. K. Mitra, Phys. Rev. E. Vol. 97, Iss. 2. 022108. 2018. DOI 10.1103/PhysRevE.97.022108.
5. R. B. Selinger, H. E. Stanley, Phys. Rev. A. Vol. 42, Iss. 8. P. 4845. 1990. DOI 10.1103/PhysRevA.42.4845.

Adsorption in structure-I clathrate hydrates described using a single Langmuir site: Evidence from all-atom Monte Carlo molecular simulations

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Clathrate hydrates are a non-stoichiometric ice-like material consisting of a hydrogen-bonded water network forming a network of cavities which contain gas molecules. Natural gas clathrate hydrate deposits can be found in the deep ocean and in tundra permafrost, where the environmental temperature and pressure conditions permit their formation. Methane clathrate hydrate, and several others, typically take on the so-called structure-I lattice structure, which is itself a solution to the Kelvin problem—i.e. a foam of approximately equal-volume bubbles with minimal inter-bubble surface area [D. Weaire, R. Phelan, Phil. Mag. Lett. 69, 107 (1994)]. Commonly, especially within the context of van der Waals-Platteeuw theory [J.H. van der Waals, J.C. Platteeuw, Adv. Chem. Phys. 2, 1 (1959)] used to describe clathrate hydrate phase equilibria, two different cavity types are modelled as Langmuir-type adsorption sites, necessitating the use of four fitted adsorption isotherm parameters [W.R. Parrish, J.M. Prausnitz, Ind. Eng. Chem. Proc. Des. Dev. 11, 26 (1972)]. This study employs all-atom Monte Carlo molecular simulations to examine the suitability of describing the structure-I clathrate hydrate cavities in terms of a single Langmuir-type adsorption site. The use of such an adsorption isotherm model would halve the number of adsorption isotherm parameters typically fitted to experimental phase equilibria. Several different gas species known to form structure-I clathrate hydrates are considered: Carbon monoxide, methane, ethane, ethene, and hydrogen sulphide. This general idea has been used previously for united-atom simulations of methane clathrate hydrate [M. Lasich, A.H. Mohammadi, K. Bolton, J. Vrabec, D. Ramjugernath, Fluid Phase Equilibr. 369, 47 (2014)], and the results of the present work demonstrate the utility and limitations of this approach using more rigorous molecular models across several different systems.

Intermediate Lattice Boltzmann-BGK method and its application to micro-flows

oral

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The Lattice Boltzmann method is supposed to be an adequate approach for the modeling of non-equilibrium flows and kinetic effects beyond the Navier-Stokes level [1]. Nevertheless, when the flow is rarefied and the role of high-order moments of the velocity distribution in a rarefied media increases the precision of conventional LB models go down. In real world, the large values of the rarefaction parameter - the Knudsen number can be observed in the micro, nano-flows, in shale gas flow inside porous media, water transport inside nano-graphene membranes [2]. The present research is aimed to develop a new LB based velocity discretization method which is able to cope with the kinetic high-order moments in the rarefied flow.

I will consider a new conservative discretization method for BGK kinetic model based on the application of the Central Limit Theorem (CLT) to the conventional LB model. In the presented discrete velocity kinetic theory we consider 1D discrete velocity local equilibrium state in a such form that this equilibrium describes the probability distribution for a sum of **N** independent and identically distributed random variables. For **N=1** case we obtain the well-known 3-velocity D1Q3 model [3], in general case we have **2N+1** velocity model. The proposed method is somewhat intermediate between the difference schemes for the Boltzmann BGK equation and the canonical LB method.

This construction has several very attractive properties. Firstly, the method is conservative. Second, according CLT the increase of **N** for this method guarantees that all the moments of the local equilibrium state will converge to local Maxwell moments. This property is important since allows us to construct the conservative difference scheme for BGK equation adjusting the precision of the highest moment by the choice of **N.** Next, the velocity grids for the method are Cartesian by the construction. Finally, some analytical properties of the equilibrium state like the moment generating function can be obtained in a nice concise form since the equilibrium distribution corresponds to the probability density for a sum of random variables.

It is shown that 5-velocity (N=2) and 7-velocity (N=3) models applied to the classical Sod shock tube problem have good stability for moderate viscosities while the conventional 3-velocity D1Q3 model (N=1) is unstable for the considered conditions. Next, the gas microflow between the parallel walls under the pressure gradient (plane Poiseuille flow) is considered for various values of the rarefaction number (Knudsen number). It is shown that the models are able to reproduce the non-equilibrium kinetic effects like the Knudsen paradox, slip velocities with excellent precision in slip and transitional regimes. The accuracy is comparable and sometimes even better than for high-order LB models with additional regularization [4]-[6]

REFFERENCES

[1] S. Succi,, Lattice Boltzmann 2038, *Europhys. Lett.*, **109**, 50001 (2015)

[2] A. Montessori, G. Falcucci, Lattice Boltzmann Modeling of complex Flows for Engeneering Applications, Morgan & Claypool publishers, 2018

[3] S. Succi, The Lattice Boltzmann Equation: For Complex States of Flowing Matter, OUP Oxford, 2018

[4] R. Zhang , X. Shan, and H. Chen, Efficient kinetic method for fluid simulation beyond the Navier-Stokes equation. Phys. Rev. E 74 046703 (2006)

[5] X-D Niu, S-A Hyodo, T. Munekata and K. Suga, Kinetic lattice Boltzmann method for microscale gas flows: Issues on boundary condition, relaxation time, and regularization. Phys. Rev. E 76 036711 (2007)

[6] A. Montessori, P. Prestininzi, M. La Rocca and S. Succi , Lattice Boltzmann approach for complex nonequilibrium flows. Phys. Rev. E 92, 043308 (2015)

Application of Time Series Analysis Technique of Box and Jenkins in Forecasting Future Sales of Nigerian Exported Crude Oil.

BY

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Abstract

This research paper was carried out in order to find out the hidden nature of revenue generated from crude oil sales abroad by Nigerian government and to forecast 12 months (January 2018 to December 2018) sales of the crude oil using crude oil sales data for January 2006 to Decembrr 2017. Crude oil is mainly the significant natural resources of the industrialized and developed economy. It can generate heat, drive machinery and fuel vehicles and airplanes. Its components are used in manufacturing chemicals as well. This was why this research paper was carried out to investigate the hidden nature of revenue generated from crude oil by Nigerian government using fox and Jenkins (1976) auto regressive integrated moving average (ARIMA) model and to forecast 12 months expected monthly sales of crude oil for the year 2018. At the end of this research, five (5) SARIMA model were developed out of which two were found te be the best and with precise forecasting power. The models are (2,1,2) (3,1,0)$\times$12, (1,1,3) (4,1,4) $\times$12 and were fish out with the help of three information criteria namely Akaike information criteria (AIC),Schwarz information critoria (SIC) and Hannan Quinn informntion criteria (HQC). the forecart of the two models mentioned above intimately forecast sales very close to the actual revenue. This means that the models absolutely understand the nature of exported crude oil revenue generated by Nigeria and as such it can be used to forecast future sales of exported crude oil by Nigeria Government with smallest amount of error, finally recommendations are offered.

Keywords: Time Series Crude Oil Fdrecasting.

Методология расчета трафика в локальных сетях ПЭВМ на основе экспериментально-численного моделирования

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Ключевые слова: трафик, Интернет, моделирование

В работе представлена методология применения экспериментально - численного подхода применительно к расчету трафика в локальных сетях ЭВМ, возникающего в результате использования служб Интернета. В настоящее время этот тип трафика является основным в сетях ЭВМ для массового пользователя, в связи с чем тема является актуальной.

Экспериментально численный метод для локальных сетей ЭВМ основан на следующих основных принципах:

- службы Интернет при работе на данной ЭВМ производят типичные для них потоки данных (так называемые элементарные потоки данных от служб Интернета). Эти потоки могут быть экспериментально измерены и их параметры могут быть определены путем статистической обработки данных.

- для потоков данных может быть принято (с точностью порядка нескольких процентов) правило суммирования нескольких потоков данных в коммутаторе.

Справедливость указанных принципов была подтверждена экспериментальными измерениями потоков данных в локальных сетях и статистической обработкой данных.

Следующим принципом является замечание, что поток данных производится непосредственно программой - службой Интернет, а пользователь только использует (активирует) программу. То есть имеется естественная декомпозиция процесса образования потока данных в локальных сетях ЭВМ: службы Интернет производят типичные потоки данных, пользователи активируют службы.

Таким образом, располагая данными об элементарных потоках данных, можно проводить моделирование активности пользователей сети - работы сотрудников предприятия (учреждения) и получать данные о потоке данных в локальной сети непосредственно как функцию активности пользователей сети, выраженных в терминах их трудовой или социальной деятельности, предпочтении тех или иных Интернет сервисов и т.д.

Представленный проект анализа данных в локальных сетях ЭВМ требует сбора и обработки большого количества разнородных данных.

Ранее были проведены эксперименты по сбору данных о характеристиках элементарных потоков локальных сетях ЭВМ. В данной статье представлены применения предлагаемого подходя для расчета потоков данных, возникающих при использовании модели работы различного числа пользователей. Модель работы пользователей также основана на экспериментальных данных о работе в сети типичных учебных групп студентов.

Литература

Филимонова, Н. А. Модель элементарного потока данных в Интернете / Н. А Филимонова // Вестник СибГУТИ. - 2013. - №2. - С. 54-68.

Methodology of traffic calculation in local PC networks based on experimental-numerical simulation

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Keywords: traffic, Internet services, local networks, modeling.

The methodology of the application of the experimental-numerical approach as applied is presented in the paper as applied to the problem of calculation of traffic in local PC networks, which arises as a result of the use of Internet services. Currently, this type of traffic is the main one in PC networks for a mass user, in connection with which the topic is practically important.

The experimental-numerical method for local computer networks is based on the following basic principles:

- Internet services when run on specific PC produce typical for them data streams (the so-called elementary data streams from Internet services). These streams can be experimentally measured and their parameters can be determined by statistical data processing.
- for data streams, the rule of summing several data streams in the switch can be adopted (with an accuracy of several percent).

The validity of these principles was confirmed by experimental measurements of data flows in local networks and statistical processing of data [1].

The next principle is the observation that the data stream is produced directly by the Internet service, and the user only uses (activates) the program. That is, there is a natural decomposition of the process of data stream generation in local PC networks: Internet services produce typical data flows, users activate services.

Thus, if elementary data streams are known, it is possible to simulate the activity of network users - the work of employees of the enterprise (institutions) and receive data about the data flow in the local network as a function of the activity of network users expressed in terms of their labor or social activity, preferences of certain Internet services, etc.

The presented approach to the data analysis in local PC networks requires the collection and processing of a large number of heterogeneous data.

Earlier, experiments were conducted to collect data on the characteristics of elementary flows of local PC networks [1]. In this paper, we use the proposed approach to calculate data streams that arise as result of activity of various number of users. The user activity model is also based on experimental data for various groups of students. Numerous results of computations will be presented.

[1] Filimonova, NA A model of an elementary data flow on the Internet / NA Filimonova // Bulletin of SibGUTI. - 2013. - №2. - P. 54-68.

Multiscale simulation of gas separation device based on thermal transpiration effect

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This paper presents numerical simulation of novel gas separation device utilizing membrane with temperature drop applied to its sides to induce thermal transpiration (Fig.1,2). To perform this simulation a new hybrid method was developed combining solution of Navier-Stokes equations at low Mach numbers at macroscale with solution of model Boltzman equation in membrane pores. Obtained results clearly indicate separation effect in such a device for three pairs of noble gases (He-Ar, He-Ne, Ne-Ar). Operation parameters for most effective separation had also been found.

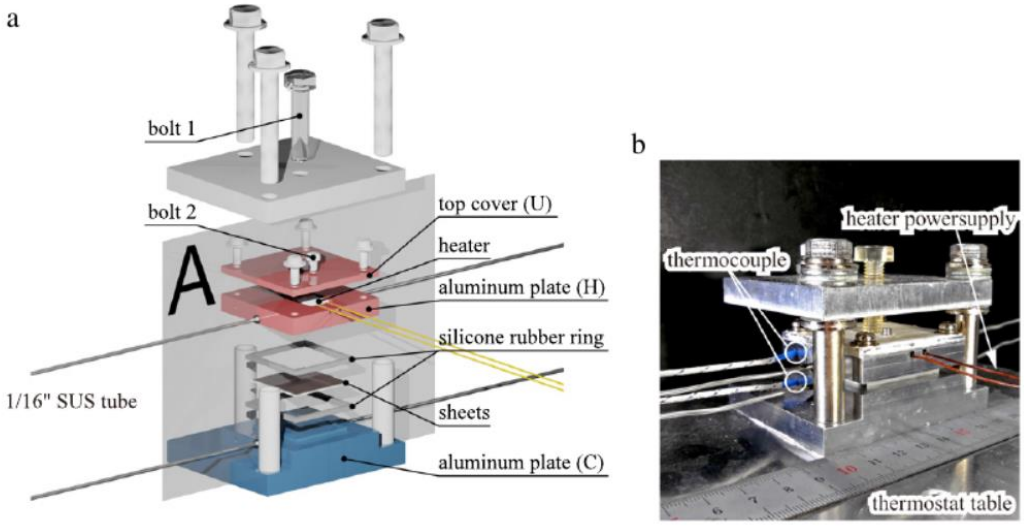

Figure 1. Schematic of gas sepation device (a) and photograph of real prototype (b).

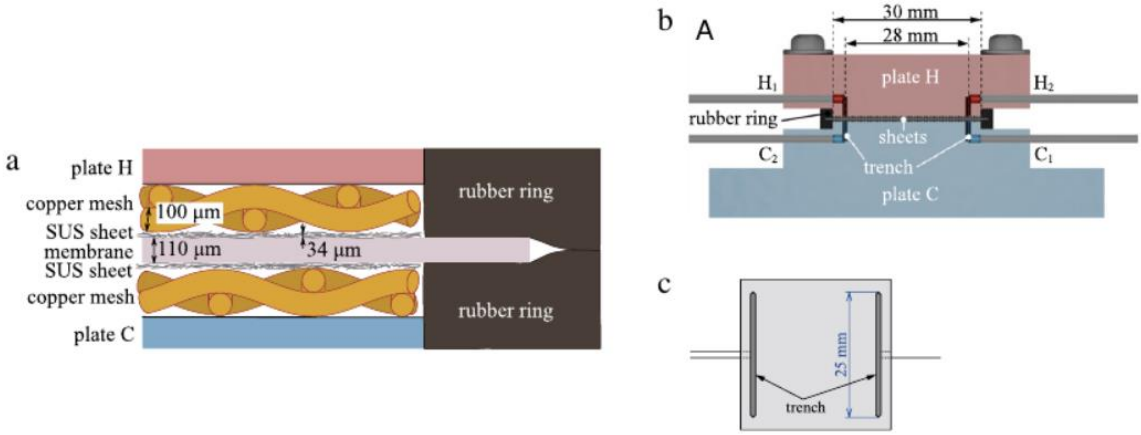

Figure 2. Sectional view of the device

Phase diagrams of polarized ultra-cold gases on attractive-U Hubbard ladders

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Recent advances in experimental technique of creation and manipulation of strongly correlated systems using ultra-cold gases in traps with varying forms and effective dimensionality of the trapping potential [1, 2] stimulates an interest in mathematical modeling of quasi-one-dimensional polarized Fermi gases at ultralow temperatures. In such systems a motion of the particles in two spatial dimensions out of three is almost completely "frozen". Moreover the spatial structure of the atomic cloud was found to be significantly different for quasi 1D cigar-shaped magnetic traps and 3D spherically symmetric traps.

In this paper we consider a quasi-one-dimensional model of a two-component Fermi gas at zero temperature on one, two and three leg attractive-U Hubbard ladders. We construct a phase diagram of a two-component spin-polarized gas in the convenient coordinates specified by chemical potential and effective magnetic field" [3-6].

We present phase diagrams for the attractive-U Hubbard model on the one leg (single chain), two-leg and three-leg ladders for various values of the onsite Hubbard attraction U, fermion density n, and hopping amplitude t (or correspondingly the 1D bandwidth $W=4t$). The phase diagram typically contains equal density phase with local bound pairs, partially polarized phase and different fully polarized phases. We obtain that the topology of the phase diagram in attractive-U Hubbard model for two, three or more legs does not qualitatively change with the increase of the number of legs, but qualitatively differs from the topology of the phase diagram of a single chain.

REFERENCES

1. *M. C. Revelle, J. A. Fry, B. A. Olsen, and R. G. Hulet* "1D to 3D Crossover of a Spin-Imbalanced Fermi Gas", Phys. Rev. Lett. 117, 235301 (2016).

2. *R. Ono*frio “Cooling and thermometry of atomic Fermi gases”, Phys. Usp. 59, 1129–1153 (2016).

3. *A. E. Feiguin and F. Heidrich-Meisner* “Pair Correlations of a Spin-Imbalanced Fermi Gas on Two-Leg Ladders”, Phys. Rev. Lett. 102, 076403.

4. *F. Heidrich-Meisner, G. Orso, and A.E. Feiguin* “Phase separation of trapped spin-imbalanced Fermi gases in one-dimensional optical lattices”, arxiv cond-mat 1001.4720, Phys. Rev. Lett. (2010).

5. *M. Yu. Kagan, S. Haas, and T.M. Rice* “Phase diagram of three-leg ladders at strong coupling along the rungs”, Physica C: Superconductivity 317-318, 185-193 (1999).

6. *E. Burovski, G. Orso, and Th. Jolicoeur* “Multiparticle Composites in Density-Imbalanced Quantum Fluids”, Phys. Rev. Lett. 103, 215301 (2009).

The Arrhenius equation demand very delicate treatment under usage in mathematical modeling schemes.

The work is devoted to a critical analysis of the widely used practice of the Arrhenius equation for the mathematic modeling and simulation of many physical and chemical processes, where under the mathematical modeling is arising an Arrhenius-type equation. All such equations by our opinion can only approximately describe the system's behavior and to create only an external resemblance with processes (below we give many examples), and it can have a negative influence for science in general. Below are presented some concrete examples (cases) for many known scientists, including N. N. Semyonov, A.G. Merzhanov, prof. Galwey, etc. Criticism and examples of "erroneous" design work are also given, including the so-called "global-kinetic mechanism". Similar situations, when theoretical models are fundamentally differ from the real situation, are very widespread in the modern science practice. We tried to formulate the questions and give answers without standard mistakes, being characteristic for the studies under consideration. We also try to demonstrate that the Arrhenius-type equations by their nature are presenting a very interesting mathematical object for some special investigations.

1. The history and special features of the Arrhenius equation
2. Arrhenius equation in the combustion theory history in general. A "phlogistic" essence of the Arrhenius equation
3. Two approaches to the Arrhenius equation usage
4. Case of academician N. N. Semenov
5. Case of prof. Galwey
6. Peculiarities of the modeling and simulation in macrokinetics
7. Case of academician Merzhhanov and his «Solid flame".
8. Case of prof. Rumanov
9. Conclusions and criteria

In 2019 year is 130-th anniversary of Svante August Arrhenius "On the rate of inversion of cane sugar under the action of acids" paper publication which is associated with the introduction to physics and chemistry of the famous equation. This equation was not inferred, but suggested, selected from several variants to describe the speed of a specific chemical reaction: the decomposition of cane sugar under the action of acid. In the article of Arrhenius 7 empirical equations from the works of different authors were cited, among which at number 5 there was an equation from the work of Van't Hoff and Schwab 1984, which is close to the modern form of Arrhenius equation:

$$k = A\exp(-E/RT). \qquad (1)$$

(k –reaction constant, A – pre-exponential factor, E – activation energy, T – temperature)

At the beginning of the 20th century the profound changes in the atoms and molecules structure understanding took place, and a modest Arrhenius' article by on a rather narrow study results "fitting" became a revolutionary milestone in the development of chemistry and other sciences. It made it possible to describe quantitatively the most complicated physicochemical processes. The Arrhenius equation began to be derived both from the point of view of the molecular-kinetic theory and more complex mathematical constructions, for example, inverse Laplace transforms, using various theoretical approaches: thermodynamic, collision theory, transition state theory, stochastic approaches. The modern bibliography on the Arrhenius equation is extensive. It turns out that the "rate constant" used in chemical kinetics is called a constant only by tradition and only formally. In fact, it is a very complex parameter, which includes many physicochemical parameters of the systems under study. This was paid special attention in the 60-70-ies of the last century (especially in connection with the study of plasma-chemical and radiation-chemical processes). In this connection, it is interesting to note that the Chancellor of Germany, Angelina Merkel, was engaged in radiation chemistry, and her doctoral dissertation was devoted precisely to the "comparison" of the so-called statistical and kinetic reaction rate constants. Many works connected with this equation concern the non-equilibrium of real processes, the presence of several temperatures and generally different constants in one elementary act, the concepts of Arrhenius and non-

Arrhenius kinetics. Thus a positive role of the equation can hardly be overestimated, because it allowed to solve many complex problems of macrokinetics.

However, we will try to demonstrate, that the so-called Arrhenius equation became an analogue of "phlogiston theory" of the 20th century. The mention of the phlogiston theory is connected in view of certain analogies with the current situation that has arisen with the modeling of the physical and chemical processes. We can recall, that one of the first theories that can be considered scientific from the point of view of modern was dedicated to burning. This is the so-called phlogiston theory (from the Greek φλογιστοζ - combustible) associated with the names of German chemists Johann Joachim Becher and Georg Ernst Stahl. Phlogiston is a hypothetical fluid, according to the authors of the theory, contained in all combustible bodies and possessing a negative mass. According to this hypothesis, combustion is represented as an expansion with the release of phlogiston, which is scattered in the air, forming a visible fire. Despite the absurdity of such views from the modern science point of view, the phlogiston theory simply and adequately described the experimental facts, was internally consistent, creative, etc. With its help many correct predictions were made and practical results were obtained. The theory was owned by the minds of scientists for more than a century, and its development played a great role in the evolution of science in general and in the creation of a special science of thermodynamics that laid the foundations of all modern science and theoretical physics, in particular (from the Boltzmann H-theorem in statistical physics to the Gibbs potential in chemistry). As an illustration, we can cite the case of the famous chemist Antoine Lavoisier, whose name is associated with the "oxygen" theory of combustion. Although Lavoisier himself used mainly the theory of phlogiston, he substantiated the successful method of bleaching sugar with activated charcoal on the grounds that the yellowish shade of sugar crystals is given by the phlogiston, which can be removed by making it switch to coal. This successful decision brought the scientist a lot of money (for the sake of justice, he and before that was one of the richest people in France). Then Lavoisier began to participate in the redemption of taxes and this led him to the guillotine of the French Revolution Now, unlike the times of Lavoisier, the level of understanding of the processes occurring during chemical reactions is now much higher.

However, the "phlogistic" essence of the Arrhenius equation is much simpler: this equation, paraphrasing the name of one famous article by E. Wigner ("The Incomprehensible Efficiency of Mathematics in the Natural Sciences") it is an "inconceivably effective mathematical" object, making possible to close almost any system of macrokinetic equations or formally "simulate" almost any макрокинетический experiment. In fairness, other functions with a strong temperature dependence (for example, a power law or a polynomial one), can be used as closing functions that describe the chemical interaction, the main thing is the presence of coefficients that can be varied to "fit" to the experimental data. But the Arrhenius exponent unlike these functions seems to have a physical and chemical meaning and the "fit" turns into "modeling", as if based on the laws of nature. Basic equations of the models based on the equations of conservation of energy, matter, components and the Arrhenius conjecture can be written in the following form:

$$\Sigma F_{phys} = \Sigma F_{chem} (\exp(-E/2RT) \qquad (2)$$

where on the right side the functions responsible for the chemical processes and containing the Arrhenius exponential for the rate of chemical reactions are summed up, and in the left – the functions responsible for the physical processes: thermal conductivity, diffusion, convection, radiation, etc. It turns out that the mathematical properties of the functions used make it possible to describe practically any experimental data in the field under consideration. Indeed, if the right and left parts of such expression are logarithmized, this operation, without changing the essence of the relationship, so "smoothes out" the features of functions that did not initially contain an exponential, which they can often be neglected. In other words, the exponent is so "strong" function for adjusting the results, that using it in such equations, you can "no bother" how accurately it was possible to describe the actual physical processes, so, paraphrasing a well-known expression, we can say that the exponent "throws out with the bathwater the baby "- a reality. It is obvious, that together with such primitive approaches and results of senseless usage of equation there were some attempts to adequate using of experimental data, but they often remained only “superficial’’ ones.

There are some concrete examples. A “dualism” is traced in works of N. N. Semenov in the field of the origin and development of the macrokinetics historically. In the late 1920s and early 1930s, Nikolai Semenov published several papers with the opposite content: a chain theory based on tracking the multiplication and death of active radical particles. The theory of a thermal explosion was based on the

fact that combustion occurs in the same laws as the breakdown of dielectrics. Another series of works led to the development of the so called thermal theory of combustion by Zel'dovich, Frank-Kamenetsky, and Todes. The term "thermal" is associated with emphasizing the main mechanism for maintaining, accelerating the physicochemical process – due to the Arrhenius temperature dependence, in contrast to the so-called "chain" mechanism associated with taking into account the real elementary reactions responsible for the combustion of gases. The fact is that the reactions between the valence-saturated molecules have enormous activation energies in comparison with the reactions involving free atoms and radicals (by tens of kcal / mole more) and the real mechanism of interaction is determined by the fast reactions of the chain carriers and by how they multiply and perish. Meanwhile, the desire to simplify the consideration of the systems of equations for the physical and chemical combustion processes, and sometimes even analytically solve these systems (simplified methods of integrating exponentials, narrow-band methods) led to the use of expressions for the reaction rate with the chemical part of the process the Arrhenius exponents for the zero or first order reactions, ignoring the real dependencies on reagent concentrations, with meaningless activation energies and pre-exponential factors chosen to be satisfactory to the experimental data. This approach now is very widespread under the name of global kinetic mechanism. For example, in [1], an empirical kinetic scheme is used for the single-stage combustion of methane with oxygen. The kinetic parameters are chosen from the experimentally measured flame velocity, and this allowed calculations of two- and three-dimensional flows, including turbulent ones.
It must be mentioned too how academician N. N. Semenov rejected the correct conception (about a chain mechanism of hydrogen and oxygen reactions at third ignition limit). According a new version, presented in Semenov's monograph [2], he suddenly believed Frank-Kamenetsky's calculations that the Arrhenius constants taken from the experiment describe combustion at high pressures well. Really the Frank-Kamenetsky's data were obtained by an Arrhenius-type treatment of the experimental results. The "discovery" of a correct view of the mechanism of combustion of gases ascribed to corresponding Member RAS, Azatyan [3] on the grounds that "the last word is more expensive than the first."

This example demonstrates one of the generally unsuccessful approaches to a modeling, when one is writing down a system of type (2) equations, assuming that the constants, Frequency Factors, Activation Energies values and other so called “enclosing” parameters will be obtained from some independent experiments or from generally accepted tables and data bases. But if the experiment data results treatment is carried out with the Arrhenius hypothesis usage we always have a vicious circle.

There is a bright analogy, proposed by V.V. Voevodskii for gaseous reaction rates. He compared the gaseous burning processes with a mountain river flowing around a great stone. A part of water mass is going over the stone the main water mass is flowing from sides. Analogously the chain mechanism is a method to overcome the high potential barriers, and the seen combustion reaction rates correspond to the active intermediate particles, free atoms and radicals, regenerating and breeding at the chain reactions. If the process is branched-chained one a summary reaction rate is determined by the so called ”double exponent”, i.e. an exponent with another exponent in power index. The modern calculation methodics allow to take into account several hundreds of reactions synchronously, but if one will “heap” the results in one pile (without dividing reactions by their cycles and mechanism). It will get an automatic ”fitting“ of results without any scientific meaning.

Below we describe some interesting examples of Arrhenius equation wrong or unsuccessful usage for reactions in condensed media.

In his monograph [5] prof. Galwey describe a strange history of degradation of the science related to the study and modeling of the changes that are occurring on heating a variety of diverse, initially solid, reactants. Shortly it can be said that there we once again see a collision of two approaches. One is based on a careful study of complex processes with calorimetric measurements, generally complemented kinetic investigations with appropriate chemical and physical observations, e.g., the effects of changes in reaction conditions, the use of microscopy, etc. The method is called TDoS (Thermal decompositions of solids). From the works of 1905 yea the earliest kinetic study of a solid-state decomposition of Silver Oxide, Ag2O and up to 80-th, this approach was actively developed and gave many important results. But from 70-th the scientists began to use a more primitive approach, so called thermal analysis (TA)….

Models of a Dependence of a Preferred Speed of Utterance of Audio Materials on Individual Indicators of Listeners

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The activity of many people involves the acquisition of a large amount of information through the sound channel of perception. This activity can be attributed to the learning process, which can be both not personified and personified.

In any case, listening to audio information creates a load on the brain, leading to the development of fatigue, loss of concentration. It, in turn, affects the effectiveness of learning and mastering the material. Adverse conditions for the perception of information flows increase work time and reduce the amount of information learned.

Thus, in order to maximize the amount of information assimilation and minimize the negative effect of information flows on the trainee, it is necessary to implement the optimal presentation of information for this trainee. Therefore, the trainees, due to individual psychophysiological characteristics, can perceive the information they provide in different ways. At the same time, in general, the question remains open regarding the ways of personifying the presentation of audio information, i.e. accounting of individual properties and indicators of the trainee in the e-learning system.

The most important parameter of the audio information output (in audiobooks, audio clips, etc.) is the rate of speech. The value of this parameter affects the assimilation of information, the time of listening to the audio, the comfort and convenience of the user.

The aim of the work is to research of a dependence of a preferred speed of utterance of audio materials on individual indicators of listeners.

The experiment is organized based on the fact that preferences are largely determined by the amount of effort spent in the process of solving a particular problem. Those, the more mental effort expended in the process of working with the object, the faster fatigue occurs and the higher the load on the body's systems, the lower will be the assessment of the preferences of the object.

Let's put the hypothesis of the research that the user's preference for the speed of speech of the audio information being monitored is determined by the strength of the nervous system, the dynamics of working capacity over time in carrying out tasks with the load, and the characteristics of the leading channel of information perception (leading perception modality).

This hypothesis is not accidental, since fatigue affects the effectiveness of training. In addition, it is important to take into account the adaptation of audio playback parameters for long-term training and the development of fatigue.

Procedure of research. The participants of the experiment were 41 students. The number of males is 32, female is 9. The average age of participants was 22.8 ± 1.6 years. To conduct the experiment, we used a tepping-test, the letterhead of S. Efremtseva's technique, a 30 second lecture audio tape on the topic "Introduction to the automation of production" with an average speed of utterance $U_0 = 78$ words/min. To play this audio, we used a player that could play it with the following speeds $0.8U_0$, $0.9U_0$, $1.0U_0$, $1.1U_0$, $1.2U_0$, $1.3U_0$, $1.4U_0$. To determine the preferences in listening to audio recordings with one or another rate of speech, a 10-point scale was used. Experiments were conducted in the classroom in the first half of the day in groups of students. After conducting the briefing and explaining the meaning of the experiment, the testees filled in the forms of S.Efremtsev's technique, passed a test tepping-test, and then the basic tepping-test was performed for 30 seconds. To assess the preferences in the speech tempo, the audio was reproduced at each of the speeds, and after listening, the tester evaluated the listening comfort at each of the playback speeds on a 10-point scale.

We will perform the regression analysis and construct a series of regressions describing the dependence of the audio playback speed on the selected indicators. These indicators describe the strength of the nervous system, the characteristics of the dynamics of performance in carrying out tasks with the load and the prevailing channel of perception of information.

As a result of the regression analysis, 3 personalized logistic models have been created, the joint use of which makes it possible to predict the preferred speed of audio playback on the scales: "speed of utterance is low" - "speed of utterance is medium" - "speed of utterance is high" - "speed of utterance is very high". Predictors of models are indicators of the strength of the nervous system and the prevailing channel of information reproduction. Besides, the classification accuracy reaches 80%.

The developed models can be used in e-learning systems for exercise a personalized control over the speed of audio information playback depending on the individual properties and indicators of the learner.

DIFFUSION AROMATIC HYDROCARBONS IN IONIC BY MD SIMULATION

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Ionic liquids (ILs) have been extensively studied as replacements to sulfolane in the separation of aromatics from alkanes. The employment of ILs could reduce energy requirements and operating costs of the aromatic extraction unit as a result of their nonvolatile character. However, the ILs studied so far have shown mass-based aromatic distribution ratios lower than the sulfolane values, which would increase the solvent-to-feed ratio in the extractor.

The MD method was applied using a modified DL_POLY_4.05 with a time step of 2 fs for study of structure and diffusion aromatic hydrocarbons in IL (dimethyl-imidazolium chloride-dmim+/Cl-) at T=400K. In the calculations cations, anions, and atoms forming the molecules of the added substance (hydrocarbons : benzene, toluene, phenol , anisole and c-hexane) ware treated as solid charged model systems with a fixed geometry. Analysis of the data allowed to establish: (1) The salvation effect in systems dmim+/Cl- - non-polar solute molecules (benzene, c-hexane) has qualitatively similar to the behavior of the hydrophobic hydration of aromatic solute molecules in liquids like water. Based on the data obtained from MSD and VAF the different diffusion mechanisms of nonpolar solute molecules in IL ware determined. (2) The salvation effect in systems ionic-liquid (dmim+/Cl-) - polar solute molecules (toluene, phenol, anisole) has qualitatively similar to the behavior of the hydrophobic hydration in liquids like water too. Based on the data obtained from MSD and VAF the different diffusion mechanisms of hydrocarbons solute molecules in IL ware determined.

Ab-initio calculations of magnetic moments and exchange integrals of $Co_{1-x}Ni_x$ alloy film on Cu(100) surface.

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One of the topical problems of modern physics is the investigation of the magnetic properties of multilayer structures in which the giant magnetoresistance effect is realized, because they prompt potential applications in data storage technologies [1]. Ni on Cu is a good epitaxial system since they both have the same fcc crystal structure with only 2.5% lattice mismatch. The growth of Co is more complicated than Ni since the equilibrium phase of bulk cobalt is hcp at room temperature. But $Co_{1-x}Ni_x$ alloy grows on Cu(100) in a well-ordered fcc structure via a layer-by-layer growth from 2 to 20 ML thickness [2].

In this work the results of a numerical first-principles calculations of the energy and magnetic characteristics for cobalt-nickel alloy on a copper surface by using VASP software package [3] by means of the Projector Augmented Wave (PAW) method are presented. The values of the total energy of various collinear spin configurations, the total magnetic moment and the magnetic moments of Ni and Co atoms are calculated. The exchange interaction integrals for the nearest and following nearest neighbors are calculated in the framework of the classical Heisenberg model.

We investigated a system consisting of a copper slab with the orientation of the surface face (100) and adsorbed on it from both sides by a ferromagnetic film of a cobalt-nickel alloy with the thickness of the films in three monoatomic layers. The multilayer structure was simulated using a periodic 2×2 36-atom supercell with the lattice constant corresponding to the copper substrate a = 3.6367 (5) Å, which we obtained as a result of calculations taking into account the optimization of the lattice parameters[4]. Ferromagnetic and six different anti-ferromagnetic configurations for "chess" and "interlaced" arrangement of Ni and Co atoms were considered. The results of our calculations demonstrates that the total energy of the multilayer structure in the ferromagnetic configuration increases with increasing Ni concentration in the alloy. The magnetic moments of atoms of both types take the greatest value in the ferromagnetic configuration in the atomic layer most distant from the substrate. The values of the exchange interaction integrals for the nearest J_1 and for the next nearest neighbors J_2 for pure metal films are positive and greater than the corresponding values in the bulk structure. From the calculation results of the exchange interaction integrals for the $Co_{0.5}Ni_{0.5}$ alloy film it follows that the constant J_1 contributes to the ferromagnetic ordering of the magnetic moments ($J_1 > 0$), and the exchange interaction constants depend strongly on the mutual arrangement of the atoms and on the choice of antiferromagnetic spin configurations.

These results can be applied in numerical simulation by the Monte Carlo methods of the nonequilibrium behavior of multilayer magnetic superstructures[5].

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1. *V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp., **60**, 762 (2017).
2. *F. Huang, M. T. Kief, G.* ***J.*** *Mankey, and R. F. Willis*, Phys. Rev. B, **49**, 3962 (1994).
3. *P. G. Kresse and J. Furthmuller*, Phys. Rev. B, **54**,11169 (1996).
4. *R. A. Kondrashov, M. V. Mamonova, E. S. Povoroznuk, V.V. Prudnikov,* Lobachevskii Journal of Mathematics, **38**, 5, 940–943 (2017).
4. *V.V. Prudnikov, P.V. Prudnikov, D.E. Romanovskiy* J. Phys. D: Appl. Phys., **49,** 235002 (2016).

Non-equilibrium Critical Behavior of the 3D Classical Heisenberg Model

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Three-dimensional classical ferromagnetic Heisenberg spin systems are traditional models for the study of critical phenomena. One of the features arisen in describing the critical behavior is the critical slowing down effect. It is associated with an anomalous increase of relaxation time t_{rel} in the system close to critical temperature T_c. As a result, a statistical system at the critical point cannot achieve the equilibrium state during the whole relaxation process. The non-equilibrium evolution in this case displays some of the peculiarities, such as aging phenomena and the memory about the initial states, as well as violation of the fluctuation-dissipation theorem (FDT) [1-3].

We present results of Monte Carlo description of features of non-equilibrium critical behavior in three-dimensional classical Heisenberg model with evolution from different initial states. Usually, we can distinguish the high-temperature initial states created at temperatures $T_0 > T_c$ and characterized by the initial magnetization $m_0 = 0$ and low-temperature initial states with $T_0 < T_c$ and $m_0 \neq 0$. Initial states with magnetization $m_0 \neq 0$ give rise to a new time scale $t_m \sim m_0^{-k}$ with the exponent $k > 0$. This time scale produces a pronounced effect on the temporal behavior of magnetization, autocorrelation function, and response function [1, 4]

Study of influence of different initial states with $0 < m_0 \leq 1$ on relaxational properties of model have been carried out. It was established realization of scaling relation for time dependence of magnetization in form $M(t, t_m) = t^{-\beta/(\nu z)} F_m(t/t_m)$, where $F_m(x)$ is the scaling function for magnetization, which has the form $F_m(x) \sim x^{1/k} \sim x^{(\theta'+\beta/\nu z)}$ at the short-time stage with $x = t/t_m \ll 1$, whereas it asymptotically approaches unity, $F_m(x \gg 1) \to 1$, at the long-time stage with $x = t/t_m \gg 1$. Values of dynamical critical exponents z = 2,035(4), θ’ = 0.490(1), and exponent k= 1.340(4) were calculated. These values of exponents are more authentic in comparison with obtained before by another methods (see [5]).

Aging effects have been revealed during study of two-time dependence of the autocorrelation function on different initial states which are characterized by the slowing down in the correlation of the system with the growth of its age t_w. We show that the slowing down of the autocorrelation function during evolution from high-temperature initial state is considerably more slow than for case of evolution from low-temperature initial state. It was established realization of scaling relation for the autocorrelation function in form $C(t, t_w, t_m) \sim t^{-2\beta/(\nu z)} F_C(t/t_w, t/t_m)$, where scaling function $F_C(t/t_w, t/t_m)$ is finite at $t_w \to 0$ and $t/t_m \to 0$. We give graphic presentation of the scaling function dependence on t/t_w for different initial states and calculate an exponents characterizing asymptotical behavior of the scaling function in long-time stage with $t/t_w >> 1$.

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1. *V.V. Prudnikov, P.V. Prudnikov, and M.V. Mamonova*, Phys. Usp., **60**, 762 (2017).
2. *V.V. Prudnikov, P.V. Prudnikov, and E.A. Pospelov,* J. Stat. Mech., **2016**, 043303 (2016).
3. *V.V. Prudnikov, P.V. Prudnikov, E.A. Pospelov, and A N. Vakilov,* Phys. Lett. A **379**, 774 (2015).
4. *P.V. Prudnikov, V.V. Prudnikov, E.A. Pospelov, and P.N. Malyarenko*, PTEP, **2015**, 053A01 (2015).
5. *H.A. Fernandes, R. da Silva, and J.R.D. de Felıcio,* J. Stat. Mech., **2006**, P10002 (2006).

Peculiarities of Non-equilibrium Critical Behavior of Site-diluted 2D Ising Model

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The collective behavior of statistical systems close to critical points is characterized by an extremely slow dynamics with anomalously long relaxation times which diverges as $t_{rel} \sim |T-T_c|^{-z\nu}$ for $T \to T_c$. Therefore, systems do not achieve equilibrium at the critical point in the course of the whole relaxation process. During this out-of-equilibrium stage aging phenomena occurs with two-time dependence of correlation $C(t,t_w)$ and response $R(t, t_w)$ functions characterized by two times: waiting time t_w and observation time $(t - t_w)$ with $t > t_w$ and $t, t_w << t_{rel}$. Non-equilibrium dynamic shows the violation of the fluctuation-dissipation theorem (FDT). It connects the correlation $C(t,t_w)$ and response $R(t, t_w)$ functions by relation: $TR(t,t_w) = X(t,t_w)\partial C(t,t_w)/\partial t_w$. The asymptotic limit $X^{\infty} = \lim_{t_w \to \infty} \lim_{t \to \infty} X(t,t_w)$, which called fluctuation-dissipation ratio (FDR) is an important characteristic of the non-equilibrium stage [1-3].

In analysis of the effect of the initial states of the system on the characteristics of the non-equilibrium critical behavior, we distinguish the high-temperature initial states formed at $T_0 > T_c$ and characterized by initial magnetization $m_0 = 0$ and the low-temperature initial states with $T_0 < T_c$ and $m_0 \neq 0$. Initial states with magnetization $m_0 \neq 0$ leads to a new time scale $t_m \sim m_0^{-k}$ with the exponent $k > 0$, which substantially affects the temporal behavior of the autocorrelation and response functions. Thus, the strong differences in the nonequilibrium critical behavior of systems relaxing from the different initial states necessitate a more detailed description of the effect of the initial value of magnetization [2, 4].

We report the results of Monte Carlo study the influence of different initial states and structural defects on the non-equilibrium critical behavior of the 2D Ising model relaxing from different initial states. The results revealed an important role of different initial values of the magnetization m_0 on the non-equilibrium critical behavior of the 2D Ising model. It has been shown that two universality subclasses corresponding to the evolution of the system from the high-temperature (with $m_0 = 0$) and low-temperature (with $m_0 = 1$) initial states with the values of the asymptotic fluctuation-dissipation ratio typical of these states can be singled out.

We also study the effect of structural defects on the non-equilibrium critical dynamics of the 2D Ising model. It has been revealed that the aging effects increase with the growth of the density of defects. In the structurally disordered systems relaxing from low-temperature initial state we obtain significant slowing down (as compared to pure systems) of correlation effects, which is associated with pinning of domain walls at structural defects. In this case superaging effect occur in the scaling behavior of the autocorrelation function. At the same time, the asymptotic values of the FDR determined by the domain dynamics in the long-term regime equals zero [5]. In the case of relaxing from high-temperature initial state, we obtain that the non-equilibrium critical behavior of weakly disordered systems with spin concentrations $p \geq 0.9$ is described by characteristics of the pure system, whereas for strongly disordered systems non-equilibrium critical characteristics are appreciably dependent on the concentration of defects owing to the crossover effects in the percolation behavior [6].

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1. *P. Calabrese and A. Gambassi*, J. Phys. A. **38**, R133 (2005).
2. *V.V. Prudnikov, P.V. Prudnikov, and M.V. Mamonova*, Phys. Usp., **60**, 762 (2017).
3. *V.V. Prudnikov, P.V. Prudnikov, and E.A. Pospelov,* J. Stat. Mech., **2016**, 043303 (2016).
4. *P.V. Prudnikov, V.V. Prudnikov, E.A. Pospelov, and P.N. Malyarenko*, PTEP, **2015**, 053A01 (2015).
5. *V. V. Prudnikov, P. V. Prudnikov, E. A. Pospelov and P. N. Malyarenko*, JETP Lett. **107**: 569 (2018).
6. *V. V. Prudnikov and O. N. Markov*, Europhys. Lett. **29**, 245 (1995)

Dimensional Crossover in Critical Behavior of Thin XY-films: Equilibrium and Non-equilibrium Properties

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The study of non-equilibrium critical behavior causes considerable fundamental and applied scientific interest. In recent years, particular interest is the study of quasi-two-dimensional systems [1], in particular, the question of the dimensional crossover in the transition from two-dimensional systems to three-dimensional [2]. In the two-dimensional XY model, the long-range order is destroyed by transverse fluctuations of the spin density at all nonzero temperatures [3]. However, this system has a topological Berezinskii-Kosterlitz-Thouless transition at $T = T_{BKT}$ and there is Berezinskii low-temperature phase $T < T_{BKT}$, where all temperatures T are critical points. There is a continuous set of fixed points of the renormalization-group transformation for the two-dimensional case and quasi-long-rage order (QLRO) is presented in system. On the other hand, the critical behavior of the three-dimensional XY-model in vicinity of T_C is described by the fixed point of «ferromagnetic-paramagnetic» phase transition and classical long-range order (LRO) is presented at $T < T_C$ [4].

The present paper presents a studying of the Kosterlitz–Thouless transition in thin films, and we gives an answer of how disappear phenomena which associated with the topological phase when films thickness N is increased. We determined the dependence of the phase transition temperature $T_{BKT}(p)$ as a function of the N. We obtained that in limit $N \to \infty$ the temperature T_{BKT} tends to T_C of three-dimensional XY-model. The obtained dimensional dependencies are in good agreement with the previous theoretical results [4].

We shown that, the spin stiffness $\rho_S(T)$ gradually decreases at the T_{BKT} from the value $\rho_S(T_{BKT}) = 2T_{BKT}/\pi$ ($N = 1$) to the value $\rho_S(T_{BKT}) = 0$ for $N \to \infty$. We revealed that a quantity $\rho_S(T_{BKT})/T_{BKT}$ has a power dependence $N^{-\sigma}$, where $\sigma = 0.875(24)$.

It was investigated the dynamical dependencies of magnetization $m(t)$ and its dispersion $D_m(t)$, second and fourth order cumulants $U_2(t)$ и $U_4(t)$ of magnetization for non-equilibrium relaxation of the system from the high-temperature and low-temperature initial states. We show dimensional crossover from the dynamic scaling dependencies of the two-dimensional XY-model to the classical dependencies of the three-dimensional system.

The reported study was supported by RFBR according to the research projects № 17-02-00279, 18-42-550003, 18-32-00814 and grants MD-6868.2018.2, MK-4349.2018.2 of the President of the Russia. The simulations were supported in through computational resources provided by the Shared Facility Center “Data Center of FEB RAS” (Khabarovsk), by the Supercomputing Center of Lomonosov Moscow State University, by Moscow Joint Supercomputer Center and by St. Petersburg Supercomputer Center of the Russian Academy of Sciences.

1. *V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp. **60**, 762 (2017).
2. *P.V. Prudnikov, V.V. Prudnikov, M.A. Menshikova, et al.,* J. Magn. Magn. Mater. **387**, 77 (2015).
3. *S.E. Korshunov*, Phys. Usp., **49,** 225 (2006).
4. *M. Hasenbusch,* J. Stat. Mech., P02005 (2009).

Disorder Aggregation by Vortices in Non-Equilibrium Critical Annealing of Two-Dimensional XY-model

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A two-dimensional systems with continuous symmetry occupy a special place among low-dimensional systems. It is well known that the long-range order is broken in these systems at any finite temperature. However, the case of the 2D XY-model is characterized by realization of topological Berezinskii–Kosterlitz–Thouless (BKT) phase transition at temperature T_{BKT}. The 2D XY-model is used to describe the behavior and the properties of a whole class of physical systems, in particular, ultrathin magnetic films and planar magnets with easy-plane anisotropy [1]. Despite extensive research [2], the influence of structural disorder on non-equilibrium critical phenomena in the 2D XY-model not finally resolved. Existing works (see ref. in [2,3]) are focused on influence of quenched disorder on critical behavior. The influence of annealed disorder and thermalisation of defects of structure subsystem on critical properties of 2D XY-model is not yet well studied.

The present work is devoted to study of influence annealed disorder on equilibrium and non-equilibrium critical behavior of 2D XY-model. It were investigated spin concentration $p = 0.9, 0.8, 0.7$ and 0.6. It were calculated temperature dependencies of equilibrium thermodynamic quantities, such as energy, magnetization, susceptibility, specific heat, spin stiffness ρ_S, and defects clusters sizes. We obtained that spin stiffness $\rho_S(T > T_S)$ is negative for disordered systems, where $T_S(p)$ is a threshold temperature.

The investigation of non-equilibrium critical relaxation with vortex dynamics are shown that disorder collecting in large clusters in the vicinity of vortices cores. This effect can be called as «disorder aggregation by vortices» and the visualization of disorder configurations (Fig. 1) is clearly demonstrates it. It were investigated features of non-equilibrium growth of large clusters in system also. Revealed effects have a strict connection with the non-equilibrium critical coarsening [4,5].

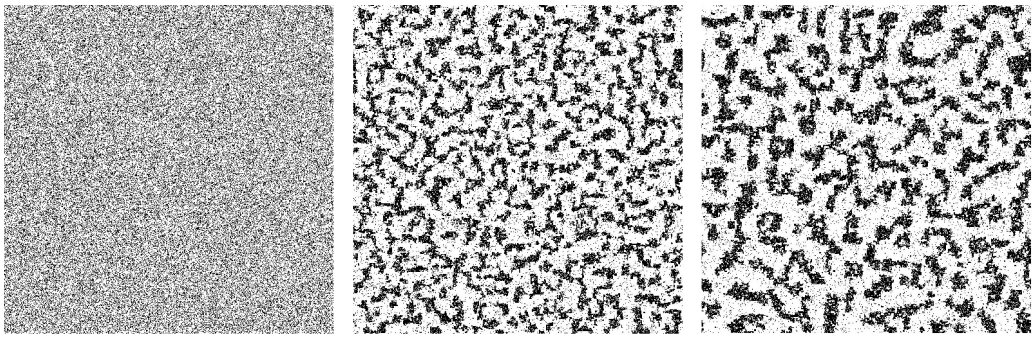

Fig. 1 Snapshot of disorder configurations in process of non-equilibrium critical relaxation for spin concentration $p = 0.8$ and linear size $L = 512$. Time moments $t = 0$, 5000 and 50000 MCS/s (from left to right).

The reported study was supported by RFBR according to the research projects № 17-02-00279, 18-42-550003, 18-32-00814 and grants MD-6868.2018.2, MK-4349.2018.2 of the President of the Russia. The simulations were supported in through computational resources provided by the Shared Facility Center "Data Center of FEB RAS" (Khabarovsk), by the Supercomputing Center of Lomonosov Moscow State University, by Moscow Joint Supercomputer Center and by St. Petersburg Supercomputer Center of the Russian Academy of Sciences.

1. *S.E. Korshunov*, Phys. Usp., **49,** 225 (2006).
2. *V.V. Prudnikov, P.V. Prudnikov, and M.V.ºMamonova*, Phys. Usp., **60**, 762 (2017).
3. *V.V. Prudnikov, P.V. Prudnikov, and I.S. Popov,* JETP **126**, 369 (2018).
4. *P.V. Prudnikov, I.S. Popov,* Solid state phenomena, **233-234**, 8 (2015).
5. *P.V. Prudnikov, I.S. Popov, V.V. Prudnikov,* J. Phys.:Conf. Series, **681,** 012015 (2016).

Acceptance ratios of Monte Carlo simulations with local updates

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We study acceptance ratios of local updates in Monte Carlo simulations of classical spin models. We derive analytic expressions for the expected value of the acceptance ratios of Metropolis and heat bath updates for a one-dimensional Ising model, and find that for the Metropolis updates, the mean value of the acceptance ratio is a linear function of the energy; for the heat bath algorithm, the dependence is close to linear outside of the low temperature range. These analytic expressions are corroborated by numeric simulations. We also report results of numeric simulations of related classical spin models: the two-dimensional Ising model, one- and two-dimensional three- and four-state Potts models, and one- and two-dimensional XY model.

BIFURCATIONS OF ZERO BALANCE STATE IN ONE BOUNDARY-VALUE PROBLEM WITH DEVIATION IN EDGE CONDITION

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Let us consider nonlinear boundary-value problem:

$$u' = \ddot{u} + \gamma u - u^3 \tag{1}$$

with edge conditions

$$u'(0,t) = 0, \tag{2}$$
$$u'(1,t) = \alpha u(x_0,t),$$

where parameters $\alpha, \gamma \in \mathbb{R}$, $x_0 \in [0,1]$. Equally with boundary-value problem (1), (2) let us consider the following system of differential equations

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

which simulates this problem. In this case edge conditions substitute for

$$u_0 = u_1, \tag{4}$$
$$u_{N+1} = u_N + \frac{\alpha}{N}u_k,$$

where $k \in [1,N]$ is determined by value x_0 in edge condition (2).

Our task of research was to find critical values of parameter $\alpha_{cr}(\gamma)$, when in system (3) with conditions (4) the trivial solution of boundary-value problem (1), (2) changes its stability. This task can be researched by two ways. One of these ways consists in the construction of characteristic equation, which can be obtained by means of Euler substitution for boundary-value problem (1), (2). As a result of this substitution there can be given a complicated transcendental equation. For this equation there can be found values α, when all roots are in the left part of complex plane and one pair of them are on the imaginary axis. In this case there will be the loss of stability for trivial solution of boundary-value problem (1), (2). The proof of this location of eigenvalues for linearized equation (1) is quite difficult. So the only way of research consists in the solving of linearized system of ordinary differential equations (3) with conditions (4). For this system values α are selected according to stability or instability of zero balance state.

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

As a result of numerical research there were found areas of values γ and α. For each of these areas there were researched the stability of zero balance state for boundary-value problem (1), (2).

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Keywords: bifurcations, nonlinear boundary-value problem, zero balance state.

Список литературы

[1] S.A. Kashchenko. About bifurcations at small perturbations in a logistic equation with delay // Model. Anal. Inform. Sist., v. 24, №2, pp. 168–185 (2017).

Wang-Landau method and coarse-graining energy spectrum

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We investigate influence of the energy spectrum partitioning on the accuracy of the Wang-Landau method. We transformed energy spectrum of one-dimensional and two-dimensional Ising model by combining 2, 4, 8 and 16 energy levels into one bin. We use exact results for the construction of the modified density of states. We found non-monotone behavior of the deviation of energy and heat capacity at high temperatures. Large level of coarse-graining leads to the large deviations and oscillations of the estimated quantities. Our results may be useful for the choose of the bin size in the simulation of the models with continuous energy spectrum.

Simulation of the entangled states generation of two qubits by using of unipolar picoseconds pulses

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Recently the superconducting circuit quantum electrodynamics is an actively developing field, in which significant progress has been achieved in the manipulation of quantum bits (qubits). One of the interesting directions in this area is the use of new generation of energy-efficient logic family for fast read-out and control of quantum registers [1,2].

In this paper, we are going to study the simplest two qubits register whose transition frequencies are located in the micro- or millimeter ranges, and the times of longitudinal and transverse relaxation are microseconds [1]. It is well known that in this field of quantum logical manipulation usually the Rabi-technique is involved. We propose here a new approach for the implementation of quantum logic which is based on the control of the qubit system by unipolar sub-nanosecond solitary-like pulses of the rectangular shape. Such kind of magnetic field pulses may be generated by fluxons in transmission lines [2]. The analysis was carried out by numerical solution of the master equation for the density matrix operator and the populations of qubit levels were calculated. It was shown that the optimal way to control a system of two qubits can be achieved when two control pulses with proper delay may be applied. Hamiltonian for two coupled flux qubits can be represented as

$$H(t) = -\frac{1}{2}\left(\varepsilon_1(t)\sigma_z^{(1)} + \Delta_1\sigma_x^{(1)}\right)\otimes I^{(2)} - \frac{1}{2} I^{(1)} \otimes \left(\varepsilon_2(t)\sigma_z^{(2)} + \Delta_2\sigma_x^{(2)}\right) - \frac{1}{2} J\sigma_z^{(1)} \otimes \sigma_z^{(2)} \qquad (1)$$

where Δ_i is tunnel splitting in the i-th qubit ($i = 1,2$), $\Delta_2 = \Delta_1 + \delta\Delta$, where $\delta\Delta << \Delta_i$, J is the interaction constant. We used square pulses $\varepsilon_i(t) = A_i\left(\theta(t + t_{in,i}) - \theta(t - t_{off,i})\right)$, where A_i is an amplitude, $t_{in,i}$, $t_{off,i}$ are the turn-on and turn-off times for the pulse, which determine the duration $\tau_i = t_{off,i} - t_{in,i}$. The relaxation dynamics of the system in the Born-Markovian approximation is described by the equation for the density matrix [3].

It is interesting to study the initialization of Bell's states, which are very important for the implementation of two-qubit quantum logic. The Bell states are four specific maximally entangled quantum states for two qubits. In this case, the intermediate states of the qubit system have the same the level populations $W_2(t) = W_3(t) \sim 0.5$. The degree of entanglement (the concurrence) of the individual qubits states is maximal: $C(\rho) \to 1$ [4]. In Fig. 2 it is shown that it is possible to select parameters for the Bell states generation. At the same time, the degree of entanglement reaches its maximum value.

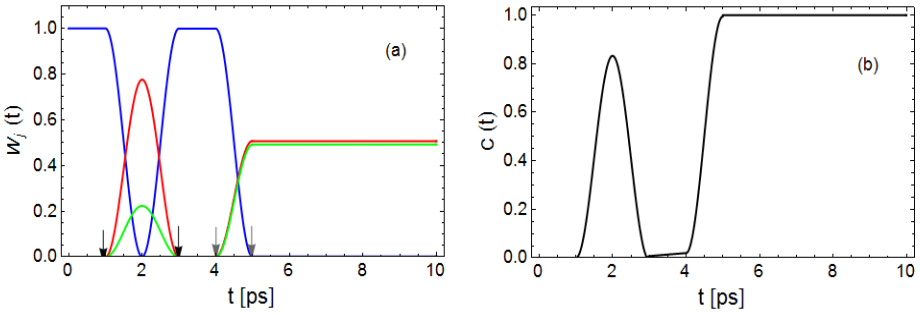

Figure 2. Evolution of the level populations *Wj* of two coupled qubits in the recording of Bell states (a) and the dynamic of the concurrence C(*t*) (b). The blue curve characterizes the behavior of $W_1(t)$, the red curve – $W_2(t)$, the green – $W_3(t)$, the black – $W_4(t)$.

In this paper, we showed that by varying the parameters of such impacts (amplitude, duration), one can realize initialization of the nonlocal entangled states. These ranges of operating parameters were obtained numerically, based on the solution of the master equation. The effects of quantum noise on these manipulations were studied and it was found that decoherence affects only when the duration of the signal is increased (i.e., at times $1/\gamma_i \sim 0.1$ μs). The degree of entanglement (the concurrence) was estimated and it was demonstrated that for Bell states it can be realized with accuracy of up to 98%, and in nonlocal states with an accuracy of 99%.

[1] M. H. Devoret and R. J. Schoelkopf, *Science* **339**, 1169-1174 (2013).
[2] D. V. Averin, K. Rabenstein, and V. K. Semenov, *Phys. Rev.* B **73**, 094504 (2006).
[3] M.O. Scully, M.S. Zubairy. *Quantum Optics* (Cambridge University Press, 1997).
[4] W. K. Wootters, *Phys. Rev. Lett.* **80**, 2245 (1998).

Modeling of heat and mass transfer in drying colloidal drops and films

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This short review deals with the mathematical modeling of heat and mass transfer in drying drops and films on a solid surface. These are open systems with variable mass that are used in various applications. Often, liquids contain dissolved or suspended substances. For example, colloidal particles that are transported by the flow of a liquid that occurs during evaporation. It is possible to control the process by controlling the intensity and non-uniformity of evaporation along the free surface of the liquid layer. This idea lies in the evaporative lithography. For instance, it is possible to influence the character of evaporation by placing a mask or a heat source over the liquid. Mathematical models are needed to learn how to obtain micro- and nanostructures of the desired shape with high accuracy. These models will predict the result depending on the parameters of the system. But first we need to understand the observed phenomena at the conceptual level. The complexity of the systems being studied lies in their nonlinear behavior. Sometimes the process is accompanied by various phase transitions ("liquid–vapor", "sol–gel", "sol–glass", etc.). Physical parameters such as viscosity and others may depend on the temperature of the liquid and the concentration of the particles. There are many approaches to mathematically describe these effects such as discrete, continuum, and semi-discrete models. It is more convenient to use a continuum approach to describe systems of relatively large volume and high concentration. In this case, the model includes the equation of continuity, the equation of motion, the convection-diffusion equation, the heat transfer equation, and the like. There is also a quasi-stationary approach where the flow rate is not time-dependent explicitly. Using the lubrication approximation simplifies some of the equations of the model. The nonlinearities associated with the curvature of the surface disappear. Such approximations are valid for slow evaporation when the two-phase boundary is almost flat (films and thin droplets). Otherwise, we have a complex case with non-stationary equations.

[1] Kolegov K. S. Formation of Ring Structures in a Drying under the Mask Film of Colloidal Solution, Bulletin of the South Ural State University, Series: Mathematical Modelling, Programming and Computer Software, 2014, vol. 7, no. 1, pp. 24–33 (In Russian).
[2] Kolegov K. S., Lobanov A. I. Mathematical Modeling of Fluid Dynamics in Evaporating Drop with Taking into Account Capillary and Gravitational Forces, Vestnik Rossiiskogo universiteta druzhby narodov. Seriya: Matematika. Informatika. Fizika, 2014, no. 2, pp. 375– 380 (In Russian).
[3] Kolegov K. S. Comparison of quasisteady and nonsteady mathematical models of fluid flow in evaporating drop with due regard for the viscosity, Vestn. Udmurtsk. Univ. Mat. Mekh. Komp. Nauki, 2014, no. 3, pp. 110–122 (In Russian).
[4] Kolegov K. S., Lobanov A. I. Comparing of a quasisteady and nonsteady mathematical models of fluid flow in evaporating drop, Computer Research and Modeling, 2012, vol. 4, no. 4, pp. 811–825 (In Russian).
[5] Kolegov K.S. Simulation of Patterned Glass Film Formation in the Evaporating Colloidal Liquid under IR Heating // Microgravity Science and Technology.— 2018.— Vol. 30, No. 1.— P. 113-120
[6] Harris D. J., Hu H., Conrad J. C., Lewis J. A. Patterning colloidal films via evaporative lithography, Phys. Rev. Lett., 2007, vol. 98, no. 14, 148301.
[7] Tarasevich Y. Y., Vodolazskaya I. V., Isakova O. P. Desiccating colloidal sessile drop: dynamics of shape and concentration, Colloid Polym. Sci., 2011, vol. 289, no. 9, pp. 1015–1023.
[8] Barash L. Yu., Bigioni T. P., Vinokur V. M., Shchur L. N. Evaporation and fluid dynamics of a sessile drop of capillary size, Phys. Rev. E, 2009, vol. 79, no. 4, 046301.
[9] Tarasevich Yu. Yu., Vodolazskaya I. V., Sakharova L. V. Mathematical modeling of pattern formation caused by drying of colloidal film under a mask, Eur. Phys. J. E., 2016, vol. 39, no. 2, 26.
[10] Georgiadis A., Routh A. F., Murray M. W., Keddie J. L. Bespoke periodic topography in hard polymer films by infrared radiation-assisted evaporative lithography. Soft Matter, 2011, vol. 7, issue 23, pp. 11098–11102.

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Computer modeling and simulation of electrically charged nano/micro-particles interaction into aqueous solution by the Brownian dissipative dynamics of their atomic counterions ensemble

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On the basis of free energy functional of charged ions and equation of diffusion of ions in self-consistent electric potential, an original method of Brownian dissipative dynamics of ions near electrically charged colloidal micro/nano-particles in aqueous solution or dusty plasma particles in the air is proposed for investigation of ionic atmosphere structure near charged surfaces, and electric interparticle force is calculated ($a<<R$, $|Q|<<|q|$, where a and q are radius and charge of small ion, R and Q are radius and charge of micro/nano-particle).

The average stationary displacement of ions obtained from this method is agreed with the Poisson-Boltzmann (PB) equation. The additional information which is not included in PB equation is the fluctuations of ionic concentration and interparticle force. The dependence of electrostatic energy and entropy of such a system on the distance between the centers of the nanoparticles is determined in the numerical experiments. The obtained results in connection with the ordinary Derjaguin-Landau-Verwey-Overbeek theory and other similar models are considered.

Numerical investigation of the critical behavior of the three-dimensional Ising model near the percolation threshold

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The question of how disorder modifies a phase transition is still not fully resolved, not with standing decades of research. Many issues remain open, even in the case of the ferromagnetic transition in the presence of quenched disorder, from the qualitative nature of the ordered phase near criticality [1,2].

The description of phase transitions is considered to be one of the most complex and urgent problems of statistical physics. The anomalously large and long-lived fluctuations of some thermodynamic quantities observed as the phase transition point approaches are characterized by strong interactions, which creates considerable difficulties in the analytical and experimental investigation of critical behavior. Computer simulation is an independent tool for investigating the abnormal behavior of a second-order phase transition [3,4], as evidenced by the progress in the development of various methods of computer simulation. Therefore, one of the important tasks is the development of computer simulation methods that depend weakly on the effects of critical slowdown.

In recent years, the study of various disordered models near the threshold of impurity percolation has become an actual and interesting problem [5,6]. In this paper we have investigated the critical properties of the Ising model near the percolation threshold. At a concentration close to critical, a cluster appears that connects the opposite sides of the lattice. At the critical concentration $p = p_c$, the largest cluster has a fractal dimension. In the theoretical description of the behavior of such systems, the concentration of defects by a small quantity can no longer be considered. That makes their theoretical description very difficult or even impossible. A Invaded cluster algorithm was proposed in [7], which is much more effective than all previous methods near the impurity percolation threshold.

In this work we investigate the critical behavior of the disordered three-dimensional Ising model with an impurity concentration close to the threshold of impurity percolation on high-performance computing systems.

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The simulations were supported in through computational resources provided by the Shared Facility Center “Data Center of FEB RAS” (Khabarovsk), by the Supercomputing Center of Lomonosov Moscow State University, by Moscow Joint Supercomputer Center and by St. Petersburg Supercomputer Center of the Russian Academy of Sciences.

[1] G. Tarjus and Vik. Dotsenko, J. Phys. A, (2002) 35, 1627.
[2] F. Krzakala, F. Ricci-Tersenghi, D. Sherrington, and L. Zdeborová, J. Phys. A, (2011) 44, 042003.
[3] V.V. Prudnikov, P.V. Prudnikov, A.S. Krinitsyn, et. al., Phys. Rev. E, (2010) 81, 011130.
[4] P.V. Prudnikov, M.A. Medvedeva, Progr. Theor. Phys., (2012) 127, 369.
[5] I. Balog, K. Uzelac, Phys.Rev.E, (2007) 76, 011103.
[6] E. Faraggi, Phys.Rev.B, (2008) 78, 134416.
[7] J. Machta, Y.S. Choi, A. Lucke, T. Schweizer, Phys.Rev.Lett., (1995) 15, 2792.

Characterization of a cluster Monte Carlo algorithm for colloidal suspensions

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The geometric particle cluster algorithm (GPCA) developed in [1] is discussed and the efficiency is analyzed by investigating various cluster size distributions. This algorithm is an extension of the GCA by Herringa and Blöte [2], the cluster algorithm by Dress and Krauth [3] as well as the method by Liu and Luijten [4]. It is capable of efficiently simulating a mixture of spherical colloids immersed in a binary liquid. Near the demixing transition of the medium, the colloidal particles interact via fluctuation-induced critical Casimir forces, that lead to interesting behavior and also has been investigated experimentally recently [5,6]. We present first results obtained in the framework of a recent Bachelor thesis [7].

[1] H Hobrecht and A Hucht, Physical Review E 92 042315 (2015)

[2] JR Heringa and HWJ Blöte, Physical Review E 57, 4976 (1998)

[3] C Dress and W Krauth, J Phys A: Math. Gen. 28, L597 (1995)

[4] J Liu and E Luijten, Physical Review Letters 92, 035504 (2004)

[5] D Bonn et al., Phys. Rev. Lett. 103, 156101 (2009)

[6] MT Dang et al., J. Chem. Phys. 139, 094903 (2013)

[7] J Verlage, Bachelor Thesis, Aug 2018 (submitted)

A COMPUTER SIMULATION OF THERMAL PROCESSES IN WATER BODIES AT DIFFERENT HYDROMETEOROLOGICAL CONDITIONS

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Water reservoirs is the most widely used type of coolers for large enterprises. Their exploitation often meets considerable problems specific for a particular basin. For small cooling basins the problems are associated with the limitation of power station performance related to a rise of the temperature of water taken off from the reservoir and for large coolers the problems are related to thermal pollution, changes in the ice-thermal regime, hydrophysical and hydrobiological processes, especially in the regions of heated water discharge. Key to the solution of a wide range of technological and ecological problems is getting comprehensive and reliable estimates of the parameters of temperature fields generated by these discharges depending on a set of technological and hydrometereological parameters.

In the present work we carry out numerical investigation of these problems using the example of the Magnitogorsk Iron and Steel Plant. This plant is one of the world's largest steel producers and a leading Russian metals company. Warm channel of this plant discharges warm water in the Magnitogorsk reservoir of the Ural River. The study is performed for different technological and hydrometeorological conditions. Since the vertical temperature distribution in such wastewater reservoirs is highly inhomogeneous, the computations should be performed in the framework of 3D model. To adapt the morphological data in a coordinate-depth format to the capabilities of the mesh generator, the reservoir bottom morphology was represented as a set of simple geometrical objects of some specified resolution, which were then introduced into the task batch file.

A code has been written to produce a batch file for grid generator of the ANSYS Fluent package from the data array describing the reservoir bottom morphology. Thus, the complex geometry of the computational domain is realized. The proposed code is of general character and is applicable to the construction of similar geometries and in other tasks. The results obtained in the calculation are the temperature and velocity fields, characteristics of turbulent pulsations at different velocities and qualitative characteristics of the heated water discharge.

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A simple description of turbulent transport in a stratified shear flow devoted to the simulation of thermohydrodinamics of inland waters

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By now, the role of inland water bodies in the processes of general circulation of the atmosphere, the ocean and land, their thermohydrodynamic and biological properties in weather forecasts, and also in climate change has been established. There are classifications of physico-mathematical models of inland water objects both in terms of spatial detailing and in terms of the described processes. 3D and 2D mathematical simulation, widely used in ocean models, is practically not used for lakes and water reservois due to the large computational resources required for these models. The most popular are one-dimensional (vertical) ones that have computational simplicity and acceptable accuracy of temperature, heat fluxes, flow velocity reproduction.

The basis of physico-mathematical simulation of thermodynamics and hydrodynamics of inland waters is RANS (Reynolds-averaged Navier–Stokes equations**)** [1]. Since this system contains unknown quantities (turbulent flows), it is necessary to involve additional hypotheses for its closure. Practically significant is the so-called κ-ε model based on the equations for the kinetic energy of turbulence κ and its dissipation rate ε. In this case, the system of Reynolds equations for the means is closed using gradient hypotheses with turbulent exchange coefficients proportional to the coefficient of turbulent viscosity. The ratio of the coefficient of turbulent viscosity to the coefficient of thermal diffusivity (the turbulent Prandtl number, Pr_T) is assumed to be constant. This, in particular, limits the description of the known effect associated with the existence of turbulence for large Richardson numbers *Ri*. At the same time, both laboratory and field measurements demonstrate the dependence of the Prandtl number on the Richardson number. In this connection, special attention in the simulation of the thermohydrodynamic regime of inland water bodies is paid to stratification and, in particular, to its role in the processes of turbulent mixing, thermocline dynamics, etc. Recently, modernized approaches to the description of geophysical turbulence, taking into account stable and unstable stratification and internal waves, are actively developing.

Authors propose geophysical turbulence models that take into account the two-sided transformation of the kinetic and potential energies of turbulent pulsations, which allow calculating, in particular, the Prandtl number dependence on the gradient Richardson number. In this paper, we present a parametrization of the turbulent exchange coefficient for the κ-ε model in order to take into account stratification in calculating the thermohydrodynamic regimes of inland water bodies.

The work was partly supported by Russian Science Foundation project 15-17-20009 and RFBR project 18-05-00292

References

[1] Monin A.S., Yaglom A.M. Statistical Fluid Mechanics: v. 1 / Moscow: Nauka, 1965. - p. 640.

Structure and Dynamics of Two-Color Random Networks with Tree-Particle Interactions

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We consider equilibrium and relaxation properties of an ensemble of exponential random graphs with vertices bearing a quenched binary variable (color). The cost function (Hamiltonian) of the ensemble implies that there is a three-point interaction between vertices. Namely, it is linear in the number of "triplets" of the same color in the system, i.e. sequences of three vertices of the same color connected with edges, with the cost of a single triplet μ being a parameter of the system.

We start with a completely random dense Erdos-Renyi graph, assign colors to the vertices, and dynamically rewire the graph edges until the equilibrium state is reached. The dynamical rules we use are based on Metropolis algorithm coupled to the cost function described above, they conserve the total number of vertices and edges as well as total degree of each vertex. Two different variations of the dynamic rules are used: the so-called Maslov-Sneppen rules, and a novel generalization of these rules which we propose here in order to avoid dynamical trapping of the system.

In the previous studies of this system it was suggested that there exists a wide range of parameter μ (a so-called plateau) in which the equilibrium number of multicolor edges stabilizes at some non-zero value which is μ-independent. The aim of this work was to study the mechanism responsible for the formation of this plateau, in particular in order to understand whether it is a true equilibrium phenomenon or a result of quenching of the system in some mestastable state. Instead, we have been able to show that the plateau does not actually exist, and in the relevant range of μ the system eventually relaxes to the state where the number of multicolor edges is essentially zero. We show, however, that the relaxation is algebraically slow both in the case of standard Maslov-Sneppen dynamic rules and in the case of generalized rules proposed here. Finally, we discuss possible systems in which Maslov-Sneppen and generalized dynamics may produce different results.

-J. Park and M. E. J. Newman, Solution for the properties of a clustered network, Phys. Rev. E 72, 026136, (2005).

-S. Maslov and K. Sneppen, Specificity and Stability in Topology of Protein Networks, Science, 296, 910 (2002).

-V. Avetisov, A. Gorsky, S. Nechaev, O. Valba, Spontaneous Symmetry Breaking and Phase Coexistence in Two-Color Networks, Physical Review E - Statistical, Nonlinear, and Soft Matter Physics. 2016. Vol. 93. No. 1. P. 012302-1-012302-7 (2016).

Universal Level Statistics of the Out-of-Time-Ordered Operator

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The out-of-time-ordered correlator (OTOC) has been proposed as an indicator of chaos in quantum systems due to its simple interpretation in the semiclassical limit. In particular, its rate of possible exponential growth at $\hbar \to 0$ is closely related to the classical Lyapunov exponent. Here we explore how this approach to quantum chaos relates to the random-matrix theoretical description. To do so, we introduce and study the level statistics of the logarithm of the out-of-time-ordered operator, $\hat{\Lambda}(t) = \ln\left(-[\hat{x}(t), \hat{p}(0)]^2\right)/(2t)$, that we dub the "Lyapunovian" or "Lyapunov operator" for brevity. The Lyapunovian's level statistics is calculated explicitly for the quantum stadium billiard. It is shown that in the bulk of the filtered spectrum, this statistics perfectly aligns with the Wigner-Dyson distribution. Our results show that the Lyapunov operator may serve as a useful tool to characterize quantum chaos and in particular quantum-to-classical correspondence in chaotic systems, by connecting the semiclassical Lyapunov growth at early times, when the quantum effects are weak, to universal level repulsion that hinges on strong quantum interference effects.

High-resolution waves and weather forecasts using adapted WAVEWATCH III and WRF models

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High-resolution waves forecast is in demand for nearshore areas and for inland water bodies. Nowadays wave models (e.g. WAVEWATCH III) are forced mostly with wind field from reanalysis with low resolution. To increase the wind input field resolution, the WRF atmospheric model can be used.

The WRF model was implemented in the area containing a middle-sized water body. The area with Gorky Reservoir was chosen as a control area. WRF simulation was performed for 4 nested domains with min cell size of 1 km. Initial reanalysis was CFSv2 winds. Different surface layer parameterizations and planetary boundary layer parameterizations were tested within WRF: MM5 similarity, Eta similarity, MYNN for Nakanishi & Niino PBL parameterization, and Large Eddy Simulation case. The results were compared with the results of the in-situ measurements held by our group.

The WRF model wind calculation results were used as wind forcing of the WAVEWATCH III wave model. A comparison of the mean wave parameters with the measured in the experiment at the Gorky Reservoir was made.

This investigation will be continued with the attempt of coupled modeling based on the automatic exchange of the calculated ocean and atmosphere parameters.

Computer modeling the self-assembly of colloidal particles into evaporating sessile drop of water-glycerol solution

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The evaporating sessile drop of binary solution is an interesting object of theoretical and experimental investigations due to its important fundamental and practice applications. Recently, the concentration Marangoni driven migration of particles in such a system was experimentally investigated [1] There was experimentally shown that the polystyrene nanoparticles were moved by toroidal vortex flow acted inside a drop, and the direction of this flow depends on solvent components types (ethanol/water, isopropanol/water, metoxypropanol/water), ratio of mixture, particle size and environmental conditions. In such a system, the thermocapillary Marangoni number is much smaller than concentration Marangoni number $Ma_C = \frac{CR}{D\eta}\left|\frac{\partial\sigma}{\partial C}\right|$ (C is concentration of mixture component, R is drop radius, D is diffusion coefficient, η is viscosity, σ is surface tension), so that the concentration gradient is a main origin of Marangoni instability.

In our case, colloidal nanoparticles self-assembly into evaporating sessile drop of binary solvent mixture water-glycerol ($C_3H_5(OH)_3$) deposited on a flat substrate is considered. The components of such a solvent have highly contrasting properties. Under normal conditions, pure liquid water has approximately a 10 000 times higher evaporation rate and viscosity a 1000 times less than pure glycerol has.

Recently, we developed the evaporation model of sessile drop of binary solvent mixture (with infinitely soluble in each other components) based on Hu and Larson solution for single solvent sessile drop and Raoult law for saturated vapor density of components of binary mixture in wide range of unidimensional molar binary concentration of the components. (The Raoult law declares that saturated vapor density of first component has a linear reducing dependence on the percent of second component presence in binary solution if this addition of second one is small enough) [2].

In this report we suggest a new physical model of dissipative particle dynamics (DPD) in drop of binary solvent mixture as a further development of recently elaborated DPD model of self-assembly into evaporating droplet of pure solvent [3] with account of phenomenological results obtained in our experiments. The output data include the trajectories of particles during drop evaporation process. The computer modeling results are compared with the previously mentioned experiments.

[1] E. L. Talbot, A. Berson, L. Yang and C. D. Bain, Internal Flows and Particle Transport Inside Picoliter Droplets of Binary Solvent Mixtures. NIP 29 and Digital Fabrication. Book of Abstracts, 307 – 312 (2013)

[2] P. Lebedev-Stepanov, A. Kobelev, S. Efimov. Evaporation dynamics and Marangoni number estimation for sessile picoliter liquid drop of binary mixture solution/ MATEC Web of Conferences – 2016. – V 84, 22. - P. 1-4.

[3] P.V. Lebedev-Stepanov and K.O. Vlasov, Simulation of self-assembly in an evaporating droplet of colloidal solution by dissipative particle dynamics, Colloids and Surfaces A : Physicochem. Eng. Aspects. 432, 132-138 (2013).

Two-dimensional words entropy calculation method

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Entropy is one of the key metrics in measuring how chaotic the considered system is. In this presentation, a new developed method for entropy calculation is being presented. Because of the original problem statement and imposed constraints, the method's application is limited to the cases where the system states are being represented as square matrices consisting of elements in an alphabet of fixed size. Both the original problem and a step-by-step method evolution will be presented and discussed, informing the listeners on encountered pitfalls and used bypassings.

The method was developed by the authors of [1] for the rod like particles' self-organization process analysis and was successfully implemented and used. Method's main idea is based on counting the appearance frequency of the unique configurations in each considered system state during the whole self-organization process. Configuration is defined as a multiset of two-dimensional words, calculated by shifting the square window of fixed size through the original matrix.

Some of the pitfalls mentioned above included the organization of effective calculations and reusing previous ones in order to minimize the computational costs and memory consumption. Effective ways of storing intermediate data mentioned here [2] are also going to be briefly discussed and explained.

References

[1] Mikhail V. Ulyanov, Yuri G. Smetanin, Mikhail M. Shulga, Andrei V. Eserkepov, Yuri Yu. Tarasevich Characterisation of diffusion-driven self-organisation of rodlike particles by means of entropy of generalised two-dimensional words // arXiv:1809.00447 [cond-mat.stat-mech]

[2] Smetanin, Yuri, Mikhail Uljanov, and Mikhail Shulga. "On Calculating the Entropy of 2D Words Over a Finite Alphabet." *2018 International Conference on Engineering Technologies and Computer Science (EnT)*. IEEE, 2018.

Ab initio calculation of multilayer magnetic structures by VASP on OpenPOWER high perfomance system

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The behaviour of multilayer magnetic structures has become of great technological importance due to the applications in magnetic storage devices. The *ab initio* calculations are widely used to calculate some characteristics of solids [1] and multilayered magnetic structures [2]. The main advantage of *ab initio* approach is independence on experimental data. Unlike the case of semi-empirical methods, there is no need for calibration or fitting parameters. Thus, *ab initio* methods can also be used to calculate the characteristics of perspective systems, i.e., for prediction of properties of materials that have not yet been developed. Mainly used packages that can perform *ab initio* calculations are VASP [3], Quantum Espresso [4], ABINIT [5]. High perfomance systems should be used for complex materials modelling with large amount of atoms in supercell.

In this paper we calculated energy and magnetic characteristics for multilayer Co/Cu[100] ferromagnetic structure by VASP on POWER architecture. We analysed perfomance of VASP package on the OpenPOWER high perfomance system with several Pascal P100 GPU units in compare with calculation on POWER8 CPU only and on system with Intel architecture. We revealed that the VASP calculations achieve maximum perfomance on OpenPOWER System with the GPUs.

We would like to thank the IBM experts, who help us to optimize VASP package for IBM Power Systems S822LC. This research was supported by the grants 17-02-00279, 18-42-550003 of Russian Foundation of Basic Research and by the grant MD-6868.2018.2 of the President of the Russian Federation. The simulations were supported by the computational resources of Shared Facility Center "Data Center of FEB RAS" (Khabarovsk) [6]. Computations were performed with the methods and techniques, which were developed under the RFBR scientific project number 18-29-03196.

1. K. Lejaeghere, G. Bihlmayer, T. Björkman, et al., Reproducibility in density functional theory calculations of solids // Science – 2016 –V. 351 – aad3000 doi:10.1126/science.aad3000

2. R.A. Kondrashov, M.V. Mamonova, E.S. Povoroznuk, V.V. Prudnikov, First-principles investigations of the atomic structure and magnetic properties of Ni and Co films on Cu substrate // Lobachevskii Journal of Mathematics – 2017 – V. 38, P. 940–943. doi:10.1134/s1995080217050225

3. G. Kresse, J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set // Phys. Rev. B – 1996 – V. 54, P 11169-11186. doi:10.1103/PhysRevB.54.11169

4. P. Giannozzi, S. Baroni, N. Bonini, et al., QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials // J. Phys.: Condens. Matter – 2009 – V. 21, P. 395502 doi:10.1088/0953-8984/21/39/395502

5. X. Gonze, B. Amadon, P.-M. Anglade, et al., ABINIT: First-principles approach to material and nanosystem properties // Comput. Phys. Commun. – 2009 –V. 180, P. 2582-2615 doi:10.1016/j.cpc.2009.07.007

6. A.A. Sorokin, S.I. Makogonov, S.P. Korolev, The Information Infrastructure for Collective Scientific Work in the Far East of Russia // Scientific and Technical Information Processing. – 2017. – V. 4, P. 302-304. doi:10.3103/S0147688217040153

Fluid flow structures in an evaporating droplet depending on ambient temperature and properties of liquid and substrate

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We investigate numerically quasi-steady internal flows in an evaporating sessile droplet. We jointly take into account the hydrodynamics of an evaporating sessile drop, effects of the thermal conduction in the drop, and the diffusion of vapor in air. The equations have been solved by finite element method using ANSYS Fluent.

Temperature distributions and the corresponding vortex structures in evaporating sessile droplets are obtained. The ‘‘phase diagrams’’ containing information on the number and orientation of the vortices depending on the ratio of substrate to fluid thermal conductivities and the contact angle, are presented and analyzed for different values of ambient temperature and for liquids of different volatility.

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Percolation and jamming of random sequential adsorption samples of large linear k-mers on a square lattice.

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We study behavior of percolation and jamming thresholds for isotropic random sequential adsorption samples by means of numerical simulations. The model with large linear k-mers on a square lattice with periodic boundary conditions is considered. We present a parallel algorithm which is very efficient in terms of speed and memory usage. We investigate the structure of the percolating and jamming states. We generalize the results of [1] for the case of periodic boundary conditions and obtain the ratio of percolation and jamming concentrations for lengths of k-mer up to 2^{17}.

[1] G. Kondrat et al., Phys. Rev. E 96, 022154 (2017).

Numerical study convex regularizations of Darcy law in the case of Rayleigh-Taylor instability

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We study problems of filtration of two immiscible liquids. We construct numerical algorithms to solve regularization for the Muskat problem and a problem of filtration of a stratified fluid with the Rayleigh-Taylor instability. Our numerical algorithms satisfy to the conservation laws. We present the results of numerical simulation of problems understudy.

Monte Carlo Simulation of Amorphous Magnets with Random Exchange Interactions

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Amorphous alloys based on rare-earth metals are of great interest due to their unique magnetic properties. In this work we report on the Monte Carlo simulation of magnetic properties of binary amorphous alloys of rare-earth metals with nonmagnetic 5d-transition metal (rhenium) which are not studied so far.

Using the Monte Carlo method within the frame of the Heisenberg model, the computer simulation of magnetic properties of pure amorphous Gd and Re-Gd amorphous alloys was performed. The model Hamiltonian contained two terms responsible for ferromagnetic exchange interaction J_1 between the nearest-neighbour Gd ions and for antiferromagnetic exchange interaction J_2 between the Gd ions in the second coordination sphere.

For pure amorphous Gd the dependence of the spin-glass transition temperature T_f on the J_1/J_2 ratio was calculated. Thus, the magnetic phase diagram for an amorphous magnet with competition of exchange interactions of different signs in the $J_1/J_2 - T$ coordinates was constructed.

In the models of the Re-Gd amorphous alloys, the spin-glass-like phase transition was also observed. With increasing concentration of Tb atoms, the transition temperature linearly increases, which is in a good agreement with the experimental results. The spin-glass transition is observed only above the percolation threshold in this system, i.e. at x>7 at. % Gd.

The temperature dependencies of spontaneous magnetization, Edwards–Anderson order parameter and magnetic susceptibility were calculated. The magnetic phase diagrams for the Re-Gd amorphous alloys were constructed which were in a good agreement with the experimental results. The magnetization curves, hysteresis loops, remanent magnetization, coercive field, spin-spin correlation functions at different temperatures are also calculated.

The magnetization relaxation after switching off the external magnetic field was studied. Our results qualitatively agree with the experimental results obtained for amorphous alloys based on rare-earth metals.

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

A variational lower bound on the ground state of a many-body system and the squaring parametrization of density matrices

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Abstract. A variational *upper* bound on the ground state energy E_{gs} of a quantum system, $E_{\mathrm{gs}} \leq \langle\Psi|H|\Psi\rangle$, is well-known (here H is the Hamiltonian of the system and Ψ is an arbitrary wave function). Much less known is the variational *lower* bound on the ground state of a many-body translation-invariant lattice system with the Hamiltonian $H = \sum_{i=1}^{N} h_i$, where local terms h_i can be obtained from h_1 by translations (and rotations, for lattices in two and three dimensions). This bound reads $E_{\mathrm{gs}} \geq N \min\limits_{\rho\in\mathbb{M}} \operatorname{tr} h_1\rho$, where $\mathbb{M}$ is some wisely chosen set of reduced density matrices ρ. The implementation of this latter variational principle is hampered by the difficulty of parameterizing the set $\mathbb{M}$, which is a necessary prerequisite for a variational procedure. The root cause of this difficulty is the nonlinear positivity constraint $\rho > 0$ which is to be satisfied by a density matrix. The squaring parametrization of the density matrix, $\rho = \tau^2/\operatorname{tr}\tau^2$, where τ is an arbitrary (not necessarily positive) Hermitian operator, accounts for positivity automatically. We discuss how the squaring parametrization can be utilized to find variational lower bounds on ground states of translation-invariant many-body systems. As an example, we consider the Heisenberg model of spins 1/2 in one and two dimensions.

References

[1] Nikolay Il'in, Elena Shpagina, Filipp Uskov, Oleg Lychkovskiy. Squaring parametrization of constrained and unconstrained sets of quantum states, J. Phys. A: Math. Theor. 51, 085301 (2018).

Computer simulation of algorithms for solving the Unilateral Matrix Polynomial Problem: average-case complexity estimation

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

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

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

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

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

The (Decisional) Unilateral Matrix Polynomial Problem (DUMP Problem) is given UMP $\mathcal{F}(X)$ to decide whether it has at least one solvent.

The work studies three algorithms for finding solvents: two λ-matrix based and exhaustive search one.

The computational experiments investigated the behavior of the algorithms for samples of the problem with matrix dimensions 2..8, degrees 2..10 and basic fields $\mathbb{F}_2, \mathbb{F}_3, \mathbb{F}_5$, and $\mathbb{F}_7$. In all cases we estimated the exact number of atomic operations needed to decide the sample of the problem.

The studies show that the number of atomic steps needed to solve the samples of the problem was exponential from matrix dimension and from the degree in average. This potentially makes the DUMP problem interesting for computer security because it's potentially hardness for quantum computers.

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Hegselmann-Krause model of opinions dynamics of interacting agents with the random noises

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We consider the Hegselmann-Krause bounded confidence model of opinion dynamics (the HK-model). We assume that the opinion of an agent is influenced not only by other agents, but also by external random noises. The case of independent normally distributed external noises is considered.

Computer modeling of deterministic and stochastic models was carried out. The properties of the models were analyzed and the difference in their behavior was revealed. We define of a confidence cluster for the stochastic model. We analyze the dependence of the number of clusters on the parameters of the problem such as the initial profile of opinions, the level of confidence, the variance of noise.

Modeling of heating in the epitaxial structure $Cd_xHg_{1-x}Te/CdTe$ a projection by the least squares method

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In work contains the results of use of the modified projective method of the least squares for modeling of unsteady heat conduction in epitaxial structure of infrared techniques $Cd_xHg_{1-x}Te/CdTe$, exposed a short laser pulse. The solution is in the form of partial sums of double Fourier series on polynoms Jacobi-Laguerre. Earlier works [1], [2] was held and discussed computing sustainability the proposed us of the modified projection method of least squares scheme for one-dimensional modeling and spatial distributions of nonequilibrium minority charge carriers, generated by external influence, after their diffusion in the semiconductor materials, and in the work [3]- the Galerkin projection method to solve stationary diffusion equation of modified Laguerre functions. This paper continues such studies: the estimate of the projection scheme of the least squares method used to calculate temperature field in epitaxial structure $Cd_xHg_{1-x}Te/CdTe$.

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1. *Seregina E.V., Stepovich M.A., Makarenkov A.M.* // J. Surf. Invest.: X-Ray, Synchrotron and Neutron Tech. 2013. V. 7. No. 6. P. 1077.

2. *Seregina E.V., Stepovich M.A., Makarenkov A.M.* // J. Surf. Invest.: X-Ray, Synchrotron and Neutron Tech. 2018. V. 12. No. 1. P. 80.

3. *Makarenkov A.M., Seregina E.V., Stepovich M.A.* // Comput. Math. Math. Phys. 2017. V. 57. No. 5. P. 802.

Conditions for quantized transport in the Thouless pump

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Abstract. The topological Thouless pump [1] is a quantum device which transfers charge in a quantized manner by performing a cycle in the parameter space of its Hamiltonian. The simplest model of the Thouless pump is the integrable Rice-Mele model describing N fermions on a one-dimensional lattice. In the original paper by Thouless, ref. [1], the quantization was proved under the assumption of adiabaticity, however, the adiabatic conditions were not discussed. A *necessary* adiabatic condition for the Rice-Mele model proven in ref. [2] stated that the cycle duration, T_N, should scale with the system size at least as fast as $\sqrt{N}$ in order to maintain adiabaticity. Here we point out that in fact the *necessary and sufficient* condition for adiabaticity is even more restrictive, $T_N = O(N)$.

Quite remarkably, the quantization is not necessarily broken simultaneously with the many-body adiabaticity. While the genuine many-body adiabaticity is sufficient for the quantization of transport [1], it may not be really necessary. In fact, two distinct modes of operation of the pump realized by the Rice-Mele model should be distinguished [2]. The first mode is a continuous one, when the pump performs one cycle after another, approaching a stationary state. In this mode the genuine many-body adiabaticity is indeed mandatory for quantization of the transferred charge per cycle. The second mode can be called a transient one: One measures the transferred charge immediately after a single cycle is completed, and then initiates the pump back in its ground state (such initialization requires some sort of external cooling). In this latter mode the quantization is present even when the many-body adiabaticity has gone completely. What is required instead is local adiabaticity independent on the system size [3].

If the Thouless pump is described by a non-integrable model, the elementary excitations propagate diffusively, not ballistically. We discuss how this fact modifies the time scale at which the quantization can be maintained despite the breakdown of many-body adiabaticity.

[1] DJ Thouless. Quantization of particle transport. *Physical Review B*, 27(10):6083, 1983.
[2] Oleg Lychkovskiy, Oleksandr Gamayun, and Vadim Cheianov. Time scale for adiabaticity breakdown in driven many-body systems and orthogonality catastrophe. *Phys. Rev. Lett.*, 119(20):200401, 2017.
[3] Sven Bachmann, Wojciech De Roeck, and Martin Fraas. The adiabatic theorem for many-body quantum systems. *Phys. Rev. Lett.*, 119:060201, 2017.

AN INFLUENCE OF DIFFERENCE OF SURFACE PROPERTIES ON AXISYMMETRIC VIBRATIONS OF AN OBLATE DROP IN AN AC FIELD

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Our work continues a series of papers devoted to the study of electrowetting-on-dielectric (EWOD) [1,2]. We are considering the forced oscillations of the incompressible fluid drop under the action of the non-uniform electric field. This electric field acts as an external force that causes motion of the contact line. The equilibrium form of drop has the form of a cylinder bounded axially by the parallel solid planes and the contact angle is right. We investigate the case of different uniform plates as district from other works [1,2], i.e. the plates have different surface (wetting etc.) properties. In order to describe this contact line motion, the modified Hocking boundary condition [3] is applied: the velocity of the contact line is proportional to the deviation of the contact angle and the speed of the fast relaxation processes, whose frequency is proportional to twice the frequency of the electric field [1,2]. The proportionality coefficient (Hocking's parameter) for each surface is different. This condition leads to damping of the oscillations, which is explained by the interaction of the contact line with a solid surface.

The solution of the problem is written as a Fourier series in eigenfunctions of the Laplace operator. The resulting system of heterogeneous equations for unknown amplitudes was solved numerically.

It is shown that, firstly, the even and odd modes spatial modes exist because of different plates. Secondly, the heterogeneity of the electric field leads to the excitation of azimuth modes.

Amplitude-frequency characteristics are plotted for different values of the parameters of the problem. For small values of the Hocking parameter, i.e. with strong interaction energy between the contact line and plate, the oscillations amplitude is small. In opposite case, the resonance amplitude of the surface forced oscillations is large and tends to infinity in the limit of fixed contact angle. Also the dynamic forms of the drop were calculated.

The deviations of the contact angle as a function of the square root of the effective amplitude are given for different Hocking parameter and field frequency. The responses obtained qualitatively agree with the experimental data.

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References

1. Alabuzhev A.A., Kashina M.A. The oscillations of cylindrical drop under the influence of a nonuniform alternating electric field // J. Phys.: Conf. Ser. 2016. V. 681, 012042.
2. Kashina M.A., Alabuzhev A.A. The dynamics of oblate drop between heterogeneous plates under alternating electric field // Microgravity Sci. Technol. 2018. V. 30, Iss. 1–2. P. 11–17
3. Hocking L. M. Waves produced by a vertically oscillating plate // J. Fluid Mech. 1987. V. 179. P. 267–281.

On the Possibility of a Numerical Solution of the Heat and Mass Transfer Problem Jointly by the Matrix Method and the Method of Generalized Powers of Bers

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In this paper, we consider some possibilities for the joint use of the matrix method and the method of generalized powers of Bers ([1], [2]) for the numerical solution of the heat and mass transfer problem by solving the problem of diffusion of minority charge carriers generated by a wide electron beam in a semiconductor target. Initially, the matrix method under consideration was used by us for the analytical solution of the problem of heat and mass transfer in a homogeneous or multilayered medium with shear, axial or central symmetry for an arbitrary number of layers [3]. Such a generality of the method is achieved due to the application of the apparatus of generalized powers of Bers, which makes it possible to obtain a solution for all the above types of symmetries of the medium in a single analytical form. Simulation is reduced to the sequential multiplication of second-order functional matrices whose components at each point are determined by the physical and geometric parameters of the current layer. The main advantage of the matrix method is that it can be used for any number of layers. It is this property of the method that makes it possible to consider of its application as a numerical one if it is artificially to split the medium into many layers.

The relative error in the computations was estimated at a uniform norm beside the analytical solution. The errors obtained at different electron beam energies and different number of mesh point were from 0.8% to 2.9%.

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1. *Bers L, Gelbart A.* // Transactions of the American Mathematical Society. 1944. Vol. 56. No. 1. P. 67-93.

2. *Gladyshev Y.A.* Metod obobshchyonnyh stepeney Bersa i yego prilozheniya v matematicheskoy fizike (Method of Generalized Powers of Bers and Its Applications in Mathematical Physics). Kaluga: Tsiolkovsky Kaluga State University, 2011, 204 p.

3. *Gladyshev Y.A., Kalmanovich V.V., Stepovich M.A.* // Journal of Surface Investigation: X-Ray, Synchrotron and Neutron Techniques. 2017. Vol. 11. No. 5. P. 1096-1100.

A Consensus Problem in Networks with Unreliable Nodes

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We consider a stochastic consensus problem in networks with unreliable nodes. We develop a new stochastic model in which some nodes can break down and repaired after some random time. Breakdowns and repairs are assumed to form an alternating process. To study the model behavior we use the theory of alternating renewal process. Under some conditions, we prove the model convergence.

Using the computer simulations we analyze the network dynamics. We study the dependence of the consensus value on the model parameters.

Direct numerical simulation of bag-breakup – mechanism of sea spray generation in strong winds

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In [1] the mechanisms of spray generation under hurricane winds were experimentally studied and it was found that for friction velocities u* > 1 m/s (at wind speeds at 10 m height exceeding 20 m/s), bag-breakup determines the contribution to the formation of large drops.

For the direct numerical simulation of the bag-breakup phenomenon, the Gerris software package was used [2, 3]. In Gerris a numerical algorithm is implemented that solves the Navier-Stokes equations for incompressible media with variable density and surface tension.

As an initial configuration for numerical simulation a drop of liquid was placed in the air flow. It was shown [4] that the droplet destruction mechanism depends on the Weber number characterizing the system $We = \frac{\rho_a v^2 D}{\sigma}$, where ρ_a – the external medium density, v – the external medium velocity, D – the initial diameter of the drop, σ – the surface tension.

A drop of water with a diameter of 1 cm (the characteristic size of the perturbation from which the bag arises) placed in the air stream at a speed of 20 m/s corresponds best to the experimental situation, such a system is characterized by the Weber number We = 54.

Modeling the dynamics of two media with very different densities, such as water and air, require a lot of computational time, so we used liquids that differ in density by a factor of 10, but to maintain the same Weber number, we changed the value of external the medium velocity.

The calculation was carried out with preservation of the Ohnesorge number, which determines the Weber numbers, under which there is a transition from one droplet destruction regime to another, and also with the preservation of the Reynolds number and the Reynolds number reduced by a factor of 10. In our simulation just as in an experiment under the action of an air stream a drop is blown into a micro-sail that bursts to form a micro-spray. As the Reynolds number decreases (with increasing viscosity of both media), the lifetime of the bag increases, in addition, the process of separating the droplets from the edge of the film changes.

Acknowledgments

Carrying out experiments themselves was supported by Russian Science Foundation (Agreement No. 14-17-00667); designing of methods of measurements including: optical and visualization scheme, methods of measurements of the air flow and wave field parameters were supported by Russian Foundation of Basic Research (No 18-55-50005, 18-05-60299, 16-05-00839); the development of the software for video processing was supported by the Grant of the President no. MK-2041.2017.5.

References

1. *Yu. Troitskaya, A. Kandaurov, O. Ermakova, D. Kozlov, D. Sergeev, S. Zilitinkevich,* 2017. Bag-breakup fragmentation as the dominant mechanism of sea-spray production in high winds. *Sci. Rep.* 7: 1614.
2. *Popinet, S.,* 2003. Gerris: a tree-based adaptive solver for the incompressible Euler equations in complex geometries. *J. Comput. Phys.* 190: 572–600.
3. *Popinet, S.,* 2009. An accurate adaptive solver for surface-tension-driven interfacial flows. *J. Comput. Phys.* 228: 5838–5866.
4. *Pilch, M., Erdman, C.A.,* 1987. Use of breakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop. *Int. J. Multiphase Flow* 13 (6): 741–757.

Wind waves modeling under hurricane wind conditions

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Tropical cyclones and hurricane phenomena directly affect the lives of people in coastal areas and can cause destruction. Good weather and sea state forecasts will make it possible to secure the population and minimize losses from such natural phenomena.

Nowadays wave forecasts are made mainly with the help of numerical wave models, e.g. WAVEWATCH III. The model solves numerically the Hasselmann equation in presence of many physical effects such as wind input, dissipation, nonlinear interactions and many others. The trial simulation of the waves generated by hurricane is implemented within WAVEWATCH III on three nested domains with grid spacing of 50 km, 15 km and 5 km, respectively. The results of the calculation of the singnificant wave height Hs show the movement the waves under hurricane conditions and the azimuthal displacement of the waves distribution. Calculated spectra in the region of high values of Hs are analyzed when different wind wave interaction parameterizations are switched on.

The CFSR reanalysis wind field from the real-case condition of the Irma hurricane that took place in the 31/08/2017 - 13/09/2018 was used as the wind forcing for WAVEWATCH III model. Wave parameters under Irma hurricane were calculated. The spectra of surface waves created by the hurricane allowed the evaluating the function of generating sprays according to empirical formulas.

COMPUTATION OF DIELECTRIC PROPERTIES OF NANO-PROBE LOCAL SURROUNDING BY SOLVATOCHROMIC SPECTRAL SHIFT MEASUREMENT OF ORGANIC DYE MOLECULE

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Computer modeling of the dielectric properties of the cucurbit [7]uril (CB[7]) cavity based on the Onsager-Liptay model [1] was carried out by analyzing the solvatochromic shift of the absorption spectrum of 1- (3-ammoniumpropyl) -4 - [(E) -2- (3,4-dimethoxyphenyl) ethynyl]pyridinium (D1) upon the formation of the inclusion complex with CB[7] in a water solution. The CB[7] cavity was considered as a polar environment into which the dye chromophore is placed. [2] Positions of the maxima of the dye absorption spectra were measured experimentally in the following solvents: methanol, ethanol, i-propanol, n-butanol and water with known dielectric and optical properties. These values were used for parametrization of the Onsager-Liptay equation. Quantum-chemical method of the combined cluster available in the Gamess-US software package was used to calculate molecular structures, dipole moments of the ground and excited states, and polarizability [2]. Original program that calculate effective molecule volume according to Van der Waals atom radii was developed to calculate the volume of dye molecule.

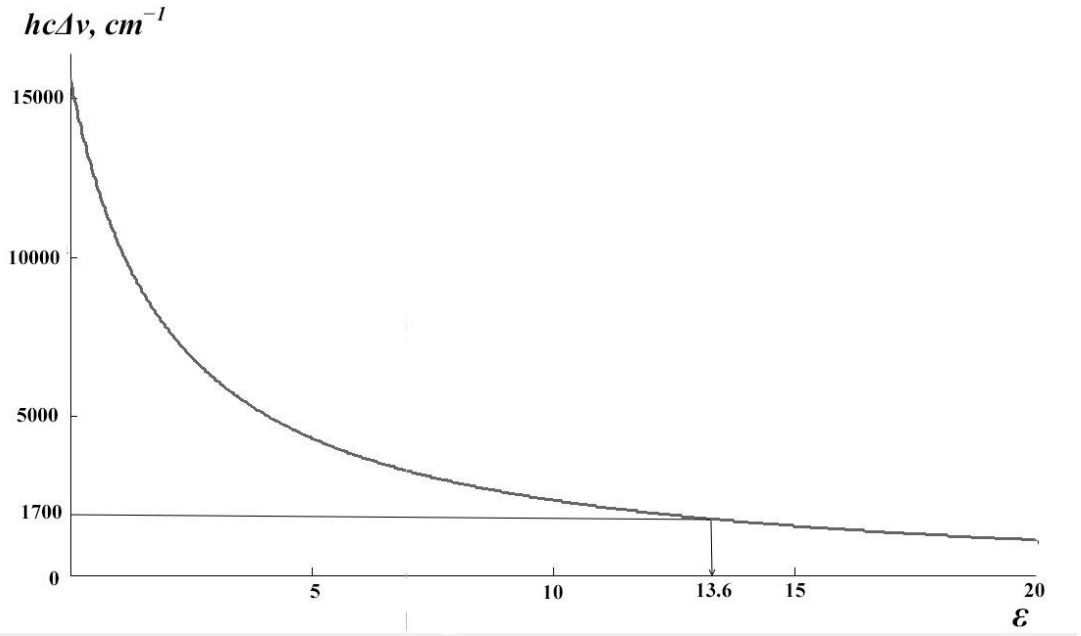

Fig. 1. Determination of the effective permittivity of the cavity of CB [7] based on the theoretical dependence of the solvatochromic shift on ε

Theoretical value of the effective dielectric permittivity of the cavity (≈13.6) is in good agreement with the literature data derived by another method. [4] Thus, we propose a new method for estimating the dielectric properties of a host molecule in a supramolecular inclusion complex according to the experimental shift of the dye molecule optical absorption spectrum due to formation of the inclusion complex with CB[7].

1. Liptay W., Sinanoglu O. (Ed.), Modern Quantum Chemistry, Part II: Interactions, Academic Press, New York, 1965. P. 282. (Chapter5).
2. Avakyan V.G, Stepko A.S. Lobova N.A., Grushnikova E. Y., Sazonov S.K/., Gromov S.P.., Plotnikov V.G.., Lebedev-Stepanov P.V.// Doklady Physical Chemistry2017. V.476 № 4 P. 406-409.
3. Christiansen O.,Koch H.,Jorgensen P. // Chem.Phys.Lett. 1995. V. 243. № 5–6. P. 409-418.
4. Khaleel I. Assaf and Werner M. Nau// Chem. Soc. Rev., 2015. V. 44. P. 394-418.

Mobile application for conducting interactive lectures on data processing

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Currently traditional passive lectures are replaced by lectures in interactive form. Interactive lecture is a form of teaching involving continuous interaction of the participants in the process under the teacher control. This lesson allows you to solve many problems that occur during traditional lectures.

Computer technology is one of the key elements of effective interactive lectures. And since the concept of the interactive lectures is becoming more common, complex hardware and software are developing. However, approach of conducting interactive lecture using computers has significant weaknesses. First of all it is the cost of equipment. Another problem is that the participants attached to the workplace, i.e. deliberately deprived of the movement possibility during operation, which can become a significant inconvenience. In this case, the solution may be found in a mobile technologies.

Despite the obvious and significant benefits, mobile learning is quite underdeveloped in the Russian Federation, although the first steps for the implementation of mobile technologies in education has already been done.

It may be noted that currently actively developing direction and disciplines associated with the data processing (machine learning, Big Data, etc.). Thus, the question remains open about the use of hardware and software for conducting interactive lectures in these subjects. In particular, existing software practically allows you to interactively carry out the study of the foundations of mathematical statistics and data processing with the direct participation of the whole group of students.

The aim of this work is to develop a mobile application for an interactive lectures on mathematical statistics and data processing. The aim is to involve all the students in the process of carrying out the assigned experiment and data collection.

In addition to develop mobile applications for smartphones and tablets for students, an application in Python for the lector's computer is developed. Using mobile application we collect data, for example, obtained as the result of any experiment. This data is sent to the server, then on the lector's computer they are read, analysed and visualized by the application.

The developed mobile application contains 4 tabs: "Survey", "Statistics", "Data processing" and "Monitoring". On the "Survey" tab there are elements that allow you to send to the server the results of any students survey and polls during lectures. On the "Statistics" tab there are elements which allow to send to the server from each student numeric values, which further are used to calculate the statistics of this sample of students. On the "Data processing" tab there are elements through which you are sending to the server the values of the predictors and the predicted variable from each student. On the "Monitoring" tab there are elements with the help of which the control of the assimilation of the examined material by students is carried out by answering the questions posed in the form of a test.

We propose the following stages of the interactive lectures on the fundamentals of regression analysis and data processing. Let the task of lesson is to identify a possible dependence of an average score for exams on the student's IQ level and an average number of hours spent preparing for the exam. In the lesson, work with applications is as follows.

1. Students open the application installed on their mobile devices, go to the tab "data processing".
2. The lector explains the task, the revealed dependence, independent variables (predictors), dependent (predicted) variable. After that, students enter the values of their IQ level, the average number of hours spent preparing for the exam and the average score for the exams. After clicking the "submit" button the entered student data is sent to the server.
3. The lector starts the application on the computer, runs a command that downloads from the server the data entered by the students. He selects the regression model.
4. The macro performs the calculation and visualizes data and results of their processing at every step. The lector commented on each step of the program. As a result, the screen displays the selected regression model, as well as information explaining the calculation of regression coefficients. For example, in the case of simple linear regression, the screen displays estimates of the regression coefficients using the method of least squares.
5. Students are asked to change the values in order to demonstrate the other results of analysis with different variations of data.
6. If necessary, students perform survey on the "survey" tab or work with statistical information on the "Statistics" tab.
7. Students go to the tab "Monitoring" and perform the test.

Stationary Schrodinger equation with density matrices instead of wave functions

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Abstract.

The stationary Schrödinger equation (SSE) can be cast in the form $H\rho_E = E\rho_E$, where H is the system's Hamiltonian and ρ_E is the system's density matrix. We explore the merits of this unconventional form of the SSE, which we refer to as SSE_ρ. For a nondegenerate energy level, ρ_E is merely a projection on the corresponding eigenvector Ψ_E. However, in the case of degeneracy ρ_E in non-unique and not necessarily pure. In fact, it can be an arbitrary mixture of the degenerate pure eigenstates. Importantly, ρ_E can always be chosen to respect all symmetries of the Hamiltonian, even if each pure eigenstate in the corresponding degenerate multiplet spontaneously breaks the symmetries. This and other features of the solutions of the SSE_ρ can prove helpful by easing the notations and providing an unobscured insight in the structure of the eigenstates, as we demonstrate for several exemplary spin systems. Eigenvalue problem for quantum observables other than Hamiltonian can also be formulated in terms of density matrices. We provide an analytical solution to one of them, $\mathbf{S}^2\rho_S = S(S+1)\rho_S$, where $\mathbf{S}$ is the total spin of N spins 1/2, and ρ_S is chosen to be invariant under permutations of spins.

Local spin exchange dynamics in random networks and graph partitioning

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We considered an equilibrium local spin exchange dynamics for the Ising model on random networks that conserves total magnetization. At low temperatures the dynamics was found not to thermalize due to the trapping of the system in particular regions of the phase space. The ground state corresponds to network partitions with a minimal number of cut edges for a given size of the cut networks, corresponding to the total magnetization value. Parallel Tempering simulations enabled us to restore thermalization and to obtain the minimum partition cost of graph partitioning from the low temperature simulations. We considered both regular random networks and Erdos Renyi networks. For the later we related the partition of the full network with a partition of the percolating cluster at nonzero magnetization. The results obtained are in good agreement with known previous results for the graph partitioning problem.

Architecture of a quantum computing platform

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Nowadays there is a major effort worldwide toward scalable quantum computers and the quantum internet, with computer scientists, physicists and software engineers that are joining forces to realize this interdisciplinary work. Quantum computers promise new possibilities for solving computing-intensive or previously not efficiently solvable problems, however quantum processors can still be used only in restrictive laboratory conditions. Thus, it was a natural decision to propose a cloud-based access to the quantum computing devices and integrate them with a high-performance computing platform. This led to the new area of quantum programming and a rapidly increasing number of companies developing their own quantum computing platforms.

In this research we develop an architecture of a quantum computing platform with the cloud interface, that is based on the original model of the nanophotonic quantum processor with integrated quantum memory and a quantum transistor [1]. At the moment the platform works with an integrated quantum simulator that implements the behavior of the underlying model [2]. As shown earlier this model is universal, i.e. it is capable of performing arbitrary quantum computations. Additionally, it allows to speed up the implementation of controlled operations, that are heavily used in most multi-qubit algorithms.

The platform has two main components: the server-side framework and the client SDK, which makes coding quantum algorithms as easy as shown in the following example.

Listing 1: Example

```
conn = kmqc.connect(endpoint, user_id, api_key)
r = conn.execute(Program(
                    kmqc.gates.X(1),
                    kmqc.gates.H(0),
                    kmqc.gates.H(1),
                    kmqc.gates.CNOT(0, 1),
                    kmqc.gates.H(0)))
```

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References

[1] S. A. Moiseev and S. N. Andrianov. A quantum computer on the basis of an atomic quantum transistor with built-in quantum memory. *Optics and Spectroscopy*, 121(6):886–896, 2016.

[2] Farid Ablayev, Sergey Andrianov, Danila Fetisov, Sergey Moiseev, Alexandr Terentyev, Andrey Urmanchev, and Alexander Vasiliev. Model of a programmable quantum processing unit based on a quantum transistor effect. *AIP Conference Proceedings*, 1936(1), 2018.

Research of the efficiency of parallel algorithms implementation of interpolation methods for scaling raster images using specialized calculators

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Abstract: This work is devoted to the study of various methods for interpolating raster images. Such methods as bicubic interpolation, bilinear interpolation, nearest neighbor method and directed interpolation are considered. The purpose of this paper is to investigate the effectiveness of applying parallel programming approaches to image scaling algorithms.
In the course of work, the above algorithms were adapted to run on Nvidia CUDA multiprocessor computers. A program is developed using C, C ++, CUDA C, which allows you to scale images in different ways and with the ability to choose the degree of parallelization of computations. As a result of the work, a study of the efficiency of parallel scaling algorithms has shown that the use of multiprocessor computing devices allows to significantly accelerate the operations of image scaling. Also in the course of the work, a comparison was made between the above methods for the speed of work and the quality of the result obtained.

Keywords: methods of interpolation of images, parallelizing an algorithm, Compute Unified Device Architecture, parallel computing, multithreaded computing, distribution of computing.

Hole distribution in a film of a ferromagnetic semiconductor in the presence of an external electric field

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The electrical manipulation of magnetism and magnetic properties has been achieved across a number of different material systems. For example, applying an electric field to a ferromagnetic material through an insulator alters its charge-carrier population.

The possibility of changing the spontaneous magnetization of a ferromagnetic semiconductor by applying an electric field. A thin film of a ferromagnetic semiconductor $(In_{0.97}Mn_{0.03})As$ 5 nm thick was placed on a substrate of other semiconductors.

In such a system, at a sufficiently high concentration Mn (on the order of several percent), the wave functions of the holes associated with neighboring ions begin to overlap, and a hole impurity band arises. Ferromagnetism is provided by the exchange interaction of holes with manganese ions by the Zener mechanism, i.e. indirect ferromagnetic interaction between ions is provided due to the *sd* - exchange of Vonsovsky-Ziner between holes and ions. The dependence of the density of states of a hole gas in the impurity band of energy, which overlaps noticeably with the valence band, is rather complicated. And for simplicity in the model calculation it was assumed that this dependence is the same as in a gas with some effective mass.

Denote by ε_{ex} the elementary energy of the exchange interaction of holes with the manganese ion, referred to the density of the particles. Then, in the model under consideration, the energy of the exchange E_{ex} interaction per unit area of the film surface is represented as:

$$E_{ex} = -\varepsilon_{ex} \cdot L \cdot \int_0^1 \left(n_+^{1/2}(z) - n_+^{-1/2}(z) \right) \cdot \left(n_-^{5/2}(z) - n_-^{-5/2}(z) \right) dz, \quad \varepsilon_{ex} > 0 \tag{1}$$

Numerical solution of the system of equations (2), (3) considering boundary conditions (4):

$$\begin{aligned} &\Delta(z) = \Omega\left(\psi(z), a(z)\right) \cdot \mathrm{Tanh}[(b/T) \cdot \Delta(z)] / q(z), \\ &\Omega\left(\psi(z), a(z)\right) = \delta \cdot \{\left((3/2) \cdot (1-\psi(z)\right)^2 + (1/2) \cdot (a(z))^2\}. \end{aligned} \tag{2}$$

$$\begin{aligned} &\frac{d^2}{dz^2}\psi = -\gamma \cdot L^2 (q(z) - 1), \quad z \in (0,1), \quad \gamma = \frac{4\pi \cdot n_-}{\chi \cdot \varepsilon_F}, \\ &q(z) = (1/2) \cdot \left((1 - \psi(z) + a(z))^{3/2} + (1 - \psi(z) - a(z))^{3/2} \right), \\ &a(z) = \delta \cdot \mathrm{Tanh}[(b/T) \cdot \Delta(z)]. \end{aligned} \tag{3}$$

$$\frac{d\psi}{dz}\Big|_{z=0} = \frac{d\psi}{dz}\Big|_{z=1} = -A \cdot L, \quad A = \frac{E}{\chi \cdot \varepsilon_F} \tag{4}$$

These equations are solved using an iterative procedure.

The computer simulation of attacks on the ring-homomorphic encryption

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The ring-homomorphic encryption allows computing on ciphertexts, generating an encrypted result which, when decrypted, matches the result of the operations as if they had been performed on the plaintext. The plaintexts are from some algebraic ring.

Thus, for ring-homomorphic encryption the following system of equation must holds:

$$\begin{aligned} D(E(m_1) \oplus E(m_2)) &= m_1 + m_2 \qquad (1) \\ D(E(m_1) \odot E(m_2)) &= m_1 \cdot m_2 \end{aligned}$$

where $m_1, m_2 \in \mathcal{M}$ are some plaintexts (from plaintexts ring $\mathcal{M}$), D and E are decryption and encryption functions, respectively.

The system of equations imposes strict security requirements on encryption. In particular, such classical attacks as the known-plaintext attack, the ciphertext-only attack, and the chosen-plaintext attack must be reviewed in ring-homomorphic context.

This work proposes the mathematical model, allowing to analyze the ability to construct secure ring-homomorphic encryption. The model consists of algebraic structures, connected by relations deduced from (1). And finally, simulation attacks on toy-sizes encryptions allow evaluating the number of operations for secret key recovery in comparison with number of operations for encryption, decryption and homomorphic computations.

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Numerical simulation of two- and three-dimensional gravity-capillary waves

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In nature wind waves of gravity-capillary range are special in many respects. Steep decimeter-range waves develop a characteristic pattern of ‘parasitic’ capillary ripples on their forward slopes. Strong viscous dissipation of centimeter-scale ripples, together with the fact that parameters of parasitic ripples are sensitive to a change in the underlying wave’s steepness, makes decimeter-range waves subject to nonlinear damping. On the other hand, decimeter waves are also subject to strong wind forcing. Understanding the dynamics of gravity-capillary waves is important for remote sensing and for studying long waves generation mechanisms, because momentum transfer from atmosphere to ocean occurs mainly due to the interaction of wind with short waves. We perform numerical simulation of gravity-capillary waves within the framework of fully nonlinear equations of motion (Euler equations) for potential waves using parameterizations for wind forcing and viscous decay. A common approach to modelling two- or three-dimensional potential flows with a free surface is to use boundary integral equation methods, which have high computational costs. Here to take an account of three-dimensional effects we employ a quasi-three-dimensional model put forward by Ruban. It is based on the method of conformal transformations and allows an efficient implementation using a Fast Fourier Transform. The model assumes narrow directional distribution of waves while not imposing any limitations on their steepness. The aim of our work is to model the dynamics of transversely modulated gravity-capillary wavetrains, and to study the effect of capillary ripples on mean wave profiles.

A new class of reinforced random walks

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We study structural properties of reinforced random walks on a regular lattice using Monte Carlo simulations. Reinforced random walk is a walk whose next step depends on its entire previous trajectory. For example, the probability of a step may depend on whether the target cite is already visited or not. This case, which we call "volume reinforcement", is extensively studied in the literature [1-4]. It is known that depending on the reinforcement parameter *a* (the ratio of probabilities to go to a visited and an unvisited target cite, respectively) there exist a phase transition between collapsed and extended trajectories, which is in many ways analogous to the coil-globule transition in polymer physics [5,6].

Here we propose a generalization of this model with both volume and surface reinforcement. That is to say, the step probability now depends on whether the target site is (a) already visited (volume reinforcement), (b) is adjacent to the visited area (surface reinforcement), (c) neither of the two. As a result, the system behavior is now governed by two parameters - those of volume and surface reinforcement. We present a sketch of the phase diagram of this system depending on the two parameters, which includes four different phases. Apart from the phases known in the volume reinforcement phase there are two new phases with anomalously developed surface. One of these new phases (which was earlier observed in a somewhat different setting in [7]) is highly similar in morphology to the so-called fractal globule conformations of polymer chains and can be used for rapid generation of such conformations.

References

1. Ordemann, Berkolaiko, Havlin, Bunde, Phys. Rev. E, V. 61 (2001).

2. Ordemann, Tomer, Berkolaiko, Havlin, Bunde, Phys. Rev. E, V. 64 (2001).

3. Foster, Grassberger, Paczuski, New Journal of Physics, V. 11 (2009).

4. Sapozhnikov, J. Phys. A 27, L151 (1994)

5. Grosberg, Khokhlov "Statistical Physics of Macromolecules," AIP Press (1994).

6. Rubinstein, Colby, "Polymer Physics", Oxford University Press (2003).

7. Tamm, Nazarov, Gavrilov, Chertovich, Phys. Rev. Letters, V. 114 (2015).

Rapid algorithm for computer simulation of free bulging process

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Free bulging testing is an innovative technique allowing one to characterize superplastic materials in conditions of hot forming. A metal blank climbed by cylindrical die is deformed by application of a gas pressure. The significant advantage of this method is that it produces a biaxial tension stress mode in the material. At the same time, complex characterization techniques based on inverse analysis are required to interpret the experimental results. Rapid and robast algorithms for simulation of the bulging process are desired in order to implement such techniques. The objective of this work is a development of semi-analytical computer model for simulation of free bulging process. The proposed model is based on membrane theory supplemented with empirical formulation constructed on a base of numerous computer simulations performed using finite element method. The model was implemented for simulation of free bulging process of a titanium sheet.

Modified asymmetric exclusion process with internal particle states

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Totally asymmetric simple exclusion process (TASEP) is an archetypic model of the transport phenomena in 1D: a linear lattice occupied by particles which hop in one direction at random provided that their hopping does not violate the excluded-volume constraint, i.e. the condition that there is no more than one particle per lattice site at any given time. We consider a following generalization of this model. Let particles have two internal states: ground and active. Activation of a particle (i.e., going from ground to active state) is a Poissonian stochastic process happening with a given fixed rate regardless of the particle's surroundings. Only active particles can move and relaxation (i.e., going from active to ground state) happens only when an active particle hops forward. If a particle tries to hop but it is prevented from that by the presence of a neighbor in the adjacent cell, it remains active. This definition generates a one-parametric class of models depending on the ratio of activation and hopping/relaxation rates. If activation is much faster than hopping, all particles are always active and the model reduces to classical TASEP. But if hopping is much faster than activation, new interesting behavior arises. In the latter case, the positions of particles in the steady state become highly correlated: a long queue of active particles tends to forming behind one in ground state, then when it finally jumps, all the queue of active particles immediately jumps, too, resulting in a long uninterrupted chain of ground-state particles, etc. We numerically study the properties of the steady state of this system on a ring (flow-density diagram, cluster size distribution, correlation functions, etc.), construct a 'cluster mean-field' theory, which qualitatively reproduces the numerical results, and discuss its possible generalization.

* - speaker

Efficient parallel algorithm for calculating the transformation matrix of the robot gripper

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Abstract: In this article the model of the multiprocessing system which allows to significantly speed up the implementation of modular algorithms for solving of direct and reverse tasks of dynamics of the industrial manipulation robot is considered. A method for the implementation of these algorithms on the established structure of the processor with shared memory is offered. Development of specialized multiprocessor field used to accelerate calculations. Produced simulation of the hardware-software complex for the problems of dynamics and estimations of an overall performance of parallel algorithm are received.

Keywords: industrial robot, kinematics of manipulator, dynamics of manipulator, parallel computing, the model of a synchronous network of processors.

Comparison of default probability models for retail loans portfolio

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Abstract: In this paper, several credit scoring models are considered for an empirical assessment of default risk factors. A unique set of data consisting of credit portfolios of several banks is used to create logistic regression models with preliminary scaling and basic methods of machine learning, which ensures the results reliability.
Keywords: Woe factor transformation, logistic regression, support vector machine, random forest, mathematical model of reserves, expected credit loss, probability of default, exposure at default, loss given default.

Algorithmic method for modeling the optimal treatment of patients with HIV

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The problem of stabilizing the level of cells of the immune system in patients with the HIV virus is considered. The mathematical model describing the dynamics of HIV in the human body is a nonlinear system of differential equations. In the work for constructing suboptimal control of the supply of drugs, the method of "extended linearization" (SDC, state dependent coefficient) is used, which makes it possible to switch from a nonlinear model to a linear model, but with parameters that depend on the state. To solve the obtained Riccati-type equation, a new method of algorithmic construction is proposed.

Development of radial turbines in low-power gas turbine engines

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Today low-power gas turbine engines, especially micro gas turbine installations (MGTI), are one of the most modern types of power generation equipment, which exceed other ones in such consumer properties as: environmental friendliness, efficiency, profitability and integrity. Microturbines are an innovative technology of independent power plant development. They find themselves in different fields of economy with an increasing quantity of consumers: industrial plants, medical centres, oil and gas industry, rural sector, recycling, electrification of autonomous regions, geological prospecting, transportable sources of power for EMERCOM, strategic and military assets.

There are advantages of micro gas turbine installations: an opportunity of performance with small load during a long period of time; a low level of polluting emissions, vibratory actions and noise; low exploitation cost, an opportunity of performance with different types of fuel excluding lubricants; high level of integrity. The main disadvantage is high cost of MGTI.

Development of new microturbines is related to high input requirements, which affect on cost of a complete installation. Cost reduction can be achieved by using of already designed turbines as prototypes and their improvements with an appliance of modern physical process modeling complex. Designers make efforts to create high-speed microturbines. Also problems, connected with supply of gasdynamic (efficiency and power values) and strength (minimal value of efficiency) parameters, are being solved simultaneously. The most frequently a design of impellers, which supply required gasdynamic parameters, is unacceptable because of strength factors in operating performance. Circumference-curved turbine blades bend back because of centrifugal forces, producing high stresses. That's why it's necessary to improve turbine impellers' geometric models, which are achieved after gasdynamic CFD-modeling or they are based on already existed prototype, considering properties of chosen material and operating performances. It's offered to organize a complex of investigational and design researches, which will allow to reduce stresses in the impeller and keep gasdynamic parameters especially coefficient of efficiency as good as possible.

First of all it's necessary to evaluate blade profile and its deviation from radial direction. Analysis of a blade radiality is realized by splitting in several cylindric sections and determination of a deflection angle. Based on received angles, geometric blade model rebuilds by turning of cylindric sections around the axis of rotation. Further, modeling of a turbine loads complex is implemented. Hazardous locations are places of blades joints with a wheel in circumference. Coefficient of efficiency is close to minimum allowed one there. Different connections are considered, which allow to reduce stresses: blades' supports based on extended fillet, triangular form, parabolical form. The most effective joint is parabolical wheel thickening towards to connections with blades in circumference. It is got by means of changing back blade surface. Using of this joint permits to achieve increment of minimum safety factor to 1.3, keeping gasdynamic efficiency parameters of the impeller.

Presented method radial turbine's design related to low-power gas turbine engines, which is based on CFD-modeling and strength analysis, allows to minimize time period and costs of new microturbines' developing process. This fact permits to make independent power engineering more accessible for consumers and profitable for the producer.

Calculation of the invariant characteristics of forced oscillations of a beam with longitudinal compression and it's phenomenological model

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In the course of a full-scale experiment with an elastic beam with longitudinal compression a large set of data was obtained. This sets contain values corresponding to both ordered oscillations and disordered oscillations specific to dynamical systems with chaotic behavior. The oscillations are excited by the exposure of alternating magnetic field. Depending on the frequency of the harmonic action the laws of motion of the beam were registered.

As a result of numerical experiments, the correlation dimension and the β-statenropy of the attractor of the corresponding dynamical system were calculated. Pseudo-phase portraits of the attractor were also constructed.

Based on the received characteristics, a phenomenological model was proposed. On the basis of a comparison of the invariant characteristics of the model and experimental data, one can draw a conclusion about the adequacy of the chosen model.

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Dynamics of spatial evolutionary games on the triangular lattice.

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We study the dynamics of a spatial evolutionary game based on the modified prisoners' dilemma[1]. We consider the game on the triangular lattice and modify rule accordingly. Dynamics is similar to those on the square lattice[2, 3]. The game features a series of sharp transitions between several regimes, controlled by the interaction parameter between players, and non-trivial geometric rearrangements of the game field. We investigate critical properties of the resulting phase transitions and present quantitative and qualitative comparison with the results of the previous study on the square lattice.

References

[1] Nowak M.A. May R.M. *Evolutionary games and spatial chaos.* Nature, 359, 1992.

[2] S. Kolotev A. Malyutin E. Burovski S. Krashakov L. Shchur. *Dynamic fractals in spatial evolutionary games.* Phys. A: Stat. Mech. and Appl., 499, 2018.

[3] S. Kolotev A. Malyutin E. Burovski S. Krashakov L. Shchur. *Interfaces in evolutionary games.* Journal of Physics: Conference Series. 955, 2018.