Book of Abstracts

XXV IUPAP Conference on Computational Physics
August 20-24, 2013, Moscow, Russia

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Preface

The Conference on Computational Physics (CCP) series is an annual international conference that is dedicated to presenting an overview of the most recent developments and opportunities in computational physics across a broad range of topical areas. The CCP series is sponsored by the International Union of Pure and Applied Physics (C20) and has been in existence since 1989. The series alternates between Europe, America and Asia-Pacific. The CCP conferences are traditionally supported by European Physical Society and American Physical Society. This year the Conference host is Landau Institute for Theoretical Physics, Russian Academy of Sciences. Details regarding the organizational structure of CCP2013 can be seen at the official conference website: http://ccp2013.ac.ru. As a major international conference, the CCP series aims to draw computational scientists from around the world, both as invited speakers and as conference participants.

The Conference covers computational physics through a series of plenary talks, which together will form a broad and accessible overview of the field. Parallel sessions with invited and contributed talks as well as Poster sessions are paying special attention to both numerical methods and physical results.

This book contains abstracts of plenary talks, invited talks, contributed talks, and poster presentations.

Conference Time Table

Time	Tuesday Aug, 20	Wednesday Aug, 21	Thursday Aug, 22	Friday Aug, 23	Saturday Aug, 24
08.30		Registration	Registration	Registration	
09.00-09.30			Plenary Talk 4	Plenary Talk 8	Plenary Talk 10
09.30-09.45		Opening			
09.45-10.30		Plenary Talk 1	Plenary Talk 5	Plenary Talk 9	Plenary Talk 11
10.30-11.00		Coffee	Coffee	Coffee	Coffee
11.00-11.45		Plenary Talk 2	Plenary Talk 6	CECAM Berni J. Alder Prize Ceremony	Plenary Talk 12
11.45-12.30		Plenary Talk 3	Plenary Talk 7		Closing 11.45-12.00
12.30-13.50		Lunch	Lunch	Lunch	
13.50-16.00		Parallel Sessions 1	Parallel Sessions 3	Parallel Sessions 4	
16.00-16.30		Coffee	Coffee	Coffee	
16.30-18.40	Registration 17.30-20.00	Parallel Sessions 2	Poster Session 1	Poster Session 2	
18.40		End of program	End of program	End of program	

List of Plenary Talks

1. Dezso Horvath, *Search for the Higgs Boson: a Numerical Adventure of Exclusion and Discovery*
2. Kurt Binder, *Simulations of Interfacial Phenomena in Soft Condensed Matter and Nanoscience*
3. Vladimir E. Zakharov, *Numerical Modeling of Ocean Waves*
4. Ali Alavi, *Quantum Monte Carlo approach to the ground state eigenvalue problem of many-electron systems*
5. Ian T. Foster, *Preparing for the Computer Revolution*
6. Wolfgang Paul, *Monte Carlo Simulations of Semi-flexible Polymers: From Single Chains to Nematic Melts*
7. Isaak M. Khalatnikov, *Numerical Methods for Partial Differential Equations and Early Days of Computational Physics*
8. Tomo-Hiko Watanabe, *Exploring phase space turbulence in magnetic fusion plasmas*
9. Carlo Pierleoni, *First-principle calculations of high pressure hydrogen*
10. Morten Hjorth-Jensen, *Living at the edge of stability, understanding the limits of the nuclear landscape: Computational and algorithmic challenges*
11. Natalia Artemieva, *Airbursts - from Tunguska to Chelyabinsk*
12. Stefan Gottloeber, *Formation of structure in the Universe*

List of Invited Talks

1. Norbert Attig, *Supercomputing Infrastructures in Europe*
2. Luca Baiotti, *Fully general-relativistic simulations of binary neutron-star mergers*
3. Marcia Barbosa, *Enhancement Flow in Nanoconfined Water*
4. Sara Bonella, *Quantum time correlation functions visa noisy Monte Carlo and classical trajectories*
5. Chin-Kun Hu, *Computational approach to synchronization of nonlinear coupled systems*
6. Nail Inogamov, *Ultrafast lasers, highly excited solids, and DFT-EAM-MD simulations*
7. Wolfhard Janke, *Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage*
8. David Landau, *A New Paradigm for Petascale Monte Carlo: Replica Exchange Wang-Landau Sampling*
9. Anthony Maggs, *Constrained statistical mechanics for charges and spins*
10. Vladimir Voevodin, *Supercomputing Center of Moscow State University: Computational Factory and Education*
11. Martin Weigel, *Simulating spin models on GPU: a tour*

PARALLEL SESSIONS I, August 21, 13:50–16:00

A.1 Monte Carlo Methods	**Red Hall**
7.1 IT & HPC for Physics and Education **4.1 Education in Computational Physics**	**Beige Hall**
1.1 Biological Physics	**Green Hall**
2.1 Hydrodynamics	**Blue Hall**

PARALLEL SESSIONS II, August 21, 16:30–18:40

D.1 Molecular Dynamics	**Red Hall**
B.1 Differential Equations	**Beige Hall**
6.1 Plasma Physics	**Green Hall**
5.1 Quantum physics and Low Temperature physics	**Blue Hall**

PARALLEL SESSIONS III, August 22, 13:50–16:00

A.2 Monte Carlo Methods	**Red Hall**
C.1 Density Functional Theory	**Beige Hall**
5.2 Quantum physics and Low Temperature physics	**Green Hall**
3.1 Astrophysics and cosmology	**Blue Hall**

PARALLEL SESSIONS IV, August 23, 13:50–16:00

A.3 Monte Carlo Methods	**Red Hall**
6.2 Plasma Physics	**Beige Hall**
5.3 Quantum physics and Low Temperature physics	**Green Hall**
7.2 IT & HPC for Physics and Education	**Blue Hall**

Sessions Schedule for Parallel Sessions.

A.1. Monte Carlo methods. August 21, Red hall, 13:50–16:00.

A.1.1	13:50–14:20	Wolfhard Janke, *Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage* (Invited Speaker)
A.1.2	14:20–14:45	Alexander Lyubartsev, *Systematic coarse-graining of molecular models by the Inverse Monte Carlo: Theory, practice and software*
A.1.3	14:45–15:10	Johannes Zierenberg, *Application of the parallel multicanonical method to lattice gas condensation*
A.1.4	15:10–15:35	Elmar Bittner, *Parallel-tempering cluster algorithm*
A.1.5	15:35–16:00	Ivanov Viktor Aleksandrovich, *Intramolecular structures in a single copolymer chain consisting of flexible and semiflexible blocks: Monte Carlo simulation of a lattice model*

A.2. Monte Carlo methods. August 22, Red hall, 13:50–15:40.

A.2.1	13:50–14:20	David P. Landau, *A New Paradigm for Petascale Monte Carlo: Replica Exchange Wang-Landau Sampling* (Invited Speaker)
A.2.2	14:20–14:50	Martin Weigel, *Simulating spin models on GPU: a tour* (Invited Speaker)
A.2.3	14:50–15:15	Prudnikov Vladimir Vasilevich, *Aging and non-equilibrium critical phenomena in Monte Carlo simulations*
A.2.4	15:15–15:40	Maria A. Medvedeva, *Monte Carlo simulation of critical properties of ultrathin anisotropic Heisenberg fims*

A.3. Monte Carlo methods. August 23, Red hall, 13:50–15:55.

A.3.1	13:50–14:15	Elci Eren Metin, *Efficient Monte Carlo Simulations of the Random-Cluster Model using a Dynamic Connectivity Algorithm*
A.3.2	14:15–14:40	Prudnikov Pavel, *Dimensional crossover in critical behavior of ultrathin magnetic fims*
A.3.3	14:40–15:05	Ryzhov Valentin Nikolayevich, *Melting Scenario of the Two-Dimensional Core-Softened System: First-Order or Continuous Transition?*
A.3.4	15:05–15:30	Pospelov Evgeny, *Ageing properties in off-equilibrium critical relaxation of 3D diluted Ising ferromagnets*
A.3.5	15:30–	Khisamutdinov Alfred, *Imitation Monte Carlo methods for*

	15:55	*Boltzmann equation problems, parallelization of the algorithms with splitting*

B.1. Differential equations and Chaos. August 21, Beige hall, 16:30–18:40.

B.1.1	16:30–17:00	Chin-Kun Hu, *Computational approach to synchronization of nonlinear coupled systems* (Invited Speaker)
B.1.2	17:00–17:20	Glyzin Sergey Dmitrievich, *Dimensional Characteristics of Multimode Diffusion Chaos*
B.1.3	17:20–17:40	Kudryavtsev Alexey Nikolaevich, *A new two-potential formalism for the Maxwell equations and its application to numerical simulation of electromagnetic processes*
B.1.4	17:40–18:00	Makarenko Andrey Viktorovich, *Estimation complexity of chaotic oscillations in aspect of the shape of their trajectories*
B.1.5	18:00–18:20	Zeitlin Michael G., *Modeling in Ensembles: Between Order and Disorder, en Route to Confinement*
B.1.6	18:20–18:40	Rumanov Edward, *Statistical Simulation for Bifurcations*

C.1. Density Functional Theory. August 22, Beige hall, 13:50–15:30.

C.1.1	13:50–14:15	Feng Yuan Ping, *Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon*
C.1.2	14:15–14:40	Jeanmairet Guillaume, *Molecular Density Functional Theory of Water*
C.1.3	14:40–15:05	Zempo Yasunari, *Optical Spectrum Analysis of TDDFT by Maximum Entropy Method*
C.1.4	15:05–15:30	Zhilyaev Petr Alexandrovich, *Ab-initio calculation of electrical and thermal conductivity of warm dense matter*

D.1. Molecular Dynamics. August 21, Red hall, 16:30–18:30.

D.1.1	16:30–16:50	Joan Adler, *Simulation of nanotube devices*
D.1.2	16:50–17:10	Zack Terranova, *Simulating the Solvation Dynamics of Ionic Liquids*
D.1.3	17:10–17:30	Ohmura Satoshi, *Ab initio Molecular-Dynamics Study of Dissociation Mechanism of Highly Charged Molecules*

D.1.4	17:30–17:50	Orekhov Nikita, *Two-phase molecular dynamic modeling of graphite melting*
D.1.5	17:50–18:10	Smirnova Daria, *Predictive molecular-dynamics models for investigation of U, U-Mo and U-Mo-Xe systems*
D.1.6	18:10–18:30	Bystryi Roman Grigorovich, *Molecular dynamics simulations of electron-ion nonideal plasmas on GPU*

1.1. Biological physics. August 21, Green hall, 13:50–15:55.

1.1.1	13:50–14:15	Andreas Tröster, *Fourier Monte Carlo Simulation of Hexatic Membranes*
1.1.2	14:15–14:40	Jerzy Bernholc, *Efficient Hybrid DFT Simulations of Solvated Biomolecules*
1.1.3	14:40–15:05	Family Fereydoon, *Large scale simulations shed new light on causes of age-related macular degeneration*
1.1.4	15:05–15:30	Negi Sunita, *Effect of calcium removal and ionic strength variation on the conformation change in calmodulin protein at physiological pH*
1.1.5	15:30–15:55	Rabinovich Alexander Lvovich, *Bond orientation properties in lipid molecules of membranes: molecular dynamics simulations*

2.1. Hydrodynamics. August 21, Blue hall, 13:50–16:00.

2.1.1	13:50–14:20	Marcia Barbosa, *Enhancement Flow in Nanoconfined Water* (Invited Speaker)
2.1.2	14:20–14:40	Dyachenko Alexandr Ivanovich, *Freak waves at the surface of deep water*
2.1.3	14:40–15:00	Lev Barash, *Approximate analytical descriptions of the stationary single-vortex Marangoni convection inside an evaporating sessile droplet of capillary size*
2.1.4	15:00–15:20	Kudryavtsev Alexey Nikolaevich, *Formation of high-gradient regions in freely-decaying and forced two-dimensional hydrodynamic turbulence*
2.1.5	15:20–15:40	Savichkin Denis, *Modeling of Rarefied Gas Flows on the Base of Numerical Solving of the Boltzmann Equation*
2.1.6	15:40–16:00	QingHong Zeng, *MMALE numerical simulation for multi-material large deformation fluid flows*

3.1. Astrophysics and cosmology. August 22, Blue hall, 13:50–15:00.

3.1.1	13:50–14:10	Luca Baiotti, *Fully general-relativistic simulations of binary neutron-star mergers* (Invited Speaker)
3.1.2	14:10–14:35	Cristina Torres, *Using a multidimensional likelihood algorithm like the Critical Coupling Likelihood to passively estimate effective transfer function like qualities in a running interferometric type gravitational wave detector*
3.1.3	14:35–15:00	Khoperskov Sergey, *Evolution of multi-component spiral disc galaxies: dynamics of gas, stars and dark matter*

4.1. Education in Computational Physics. August 21, Beige hall, 15:20–16:00.

4.1.1	15:20–15:40	Joan Adler, *I want to simulate problem X*
4.1.2	15:40–16:00	Salagaram Trisha, *Simplied pseudopotential problems for the classroom*

5.1. Quantum physics and Low Temperature Physics, August 21, Blue hall, 16:30–18:15.

5.1.1	16:30–17:00	Anthony Maggs, *Constrained statistical mechanics for charges and spins* (EPS Invited Speaker)
5.1.2	17:00–17:25	Satanin Arkady Mikhailovich, *Mesoscopic fluctuation of a qubit population in a biharmonic driving field*
5.1.3	17:25–17:50	Ehsan Khatami, *Fluctuation-dissipation theorem in isolated quantum systems out of equilibrium*
5.1.4	17:50–18:15	Larkin Ivan Anatolevich, *Dynamics of Two-dimensional Electron Gas in Non-uniform magnetic field*

5.2. Quantum physics and Low Temperature Physics, August 22, Green hall, 13:50–16:00.

5.2.1	13:50–14:20	Sara Bonella, *Quantum time correlation functions via noisy Monte Carlo and classical trajectories* (Invited Speaker)
5.2.2	14:20–14:45	Fedorova Anotonina N., *Quantum Modeling: from Coarse Graining to a Tower of Scales*
5.2.3	14:45–15:10	Ryabushkin O.A., *Concept of equivalent temperature of the nonlinear-optical crystal interacting with nonuniform laser radiation*

5.2.4	15:10–15:35	Konyashkin A.V., *Novel method for identification of intrinsic vibration modes in piezoelectric crystals*
5.2.5	15:35–16:00	Baranov A.I., *The equivalent temperature model in process of nonlinear conversion of laser radiation*

5.3. Quantum physics and Low Temperature Physics, August 23, Green hall, 13:50–15:55.

5.3.1	13:50–14:15	Wahnon Perla, *New Generation of More Efficient Solar Energy Materials: Quantum Modeling and Experimental Realizations*
5.3.2	14:15–14:40	Baturin Vladimir Sergeevich, *On structural and electronic properties of small silicon nanoclusters*
5.3.3	14:40–15:05	Sugimoto Soichiro, *Smoothed Particle Method for the Real-Space Electronic Structure Calculation*
5.3.4	15:05–15:30	Lozovik Yurii Efremovich, *Quantum Monte Carlo Simulations of Quantum Crystals and Supersolids*
5.3.5	15:30–15:55	Zeitlin Michael G, *The Topological Qubit: Quantum Evolution via Sheaves*

6.1. Plasma physics, August 21, Green hall, 16:30–18:40.

6.1.1	16:30–17:00	Inogamov Nail' A., *Ultrafast lasers, highly excited solids, and DFT-EAM-MD simulations* (Invited Speaker)
6.1.2	17:00–17:25	Lee Ricketson, *Entropy-based accelerated Monte Carlo methods for Coulomb collisions*
6.1.3	17:25–17:50	Kuznetsov Viktor Iosifovich, *Nonlinear oscillations in the Knudsen plasma diodes*
6.1.4	17:50–18:15	Perepelkina Anastasia Urevna, *Numerical simulation of Weibel instability in laser interaction with plasma*
6.1.5	18:15–18:40	Saitov Ilnur, *Ab initio calculation of dielectric properties of shocked xenon*

6.2. Plasma physics, August 23, Beige hall, 13:50–15:30.

6.2.1	13:50–14:15	Petrosyan Arakel, *Large eddy simulations of compressible magnetohydrodynamic turbulence in space plasma. Model developments and validations*
6.2.2	14:15–14:40	Shevelev Mark, *Numerical simulations of the Kelvin-Helmholtz instability development in a bounded supersonic plasma flow*

6.2.3	14:40–15:05	Morozov Igor Vladimirovich, *The method of Wave Packet Molecular Dynamics for warm dense matter and nonideal plasma simulations*
6.2.4	15:05–15:30	Viacheslav Belyi, *Model kinetic description for many-component plasma*

7.1. IT and HPC for Physics and Education, August 21, Beige hall, 13:50–15:20.

7.1.1	13:50–14:20	Voevodin Vladimir, *Supercomputing Center of Moscow State University: Computational Factory and Education* (Invited Speaker)
7.1.2	14:20–14:40	Budaev Denis, *Development of software for managing network resources based on the approach of software-configurable network*
7.1.3	14:40–15:00	Hong Guo, *A Communication Algorithm for the Patch-based Multiblock Structured Mesh Applications*
7.1.4	15:00–15:20	QingKai Liu, *Patch-based Computing for Large Scale Unstructured Mesh Applications*

7.2. IT and HPC for Physics and Education, August 23, Blue hall, 13:50–16:00.

7.2.1	13:50–14:20	Norbert Attig, *Supercomputing Infrastructures in Europe* (Invited Speaker)
7.2.2	14:20–14:45	Petrov Konstantin, *Automatic code generation for scientific computing*
7.2.3	14:45–15:10	Liu Xu, *Building Parallel SPH Programs with a Unified Infrastructure*
7.2.4	15:10–15:35	Cohn Ilya, *Experimental research automation system*
7.2.5	15:35–16:00	Moskovsky A., *RSC scalable and energy efficient HPC solutions: applications in solving computational physics problems*

Sessions Schedule for Poster Sessions

Poster Session 1, Thursday, August 22, 16:30–18:40

P1.1. Ahn Sul-Ah, *A detailed Numerical Analysis for High-T_c Superconductivity Phase Diagram Based on the Slave-Boson Representation of t-J Hamiltonian*

P1.2. Barash Lev, *PRAND: GPU accelerated parallel random number generation library*

P1.3. Bock Johannes Gerhard, *Kinetic Growth Random Walks*

P1.4. Bondareva Anna, *Radiation damage thin coating of silicon carbid*

P1.5. Brusentseva Svetlana V., *Numerical analysis and forecasting nonlinear dynamics of chaotic systems using chaos theory methods. Application to neurophysiology and econophysics.*

P1.6. Ciftja Orion, *Monte Carlo simulation of correlated electronic liquid crystalline phases*

P1.7. da Silva Ricardo Lopes, *Nanoring bilayer*

P1.8. Davidova Larisa, *Sync and anti-sync in a system of coupled oscillators*

P1.9. Dickman Adriana Gomes, *A Lattice Model for Malaria Transmission: mean-field approach and simulation*

P1.10. Dorosz Sven, *Fluctuation Relations and Crystallization*

P1.11. Elizarova Tatiana Gennagyevna, *Numerical simulation of turbulent flow in Taylor-Green vortex decay*

P1.12. Fazleev Nail, *First principles study of properties of the oxidized Cu(100) and Cu(110) Surfaces*

P1.13. Furukawa Nobuo, *Quasi Long Range Order of Defects in Frustrated Antiferromagnetic Ising Models on Spatially Anisotropic Triangular Lattices*

P1.14. Glushkov Alexander V, *Numerical modeling of atomic and nuclear systems inan intense laser field and resonance phenomena in heavy ions collisions*

P1.15. Ishkhanyan Hayk, *Electron spectrum of a double-wall carbon nanotube within the frame of the nonlinear Schrödinger equation*

P1.16. Ivanova Tatiana Alekseevna, *Effect of nitrogen impurity on the structural, mechanical and phonon properties of diamond from first- principle study*

P1.17. Kaurav Netram, *Pressure induced structural phase transition and lattice dynamics in thallium-V compounds*

P1.18. Khilkov Sergey, *Numerical simulation ofspin distribution evolution for super-paramagnetic materials*

P1.19. Kim Sangrak, *Validity of Molecular Dynamics Simulations for Soft Matter*

P1.20. Menshutin Anton, *Scaling in the Diffusion Limited Aggregation Model: towards ultimate growth probability*
P1.21. Murtazaev Akai Kurbanovich, *Frustrations and phase transitions in the Ising model on square lattice*
P1.22. Shul'man A. Ya., *Self-consistent mean-field approximation in the density functional theory of many-electron unbounded systems*
P1.23. Vali Rashid, *Effects of the in-plane magnetization on the conductance properties of the topological insulator ferromagnet/insulator/superconductor junctions*
P1.24. Russkov Alexander, *Analysis of cloud computing application in scientific centre*
P1.25. Voznesenskiy Mikhail, *Computer Simulations of Self-Assembled Mesocrystals formed by Iron Oxide Nanocubes*

Poster Session 2, Friday, August 23, 16:30–18:40

P2.1. da Silva Ricardo Lopes, *The influence of the vacancies in the magnetic skyrmion lattice*
P2.2. Elizarova Tatiana Gennagyevna, *Regularized shallow-water equations as a model for a solitary wave generation*
P2.3. Iskakova Kulpash, *About the energy levels of GaAs*
P2.4. Ivanov Momchil Nikolaev, *Polymer Adsorption onto a Stripe-Patterned Surface*
P2.5. Magnitskaya Maria Viktorovna, *Pressure-induced semiconducting behavior of calcium from ab initiocalculations*
P2.6. Menshutin Anton, *How to make large computer simulation user friendly: one practical example*
P2.7. Najafi Amin, *The Fluctuation-Dissipation Theorem of Topological Defect Colloidal Particles's energy on 2D Periodic Substrates: A Monte Carlo Study of thermal noise-like fluctuation and diffusionlike Brownian motion*
P2.8. Nepeina Ksenia, *Automatic post processing algorithm for passive seismic monitoring data*
P2.9. Osipchuk Igor, *Calculations of the direct and compound reactions of neutrons with nuclei*
P2.10. Petrov Vladimir, *Models and solutions of quasi 2D turbulence with chemical reactions*
P2.11. Popov Ivan Sergeevich, *Non-equilibrium critical dynamics of pure and diluted 2D XY model*
P2.12. Posvyanskii D.V., *True self-consistent solution of Kohn-Sham equations for infinite systems with inhomogeneous electron gas*

P2.13. Prepelitsa Georgy Petrovich, *Computational modelling dynamics of quantum and laser systems and backward-wave tubes with elements of a chaos*

P2.14. Rahimi Seyed Ali, *Measurement of Radon Concentration of Air Samples and Estimating Radiation Dose from Radon in SARI Province*

P2.15. Sako Tokuei, *Angular correlation and genuine- and conjugate-Fermi holes in two-electron atomic systems*

P2.16. Satanin Arkady Mikhailovich, *Calculation of optical properties of semiconductor nanocrystals in the framework of density functional theory using GPU parallel programming*

P2.17. Stornes Morten, *Optimal Paths in Random Resistor Networks*

P2.18. Svitenkov Andrew Igorevich, *Nonlocal correlation functions and an integral model for nanomechanical properties of nanostructural complexes*

P2.19. Turansky Robert, *Reference system for scanning probe tip fingerprinting*

P2.20. Vakilov Andrei, *Monte Carlo renormalization group of dilute 3D Ising dynamics*

P2.21. Vali Rashid, *Effects of the perpendicular magnetization on the nonlocal transport properties of the topological insulator ferromagnet/insulator/superconductor/insulator/ferromagnet junction*

P2.22. Valuev Ilya, *Numerical Integration of Quantum Dynamics in the Floating Multiple Gaussians Basis*

P2.23. Vaschenko Vladimir Nikolaevich, *Numerical modeling and forecasting the geophysical (atmospheric and hydroecological) systems dynamics by using the non-linear prediction and chaos theory methods*

P2.24. Vinnikov Vladimir Vladimirovich, *Numerical simulation of dark flight trajectory and dispersion ellipse for meteorites*

P2.25. Voznesenskiy Mikhail, *Simulation of small quantum systems by Path Integral Numerical Methods*

Search for the Higgs Boson: a Numerical Adventure of Exclusion and Discovery

Dezső Horváth
(on behalf of the CMS Collaboration)

Wigner Research Centre for Physics, Institute for Particle and Nuclear Physics, Budapest, Hungary
and
Institute of Nuclear Research (Atomki), Debrecen, Hungary

Abstract*:*

The Standard Model, the theory of particle physics was established 40 years ago and it seems to describe all experimental data very well. All of its elementary particles were identified and studied apart from the Higgs boson until 2012. For decades many experiments were built and operated searching for the Standard Model Higgs boson and finally, the two main experiments of the Large Hadron Collider at CERN, CMS and ATLAS in 2012 observed a new particle with properties close to those predicted for the Higgs boson. In this talk we describe the search process at LEP, the Large Electron Positron collider, and the discovery at LHC, the latest results, with special emphasis on the numerical methods used.

Simulations of Interfacial Phenomena in Soft Condensed Matter and Nanoscience

Kurt Binder
Institut für Physik, Johannes Gutenberg-Universität Mainz,
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June 19, 2013

Abstract

Computation of interfacial free energies between coexisting phases (e.g. saturated vapor coexisting with liquid) is a fundamental problem of classical statistical mechanics: the standard approach (dating back to van der Waals, Ginzburg-Landau, Cahn-Hilliard $\cdots$) is based on the continuation of the free energy of homogeneous states throughout the two phase coexistence region. Beyond mean field this continuation does not exist, nor does an "intrinsic profile" of the interface exist! These problems can be overcome by computer simulation: one popular method is based on sampling the order parameter distribution function in the two-phase coexistence region, which yields information on the surface tension of planar interfaces (from "slab configurations") and of curved interfaces (from states containing "droplets"), elucidating the problem of the "Tolman length". Another method (suitable also for solid-liquid interfaces) analyzes the capillary wave broadening or the capillary wave spectrum; all these methods require a careful assessment of finite size effects. Related problems occur for excess free energies due to walls, needed to describe wetting phenomena, capillary condensation, heterogeneous nucleation, etc. As an example, a thermodynamic integration method (based on "mixing" systems with and without walls) will be described, and an application to understand phase separation in nanoconfinement will be mentioned.

Vladimir E. Zakharov, University of Arizona, USA – "Numerical Modeling of Ocean Waves"

Quantum Monte Carlo approach to the ground state eigenvalue problem of many-electron systems.

Ali Alavi
University of Cambridge
UK

Abstract

The ground-state eigenvalue problem posed by the electronic Schrödinger equation can be cast as a stochastic process involving an annihilating population of positive and negative walkers that inhabit Slater determinant space [1]. The population of walkers evolve according to a simple set of rules (akin to a “game of life”), which are derived from the underlying imaginary-time Schrödinger equation, such that the long-time distribution of the walkers matches the exact ground-state eigenvector. We show that this algorithm has a remarkable *emergence* characteristic, akin to symmetry-breaking phase transitions in classical statistical mechanical systems.

The use of Slater determinants obviates the usual Fermion sign problem of diffusion Monte Carlo (namely the collapse onto Bosonic wavefunctions), but instead introduces a different sign problem associated the fact that the off-diagonal Hamiltonian matrix elements are both positive and negative. This sign problem however can be solved through a combination of walker annihilation and a “survival of the fittest” criterion [2] (the latter greatly reducing the dependence of the algorithm on walker annihilation). The method provides a way to compute *exact* electronic energies within a specified *N*-electron basis set. We will give examples of the algorithm at work in real systems in sizeable basis sets, ranging from atomic ionization potentials and electron affinities[3], dissociation energies of diatomic molecules[4], the uniform electron gas [5], and a first application to real solids[6].

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Preparing for the Computer Revolution

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Computer pioneer Alan Kay has asserted (most recently in 2007) that "The Computer Revolution Hasn’t Happened Yet." That may seem a strange statement to make some 60 years after the surely revolutionary ENIAC, and the subsequent 12+ orders of magnitude increase in computing capability. Kay was referring, however, to what he sees as the yet-unrealized potential for the computer to act as a true intelligence amplifier. In this talk, I examine Kay's vision, asking: Was he right in his assessment? Is this computer revolution imminent? How will we know when it arrives, and how will life be different? How can we accelerate its arrival?

Wolfgang Paul, University of Halle-Wittenberg, Germany – "Monte Carlo Simulations of Semi-flexible Polymers: From Single Chains to Nematic Melts"

Numerical Methods For Partial Differential Equations and Early Days of Computational Physics

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In this talk I will describe some of the finite difference methods of numerical integration for hyperbolic and parabolic differential equations, which were developed in 1951 within the framework of the Soviet atomic project. Later the results played a basic role in constructing most of known implicit finite difference methods, which are widely used in scientific research and engineering. I will present the implicit difference schemes and the marching computations in the form, in which they were derived for the first time.

Exploring phase space turbulence in magnetic fusion plasmas

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Plasma turbulent transport is one of the most important issues in the magnetic fusion research, and the most challenging target in numerical simulations of fusion plasmas. While fusion plasma confinement has achieved the break-even condition or beyond, comprehension of the turbulent transport is still demanded toward more reliable prediction for future experiments. Direct numerical simulations of plasma turbulence are expected to provide physics-based understandings on the transport properties and its mechanism.

As the magnetic fusion plasma with high temperature of several keV is almost collisionless beyond applicability of the fluid approximation, gyrokinetic simulations solving time-evolution of distribution function on the phase space have been developed, extending a concept of turbulence onto the velocity space. Indeed, a drift wave turbulence simulation manifests cascades of fluctuations of the distribution function from macro to microscopic velocity scales.

The gyrokinetic turbulence simulation clarifies that optimization of a confinement magnetic field and particle orbits leads to turbulent transport reduction through enhancement of a self-generated sheared (zonal) flow, and confirms a theoretical guideline for designing non-axisymmetric toroidal confinement fields. More recent studies are devoted for validation of the gyrokinetic simulations against experiments, and demonstrate their reasonable agreements and feasibility for numerical prediction of transport.

The state-of-the-art peta-scale gyrokinetic simulations utilizing the K computer enable us to investigate multi-scale turbulent transport in fusion plasmas, where the two major topics are addressed; relaxation of a macro-scale temperature profile due to micro-scale turbulent transport, and ion- and electron-scale transport driven by plasma turbulence with a variety of spatio-temporal scales.

First-principle simulations of high pressure hydrogen

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First principle simulations results are crucial for the present understanding of the physics of hydrogen under extreme conditions of pressure and temperature. I will present a critical overview of those methods for Dense Hydrogen and describe some recent results [1]. In particular I will focus on recent developments to include nuclear quantum effects and how standard methods need to be modified accordingly. Finally I will illustrate predictions for the Metal-Insulator transition in liquid hydrogen[2,3,4] and for molecular and atomic crystalline hydrogen[5,6,7].

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Living at the edge of stability, understanding the limits of the nuclear landscape: Computational and algorithmic challenges.

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To understand why matter is stable, and thereby shed light on the limits of nuclear stability, is one of the overarching aims and intellectual challenges of basic research in nuclear physics. To relate the stability of matter to the underlying fundamental forces and particles of nature as manifested in nuclear matter, is central to present and planned rare isotope facilities. Important properties of nuclear systems, which can reveal information about these topics are for example masses, and thereby binding energies, and density distributions of nuclei. These are quantities, which convey important information on the shell structure of nuclei, with their pertinent magic numbers and shell closures or the eventual disappearance of the latter away from the valley of stability. Neutron-rich nuclei are particularly interesting for the above endeavor. As a particular chain of isotopes becomes more and more neutron rich, one reaches finally the limit of stability, the so-called dripline, where one additional neutron makes the next isotopes unstable with respect to the previous ones. The appearance or not of magic numbers and shell structures, the formation of neutron skins and halos can thence be probed via investigations of quantities like the binding energy or the charge radii and neutron rms radii of neutron-rich nuclei. In this talk I will present some recent calculations on properties of oxygen, calcium and nickel isotopes towards their corresponding driplines and point to new experiments. In particular I will focus on ground state properties and excited states, with an emphasis on the role of two- and three-body forces using first principles methods like large scale diagonalization approaches, coupled-cluster theory, in-medium Similarity Renormalization group and diffusion Monte Carlo. I will also try to outline present and futurechallenges to nuclear many-body theory and how to understand the above properties in terms of the underlying forces. The computational challenges will be outlined as well, with an emphasis on various methods together with additional applications to systems from solid state physics like quantum dots and infinite homogeneous matter like neutron star matter or the electron gas in two and three dimensions.

Airbursts - from Tunguska to Chelyabinsk

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Airburst (incorrectly called an “explosion”) is a sharp release of meteoroid’s energy into the atmosphere causing generation of strong blast waves. Airbursts are closely related to meteoroid’s fragmentation which occurs if a dynamic loading exceeds meteoroid strength. The 1908 Tunguska event represents the largest recorded example of an airburst event on Earth to date, with a magnitude estimates ranging from 3 to 5 Mt up to ~10–20 Mt [1-3]. Recent airburst above Chelyabinsk area was probably the largest since the Tunguska time with estimated energy of 100-500 kt. Theoretical calculations coupled with ground- and satellite-based observations of airbursts suggest that the Earth is struck annually by a objects of energy 2–10 kt [4,5].

Numerical methods and hydrocode in use. Methods describing meteoroid’s motion through the atmosphere include: 1) a system of differential eqs. to describe describing deceleration, ablation, and fragmentation into separate fragments [6] or “pancaking” [7]; 2) full-scale hydrodynamic modeling of a high-velocity gas flow (Mach number ~ 50) around the meteoroid [2,3,6]. SOVA code [8] is a 3D Eulerian code that models multidimensional, multi-material, large deformation, strong shock wave physics. SOVA includes a general treatment of viscosity for modeling viscous flow with Newtonian or Bingham rheology. Compared to other hydrocodes used to model high-velocity impacts SOVA has the advantage of including a two-phase hydrodynamics procedure that describes condensed particles and their momentum-energy exchange with gas.

Tunguska event 1908. The peculiar butterfly shaped pattern of the surface damage has been explained by an interaction of atmospheric shock waves with the surface and has been reproduced repeatedly in experiments and in three-dimensional physical models. Models and observations of Shoemaker-Levy 9 comet impact on Jupiter in 1994 helped to understand what happened to the Tunguska body. First of all, it was deformed, disrupted, and transformed into tiny droplets as it entered the atmosphere. The hot rarified atmospheric wake worked like a chimney forcing numerous particles into the upper atmosphere. A 400-km-diameter plume was formed within a few minutes and then splashed back spreading the projectile material along the dense lower atmosphere to distances of up to several thousand kilometers. Substantial amounts of water-vapor have been transported from the troposphere into the usually cold and dry mesosphere. Strong upper atmospheric winds transported this giant cloud all the way to Northern Europe within ~20 hours, creating extremely bright polar mesospheric clouds.

Chelyabinsk event 2013. On the early morning of February 15, 2013, thousands of people observed a bright flash in the sky over the city of Chelyabinsk. The flash was followed by a powerful sonic boom which destroyed windows across the area of ~ 5000 km^2 injuring more than 1500 people. Numerous video recordings of the event have allowed to reconstruct the trajectory and fragmentation history. The size (15-20 m) and energy of meteorite (100-500 kt) were estimated based on its infrasound signal, the energy of the brightest flash, and ground effects. Only a small fraction of the total mass was found near Chelyabinsk — mainly just tiny pieces with the largest fragment weighting ~3 kg.

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Formation of structure in the Universe

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In 1965 Arno Penzias and Robert Wilson detected the cosmic microwave background radiation. More than 13 billion years ago this radiation was imprinted on the sky, only a few 100,000 years after the Big Bang. In 1992 the COBE satellite detected anisotropies in the temperature of the CMB radiation. Meanwhile these temperature fluctuations are measured with very high precision by satellites (WMAP, Planck) as well as many ground based observations. The measured temperature fluctuations tells us that shortly after the Big Bang the Universe was almost homogeneous with tiny density fluctuations of the order of 10^{-5}. Comparing the power spectrum of measured density fluctuations with models the cosmologists concluded that the Universe is spatially flat and consists at present of about 68 % of some unknown Dark Energy, 27 % of also unknown Dark Matter and 5% of baryons.

In the evolved universe one can directly observe the distribution of baryons and indirectly (gravitational lensing, velocity measurements) the distribution of Dark Matter. We see huge clusters of galaxies with masses up to a few 10^{15} solar masses in the knots of the cosmic web which is build by galaxies in a wide range of masses from tiny dwarfs (10^9 solar masses) to massive ellipticals (10^{13} solar masses). All these structures have been formed out of the tiny fluctuations generated during the early inflationary phase and measured in the CMB background.

During the last two decades our understanding of the evolution of structure in the universe grew substantially. Due to the non-linear nature of the gravitational dynamics and the complicated gas-astrophysical processes numerical simulations on modern supercomputers have been the driving force behind much of this theoretical progress. Dark matter only simulations of the evolution of large cosmological volumes use thousands of cores of the largest supercomputers in parallel. In the analysis of these simulations assumptions must be made about the observable objects (galaxies) which are hosted by the dark matter halos. Gas-dynamical simulations allow to include the formation of stars but such simulations are much more demanding both in computational resources as well as in the number of physical processes which must be considered in addition to the gravitational clustering. This includes radiative cooling of the gas, star formation and the feedback of the stars. But also magnetic fields, supermassive black holes, and many other processes might be important.

Cosmological simulations must cover a large dynamical and mass range. A representative volume of the universe should be large, but this comes at the expense of the resolution. To overcome this problem a new, and almost orthogonal but yet complementary, approach to cosmological simulations has been introduced over the last few years. This consists of using observations of the nearby universe as constraints imposed on the initial conditions of the simulations. The resulting constrained simulations serve as a numerical laboratory of the nearby universe where small scale structures can be studied in detail.

Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage

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We analyze the adsorption propensity of a single polymer confined in a spherical cage with attractive walls [1,2]. The polymer is modeled in a coarse-grained continuum formulation by 12-6 Lennard-Jones interactions among the monomers and a very weak bending energy. By means of extensive parallel tempering and multicanonical Monte Carlo simulations it is shown that the system exhibits a rich phase diagram in the adsorption strength-temperature plane, ranging from highly ordered, compact to extended, random coil structures and from desorbed to partially or even completely adsorbed conformations. These findings are identified by canonical and microcanonical analyses techniques using different energetic and structural observables such as the gyration tensor and universal shape parameters that characterize the asphericity of a typical polymer conformation. The talk concludes with a discussion of the similarities and differences to a polymer adsorbing to a solid attractive substrate [3] or to a fluctuating attractive membrane [4], allowing for a back-reaction of polymer and substrate degrees-of-freedom.

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Systematic coarse-graining of molecular models by the Inverse Monte Carlo: Theory, practice and software.

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Molecular simulations of many phenomena related to biomolecular systems, soft matter and nanomaterials requires consideration of length scales above 10 nm and time scales longer than 1 mks, which necessitates the use of coarse-grained (low resolution) models, when each site of the model represents a group of atoms, and the solvent is often omitted. While many of coarse-grained models used in different studies in recent years relay on empirically parameterized interaction potentials, the multiscale approach is based on determination of coarse-grained potentials from atomistic (high resolution) simulations.

In this presentation a multiscale modeling approach based on the inverse Monte Carlo method is discussed, in which radial distribution functions (RDF) and distributions of internal degrees of freedom of molecular structure, obtained in high-resolution atomistic simulations, are used to reconstruct effective potentials which reproduce the same structural properties within low-resolution coarse-grained model. The statistical-mechanical equations expressing canonical properties such as RDFs in terms of potential parameters can be inverted and solved numerically according to the iterative Newton scheme [1]. The approach is illustrated on several examples of varying complexity: ionic solution; ionic liquids, coarse-grained lipid model, coarse-grained DNA model. We demonstrate further how effective potentials, derived exclusively from atomistic simulations, can be used to model such phenomena as lipid self-assembly, formations of vesicles and other ordered structures at varying lipid composition and concentration of different components. The problem of transferability and thermodynamical consistency of effective potentials obtained at different thermodynamic conditions is also discussed. Finally, a novel software MagiC [2] implementing the inverse Monte Carlo method for computation of effective potentials for coarse grained models of arbitrary structure from atomistic trajectories is presented.

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Application of the parallel multicanonical method to lattice gas condensation

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We present the speedup from a novel parallel implementation of the multicanonical method on the example of lattice gas in two and three dimensions. In this approach, all cores perform independent equilibrium runs with identical weights, collecting their sampled histograms after each iteration in order to estimate consecutive weights. These weights are distributed onto all cores again, repeating the procedure until the weights are converged. This procedure benefits from a minimum of communication while distributing the necessary amount of statistics efficiently. The final time series is obtained from independent simulations with the converged weights.

Using this method allows us to study the temperature dependence for a variety of large and complex systems. In this case, a gas is modeled by particles on the lattice that interact only with their nearest neighbors. For a fixed density this model is equivalent to the Ising model with fixed magnetization. We compare our results to an analytic prediction for equilibrium droplet formation, showing that a single macroscopic droplet forms only above a critical density.

Parallel-tempering cluster algorithm

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Using our new flexible and powerful method for systematic investigations of second-order phase transitions, introduced in Phys. Rev. **E 84** (2011) 036701, we revisit the two-dimensional 3- and 4-state Potts model and the three-dimensional XY model. The combination of the replica-exchange algorithm with cluster updates and an adaptive routine to find the temperature range of interest around the critical point, proved to be very efficient, robust and easy to use.

Intramolecular structures in a single copolymer chain consisting of flexible and semiflexible blocks: Monte Carlo simulation of a lattice model

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We study the conformational properties of a single multiblock copolymer chain consisting of flexible and semiflexible blocks. Monomer units of different blocks are equivalent in the sense of the volume interaction potential, but the intramolecular bending potential between successive bonds along the chain is different. We consider a single flexible-semiflexible regular multiblock copolymer chain with equal content of flexible and semiflexible units and vary the length of the blocks and the stiffness parameter. We perform flat histogram type Monte Carlo simulations based on the Wang-Landau approach [1] and employ the bond fluctuation lattice model, for which the phase diagram for flexible chains has been determined [2] using the Wang-Landau simulation method and for which the state diagram of semiflexible chains has been determined by use of expanded ensemble simulation techniques [3].

We present our data on different non-trivial globular morphologies which we have obtained in our model for different values of the block length and the stiffness parameter. We demonstrate that the collapse can occur in one or in two stages depending on the values of both these parameters and discuss the role of the inhomogeneity of intraglobular distributions of monomer units of both flexible and semiflexible blocks. For short block length and/or large stiffness the collapse occurs in two stages, because it goes through intermediate metastable structures, like a dumb-bell shaped conformation. In such conformations the semiflexible blocks form a cylinder-like core, and the flexible blocks form two domains at both ends of such a cylinder. For long block length and/or small stiffness the collapse occurs in one stage, and in typical conformations the flexible blocks form a spherical core of a globule while the semiflexible blocks are located on the surface and wrap around this core.

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A new paradigm for petascale Monte Carlo simulation: Replica exchange Wang–Landau sampling*

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Abstract. We introduce a generic, parallel Wang–Landau method that is naturally suited to implementation on massively parallel, petaflop supercomputers. The approach introduces a replica-exchange framework involving densities of states that are determined iteratively for overlapping sub-windows in energy space, each via traditional Wang-Landau sampling. The advantages and general applicability of the method are demonstrated using thousands of cores for several quite different systems (possessing either discrete or continuous degrees of freedom) including those with complex free energy landscapes and topological constraints.

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Simulating spin models on GPU — a tour

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Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses.

In this overview lecture I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards-Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis [1, 2] and cluster updates [3], as well as computional tricks such as multi-spin coding are taken into account.

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Aging and non-equilibrium critical phenomena in Monte Carlo simulations

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The collective behaviour of statistical systems close to critical points is characterized by an extremely slow dynamics which, in the thermodynamic limit, finally prevents them from relaxing to an equilibrium state after a change in some thermodynamic parameters. The non-equilibrium evolution following this change displays some of the features typically observed in glassy materials, such as ageing and violation of the fluctuation-dissipation theorem (FDT)[1]. It can be monitored through determination of dynamic susceptibilities and correlation functions of the order parameter, the scaling behaviour of which is characterized by universal exponents, scaling functions, and amplitude ratios. This universality allows one to calculate these quantities in suitable simplified models and Monte Carlo methods are a natural way for this analysis. We review here some of the theoretical results of computations that have been obtained in recent years for universal quantities, such as the fluctuation-dissipation ratio, associated with the non-equilibrium critical dynamics, with particular focus on the 3D pure and diluted Ising models with Glauber dynamics.

We analyse an influence of critical fluctuations, different non-equilibrium initial states and presence of nonmagnetic impurities in spin systems on two-time dependence of correlation and response functions on characteristic time variables as waiting time t_w and time of observation $t - t_w$ with $t > t_w$. It is demonstrated the two ways of Monte Carlo calculations of response functions with application of small external random magnetic fields and without its through calculation of some complicated correlation functions [2]. We discuss the obtained values of non-equilibrium exponents for autocorrelation and response functions and values of the universal long-time limit of the critical fluctuation-dissipation ratio X^{∞}. Analysis of simulation results show that the insertion of disorder leads to new values of with $X^{\infty}_{\rm diluted} > X^{\infty}_{\rm pure}$.

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Monte Carlo simulation of critical properties of ultrathin anisotropic Heisenberg films

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The dimensional crossover of magnetic properties from two-dimensional to three-dimensional character in magnetic multilayers has currently attracted much interest as a result of both technological and fundamental importance [1]. Of particular interest is the critical behavior of magnetic thin films for which the dimensionality d is not well established. It is interesting to consider how magnetic properties such as the magnetization m, magnetic susceptibility χ, and critical temperature T_c depend on the thickness of the film.

The anisotropic Heisenberg model studied is described by the following Hamiltonian [2]:

$$H = -J \sum_{ij} [(1-\Delta)(S_i^x S_i^x + S_i^y S_i^y) + S_i^z S_i^z], \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a unit vector in the direction of the classical magnetic moment at lattice site i, the sum is extended over nearest-neighbor pairs on the cubic lattice, $J > 0$ being the exchange constant, and Δ characterizes the amount of anisotropy. $\Delta = 0$ is the isotropic Heisenberg case, $\Delta = 1$ the Ising case. In order to study the critical properties of anisotropic Heisenberg magnets we thus made Monte Carlo calculations, studying cubic lattice with periodic and free boundary conditions are used for the in-plane and out-plane directions, respectively. The anisotropy constant for different sizes of the film is chosen from experimental studies of thin films of Ni(111)/W(110) [3]. The anisotropy constant is chosen proportional to the temperature corresponding to the critical temperatures of films to different thickness.

The simulation are carried out for simple cubic films of size $N_s = L \times L \times N$ where $L \times L$ represents the number of sites (spins) in each layer of the film and N is the number of layers. The spin configurations of the films are updated using the Swendsen-Wang algorithm. As a starting configuration we always used a completely ordered ferromagnet. We measured the total magnetization $m = \langle (1/N_s) | \sum \mathbf{S}_i | \rangle$, out-plane magnetization $m_z = \langle (1/N_s) \sum S_i^z \rangle$, the in-plane magnetization $m_{||} = \langle (m_x^2 + m_y^2)^{1/2} \rangle$ where angle brackets denote the statistical averaging. To estimate the critical temperature T_c was calculated temperature dependence of the susceptibility $\chi \sim [\langle m^2 \rangle] - [\langle m \rangle]^2$ for different lattice size. The position of the susceptibility maximum allowed to estimate range of values of the critical temperature. To clarify the critical temperatures were calculated temperature dependence of the forth order Binder cumulant.

In this work from the temperature dependence of the magnetization near the critical point $m \sim (T_c - T)^\beta$ values have been estimated the critical exponent β for different thickness of the magnetic film. From this dependence was found the crossover from two-dimensional Ising model to three-dimensional Heisenberg model with increasing film thickness. For a strong anisotropy we observed the spin reorientation transition. In the experimental and theoretical studies devoted to the study of single-layer magnetic materials, it is predicted that the orientation of the spin transition is a weak first-order transition.

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Efficient Monte Carlo Simulations of the Random-Cluster Model using a Dynamic Connectivity Algorithm

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The simulation of spin models close to points of continuous phase transitions is heavily impeded by the occurrence of critical slowing down.
A number of cluster algorithms usually based on the Fortuin-Kasteleyn representation of the Potts model and suitable generalizations for continuous-spin models has been used to increase simulation efficiency. The first algorithm making use of this representation, suggested by Sweeny in 1983, has not found widespread adoption due to problems in its efficient implementation. It has been shown recently, however, that it is indeed more efficient in reducing critical slowing down that the more well-known variants due to Swendsen/Wang and Wolff. Here, we discuss an efficient implementation of Sweeny's approach using recent algorithmic advances in dynamic connectivity algorithms, and show how these can be used for efficient simulations in the random-cluster model. An extension of this approach, which is also efficient for first order phase transitions, is the combination of the random cluster model and multicanonical simulations. In this framework, we directly sample the combined geometrical bond- and cluster-number density of states of the model. By construction, this approach does not suffer from any (hyper-)critical slowing down.

Dimensional crossover in critical behavior of ultrathin magnetic films

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An understanding of critical phenomena in low dimensional structures can be acquired from a study of ultrathin films in which one dimension, the film thickness N, is systematically reduced. The magnetic behavior of ultrathin films has become of great technological importance due to the applications in magnetic storage devices [1]. Magnetic order in ultrathin ferromagnetic films is very complex due to a strong influence of the shape and the magnetocrystalline anisotropies of the sample. In the past 20 years, a considerable amount of experimental results on different aspects of magnetism in ultrathin films has appeared [2]. Nevertheless it is difficult to reach general conclusions even in seemingly basic things such as the kind of magnetic order at low temperatures. In view of this complexity, theoretical work on simplified models and computer simulations are essential for rationalizing and guiding new experimental work.

In this study, our aim is to give a complete picture of the magnetic phase transition in thin films structures. We have studied the magnetic behavior of anisotropic Heisenberg thin films [3] using extensive Monte Carlo simulations. We have found the dimensional crossover of magnetization m and susceptibility χ from 2D to 3D like with increasing film thickness. Estimated values of the critical exponent β for different thickness demonstrates crossover from 2D Ising universality class to 3D Heisenberg through 3D Ising class.

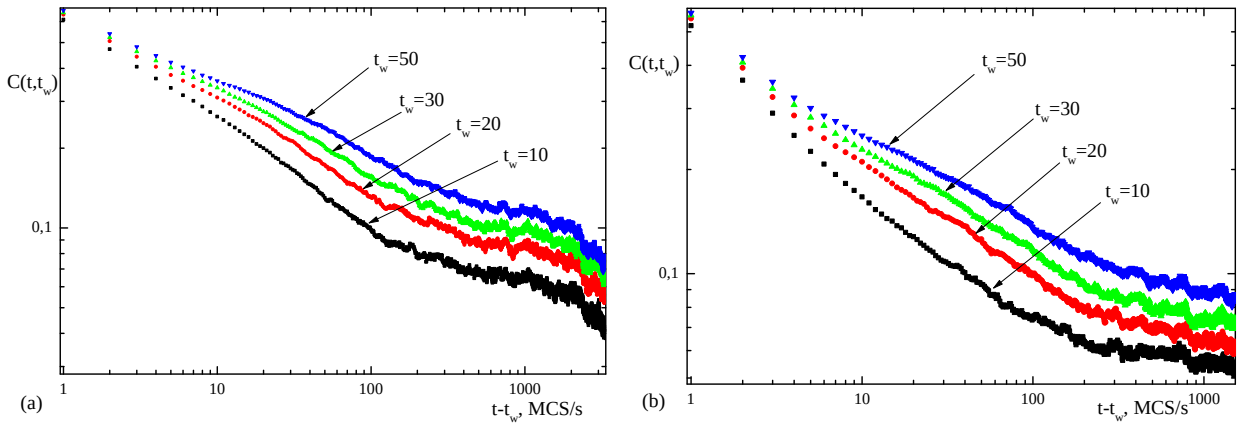

Fig.1 Aging in autocorrelation function $A(t, t_w)$ for (a) $N = 2$ and (b) $N = 4$

Presence of surfaces breaks lattice symmetries, and this can lead to many surprising and unexpected effects out of equilibrium [4]. The influence of non-equilibrium initial states on critical dynamic behavior of ultrathin magnetic and metamagnetic films have studied by short-time dynamics method [5]. Aging effects were discovered for non-equilibrium regime $t - t_w \gg t_w$ (Fig.1).

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Melting Scenario of the Two-Dimensional Core-Softened System: First-Order or Continuous Transition?

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We present a computer simulation study of the phase behavior of two-dimensional classical particles repelling each other through an isotropic core-softened potential [1-4]. As in the analogous three dimensional case [1-4], a reentrant-melting transition occurs upon compression for not too high pressures, along with a spectrum of water-like anomalies in the fluid phase. However, in two dimensions in the low density part of the phase diagram melting is a continuous two-stage transition, with an intermediate hexatic phase. All available evidence supports the Kosterlitz-Thouless-Halperin-Nelson-Young scenario for this melting transition [5-7]. On the other hand, at high density part of the phase diagram one first-order transition takes place. We expect that such a phenomenology can be checked in confined monolayers of charge-stabilized colloids with a softened core and water confined between two hydrophobic plates.

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Ageing properties in off-equilibrium critical relaxation of 3D diluted Ising ferromagnets

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The non-equilibrium relaxation of magnetic systems close to critical point demonstrates a wide range of interesting phenomena such as critical slowing down, ageing properties, and violation of the fluctuation-dissipation theorem (FDT). According to dynamical scaling the relaxation time $t_{rel} \to |T - T_c|^{-z\nu}$ and magnetic system does not achieve an equilibrium state at critical point. During out-of-equilibrium stage of dynamics for $t \ll t_{rel}$ ageing phenomena occur with two-time dependence of correlation and response functions on characteristic time variables as waiting time t_w and time of observation $t - t_w$ with $t > t_w$ [1]. It was shown that the time correlation function decays more slowly with increasing waiting time t_w.

The relationship between time correlation function $C(t, t_w)$ and response function $R(t, t_w)$ can be written as

$$R(t, t_w) = \frac{X(t, t_w)}{T} \frac{\partial C(t, t_w)}{\partial t_w}, \tag{1}$$

where $X(t, t_w)$ is so called fluctuation-dissipation ratio (FDR). FDT states that $X(t, t_w) = X(t - t_w) = 1$ in equilibrium.

Using Monte-Carlo simulations we have investigated ageing properties of three-dimensional Ising model with point-like nonmagnetic impurities. The spin concentrations p were taken as equal to $p = 1,\ 0,8$ and $0,6$. The investigations were carried out on cubic lattices. We used a high-temperature initial state with small initial magnetization $m_0 \ll 1$. Analysis of autocorrelation function behavior showed the realization of ageing in systems during out-of-equilibrium stage of dynamics for each spin concentration.

For checking violation of FDT we have used two ways to find fluctuation-dissipation ratio. Firstly, using Metropolis dynamics, we simulated Ising model in the presence of small bimodal random magnetic field h on lattice after t_w with distribution $< h >= 0$ [2]. In this way FDR can be calculated using integrated susceptibility $\chi(t, t_w)$ and final expression is

$$X(t, t_w) = -\lim_{C \to 0} \frac{\partial (T\chi(t, t_w))}{\partial C(t, t_w)}. \tag{2}$$

As result of investigations we obtained the following values of FDR: $X^{\infty}(p = 1) = 0,391(12)$, $X^{\infty}(p = 0,8) = 0,419(11)$ and $X^{\infty}(p = 0,6) = 0,443(6)$.

Another way of FDR definition is to calculate the response function $R(t, t_w)$ and derivative of correlation function without the use of the random magnetic field h. In this case FDR can be estimated through calculation of some complicated correlation functions as [3]

$$X(t, t_w) = TR(t, t_w)/(\frac{\partial C(t, t_w)}{\partial t}) = \frac{\sum_{i=1}^{N} < \sigma_i \left[\sigma_k(t_w + 1) - \sigma_k^{Weiss}\right] >}{\sum_{i=1}^{N} < \sigma_i(t)(\sigma_i(t_w + 1) - \sigma_i(t_w)) >}. \tag{3}$$

The sum in this expression includes all sites at the lattice, σ_i is spin value at site i. $\sigma_i^{Weiss} = tanh(1/T \sum_{<j \neq i>} \sigma_j)$ (where sum pass through neighboring spins around site i). The obtained final values of FDR are $X^{\infty}(p = 1) = 0,381(16)$, $X^{\infty}(p = 0,8) = 0,426(10)$ and $X^{\infty}(p = 0,6) = 0,451(10)$. Thereby, it was proved the violation of FDT in disordered three-dimensional Ising model and was shown that the non-equilibrium critical dynamics of this model is characterized by new universal FDR with $X^{\infty}_{disorder}(p < 1) > X^{\infty}_{pure}(p = 1)$.

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Imitation Monte Carlo methods for Boltzmann equation problems, parallelization of the algorithms with splitting.

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The talk examines a system of pairwise interaction particles, which models a rarefied gas in accordance with the nonlinear Boltzmann equation, the master equations of Markov evolution of this system and corresponding numerical Monte Carlo methods. Selection of some optimal method for simulation of rarefied gas dynamics depends on the spatial size of the gas flow domain. For problems with the Knudsen number Kn of order unity quite adequate and competitive are "imitation", or "continuous time", Monte Carlo methods ([1]). However if $Kn \leq 0.1$ (the large sizes) , excessive punctuality, namely, the need to see all the pairs of particles in the latter, leads to a significant increase in computational cost(complexity). We are interested in to construct the optimal methods for Boltzmann equation problems with large enough spatial sizes of the flow. Speaking of the optimal, we mean that we are talking about algorithms for parallel computation to be implemented on high-performance multi-processor computers. The characteristic property of large systems is the weak dependence of sub-parts of each other at a sufficiently small time intervals. This property is taken into account in the approximate methods using various splittings of operator of corresponding master equations. In the talk, we develop the approximate method based on the splitting of the operator of master equations system "over groups of particles" ([2]). The essence of the method is that the system of particles is divided into spatial subparts which are modeled independently for small intervals of time, using the precise"imitation" method. The type of splitting used is different from other well-known type "over collisions and displacements", which is an attribute of the known Direct simulation Monte Carlo methods. The second attribute of the last ones is the grid of the "interaction cells", which is completely absent in the imitation methods. The main of talk is parallelization of the imitation algorithms with splitting using the MPI library. New constructed algorithms are applied to solve the problems: on plane Poiseuille flow in the field of external forces and on propagation of the temperature discontinuity. In particular, on the basis of numerical solutions, comparative estimates of the computational cost are given for all algorithms under consideration.

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Computational approach to synchronization of nonlinear coupled systems*

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Synchronization appears in many natural phenomena, such as neural oscillation, coherent motion of birds and fishes, etc. In this talk, I briefly review some developments in computational approach to synchronization in nonlinear coupled systems. The topics under discussion include: (1) synchronization and coherence in thermodynamic coupled map lattices with intermediate range coupling [1], (2)synchronous chaos in coupled map lattices with small-world interactions [2], (3) synchronization for systems on scale-free networks [3], (4) universality and scaling in transition to synchronous chaos with local-global interactions [4], (5) synchronized state of coupled dynamics on time-varying networks [5], (6) influence of noises and delay on the synchronization of the stochastic Kuramoto model [6], (7) paths to globally generalized synchronization in scale-free networks [7], (8) stepwise transition to higher degrees of coherence in a random network of phase oscillators [8].

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Dimensional Characteristics of Multimode Diffusion Chaos

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Some parabolic systems of the reaction-diffusion type exhibit the phenomenon of diffusion chaos. Specifically, when the diffusivities decrease proportionally, while the other parameters of a system remain fixed, the system exhibits a chaotic attractor which dimension increases indefinitely. Various finite-dimensional models of diffusion chaos are considered that represent chains of coupled ordinary differential equations and similar chains of discrete mappings. A numerical analysis suggests that these chains with suitably chosen parameters exhibit chaotic attractors of arbitrarily high dimensions.

"Reaction – diffusion" systems are an important class of nonlinear dynamical systems in which spatially inhomogeneous oscillation modes are due to the presence of the diffusion component. Such systems are often encountered in physical, biochemical and population dynamics applications. By diffusion chaos we understand the strange attractor of the system "reaction - diffusion" non-trivially depending on the space variable. Currently, there are two concepts of diffusion chaos: low-mode and multimode chaos. The first of these can occur when diffusion parameter values are average and the second occurs when the diffusion parameter tends to zero.

The interest for low-mode chaos was inspired by the well-known works by E.Lorenz, D.Ruelle and F. Takens and then by Y. Kuramoto. The general question raised there is if it is possible to find a correspondence between stochastic regimes in a distributed dynamical system with infinite-dimensional phase space and strange attractors in finite-dimensional model system. There are many papers describing the situations where the answer is positive.

We consider the growth of the Lyapunov dimension of the attractor of the evolution system as the diffusion coefficient decreases to be one of the features of multimode diffusion chaos. In the work a number of parabolic boundary value problems are analyzed numerically and it shows that the phenomenon occurs. The Ginzburg-Landau equation is considered for different parameter values. We present an extended numerical experiment for generalized Klein-Gordon equation which illustrates the feasibility of Landau-Sell scenario.

A new two-potential formalism for the Maxwell equations and its application to numerical simulation of electromagnetic processes

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A new formulation of electromagnetic field equations based on the use of two vector potentials and two scalar potentials is proposed. This formulation allows the Maxwell equations both in vacuum and in a material medium to be written in the form of a hyperbolic system possessing a number of desirable properties. In particular, in contrast to the original Maxwell equations, the new system of equations consists only of evolutionary equations and does not include relations having the character of differential constraints. Such differential constraints (divergence-free conditions for electric and magnetic field) lead to significant difficulties when the Maxwell equations in the standard formulation are solved numerically with finite-difference methods. All eigenvalues of the Jacobi matrix of the derived system of equations corresponds to physical modes propagating with the velocity of light; there are no non-physical modes corresponding to the zero eigenvalue and obtained in the frequently used approach where only equations containing vector field rotors are solved, whereas equations with divergence are ignored. The relativistic invariance of the new formalism is shown.

All these facts allow powerful advanced shock-capturing methods based on approximation of spatial derivatives by upwind differences to be used to solve the new system numerically. Examples of numerical simulations of propagation of electromagnetic waves by solving the equations in the new formulation are given. One of the high-resolution numerical methods, a fifth-order WENO (Weighted Essentially Non-Oscillatory scheme, is employed and the results obtained are compared with the standard second-order FDTD (finite-difference time-domain) method. It is demonstrated that such a numerical approach allows the solution to be obtained with high accuracy, including problems that involve jumps of material properties of the medium.

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Estimation complexity of chaotic oscillations in aspect of the shape of their trajectories

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The concept of the "*complexity*" of any object is its important of information-structural characteristic, and is one of the fundamental scientific concepts [1, 2]. Is no exception and a more narrow concept of the "*complexity of dynamic process*". With it linked the predictability and information capacity of processes. It is part of the many criteria for classifying the processes as deterministic, chaotic, stochastic. However, along with this, questions of definition and calculation the complexity of dynamic processes remains of methodologically open [2].

In this report, we proposed an original approach to the evaluation and analysis the complexity of chaotic sequences – through the study of their structural properties in the aspect of the forms of their trajectories in the terms of symbolic CTQ-analysis (the so-called TQ-complexity). The developed tools (based on Wolfram Mathematica) allows methods of computational physics us to study various phenomena in nonlinear multi-dimensional dynamical systems (including a network of oscillators with an arbitrary topology and configuration of the lattice).

Earlier, in the papers [3, 4], was presented computationally oriented method of symbolic CTQ-analysis, which allows a detailed study of the shape (structure of geometry) sequences $\{\mathbf{s}_k\}_{k=1}^{K}$ in the space $\mathrm{S}\times\mathrm{K}$, $\mathbf{s}\in\mathrm{S}\subset\mathbb{R}^N$, $k\in\mathrm{K}\subseteq\mathbb{N}$, $K\geq 3$. In coding a sequences $\{\mathbf{s}_k\}_{k=1}^{K}$ for each of its nth component ($n=\overline{1,N}$) is formed corresponding to a sequence of terms $\{T_k^{\alpha\varphi}|_n\}_{k=1}^{K}$ [3]. The transition $T_k^{\alpha\varphi}|_n\to T_{k+1}^{\alpha\varphi}|_n$ corresponds to the characters $Q^{\alpha\varphi}|_n$ that are are included in the alphabet $\mathrm{Q}_o^{\alpha\varphi}$.

In paper [3] put into consideration of the symbolic TQ-image of sequences $\{\mathbf{s}_k\}_{k=1}^{K}$, which formally defined an graph $\Gamma^{TQ}|_n=\left\langle \mathrm{V}^{\Gamma}|_n, \mathrm{E}^{\Gamma}|_n\right\rangle$, at wherein the vertex $\mathrm{V}^{\Gamma}|_n\subseteq\mathrm{T}_o^{\alpha\varphi}$, and the edges $\mathrm{E}^{\Gamma}|_n\subseteq\mathrm{Q}_o^{\alpha\varphi}$.

The complexity of chaotic trajectories in the framework of the approaches, possibly to evaluate on measures the complexity of of the graph $\Gamma^{TQ}|_n$: *degenerate* (DM) – by count of vertices and edges; *weighted* (WM) – subject to the specific value of complexity of $T^{\alpha\varphi}|_n$ and $Q^{\alpha\varphi}|_n$ symbols. Based on the fact that $\Gamma^{TQ}|_n$ – a weighted graph, each of the measures has two implementations: *topological* and *metric*. The metric is defined by the Boltzmann-Shannon entropy (for a DM) and Renyi (for a WM). By analyzing these measures, it is possible an study various aspects of the structure of chaotic attractors in nonlinear multi-dimensional dynamical systems.

In this paper, a numerical study the TQ-complexity of the trajectories of Rössler system:

$$\dot{x}=-y-z,\ \dot{y}=x+p\,y,\ \dot{z}=q+z(x-r),\ p=0.2,\ q=0.1,$$

for cases band-type $r=r_b=4.4$ and screw-type $r=r_s=12$ chaos. The results are compared with previously obtained data on the structure of these attractors [4].

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Modeling in Ensembles: Between Order and Disorder, en Route to Confinement

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A fast and efficient numerical-analytical approach is proposed for the description of complex behaviour in non-equilibrium ensembles both in the BBGKY framework and in a number of its Vlasov-Poisson/Maxwell reductions. We construct a multiscale representation for the hierarchy of partition functions by means of the variational approach and multiresolution decomposition. Numerical modeling shows the creation of various internal structures from fundamental localized (eigen)modes. These patterns determine the behaviour of plasma. The Waveleton, localized (meta) stable long-living pattern with minimal entropy and zero measure, is proposed as a possible model for the energy confinement state (the fusion state) in plasma.

Statistical Simulation for Bifurcations

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Numerical simulation in critical domain (near a bifurcation) is considered to be unreliable since the results are reproduced unsatisfactorily. Because of large susceptibility there [1], smooth variations of parameters lead to disordered jumps in solution to the set of equations in question. Indeed, we deal with finite-difference equations, and the rounding, unavoidable in the course of calculations, acts as an uncontrolled noise. When close enough to the bifurcation, the variance of random pulsating is comparable to the mean value of the considered quantity as is the case in fully developed turbulence. To overcome this difficulty we propose addition of a small random function of time, e.g. white noise, to a constant source (pumping). Thereby the simulation approaches experimental situation. The solutions to Langevin equations [2] thus obtained are also random functions of time and require statistical reprocessing. Their properties, with the exception of intensity, are independent of the initial noise, and soft modes prevail in their spectrum. In the space of states, a complicated critical attractor appears instead of the limit point. We study this critical chaos [3,4], compare it to the dynamical one [5,6] and give examples of statistical description of bifurcations.
To forecast a future (in particular, predict catastrophes) the method of *compressive sensing* [7] was proposed [8,9]. There completely unknown set of equations of the general form

$$dx_i / dt = f_i(x_1, x_2, \ldots), \quad i = 1,2,\ldots$$

(i.e. with unknown right-hand sides) is reconstructed by using time series, in particular, experimental data. Right-hand sides of the equations are represented as power series in all the dependent variables. The coefficients of such expansion should be determined by compressive sensing. There is a code [7] for the determination. When the equations have been reconstructed one can find bifurcations (catastrophes) of their solutions. However, the authors [9] note difficulties appearing if the number of equations, i.e. variables, becomes large or time series are distorted by noise. In contrast, we suggest just adding the noise as a way to help predict catastrophes. We show that bifurcations of steady-state operation for a man-made or natural system can be predicted due to the onset of soft modes in the system's noise spectrum, see [10].
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Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon

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To enable many applications of topological insulators, it is necessary to open a surface energy gap and keep the Fermi energy inside the bulk gap. A two-step doping process, magnetic followed by charge or vice versa, is required to produce insulating massive surface states in topological insulators. Using first-principles calculations based on density funtional theory, we demonstrate here simultaneous magnetic and hole doping achieved with a single dopant, carbon, in Bi_2Se_3. Carbon substitution for Se (C_{Se}) results in an opening of a sizable surface Dirac gap (up to 85 meV), while the Fermi level (E_F) remains inside the bulk gap and close to the Dirac point at moderate doping concentrations. This *one-step* approach is possible because carbon doping simultaneously introduces localized spin moments and holes. The strong localization of 2*p* states of C_{Se} favors spontaneous spin polarization via a *p*-*p* interaction and formation of ordered magnetic moments mediated by the surface states. This dual function of carbon doping suggests a simple and effective way to realize insulating massive topological surface states.

Keywords: topological insulator, first-principles calculation, Bi_2Si_3, carbon-doping

Molecular Density Functional Theory of Water

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The determination of the solvation free energy and the microscopic structure of complex solutes in molecular solvent is an important problem for the understanding of chemical and biological systems. This can be done by the use of molecular simulations techniques such as Monte Carlo and Molecular Dynamics with explicit molecular solvent molecules to sample the microscopic solvent configurations. The use of thermodynamic integration techniques such as umbrella sampling enables to evaluate the free energy of the system. Another route is to employ implicit solvent methods, which do not consider explicitly all the instantaneous microscopic configurations of solvent molecules but instead treat it in a continuous way, while still taking into account its molecular nature. The computational cost of the implicit methods is then much lower than the one of molecular simulations. Molecular density functional theory [1] (MDFT), an implicit solvent method that can predict both microscopic structure and thermodynamic properties of any solute in a molecular fluid is introduced. Molecular DFT has many features in common with electronic density functional theory; they will be highlighted in this presentation. This theory relies on the fact that the grand potential of a molecular fluid submitted to an external potential could be written as a functional of the position and orientation solvent density. The exact free energy functional is obviously not known but approximations can be proposed. Due to the tetrahedral order of the fluid, the study of water raises particular problems that require some extra corrections [2]. A functional appropriate to liquid water [3] will be proposed and some results on the hydration properties of a set of solutes (atomic, molecular, charged and non charged) in water will be presented to prove the validity of the approximations made.

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Optical Spectrum Analysis of TDDFT by Maximum Entropy Method

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In computational materials science, meanwhile, many improvements are introduced to DFT as advanced techniques. As one of these improvements, Time Dependent Density Functional Theory (TDDFT) has been a focus of attention recently, which is also introduced in our materials research. In our calculations, the real-time and real-space technique is adopted in solving equation by the finite difference approach. Within the framework of this approach, the wave functions are evolved with the perturbed initial wave function. In the traditional method, the optical strength function is obtained from the frequency Fourier transformation of the dynamic dipole moment.

In frequency domain, however, we can introduce the maximum entropy method (MEM), by which we can obtain a fairly good resolution with a relatively small number of time-series data. This MEM is applied to the spectrum analysis of time-series data of the dipole moment, which is calculated by TDDFT. In our paper, we adopt Burg's MEM method to compute a best possible spectrum, which is based on the relationship that the known autocorrelation are connected with the power spectrum by a Fourier transform. The major issue of MEM for the spectral estimation is to determine the number of autocorrelation samples. We use Akaike's final prediction error.

We have applied this MEM to the several spectrum analyses to investigate the calculation efficiency, which is compared to FFT. For demonstration, we calculate the dipole moment of an ethylene molecule up to 20,000 steps with $\Delta t = 4.84 \times 10^{-5}$ fs. The optical strength functions are calculated by FFT and MEM. Both calculations provide a fairly good spectrum results with this time steps. As a result, however, we figure out the advantage of MEM. The 1/4-1/2 series of data are enough for MEM to obtain the similar spectrum by FFT, although the real time evolution of real-time TDDFT consumes a lot of computational resources. In the presentation, we will show the results of MEM applications to several organic materials and those spectra.

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Ab-initio calculation of electrical and thermal conductivity of warm dense matter

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Warm dense matter (WDM) can be attributed to the state of matter at near-solid densities and temperature between 1 eV and 100 eV. Such conditions are believed to exist in the core of giant planets such as Jupiter and Saturn. Investigation of WDM is important for number of technological applications such as surface treatment at nanoscale (see for example [1]), laser deposition, creating plasma sources of X-rays and development of Inertial Confinement Fusion.

In this work, we present a direct calculation of thermal conductivity based on density functional theory and the Kubo-Greenwood formula [2, 3, 4, 5]. This method proved to be useful for modeling the transport properties in a wide range of densities and temperatures [5]. Two cases are considered: equilibrium, where temperature of electrons (T_e) equals temperature of ions (T_i) and nonequilibrium T_e » T_i. Electrical and thermal conductivity of aluminum and gold, typical s- and d- metals, is examine The calculations are performed for both liquid and solid phases in the range of Te from 0 to 6 eV.

Calculation of transport properties requires accurate determination of the electronic structure. This imposes a limit on the number of atoms considered so advanced calculations are conducted for 2000 atoms [6]. To perform typical calculations require the use of 1000 cores on a supercomputer, and 100 GB of memory per node.

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Simulation of nanotube devices

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Nanotube devices are already far beyond science fiction, and atomistic simulations of their behaviour are proceeding apace. I will discuss my group's recent results of the effects of boundary conditions and tension on the behaviour of vibrating nanotubes for mass sensor applications.

An important next stage is to enable such simulation in an easy to use application for non-experts and I will discuss our progress towards this goal.

Zack Terranova
University of Notre Dame
Ph.D. Student, expected completion May 2014
Passport:
U.S. Passport; Date of expiration: 24 October 2022;
I anticipate no issues to obtain a visa for Russia in a seven day timeframe
CCP Poster Presentation:
Title: Simulating the Solvation Dynamics of Ionic Liquids
Authors: Z. L. Terranova and S. A. Corcelli
Affiliation: University of Notre Dame

Abstract:

Molecular dynamics simulations of coumarin 153 (C153) in imidazolium based ionic liquids (ILs) are performed to shed insight into solvation dynamics and compare directly with experimental studies. Solvation dynamics in ILs reveal very complex kinetics over a range of time scales, spanning from femtoseconds to tens of nanoseconds. In order to draw conclusions about the nature of these dynamics an extensive amount of simulation time is necessary for the response function to converge, requiring at least 5 microseconds of MD simulations per ionic system. By employing various decomposition techniques on the simulated solvation dynamic response on a representative set of ILs it is possible to deduce information about the local environment and factors responsible for solvation dynamics and identify any trends that may exist. Thus far, preliminary analysis of the structure in the vicinity of C153 has revealed preferential solvation by the cations despite typically being larger than the anions. However when separating the solvation response into its respective components, it is the smaller and more distant anions that are responsible for a majority of the short and long time response to the sudden charge perturbation. Obtaining insight of solvent dynamics is crucial for our understanding of solvent effects on chemical reactions. Given the multitude of possible combinations of cations and anions, it is absolutely necessary to understand the molecular interactions that are responsible for the macroscopic physicochemical properties of interest.

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(2) **Supplemental Information:** http://zackterranova.com/research

Ab initio Molecular-Dynamics Study of Dissociation Mechanism of Highly Charged Molecules.

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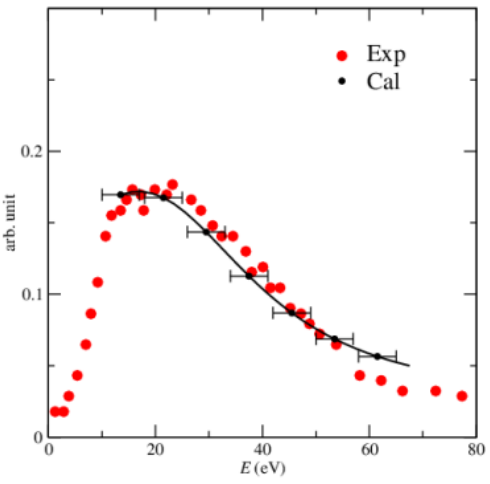
With the advent of free electron laser (FEL) such as Extreme Ultraviolet FEL and X-Ray FEL, many interesting phenomena in which atoms or molecules are highly excited due to the strong laser fields were observed. When a molecule is irradiated by intense laser, holes are proliferated through the Auger cascade and the molecule takes highly charge. The highly charged molecular ions are quite unstable due to the coulomb repulsive force and typically destroyed on a subpicosecond time scale. The fragment ions may convey information about molecular shape because they reflect geometric structure of the parent molecule just before dissociation. Recently, dissociation (Coulomb explosion) of several highly-charged aromatic molecules has been investigated by position-sensitive time-of-flight measurements. However details of the dissociation mechanism of these molecules are still unknown. Coulomb explosion mechanisms for polyatomic molecules are expected to be complicated for several reasons. First, a variety of ionic molecular fragments can be produced and there are many possible dissociation channels.

In order to clarify the atomic dissociation mechanism in the coulomb explosion of highly-charged molecules, we perform *ab initio* molecular dynamics simulation based on density functional theory. The cluster simulations for charged system were carried out using cluster boundary conditions which were imposed using the method of Martyna and Tuckerman [1]. From our simulation, it is found that molecular dissociation occurs through several stages. First, hydrogen atoms dissociate from the molecule, and then the molecule breaks into small fragments. Figure shows the kinetic energy distributions of H^+ ions of coulomb explosion of Bromo-phenol. The simulation results are good agreement with experimental results. In this study, we will discuss about the charge-state dependence of the dissociation mechanisms in coulomb explosion of several types of aromatic molecules.



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Two-phase molecular dynamic modeling of graphite melting

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For many years the graphite melting curve has been the object of essential debates due to large discrepancies in experimental data. We report here the two-phase molecular dynamic simulations of graphite melting with the semiempirical bond-order potential AIREBO. In the pressure range up to 14 GPa the graphite melting line is obtained and properties of liquid carbon are investigated. For the superheated graphite the melting front velocity dependencies on temperature are calculated to verify the melting temperatures values. The influence of the defect formation in superheated crystal on melting process is considered. Different melting regimes are revealed. The results provide a possible way to resolve the long-standing question for the reasons of large discrepancies in experimental data.

Predictive molecular-dynamics models for investigation of U, U-Mo and U-Mo-Xe systems

Daria Smirnova, Alexey Kuksin, Sergey Starikov, Vladimir Stegailov

Joint Institute for High Temperatures of Russian Academy of Sciences

Uranium alloys are now under active investigation as possible fuels for future fast and research reactors. Understanding the radiation damage effects on the fuel stability is one of the major challenges to be solved on the way to effective and safe fuel design. A description of radiation damage requires knowledge of the atomistic mechanisms of defect generation in solids. In case of uranium the radiation defect properties still have not been sufficiently studied either for pure U or for metallic uranium compounds, including uranium-molybdenum (U–Mo). Therefore reliable models of radiation damage in nuclear fuels are required to explain essential physical effects (point defects clustering, interaction with dislocation loops, grain boundaries etc) and make predictions about the materials characteristics. In this work the atomistic and molecular-dynamics models of pure U and prospective high density U-Mo fuel alloys are proposed. Also a set of new many-body interatomic potentials created especially for predictive modelling and simulation of these nuclear fuels is introduced and discussed [1,2]. The potential functions are fitted to the values of *ab initio* interatomic forces, energies and stresses. The models proposed are validated to be applicable for study of the following issues:

1) Structure of orthorhombic α-U, bcc γ–U, bcc Mo, U_2Mo compound and bcc U-Mo fuel alloys (containing from 7 to 12 wt.% of Mo).
2) Elastic constants, melting temperatures, thermal expansion and room-temperature isotherms of the components of U-Mo system; Grűneisen parameter for liquid and solid U.
3) The point defect (SIA, vacancy) formation energies for pure U and Mo.

The potentials developed are aimed to study the evolution of radiation defects in U and U-Mo fuels. For example, the point defects diffusion mechanisms in U-9Mo are considered and some comparison between the defect diffusivities in pure bcc U and in bcc U-9Mo is made. The potentials also give an opportunity for simulation of fission products (namely Xe) behavior in U, Mo and U-Mo.

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Molecular dynamics simulations of electron-ion nonideal plasmas on GPU

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Graphical procession units (GPUs) have shown their particular efficiency for classical molecular dynamics (MD) simulations [1,2,3]. In the case of long range interaction (Coulomb or gravitational) the so-called N-body problem is solved numerically which requires a relatively small amount of GPU memory and a large amount of computations. Such kind of algorithms fit the GPU architecture perfectly and allows one to achieve a significant performance gain (about 10 times comparing Intel Xeon X5670 CPU and Nvidia Tesla C2050 GPU).

In this work we applied GPU-accelerated MD simulations to study the electron-ion plasma generated by irradiation of nanosized metallic clusters by femtosecond laser pulses. Provided that the laser intensity is moderate (10^{13} – 10^{16} W/cm^2) the plasma becomes nonideal with the ratio of the mean potential to kinetic energy about unity. Electron plasma oscillations, electron-ion collisions, relaxation rates in such nonideal nanoplasma are of particular interest in view the size effects essential for the cluster plasma [3].

The use of GPUs allowed us to increase the number of particles by two orders of magnitude and to observe transitions of the electron oscillation spectra in the cluster plasma ranging from 55 to 10^5 ions. The dependence of frequency and damping of different collective plasma oscillation modes including Mie and Langmuir oscillations are presented. Influence of the choice of interaction potential is discussed.

GPU-accelerated program is also suitable for other problems of strongly coupled plasma. The example of convenient task is researching of equation of states of plasma. Computational aspects of this problem are discussed.

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Fourier Monte Carlo Simulation of Hexatic Membranes

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Abstract. Hexatic membranes are extremely difficult to study both in theory as well as in simulations based on conventional real space algorithms. We present new results for the flat phase of hexatic membranes using a unique simulation approach based on an recently developed optimization [1] of our Fourier Monte Carlo algorithm [2, 3]. In our present treatment, the case of hexatic membranes is found to closely resemble that of solid membranes for which our algorithm has already proven to be quite successful [1]. This success is based on tuning the Monte Carlo acceptance rates separately for each wavevector, which enables us to drastically reduce critical slowing down and thus observe critical behavior with excellent statistical accuracy. The resulting simulation scheme provides a new tailor-made approach to study critical behavior of systems with long-range interactions.

In detail, we calculate correlation function $< |f(q)| >^2 = G(q)$ and the related mean squared displacement $< (\Delta f)^2 >$ of the membrane's out-of-plane deformations in the Monge parametrization and give a detailed finite size scaling analysis of these data. For hexatic membranes, our simulations yield evidence for a logarithmic singularity of the critical exponent $\eta = 0_{\log}$. For the solid case, our numerical estimate for η is markedly smaller than that derived from other recent simulations [4], and we find clear evidence against "intrinsic ripples", whose existence has recently been claimed in the graphene-related literature [5].

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Efficient Hybrid DFT Simulations of Solvated Biomolecules

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One of the most important challenges in quantum simulations of biomolecules is efficient and accurate inclusion of the solvent, because the solvent atoms usually far outnumber those of the solute. We have developed a hybrid method that allows for explicit quantum-mechanical treatment of the solvent at low computational cost. It combines Kohn-Sham (KS) density functional theory (DFT) with orbital-free (OF) DFT. KS DFT is used to describe the biomolecule and its first solvation shells, while the OF DFT is employed for the rest of the solvent. The OF method scales linearly with the number of atoms and is capable of handling 10^5 solvent molecules on current supercomputers, while taking only a small percentage of the total computational time. The compatibility between the KS and OF DFT methods enables seamless integration between the two. In particular, the flow of solvent molecules across the KS/OF interface is allowed and the total energy is conserved. This method is implemented in the RMG (real-space multigrid) code, which employs grids for efficient parallelization and multigrid preconditioning for convergence acceleration.

The hybrid method has been used to investigate the binding of copper ions to proteins involved in prion (PrP) and Parkinson's diseases, and to study an experimental drug for Alzheimer disease. Our results for PrP show how this protein binds multiple copper ions while undergoing complex structural rearrangements and becoming more resistant to misfolding and thus to initiation of the prion disease. For alpha-synuclein, the Parkinson's disease (PD) protein, we show that copper binding modifies the protein structurally, making it more susceptible to misfolding -- an initial step in the onset of PD. In Alzheimer disease (AD), a drug based on a copper chelator shows significant promise in clinical trials. We investigated the mechanism of its action and found a low-activation-energy pathway for copper removal from amyloid-β, the principal protein involved in AD.

Very recently, we have adapted the RMG method to the latest generation of supercomputers that use multicore CPUs and high-performance accelerators (GPUs). Our latest implementation uses one MPI process per node, rather than one per core. It achieves intra-node parallelization through POSIX threads and OpenMP, and efficiently distributes the computational load between CPUs and GPUs, while minimizing costly data transfers between CPU and GPU memories. The revamped code scales to over 100,000 CPUs and 10,000 of GPUs, and easily reaches multi-petaflop performance.

Abstract for a contributed talk submitted to the
Conference on Computational Physics 2013

Topic: Statistical Physics & Complexity

Large-scale simulations shed new light on causes of age-related macular degeneration

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Age-related macular degeneration (AMD) is a debilitating eye disease and the leading cause of blindness in adults. We have developed a large-scale statistical mechanical model of the retina and studied the growth, patterning and progression of AMD. The computational approach allowed us to explore and quantitatively test many more combinations of hypotheses and parameter choices than would have been experimentally feasible. Our results suggest that new mechanical instabilities due to adhesion failure at the cell level are the dominant cause of the initiation and progression of neovascularization in AMD. This unexpected finding demonstrates the power of computational modeling approaches for studying complex biological system. Our findings will have a significant effect on the future development of targeted intervention strategies and clinical treatment of AMD.

Coauthors: A. Shirinifard, J. Glazier, M. Swat, Y. Jiang, J. Scott Gens, Y. Jiang, H. Grossnicklaus

EFFECT OF CALCIUM REMOVAL AND IONIC STRENGTH VARIATION ON THE CONFORMATION CHANGE IN CALMODULIN PROTEIN AT PHYSIOLOGICAL pH

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ABSTRACT

It is well known that there are many conformational sub-states of proteins which are determined by their folded structures. External factors like solvent type, temperature, pH and ionic strength play a very important role in this conformational sampling of the protein. In this manuscript, we investigate the response of the Calmodulin (CaM) protein as a function of calcium removal and ionic strength at physiological pH. CaM plays a very important role in different physiological processes as it can bind to a variety of other proteins. One hundred nanosecond simulations are carried out on the extended form of CaM. Changing the ionic strength came out to be one of the possible routes for observing a conformation change in the protein. This behavior is similar to the conformation change observed in our previous study where a change in the pH was observed to trigger a conformation change in this protein. As the calciums are removed from the protein, the protein is observed to become more flexible and acquires a more compact form as compared to its extended initial structure. The N and the C-lobes are observed to come as close as to a distance of 20-25 Angstroms. At a lower ionic strength of 150 nM, this conformation change is observed to take place at a much shorter time duration.

Bond orientation properties in lipid molecules of membranes: molecular dynamics simulations

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Rapid development of computer power during the last decade has made molecular simulations of lipid membranes feasible for many research groups, which, together with the growing general interest in investigations of these very important biological systems has lead to tremendous increase of the number of research on the computational modeling of lipid membranes [A.P. Lyubartsev, A.L. Rabinovich, *Soft Matter*. 2011. V.7. No.1. P.25-39; A.L. Rabinovich, A.P. Lyubartsev, *Polymer Science. Ser.C.* 2013. V.55. No.1. P.162-180]. Natural membranes (biomembranes) are very complex heterogeneous systems consisting of many different molecules which are involved in a variety of cellular processes. The most commonly occurring chains of lipid molecules have 12 to 24 carbons and may contain 1 - 6 carbon - carbon double bonds of the *cis*-configuration in different positions. The polyunsaturated chains are of great importance in structure and functioning of natural membranes At the same time, full understanding of the effects of lipid unsaturation on various physical properties of membranes at the molecular level, affecting their functioning, is not yet achieved. Molecular dynamics and Monte Carlo computer simulations of various lipid membrane systems allow elucidating the detailed relations between the chemical structure and physical properties of various lipid molecules and membrane inclusions, to explain individual peculiarities of natural objects, to make forecasts concerning their behavior, etc. An understanding of the molecular basis of various physical properties of lipids allows one to narrow down the list of hypotheses under consideration about the possible functions of various components (such as acyl chains) in lipid membranes, e.g., the maintenance of proper bilayer fluidity and permeability, of the activity of membrane-bound enzymes, etc.

Series of molecular dynamics simulations of 16 hydrated liquid crystalline phase phosphatidylcholine bilayers were carried out in order to investigate systematically the role of double bonds in physical properties of lipid membranes. The simulation boxes were filled by 64 lipid molecules per monolayer and 30 water molecules per lipid. The two hydrocarbon tails, the glycerol section and the head group of the lipid molecules were treated in accordance with their known chemical structure. All hydrogen atoms were explicitly included in the computations. Phosphatidylcholine molecules contained 1 – 6 *cis* double bonds in unsaturated chain *sn*-2 (with 18, 20 or 22 carbons) and saturated *sn*-1-chains (with 16 or 18 carbons). The 16 unsaturated pure bilayer systems were coupled to an external temperature bath of 303 K and a pressure bath of 1 atm. After 20 ns relaxation trajectories the MD production runs of 80 ns were executed for all bilayer systems.

Different equilibrium structural and dynamic properties of the bilayers were defined, such as profiles of C-C and C-H bond order parameters of lipid molecules with respect to the bilayer normal, the orientational fluctuations of these bond vectors (probability density distributions of C-C and C-H bond orientations), the root mean square values of the positional fluctuations of all lipid atoms relative to the average atomic coordinates, etc. It was shown that the study of anisotropy degree of probability density distributions of bond orientations allows distinguishing extended regions with different types of angular fluctuations of bonds in a membrane formed by lipid molecules with unsaturated chains. The computed properties were compared with available experimental data and discussed in relation to their possible role in the biological functioning of membranes.

This work has been supported by grant No. 1642.2012.4 for leading research schools of Russian Federation; grant No. 10-03-00201 of Russian Foundation for Basic Research; grant No. 310465 of the seventh framework programme (FP7) of the European Community.

Enhancement Flow in Nanoconfined Water

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We investigate through non-equilibrium molecular dynamic simulations the flow of core-softened fluids inside nanotubes. Our results reveal a anomalous increase of the overall mass flux for nanotubes with sufficiently smaller radii. This is explained in terms of a transition from a single-file type of flow to the movement of an ordered-like fluid as the nanotube radius increases. The occurrence of a global minimum in the mass flux at this transition reflects the competition between the two characteristics length scales of the core-softened potential. Moreover, by increasing further the radius, another substantial change in the flow behavior, which becomes more evident at low temperatures, leads to a local minimum in the overall mass flux. Microscopically, this second transition results from the formation of a double-layer of flowing particles in the confined nanotube space. These special nano-fluidic features of core-softened particles closely resemble the enhanced flow behavior observed for liquid water inside carbon nanotubes.

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Freak waves at the surface of deep water

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Abstract

We present generalization of the improved Zakharov equation for the "almost" 2-D water waves at the surface of deep water. When considering waves slightly inhomogeneous in transverse direction, one can think in the spirit of Kadomtsev-Petviashvili equation for Korteveg-de-Vries equation taking into account weak transverse diffraction. Equation can be written instead of classical variables $\eta(x,y,t)$ and $\psi(x,y,t)$ in terms of canonical normal variable $b(x,y,t)$:

$$i\frac{\partial b}{\partial t} = \hat{\omega}_{k_x,k_y} b + \frac{i}{4}\hat{P}^{+}\left[b^{*}\frac{\partial}{\partial x}({b'_x}^{2}) - \frac{\partial}{\partial x}(b^{*\prime}_x \frac{\partial}{\partial x} b^2)\right] - \\ -\frac{1}{2}\hat{P}^{+}\left[b\cdot\hat{k}(|b'_x|^2) - \frac{\partial}{\partial x}(b'_x \hat{k}(|b|^2))\right].$$

This equation is very suitable for robust numerical simulation. Due to specific structure of nonlinearity in the Hamiltonian the equation can be effectively solved on the computer. It was applied for simulation of sea surface waving including freak waves appearing.

Approximate analytical descriptions of the stationary single-vortex Marangoni convection inside an evaporating sessile droplet of capillary size

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Three versions of an approximate analytical description of the stationary single vortex Marangoni convection in an axially symmetrical sessile drop of capillary size are studied for arbitrary contact angle and compared with the results of numerical simulations. The first approach is heuristic extension of the well-known lubrication approximation. Two other new descriptions are developed for arbitrary contact angle and named $n\tau$- and rz-description. They are free from most of restrictive assumptions of the lubrication approach. For droplets with large contact angles they result in better accuracy compared to the heuristic extension of the lubrication approach, which still gives reasonable results within the accuracy 10–30 per cent. For droplets with small contact angles all three analytical descriptions well agree with the numerical data.

[1] L.Yu. Barash, submitted to Phys. Rev. E., arXiv: 1308.0342

Formation of high-gradient regions in freely-decaying and forced two-dimensional hydrodynamic turbulence

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Freely-decaying and forced two-dimensional hydrodynamic turbulence is simulated numerically with a Fourier pseudospectral method using both conventional multiprocessor and graphical clusters. The Euler equation with hyperviscosity is solved to study statistical characteristics of turbulence. In numerical experiments with grid resolution up to 8192 × 8192 a Kraichnan-type turbulence spectrum, $E(k) \sim k^{-3}$ is observed over a few decades in the direct-cascade region of the spectral space. A spatial filtration procedure is used to establish that the main contribution to the spectrum comes from the sharp vorticity gradients in the form of vorticity quasi-shocks. Though the collapse as the process of singularity formation in a finite time is forbidden in two-dimensional hydrodynamics, but there is a strong tendency to the emergence of high-gradient regions. As it follows from our numerical experiments, vorticity gradients increase by more than two orders of magnitude during computation.

Such quasi-singularities are responsible for a strong angular dependence of the spectrum owing to well-localized (in terms of the angle) jets with minor and/or large overlapping. In each jet, the spectrum decreases as k^{-3}, which yields the Kraichnan spectrum after averaging over the angle. The behavior of the third-order structure function accurately agrees with Kraichnan direct cascade concept corresponding to a constant enstrophy flux. It is shown that the power law exponents ζ_n for higher structure functions grow more slowly than the linear dependence of n, which testifies to turbulence intermittency.

Thus, the main result of this investigation is the fact that the Kraichnan-type power-law spectrum is formed owing to quasi-singularities, which appear in solving the Cauchy problem for the two-dimensional Euler equation.

This work was supported by the grant of the Government of the Russian Federation for state support of academic research performed under supervision of leading scientists in Russian educational institutions of higher professional education (Agreement No. 11.G34.31.0035).

Modeling of Rarefied Gas Flows on the Base of Numerical Solving of the Boltzmann Equation

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The traditional approach of gas flow modeling is based on Euler or Navier-Stocks equations. This approach is relevant if the mean free path of molecules is small compared to specific size of flows, whereas the rarefied gas effects are not important. However, due to development of micro devices in various application areas, at the present time interest in rarefied gas modeling has been increasing. A kinetic approach is required to describe the rarefied gas flows. The basis of the kinetic theory of gases is the Boltzmann kinetic equation.

The complexity and non-linearity of the Boltzmann equation cause many researchers to use alternative approaches. One of these is the Direct Simulation Monte-Carlo (DSMC) method. However, because of high level of statistical noise the Monte-Carlo methods are not very efficient for simulating slightly disturbed flows, which are typical for microdevices. Other prevalent approaches are based on using model kinetic equations where the right term of the Boltzmann equation – the collision integral – is replaced by simpler relaxation forms with less computational complexity. Nevertheless, the reliability of results obtained by these methods is unknown.

Nowadays, the growth of the power of modern computation systems made it possible to solve the Boltzmann kinetic equation directly without any simplifications. In the present work we solve the Boltzmann equation by finite-difference method with application of the conservative projection method for calculation of the collision integral [1]. The last method ensures that the laws of conservation of mass, momentum and energy are strictly observed, and the collision integral of the Maxwellian distribution function is equal to zero. Real molecular potentials can be used in simulation. The method can be applied to a single component gas, a gas mixture [2] and a gas with internal degrees of freedom [3].

On the basis of the conservative projection method the problem-solving environment (PSE) designed for simulation of rarefied gas flows was developed. The PSE allows one to perform calculations on personal computer, including the use of graphics processors [4]. Complex two- and three-dimensional problems are computed on multi-processor clusters.

In course of development of the program code some bottlenecks were located using performance analyzers. The code was optimized by using of SSE and AVX instructions that gives about 40-50% increase of the speed of computations. A version adapted to Intel MIC architecture is now under development.

The work presents the results of simulation of some slightly disturbed flows as well as supersonic flows. Examples of slightly disturbed flows show modeling of Knudsen pump and its multistage modification. The accuracy of obtained results is proved by parametric computations and is limited only by the available computational resources.

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MMALE numerical simulation for multi-material large deformation fluid flows

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Multi-material large deformation fluid flows exist frequently in astrophysics, weapon physics and inertial confinement fusion (ICF) fields. There are two important characteristics in these kinds of flow phenomena. One is the violent movement of the fluid, which leads to large deformation of fluid field. The other is the existence of multi-material and the distortion of the interface between different materials.

Multi-material arbitrary Lagrangian-Eulerian (MMALE) methods are employed widely in the computation of multi-material and large deformation fluid flows. In these methods, mixed cells are introduced and the material interfaces are permitted to cross computational cells. Here mixed cells are cells including two or more kinds of materials. The introduction of mixed cells make the computational code robust, while keep the computational results as accurate as possible. To handle the material interfaces in mixed cells, MOF interface reconstruction method is used in MMALE simulations.

A test case deals with the well-known Rayleigh-Taylor instability. The computational domain is the rectangular box [0,1/3]x[0,1] with is paved with 34x100 cells. The initial set up consists of two immiscible fluids which are separated by a perturbed interface, whose equation writes $y_i(x) = 0.5 + 0.01\cos(6\pi x)$. The heavy fluid is located above the light one. The densities of the two fluids are $\rho_h = 2$ and $\rho_l = 1$. The same polytropic index $\gamma = 1.4$ is shared by the two fluids. A downward gravity field is applied, $\boldsymbol{g} = (0, -0.1)^t$. We have plotted in Fig.1 the grid and interface at times t=7, t=8 and t=9.

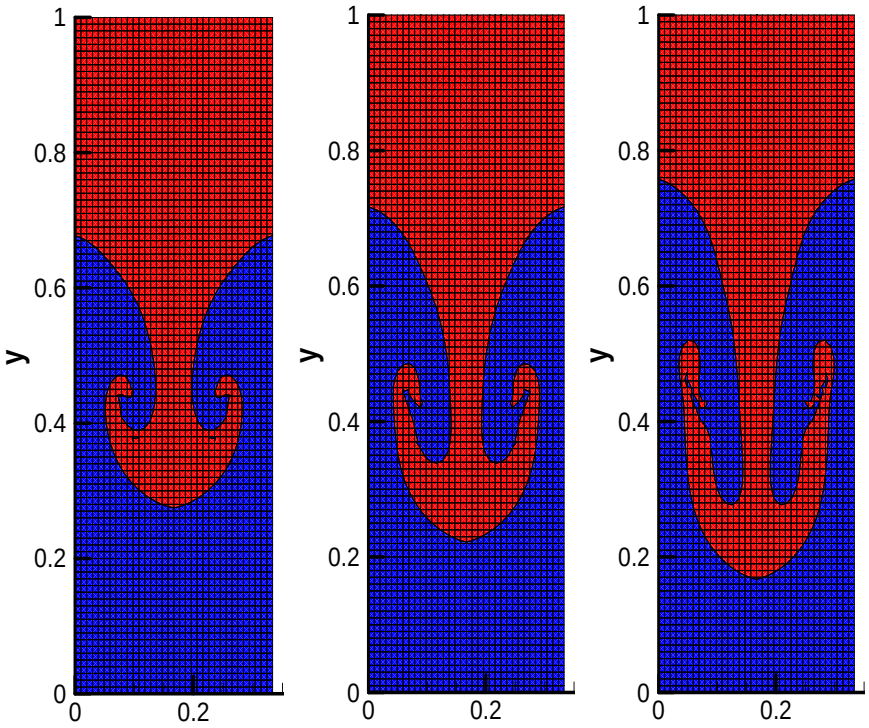

Fig.1 Rayleigh-Taylor instability. Snapshots of the grid and interface at times t=7, t=8 and t=9

Fully general-relativistic simulations of binary neutron-star mergers

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I will present our results on **three-dimensional general-relativistic simulations of binary neutron-star coalescence and merger**, and of the subsequent formation and evolution of the merged object (black-hole) surrounded by a possibly massive self-gravitating disc, which may be the **engine of short gamma-ray bursts** (GRBs). I will focus also on the numerically extracted **gravitational radiation** and on the comparison with the results of independent codes and analytic approximations.

Neutron stars (NSs) are very compact objects formed in the gravitational collapse of massive stars. NSs are at the center of many fascinating phenomena in the Universe, including gamma-ray bursts, supernova explosions, pulsars, and gravitational waves. A large fraction of the current astrophysical research topics in the world focuses on one of the above phenomena.

Binary neutron star systems (BNSs) are especially interesting for two main reasons:

1) BNSs are very strong sources of gravitational waves. By measuring the gravitational signal from BNSs we can – among many other things – get information about the structure and equation of state of NSs; this is actually a prime possibility to investigate the properties of ultra-high density matter, because NS-like densities are not reproducible in laboratory experiments.
2) BNSs are thought to be the engine powering one type of GRBs.

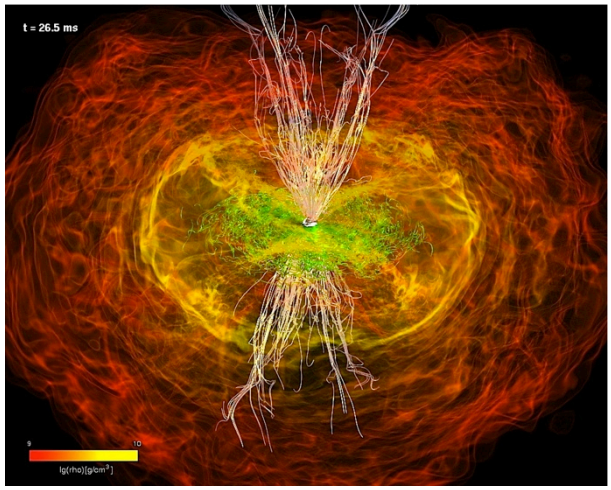

Figure. A snapshot of the formation of a large-scale ordered magnetic field after the merger and collapse of a BNS. Its structure includes a funnel, in which a GRB jet may be launched. Shown with a color-code map is the rest-mass density, over which the magnetic-field lines are superposed. Green lines sample the magnetic field in the disc and on the equatorial plane, while white lines show the magnetic field outside the disc and near the BH spin axis.

A subclass of "short hard" GRBs (lasting less than 2s and with a hard spectrum) are thought to originate from the merger of BNSs. The typical scenario is based on the assumption that a system composed of a rotating black hole (BH) and a surrounding massive torus is formed after the merger of NS-NS or NS-BH binaries. If the disc has a mass greater than 0.1 solar masses, it could supply the large amount of energy involved in GRBs by magnetic-field and neutrino processes.

Furthermore, we report on our study on the tidal effects due to the finite size of neutron stars and on how they can produce a detectable signature in gravitational signals that are likely to be observed by ground-based gravitational wave detectors such as Advanced LIGO. The observation of these tidal effects presents the possibility of measuring neutron star properties which in turn will constrain models for the neutron-star EOS.

Author: Cristina Torres

Title:

Using a multidimensional likelihood algorithm like the Critical Coupling Likelihood to passively estimate effective transfer function like qualities in a running interferometric type gravitational wave detector.

Co-authors:

Cesar Augusto Costa, Instituto Nacional de Pesquisas Espaciais, Sao Jose dos Campos, Brasil

Abstract:

The effective spectrum of a gravitational wave (GW) detector without signals present, is the product of instrumental noise sources. Different components of the spectrum are related to different sources of noise. Using a high dimensional likelihood algorithm, like the Critical Coupling Likelihood method one should be able to probe the properties of instrumental noise. This passive probing of the system inputs and outputs, in principle, allows for the measurement of noise propagation without disturbing the running state of a GW detector. From the results of this probing one can infer the average strength of coupled noise as a function of detector frequency. This information along with basic calibration information of individual GW detector components can be used to create a pseudo-transfer function (PTF). These PTFs reveal the manner in which noise sources external to the GW detector manifest themselves in the final output of the GW detector. Computing a rigorous traditional transfer function for a series of non-linear systems in a live GW detector is not possible without disturbing the operational state of the detector. Using passively obtained PTFs, one would hope to be able to make incremental improvements to a GW detector thereby improving its noise suppression capabilities. We plan on introducing one particular method for creating these pseudo-transfer functions which should describe noise coupling in a live GW detector.

Evolution of multi-component spiral disc galaxies: dynamics of gas, stars and dark matter.

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We present a numerical N-body/hydrodynamics code for investigating the evolution of disc galaxies in the context of secular processes and ISM transformation. Hydrodynamical equations were solved using TVD-MUSCL scheme with the extended thermodynamics, magnetic field and the possibility of the multi-species simulations. N-body approach was used for describing of the dynamics of stellar particles, DM halo particles and/or dust grains. The gravitational potential was calculated by FFT. The whole code was adopted for the parallel application using MPI standard. A two different kinds of decomposition were applied for calculation the hydrodynamical and Poisson equations. We briefly discuss recent results in simulations of the hydrodynamic processes involved in the formation of a galactic spiral pattern, the evolution of gas-dust clouds and other possible applications of the code. Our numerical experiments were performed using supercomputers of the Moscow State University — Lonomosov and Chebyshov (NIVC MSU).

I want to simulate problem X

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My Computational Physics class for some 20 beginning graduate students has a project component. It is relatively easy to find simulation projects loosely connected to one's research area. I can easily propose projects on atomistic simulations of condensed matter or statistical physics that are relevant, interesting and can be completed with the appropriate effort.

In my (idealistic or crazy) attempts to extend Computational Physics education in our department beyond "my areas", my recent computational physics classes have included students from areas such as relativity, optics, plasma physics and types of quantum physics. These topics fall outside of my expertise in either topic or algorithm (or both). The students (not unreasonably) expect projects in these areas. In some cases their supervisors hope said projects will jumpstart a computational component in their research groups, a challenge I cannot refuse. I also enjoy beginning new directions. I will present some of these projects, and describe our pitfalls and successes.

Simplified pseudopotential problems for the classroom

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Abstract. In the computational quantum mechanical study of condensed matter systems *ab initio* methods have been used for many decades to accurately predict properties of crystalline solids such as equilibrium lattice constants, band structure, optical properties, elastic constants, etc. In the early 80's and 90's many research groups developed their own programs to perform *ab initio* calculations. In doing so, generations of research students and postdoctoral fellows acquired useful, transferable skills. Over time however, collaborations between various research groups within academia and in industry have resulted in the creation of more than 50 open-source and commercial software packages. These software packages are widely used today for condensed matter research by students who, unfortunately, often have have very little understanding of the theoretical framework, and algorithmic and programming details of these codes. To address this shortcoming, our research group has embarked on a programme to devise a range of simplified computational problems appropriate for the classroom, which can be used to teach undergraduate students about particular theoretical and numerical aspects of the electronic structure method. These problems are easily programmable. In this presentation, we will focus on the pseudopotential method, which is an important ingredient in modern *ab initio* methods. Whereas the full implementation of this concept in a real electronic structure code requires complicated numerical methods, e.g. accelerated convergence to selfconsistency including the interactions between all the electrons in the system, we show that the essential principles of the pseudopotential can, nevertheless, be presented in a simpler class of problems, which can readily be coded by students.

Constrained statistical mechanics for charges and spins

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The statistical mechanics of constrained systems has been developed to describe the properties of exotic frustrated magnetic materials, such as spin-ice. At the same time very similar mathematical tools have been used to create local simulation algorithms for charged systems.

We bring out analogies between the approaches in the two communities, and discuss the effective dynamic equations generated in Monte-Carlo simulations of constrained systems. We will also discuss analogies to quantum electrodynamics and the Dirac procedure and look for analogies to gauge invariance in the effective dynamics.

Mesoscopic fluctuation of a qubit population in a biharmonic driving field

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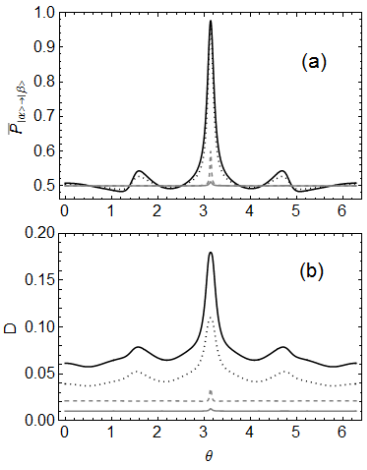
It is well known that the conductance of disordered systems at low temperatures manifests mesoscopic fluctuations, due to interference of electron waves [1]. The large size of the electron trajectories makes the interference corrections to the conductance is very sensitive to the configuration of impurities in low-dimensional systems (a film or a wire): it is enough to move one impurity at a distance of the order of the wavelength of an electron to significantly alter the interference of electron waves. Conductance one-dimensional system is sensitive especially to the impurity configurations because in this case the returnable path of the electrons always pass the same scatterers [2].

In the present paper the mesoscopic fluctuations of the transition probability between the ground and excited states of a superconducting Josephson qubit excited by a superposition of two radio pulses is investigated both numerically and analytically. The Hamiltonian of the qubit is: $H(t)=\left(\varepsilon(t)\sigma_z+\Delta\sigma_x\right)/2$, where $\varepsilon(t)$ - a time-dependent control parameter, Δ - tunneling splitting of levels. It is assumed that initially a qubit is in the ground state, and the transitions to the exited level are induced by an external biharmonic driving field $\varepsilon(t)=\varepsilon_0+A(\cos\omega t+\gamma\cos(2\omega t+\theta))$, where ε_0 is dc and A is ac components of the driving amplitude; γ and θ - are relative amplitude and phase of mixing pulses. In the adiabatic approximation the qubit can be in states $\phi_{\pm}(t)$ with the energies $E_{\pm}(t)=\pm\sqrt{\varepsilon(t)^2+\Delta^2}$. When the control field is changed such a way that the anticrossing levels $E_{\pm}(t)$ takes place then the Landau-Zener transitions between them may be induced [3]. The rate of the Landau-Zener transitions can controlled by the amplitudes and relative phase of the pulses [4]. By analogy with the theory of mesoscopic systems, we can see that the number of quasicrossings adiabatic levels (number of transitions) during the external field time is analogous to the number of s scatterers which are placed on the length of the wire. For a fixed pulse duration phase is responsible for changing the configuration of the scatterers, and the total duration of the signal behaves like a length of wire.

The transition probabilities between the qubit levels, taking into account the phase noise, are found by solving the equation for the density matrix. The figure shows the results of numerical calculation of transition probabilities (a) and the dispersion (b) depending on the relative phase difference θ. It is shown the transition probabilities and variances depending on the relative phase difference θ for different values of the phase noise of Γ: Γ = 0.0001, black, black dotted Γ = 0.001, gray dotted Γ = 0.01, a gray Γ = 0.1. As can be seen, the noticeable fluctuation in the value of the relative phase $\theta=\pi$. With an increase in the rate of phase relaxation is observed suppression fluctuations similar to the mesoscopic systems. Also the behavior of the fluctuations intensity at different durations of the signal τ has been studied. It is shown that strong mesoscopic fluctuations occur on time scales shorter than the time dephasing ($\tau<1/\Gamma$), whereas at the long-time ($\tau>1/\Gamma$), the variance is completely suppressed. This fact enables us once again emphasize the analogy with the mesoscopic, consisting in the fact that the dependence of the fluctuations of the population of the qubit on the pulse duration is similar to the behavior of conductivity fluctuations on the length of the wire.



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Title:
Fluctuation-dissipation theorem in isolated quantum systems out of equilibrium

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US institution: University of California, Davis

Co-authors and their institutions:
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Mark Srednicki (University of California, Santa Barbara)
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Abstract:
We examine the validity of fluctuation-dissipation relations in isolated quantum systems taken out of equilibrium by a sudden quench. We focus on the dynamics of trapped hard-core bosons in one-dimensional lattices with dipolar interactions whose strength is changed during the quench. We find that fluctuation-dissipation relations hold if the system is nonintegrable after the quench. They also hold if the system is integrable after the quench if the initial state is an equilibrium state of a nonintegrable Hamiltonian. However, they fail if the system is integrable both before and after quenching.

References to your relevant published papers:

E. Khatami, G. Pupillo, M. Srednicki, and M. Rigol
"Fluctuation-dissipation theorem in an isolated system of quantum dipolar bosons after a quench"
Accepted in Phys. Rev. Lett. (to appear online July 31), preprint: arXiv:1304.7279

The Topological Qubit: Quantum Evolution via Sheaves

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We consider some generalization of the theory of quantum states, which is based on the analysis of long standing problems and unsatisfactory situation with existing interpretations of quantum mechanics/Local Quantum Field Theory. We demonstrate that the consideration of quantum states as sheaves can provide, in principle, more deep understanding of some well-known phenomena. The key ingredients of the proposed construction are the families of sections of sheaves with values in the proper category of the functional realizations of infinite-dimensional Hilbert spaces with special (multiscale) filtrations decomposed into the (entangled) orbits generated by actions/representations of internal hidden symmetries. In such a way, we open a possibility for the exact description of a lot of phenomena like entanglement and measurement, wave function collapse, self-interference, instantaneous quantum interaction, Multiverse, hidden variables, etc. In the companion paper we consider the machinery needed for the generation of a zoo of the complex quantum patterns during Wigner-Weyl-Moyal evolution together with constructive algebraic control.

Dynamics of Two-dimensional Electron Gas in Non-uniform magnetic field.

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We have theoretically studied dynamics of the two-dimensional electron gas (2DEG) placed in a strong laterally non-uniform magnetic field, which appears due to ferromagnetic film on the top of heterostructure.

It is shown that lateral inhomogeneity of a strong magnetic field allows itself “magnetic gradient” or special magnetic-edge magnetoplasmons due to complex lateral structure of magnetic field distribution. This mechanism is different from usual “density gradient” edge magnetoplasmons.

We have solved self-consistently Poisson equation for non-uniform density distribution of the 2DEG for realistic heterostructure together with hydrodynamic equation of 2D Fermi liquid. As a result eigen value problem has been obtained that corresponds to the motion of charge density wave perpendicular to magnetic gradient. It is shown that for non-monotonic distribution of magnetic field “magnetic gradient” magnetoplasmon may move in both directions.

To solve eigen value problem we have compared two types of numerical approaches: (i) grid method that diagonalizes large Hermitian matrix and (ii) semi-analytical approach that expand each eigen mode on the set of orthogonal functions. Proper choice of parameters of the basis permits to reduce size of the matrix substantially preserving reasonable accuracy.

Quantum time correlation functions via noisy Monte Carlo and classical trajectories

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Abstract

Starting from a path integral representation, we show that, in its linearized form, Schofield's expression for the correlation function can be efficiently computed by averaging appropriate functions of coordinates and momenta over a set of classical trajectories [1]. The initial conditions for these trajectories are obtained from an exact representation of the quantum thermal density. To tame the effect of a phase factor, in this representation we use a cumulant expansion leading to a form for the density which can only be estimated numerically. To solve this difficulty, we adapt to our case advanced Monte Carlo methods for ``noisy" probability densities [2,3]. The efficiency of the algorithm is demonstrated by calculating the dynamic structure factor for a realistic model of liquid Neon [4]. We also show, by computing the gas phase infrared spectrum of a set of test molecules, that the method converges with a number of trajectories similar to that of other commonly adopted quasiclassical schemes that fail when applied to this calculation.

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Quantum Modeling: from Coarse Graining to a Tower of Scales

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We present a family of methods which can describe complex behaviour in quantum ensembles. We demonstrate the creation of nontrivial (meta) stable states (patterns), localized, chaotic, entangled or decoherent, from the basic localized modes in various collective models arising from the quantum hierarchy described by Wigner-like equations. The advantages of such an approach are as follows: i). the natural realization of localized states in any proper functional realization of (Hilbert) space of states, ii). the representation of hidden symmetry of a chosen realization of the functional model describes the (whole) spectrum of possible states via the so-called multiresolution decomposition. Effects we are interested in are as follows: 1. a hierarchy of internal/hidden scales (time, space, phase space); 2. nonperturbative multiscales: from slow to fast contributions, from the coarser to the finer level of resolution/decomposition; 3. the coexistence of the levels of hierarchy of multiscale dynamics with transitions between scales; 4. the realization of the key features of the complex quantum world such as the existence of chaotic and/or entangled states with possible destruction in "open/dissipative" regimes due to interactions with quantum/classical environment and transition to decoherent states. The numerical simulation demonstrates the formation of various (meta) stable patterns or orbits generated by internal hidden symmetry from generic high-localized fundamental modes. In addition, we can control the type of behaviour on the pure algebraic level by means of properly reduced algebraic systems (generalized dispersion relations).

Concept of equivalent temperature of the nonlinear-optical crystal interacting with nonuniform laser radiation

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Crystal temperature control with high precision is necessary condition for the efficient conversion of laser radiation in critically phase matched nonlinear-optical processes. However till now methods for precise temperature control of crystals heated by laser radiation are not devised. Conventional techniques imply temperature measurement of air surrounding nonuniformly heated crystal. These methods cannot ensure sufficient accuracy due to high air temperature gradient in the vicinity of the crystal surface. Moreover in process of laser frequency conversion changes occur of crystal-air heat transfer coefficient as well as optical absorption coefficients at pump and converted radiation wavelengths. Thus nonlinear-optical crystal temperature measurement and control is topical problem in laser physics.

Present work is dedicated to both the theoretical model elaboration and experimental performance of the precise temperature measurement of crystal nonuniformly heated by laser radiation. Acousto-resonance spectroscopy technique is employed for these purposes. The idea of simultaneous combination of optical and acoustical measurements proved to be fruitful [1-3]. The reason is that all nonlinear-optical crystals possess piezoelectric properties. As follows both direct noncontact excitation and detection of acoustical vibrations in crystals can be performed by using external radiofrequency (RF) electric field. Piezoelectric resonance is observed when the electric field frequency f coincides with the crystal intrinsic vibration mode frequency Rf_{n} (n – mode index). Recently novel concept of "crystal equivalent heating temperature $\Delta\Theta_{\mathrm{eq}}(P)$" has been introduced in laser physics [1]. This concept is based on experimental determination of the piezoelectric resonance frequencies $Rf_n(\mathrm{T})$ dependence on crystal uniform temperature T and theoretical model of the crystal nonuniform heating by laser radiation of power P. Crystal nonuniform temperature change $\Delta\mathrm{T}_{\mathrm{cr}}(x,y,z,P)$, which is calculated, is then substituted by $\Delta\Theta_{\mathrm{eq}}(P)$ value that is independent on coordinates. The $\Delta\Theta_{\mathrm{eq}}(P)$ is directly measured from the piezoelectric resonance frequency shift $\Delta Rf_n(P)$ for the given laser power distribution $P(x,y,z)$. Crystal true thermodynamic temperature distribution is expressed: $\mathrm{T}_{\mathrm{cr}}(x,y,z,P)=\mathrm{T}_0+\Delta\Theta_{\mathrm{eq}}(P)+\delta\mathrm{T}(x,y,z,P)$. Here T_0 is crystal temperature at P=0. Using the proposed mathematical model of the crystal heating by laser radiation it was shown that temperature nonuniformity inside the crystal satisfies the following condition $\delta\mathrm{T}(x,y,z,P)<<\Delta\Theta_{\mathrm{eq}}(P)$ [2]. Here mathematical problem definition and solution are based on variation principle. Mechanical and electrical boundary conditions should be specified for calculating motion state of the medium. Electrical boundary conditions of the first type suggest specification of the surface charge density $\bar{\sigma}$ and those of the second type suggest specification of the electrical potential φ. The following expression for the action functional can be written.

$$L_0(u_i,\varphi)=\int_{t_0}^{t}\left[\iiint_{\Omega}\left(\frac{1}{2}\rho\dot{u}_i^2-\frac{1}{2}c_{ijkl}S_{ij}S_{kl}+\frac{1}{2}\varepsilon_{ij}E_iE_j\right)d\Omega\right]dt+\int_{t_0}^{t}\left[\iint_{\Gamma_f}\bar{F}_iu_i\,dA-\iint_{\Gamma_D}\bar{D}_in_i\varphi\,dA+\iint_{\Gamma_u}T_{ij}n_j(u_i-\bar{u}_i)\,dA-\iint_{\Gamma_\varphi}D_in_i(\varphi-\bar{\varphi})\,dA\right]dt\cdot$$

Here D_i – electric displacement vector; $E_i=-\partial\varphi/\partial x_i$ – electric vector; c_{ijkl} – tensor of elastic constants of the sample; e_{ijk} – tensor of piezoelectric modules; ε_{ij} – dielectric tensor; S_{ij} – strain tensor; T_{ij} – stress tensor; ρ – density of the sample; u_i – components of mechanical displacement of the sample points; F_i – force; n – normal vector; $d\Omega$ – volume element; dA – surface (boundary) element; t – time; Γ denotes boundary; horizontal bar above function denotes its value at the boundary. For the case of natural boundary conditions the derivation of equations for crystal intrinsic modes was made. It was shown that for all unknown functions (mechanical displacement and electric potential) the dependence on time is harmonic and is characterized by the certain frequency. The last one is the intrinsic vibration mode frequency. After calculating the eigenfrequencies and spatial distributions of the functions u_i, φ the piezoelectric resonance thermal shifts are calculated using known dependence of the elastic constants $c_{ijkl}(\mathrm{T})$ on crystal uniform temperature. Nonuniform temperature distribution inside the crystal results in additional piezoelectric resonance frequency shifts. The reason for that is spatial dependence of the elastic constant values, which is typical for the case of crystal nonuniform heating.

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Novel method for identification of intrinsic vibration modes in piezoelectric crystals

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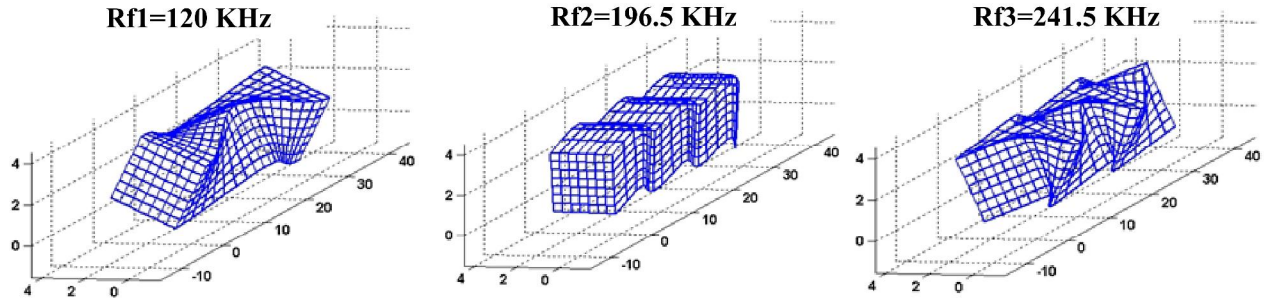
Variety of practical applications of dielectric piezoelectric crystals in scientific experiments as well as in everyday life can be compared with that of semiconductor crystals. Moreover novel surprising applications of piezoelectric crystals in nonlinear optics have only recently been established [1, 2]. With respect to development of theoretical models that can explain behavior of the crystal in certain experimental conditions the considerable retardation is the case in relation to semiconductor physics and semiconductor devices. One of the most important property of piezoelectric crystals that is exploited consists in explicit response (piezoelectric resonance at certain frequencies Rf_n, n-mode index) to the applied radiofrequency electric field. However microscopic model of this unique phenomenon is not developed so far. Moreover there is no macroscopic model that can describe dependence on frequency of line forms of experimentally observed piezoelectric resonances. Discrepancy of line form amplitudes and widths experimentally measured in certain crystal can substantially vary. Great amazement arise the fact that quantity of resonances calculated from model approximation doesn't correspond to the quantity of measured ones [3]. Number of resonances obtained from theory can exceed that of experimentally measured by more than a factor of ten. Problem of large quantity of calculated modes and its identification becomes more complicate because one experimentally measure mode can be at the same time attributed to several calculated modes that are close in frequency. In practice because of unavoidable experimental errors it is impossible to identify reliably the experimental mode with calculated one. In case of mode identification mismatches the calculation of physical parameters of the crystal using experimentally measured piezoelectric resonance frequencies becomes impracticable. For authentic determination of the elastic and piezoelectric constants, which amount depends on the crystal symmetry, the number of identified modes should be several times higher than that of nonzero elastic and piezoelectric constants.

In present paper we introduce novel method for identification for resonance modes in piezoelectric crystal. This method is based on recently proposed theoretical model of piezoelectric resonance frequencies dependence on temperature $Rf_n(T)$. Calcualtion of Rf_n is based on Lagrange-Hamilton variation principle. Lagrangian for piezoelectric crystal includes not only potential energy of deformed crystal together with kinetic energy of vibrating points but also the energy term related to piezoelectric properties. For calculating the dependence of piezoelectric resonance frequencies on temperature we used crystal temperature dependent tensors: elastic, piezoelectric and dielectric. For mathematical solving the components of the sample points mechanical displacement as well as electrical potential should be expanded in some set of basis functions. As a result, the Lagrangian is dependent on the expansion coefficients and equations for the eigenmodes are obtained by Lagrangian differentiation in the components. Below calculation results of three intrinsic vibration modes are shown. Calculations were performed for quartz crystal 3×3×30 mm^3 cut along crystallographic axes



Comparison of temperature dependencies of the measured and calculated resonance frequencies reveals reliable method for identification of vast majority of the experimentally measured resonance modes. It should be emphasized that amplitudes of the experimentally measured piezoelectric resonances strongly differ from each other and mathematical criteria for theoretical analysis of intrinsic vibration mode amplitudes aren't devised so far.

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The equivalent temperature model in process of nonlinear conversion of laser radiation

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In laser optics nonlinear frequency conversion proved to be one of the most important branch. Thanks to development of nonlinear optics one can obtain new powerful laser sources in different spectral ranges. The usage of nonlinear-optical frequency conversion is rather broad. It spreads from medical applications and biophotonics to inertial confinement fusion and precise micromachining. Stability and uniformity of crystal temperature is fundamental demand for efficient nonlinear frequency conversion in terms of critical phase matching. However if we for example consider second harmonic generation process than in practice taking into account optical absorption α at both pump wavelength λ_1 and converted laser radiation λ_2 wavelength it is almost impossible to achieve such conditions. One can observe high temperature gradient in radiation propagation direction not only due to absorption coefficient difference (in most cases $\alpha(\lambda_2) > \alpha(\lambda_1)$) but also due to nonlinear conversion. Because of the last one the pump power P_1 decreases and second harmonic power P_2 increases along the crystal. Yet, to the present day the problem of measuring and maintaining nonuniform temperature distribution inside nonlinear-optical crystal in terms of laser frequency conversion has not been solved.

In this paper we present theoretical model of crystal temperature calculation in terms of nonuniform heating by laser radiation. Also we compare the true thermodynamic temperature $T_{cr}(x,y,z,P_1,P_2)$ with measurable parameter $\Delta\Theta_{eq}$ – the equivalent temperature of nonlinear-optical crystal heated by laser radiation that we have recently introduced in laser physics [1-3]. Thanks to the fact that all nonlinear-optical crystals are piezoelectric materials one can excite and detect acoustic vibrations in direct manner. This feature allowed us to introduce the concept of equivalent temperature. In work [2] the temperature distribution in crystal was calculated according to 2-dimension model of distribution of laser radiation propagating through the crystal. Still longitudinal gradient of the crystal temperature wasn't taken into account. However in processes of frequency conversion of laser radiation there is always longitudinal temperature nonuniformity in crystal. In many practical applications longitudinal temperature gradient can be considerably high and thus phase matching conditions along the crystal length may be violated. This effect exhibits dramatically in so-called periodically poled nonlinear optical crystals such as periodically poled lithium niobate (PPLN) and periodically poled potassium titanyl phosphate (PPKTP). Longitudinal temperature gradient in periodically poled crystals is very essential in terms of conversion phase matching because it has strong influence on nonlinear conversion efficiency. Three-dimensional heat conduction equation with the heat sources is well-known and can be written in form: $\kappa\nabla^2 T(x,y,z) = \alpha(\lambda_1)P_1(x,y,z) + \alpha(\lambda_2)P_2(x,y,z)$. Here κ is heat conduction coefficient. Also we have to write boundary conditions in terms of convective heat transfer between crystal and air: $\kappa\left.\frac{\partial T(x,y,z)}{\partial n}\right|_{\partial V} = h^T(T_{air} - T_{cr})\big|_{\partial V}$. Here h^T is heat transfer coefficient, T_{cr} and T_{air} are crystal and air temperature at the interface respectively, n is normal vector to the crystal surface. Experimental values of optical absorption coefficients $\alpha(\lambda_1)$ and $\alpha(\lambda_2)$ and heat transfer coefficient h^T are obtained by measuring kinetics of the crystal equivalent temperature when crystal is irradiated by λ_1 wavelength, λ_2 wavelength, and by the sum of λ_1 and λ_2 [3]. After calculating temperature distribution $T(x,y,z,P_1,P_2)$ in crystal the problem of calculating piezoelectric resonance modes of nonlinear-optical crystal with nonuniform temperature distribution is solved. In order to solve this considerably complicated problem variation principle is used as in [1, 2]. Experimental verification of the proposed three-dimensional model of the crystal heating is performed by measuring the dependence of the equivalent temperature on pump laser power P_1 and converted laser power P_2.

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New Generation of More Efficient Solar Energy Materials: Quantum Modeling and Experimental Realizations

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The intermediate band (IB) solar cell has been proposed as a novel device structure which could enhance photovoltaic efficiency, thanks to the cooperation of two sub-bandgap energy photons which allows the full excitation of an electron across the whole bandgap of a semiconductor[1]. To realize this principle we have proposed in recent years, on the basis of quantum mechanical calculations, several materials where a metal or heavy element substitutes an atom in a known semiconductor with appropriate band gap, creating inside the band gap a partially filled band[2]. This new intermediate band, allows the absorption of low energy photons inside the gap increasing the photo-current and also maintaining the photo-voltage.

We present here compounds derived from different families of sulphides semiconductors, mainly spinels thin film and layered compounds:

- In_2S_3 and other sulphides containing octahedral In. The V-doped In_2S_3 material is particularly promising. We have synthesized it in nanocrystalline form and shown that its optical absorption spectrum has the features predicted by quantum calculations[3]. Recent photocatalytic tests made with it show that the V dopant extends its spectral response down to the IR range without increasing recombination.

- Octahedral Sn^{IV} layered sulphide and other similar compounds show also, according to theoretical modeling the formation of an IB with the desired characteristics when transition metals are introduced at Sn sites. The Van der Waals cleavage plane (0001) of these layered semiconductors is characterized by hexagonal arrays of close packed chalcogenide ions which are covalently bound within X-M-X sandwiches. This is an ideal substrate to study fundamental aspects of the metal/semiconductor interaction. The experimental synthesis of such sulphide show optical absorption spectra matching again the expectations for an IB material[4].

An overview of these systems, including results obtained on them using high level, state-of-the-art quantum calculation methods will be presented. Experimental results obtained for such novel IB materials matching in all cases the theoretical predictions.

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On structural and electronic properties of small silicon nanoclusters

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The small nanoclusters are very promising objects for the development of opto- and nanoelectronics, mostly because of their compatibility with currently dominating silicon-based technology of microelectronics. In this regard, the problem of production clusters with predetermined features is crucial. Since physical properties are determined by structure, a lot of effort had been put to develop methods of finding low-energy structures of atomic systems.

For large clusters (with sizes >5nm) it is well known experimentally, that their core has the structure of bulk sample, but for small ones the arrangement of atoms strongly depends on number of atoms.

In present work we will focus on the global optimization method based on combining evolutionary algorithms with sequential refinement of atomic interaction models. We use the USPEX code as the implementation of evolutionary algorithm for it has proved to be successful in solving many solid-state problems. [1] This code implies the creation of 'generation' of structures with subsequent local optimization. For this optimization we used the empirical potentials on the first steps of our calculation, and the ab-initio relaxation on the final steps. It allowed to save the CPU time without significant loss of accuracy.

As a result we calculated the stable structures of Si_n with n = 4...13 and of passivated clusters $Si_{10}H_{2m}$ (m=6,8,11). These structures showed excellent agreement with available experimental data [2] and earlier calculations performed by different optimization methods [3]. Further possibilities to accelerate cluster structure prediction are discussed. Authors are grateful to Ministry of Education and Science of Russia, Russian Academy of Sciences, and Russian Foundation for Basic Research for partial support of this research.

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Smoothed Particle Method for the Real-Space Electronic Structure Calculation

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In large-scale calculation such as hydrodynamics analysis, Smoothed Particle Hydrodynamics (SPH) is used as a typical mesh free particle method, and is very convenient and applicable for dealing with complex shapes, large deformations, and free surfaces. Currently, SPH is used in various fields for solving non-hydrodynamic partial differential equations such as the wave equation, Maxwell's equations, and Poisson's equation. However, it lacks sufficient accuracy. To realize a similar level of accuracy, many more particles are necessary than mesh points in the finite difference method (FD). Thus, it has not been evaluated sufficiently in quantum mechanical problems, because they require fairly high accuracy. As a higher-accuracy method in an improved method of SPH, Modified Smoothed Particle Hydrodynamics (MSPH) has recently been developed. Although various improved versions of SPH have been proposed, it is reported that MSPH has higher accuracy than other versions.

We have applied MSPH to quantum mechanical problems. The Schrödinger equation of a harmonic oscillator and the hydrogen atom are solved. Since we can analytically obtain exact solutions for these problems, it is quite efficient to evaluate MSPH in the quantum mechanical problems. The calculated results for MSPH are in good agreement with the analytical solutions. As a result, we have successfully shown that MSPH is efficient, and can therefore be applied to quantum mechanical problems with adequate accuracy. The results of using this method are also compared with those of the traditional FD and the standard SPH. The accuracy, however, depends on the arrangement of the particles. To obtain high accuracy, many particles should be distributed in the area where the wave function changes significantly.

In this paper, we demonstrate the importance of non-uniform particle distribution. Since the electron density of molecules is localized for example, fewer particles are necessary in the low electron density region and many particles are distributed in the high electron density region. We have introduced the smooth particle arrangement based on the electron charge density, and show the efficiency of MSPH in the electronic structure calculations.

Quantum Monte Carlo Simulations of Quantum Crystals and Supersolids

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Strong correlation regime and quantum phase transition*s* into crystal phase controlled by the density are studied for a set 2D quantum systems and clusters - dipole Bose atoms*,* dipole exciton*s* and Rydberg atoms by *Q*uantum Monte Carlo simulations.
Essential peculiarities in excitation spectra, in structure and condensate depletion with density will be discussed. We have studied also the possible existence of a supersolid phase of a two-dimensional dipolar crystal using quantum Monte Carlo methods at zero temperature. Our results show that the commensurate solid is not a supersolid in the thermodynamic limit. The presence of nonequilibrium vacancies or interstitials turn the solid into a supersolid phase even when a tiny fraction of them are present. The residual interaction between vacancies is repulsive making a *quasi-equilibrium* dipolar supersolid possible. The ground state of the system is not the supersolid with defects but ideal crystal. But there is large energy barrier between these two states. So supersolid with defects is metastable state.

A mesoscopic system of dipolar bosons trapped by a harmonic potential is considered.
The system has a number of physical realizations including dipole excitons, atoms with large dipolar moment, polar molecules, Rydberg atoms in inhomogenious electric field.
In dimensionless units the system is described by two control parameters, the number of particles and the strength of the interparticle interaction. We have shown that when the interparticle interaction is strong enough a mesoscopic crystal cluster is formed. As the strength of interactions is decreased a multi-stage melting takes place. Off-diagonal order in the system is tested using natural orbitals analysis. We have found that the system might be Bose condensed even in the case of strong interparticle interactions. There is a set of parameters for which a spatially ordered structure is formed while simultaneously the fraction of Bose condensed particles is non zero. This might be considered as a realization of a mesoscopic supersolid.

Crystallization of Rydberg gas and mesoscopic clusters of Rydberg atoms due to van der Waals repelling (instead of van der Waals attraction of atoms in ground state) is discussed.
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Ultrafast lasers, highly excited solids, and DFT-EAM-MD simulations

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Nowadays ultrafast infrared, optical and X-ray lasers have many applications from technology to medical treatments like cutting, drilling, micromachining of electronic devices, changes in colorizing and wettability due to appearance of nanoscale surface structures, keratotomy, LASIK, Epi-LASIK, CLEAR surgery and so on. Ultrafast means that duration of laser pulse τ_L is of the order of few picoseconds 10^{-12} s [ps] and less, down to few light oscillations. For infrared light with photon energy $h\nu = 1$ eV a period of oscillation is 0.7 fs; 1 fs = 10^{-15} s. In mentioned applications energies transferred to matter are in the range 0.1-1 eV/atom. A heated layer is extremely thin 10-100 nm, 30-300 interatomic spacings. Energy of pulse is absorbed by electron subsystem in intraband and/or interband transitions depending on electronic spectra of material and energy $h\nu$. Absorption strongly excite electrons, their temperatures T_e are 1-10 eV in our applications. Later electron-ion (e-i) relaxation, lasting few ps, equalizes electron and ion temperatures. To understand the processes, knowledge about equation of state (EOS), electron heat conduction coefficient κ, and e-i coupling parameter α, defining rate of e-i thermalization, is necessary for conditions of highly excited electron states of solids and liquids. EOS, κ, and α are applied to describe heating, melting, and motion of an irradiated target. We use DFT (Density Functional Theory) and kinetic equations to find energy, pressure (EOS), and kinetic characteristics (κ, α) of excited states. Those data are employed to run our hydrodynamic code. DFT is also used to find many-body interaction potential in frame of embedded atom model (EAM). Our EAM depicts all important parameters – bulk and shear modulus, vacancy formation energy, melting curve and so on. EAM potential is employed in large scale multi-processors molecular dynamics (MD) simulations. Combined hydrodynamic and MD codes describe full picture of many interlinked processes at different spatiotemporal scales from fs to ns. The processes are: absorption by electrons, conductive heating, e-i relaxation, hydromotion under action of electron and ion pressures, generation of superstrong elastic shocks (we have proved that ultrafast action keeps crystal in elastic uniaxially compressed state even near ultimate strength of solids), strong foaming of molten metals, and freezing of foam with creation of nanoscale structures containing ultrasmall bubbles frozen in solid matrix and frozen remnants of membranes of broken foam. The report gives a review of modern situation and is based on our recent papers:

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Entropy-based accelerated Monte Carlo methods for Coulomb collisions

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Abstract: We present a computational method for the simulation of Coulomb collisions in plasmas that significantly improves upon our earlier hybrid method, which combines a Monte Carlo particle scheme and a fluid dynamic solver in a single uniform method across phase space. The hybrid method represents the velocity distribution function f(v) as the sum of a Maxwellian M(v) and a collection of discrete particles g(v). M evolves in space and time through fluid equations, and g through a Monte Carlo particle in cell (PIC) method. Interactions between M and g are mediated by mean fields and simulated collisions. Computational resources are reallocated by (de-)thermalization processes that move particles from g to M and vice versa. We present a new algorithm for performing these (de-)thermalizations that is more accurate and rigorously justifiable than previous efforts. This new algorithm assigns a passive scalar to each simulated particle that approximates a ``relative entropy.'' Particles are thermalized (dethermalized) when this quantity is sufficiently small (large). We present results from numerical simulations of two test problems - a two temperature Maxwellian and a bump-on-tail distribution, finding a computational savings between a factor of 5 and 20 over PIC.

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Nonlinear oscillations in the Knudsen plasma diodes

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Time-dependent processes occurred in planar plasma diodes are considered. We suppose that the electrons and ions leave the emitter surface with a prescribed velocity distribution functions (DF) and travel collisionlessly between electrodes due to a self-consistent electric field. The theory of nonlinear oscillations in the Knudsen diode with surface ionization (KDSI), where the emitted electrons and ions have the half-Maxwellian DF, is presented. The Knudsen thermionic energy converter and *Q* machine are examples of the KDSI. Both devices exhibit the nonlinear oscillations of the electron current with large amplitude.

The details of time-dependent processes in the vacuum diode, where DF of emitted electron is close to the monoenergetic one, are studied. About 30 years ago, the vacuum diode with directed electron beam has attracted attention in connection with the creation of high power microwave generators such as vircators, reditrons, and reflecting triodes. Under certain conditions, highly nonlinear oscillations can arise the diode. This process is accompanied by an intense energy exchange between the electrons and the time-dependent electric field. As a result, a fraction of energy of the electron beam is transferred to the virtual cathode oscillations, the energy of which is converted into electromagnetic radiation. There is intense energy exchange between charged particles and the electric field in all devices mentioned. This results in a strongly non-equilibrium DFs and even its disruption. In order to describe correctly such processes the kinetic and Poisson equations should be solved.

In the investigations, we extensively use our E,K-code. The code involves the fact that, in the collisionless case, the velocity DF is conserved along the trajectory of each particle. To calculate the DF in a node of the spatiotemporal grid, a number of trajectories of the test particles is computed. The main feature of the method is a calculation of the trajectory of any particle backward in time to the moment when the trajectory reaches the emitter surface. As a result, from a given arrival velocity u, the velocity and time when a particle is injected from the emitter are determined, as well as the value of the DF at the velocity u. In order to guarantee the accuracy in calculating the DF and its moments, the velocity step is chosen such that the difference between two DF-values for neighboring trajectories does not exceed a certain value. The particle density distributions over space being obtained, the Poisson equation is solving. At each time step, iterations of kinetic and field units are performed in order to obtain a self-consistent solution.

The complete theory of the nonlinear oscillations within the KDSI has been created. These oscillations are characterized by periodic sequences of two types of stages: the slow (related to the slow motion of the ions) and fast (compared with the time an electron takes to travel the electrode distance d) ones. When calculating the slow stage we suppose that the electrons overcome the gap d before the ions move over the distance of the Debye length λ_D. Then it can be considered, that to the moment when ions moved over distance about λ_D, the electrons and electric field in the electrode gap have already a time to redistribute and conform with a given ion distribution. Therefore the timescale is selected to be the time for ion to travel λ_D. At each step the electron and electric field distributions for a given ion background are determined as a stationary problem. This task as a rule has several solutions. The potential distributions that can be realized as well as their stability properties, are analyzed by the η,ε-diagram technique. At certain instants during the slow stage the Pierce type instability arises, and a fast stage starts. Here the timescale is selected to be the time for an electron to travel λ_D. During this stage, the ion distribution may be considered as the unchanged one. Oscillation process occurs with severe rearrange of a potential distribution and deep modulation of electron current. In the course of oscillations, electrons intensively transfer their energy to ions via the electric field. Fast ion beams form. Various nonlinear structures: the moving virtual cathode and double layer, as well as the structures, generated when electrons are trapped into the potential well, that being forming during the fast stage of the oscillations, are studied.

The details of oscillation process in the vacuum diode with monoenergetic electron flow are studied. A threshold when the oscillations arise exists as in the KDSI. Regions, within which several oscillation solutions can exist, are discovered. The amplitude of oscillations as a function of the beam current is built. Physical phenomena and structures inherent in the nonlinear oscillations are studied in details. A phenomenon of the sharp jumps in the temporal dependencies of convection current is discovered and clarified. The reason why the long-lived electrons come into being is clarified.

Numerical simulation of Weibel instability in laser interaction with plasma

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Weibel instability [1] is known to arise in systems with anisotropic particle velocity distribution. It leads to the growth of the magnetic field in form of thin (scale typically approximates to the skin length) filaments, which may further form stable large-scale magmetic fields in plasma. The condition for the instability arises in laser interaction with overdense plasma. Electrons accelerated by the pulse form a anisotropic system of a relativistic beam and plasma background, and the charge current filaments are formed. This mechanism lessens the efficiency of laser pulse energy transfer to electron acceleration due to energy loss for magnetic field formation.

The current study is dedicated to the investigation of energy transport to magnetic fields in such system with the use of numerical simulation. The simulation serving such purpose should take into account the three dimensional nature of the phenomena, have enough spacial and time resolution to show the fastest growing instability modes and be able to cover the size of a characteristic laser-plasma system in question.

We use the CFHall code [2]. It is based on the novel Locally-Recursive non-Locally Asynchronous algorithms. By taking account of the memory subsystem hierarchy it greatly decreases the time needed for simulation both on the massively parallel computer clusters and common desktop machines. The benefit for the current study is the ability to use enough cell resolution to provide several cells per smallest predicted filament structure in a 3D3V simulation.

While the three-dimensional small-scale scale filament structure can be neither observed by current experimental equipment, nor described comprehensively in the terms of known theoretical frameworks, the numerical experiment provides an insight to the mechanism of the instability process and provides estimates of the important output values (such as the ratio of energy converted to magnetic fields) depending on the control parameters.

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Ab initio calculation of dielectric properties of shocked xenon.

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The reflectivity of shocked xenon was measured in the experiments of Mintsev and Zaporoghets in 1989 for wavelength $\lambda = 1064$ nm [1] and further for $\lambda = 694$ nm and $\lambda = 532$ nm [2]. But there is no adequete theoretical explanation of these reflectivity results in frames of the standard methods of nonideal plasma theory. As it was shown in [3], the Drude model, with collisional frequency in Born approximation, gives reflectivities that are 2.5 – 3 times larger than the measured values at low densities. The results of other approaches to the collision frequency calculation also can't provide better explanation of steep slope of reflectivity drop with decreasing of density. As it was shown in [3] the assumption of significant width to the shock front gives a good agreement with the experimental data. However, there are no evidences of this effect in experiment. The values of reflectivity of xenon plasma, calculated by Desjarlais [4], are obtained in frames of the approach of quantum molecular dynamics, based on the finite temperature density functional theory; Kubo-Greenwood formalism is used for calculation of the optical properties. In comparison with [3] in [4] shock has an ideal step profile. The approach, used in this work, is approximately the same with method in [4]. However, in contrast to pseupotential in [4] (PAW Xe 07Sep2000), in given work the improved Projector Augmented Wave (PAW Xe_GW 08Jan2009) pseupotential is used. The advantages of this potential in comparison with (PAW Xe 07Sep2000) for calculation of shocked liquid xenon Hugoniot were first shown in [5]. The formula for longitudinal part of the dielectric tensor [6] is used, which is more accurate than the Kubo-Greenwood formula for transverse part of the dielectric function in frames of PAW method. The agreement of obtained results in this work with experimental data [1, 2] is much better than in [4].

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LARGE EDDY SIMULATIONS OF COMPRESSIBLE MAGNETOHYDRODYNAMIC TURBULENCE IN SPACE PLASMA. MODEL DEVELOPMENTS AND VALIDATIONS

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Numerical simulation of compressible turbulent magnetohydrodynamic (MHD) flows is an effective tool for study of flows of charged fluid of astrophysical, helio and geophysical plasma (for instance, solar corona expansion, solar wind, flows in the solar convection zone, turbulence in interstellar matter), that is beyond the reach of direct experimental study. Complete information about turbulent fuid flow can be obtained by means of direct umerical simulation (DNS) that lies in numerical solution of full nonstationary system of equations. That approach allows resolving all scales of charged fluid flows and does not require special closures for magnetohydrodynamic equations. However, direct numerical computation of MHD-turbulence faces fundamental difficulties concerned with large hydrodynamic and magnetic Reynolds numbers typical for studied processes, because in that case the number of degrees of freedom of turbulent flow is large and minimal number of mesh points must be so large that application of direct numerical simulation for study of turbulent flows with real Reynolds numbers is limited by available computational resources. Large eddy simulation (LES) approach describes approximate turbulence dynamics, where the large-scale part of turbulent fowl is computed directly, while the small-scale one is simulated. Possibility of using filtration operation in LES for decomposition of turbulent flow characteristics into large-scale and small-scale parts is due to sufficient isotropy, homogeneity and universality of small scales of turbulent flow In present work. Large Eddy Simulation (LES) technique for study of compressible magnetohydrodynamic turbulence is developed. The filtered equations of magnetohydrodynamics of compressible fluid are obtained with use of mass-weighted filtering procedure (Favre filtering). Favre filtered equations for large-scale component of turbulence include subgrid scale terms describing subgrid phenomena. For the case of polytrophic fluid these terms represent combination of subgrid stresses already known from studying incompressible magnetohydrodynamic turbulence and compressible turbulence of neutral fluid. Different models of closures for subgrid terms appearing after filtration of initial equations of magnetohydrodynamics of compressible fluid are developed. The results of numerical direct numerical simulation (DNS) computations and various subgrid closures for LES approach are demonstrated; analysis and comparison of obtained results are carried out. It is shown that subgrid scale closure models suggested in this work provide sufficient dissipation of kinetic and magnetic energy and reduce computational efforts at simulation of compressible magnetohydrodynamic turbulence. In this work LES method for modeling of compressible decaying MHD turbulence is applied for various similarity parameters, namely, magnetic Reynolds numbers, hydrodynamic Reynolds numbers and Mach numbers. Numerical study is performed for five subgrid-scale closures for MHD case: the Smagorinsky model, the Kolmogorov model, the cross-helicity model, the scale-similarity model and mixed model. The comparison between LES and DNS results is carried out regarding the time evolution of kinetic and magnetic energy, cross felicity, sub grid-scale and molecular dissipations for kinetic and magnetic energy, turbulent intensities and quantities that describe anisotropy of flow, that is, skewness and kurtosis of velocity and magnetic field. It is shown that some subgrid-scale models proposed in the work provide sufficient dissipation of kinetic and magnetic energy, reduce computational efforts and produce adequate results of magnetohydrodynamic turbulent modeling for various values of similarity parameters of flows. In the whole, the best results are demonstrated by the Smagorinsky model for MHD case and the model based on cross-helicity. The scale-similarity model do not provide sufficient dissipation of both kinetic and magnetic energy, and it is necessary to use this subgrid-scale closure only together with eddy viscosity model (for example, with the Smagorinsky model), that provided a basis idea for mixed model. Thus, LES method has good future trends for research of compressible magnetohydrodynamic turbulence.

Numerical simulations of the Kelvin-Helmholtz instability development in a bounded supersonic plasma flow

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In the frame of a semi-infinite flow model, the supersonic flows $M_S \equiv U / C_S > 2$ (U_0 – the flow speed, C_S – the ion sound speed) are well known to be stable (Miura & Pritchett 1982). However, the semi-infinite flow model is an appropriate approximation only of the oscillations with the wave length shorter than the flow thickness. Thus, in order to investigate the stability of the long wave oscillations, one has to allow for the finite thickness of the flow.

We have carried out a linear stability analysis of the flow of a finite thickness using two models: a three-layered slab flow model (Burinskaya et. al. 2011), and a cylindrical flow model (Shevelev & Burinskaya 2011). In both cases we have proved for the K-H instability to grow for a sufficiently large sound Mach numbers, $M_S \gg 2$.

Our recent studies are concentrated on a nonlinear evolution of the K-H instability. The process of a vortices formation is of a great importance in a momentum and density transport from the flow to the surrounding medium. To simulate evolution of the MHD K-H instability we have implemented a numerical algorithm based on HLL-like (Harten et al. 1983) scheme to calculate monotonic and high-resolution flux approximations and flux-corrected transport (FCT) approach (Zalesak 1979, DeVore 1998) to result in TVD close monotonic high-order scheme. Simple and robust computational code has given us an opportunity to examine the nonlinear stage of the K-H instability development initiated from the periodic perturbations or pure noise. We have accomplished a series of numerical simulation for the slab flow in a longitudinal magnetic field to study the K-H nonlinear dynamics.

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The method of Wave Packet Molecular Dynamics for warm dense matter and nonideal plasma simulations

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Interaction of strong laser pulses and particle beams with condensed matter produce special (extreme) states of the mater such as warm dense matter and nonideal plasmas. Study of particle dynamics at such states can hardly be done analytically and require appropriate computer simulation techniques.

The method of molecular dynamics (MD) is widely used to study nonideal plasmas with electrons and ions treated classically. At the same time the use of electron-ion pseudopotentials in the classical MD simulations restricts the applicability of this method to high temperatures, high ionization degrees and near equilibrium states. relaxation rates.

Computational methods based on the Density Functional Theory (DFT), applied to both warm dense matter and plasma simulations, are much more computationally demanding than the classical MD. Moreover, these methods are mostly not capable to handle the dynamics of electrons.

The Wave Packet Molecular Dynamics/Wave Packet Mote-Carlo methods (WPMD/WPMC) introduce quantum features in terms of classical electron dynamics. Within these methods the ions are treated classically whereas the electron quantum dynamics is approximated by propagation of wave packets [1], parameterized by a small number of dynamic variables. The exchange interaction between electrons of the same spin in the Hartree-Fock limit can be taken into account using antisymmetrized wave packets [2].

Poor accuracy for electronic bound states at ions and spreading of wave packets for weakly bound electrons are known problems of the existing WPMD models for nonideal plasmas [3,4]. We address both issues using a new technique based on multiple Gaussian expansion of the single-electron wave function, which is called Split Wave Packet Molecular Dynamics (SWPMD) [5]. Calculations of the ground state energies of small atoms and molecules show that this method provides better accuracy than the original WPMD. Representing an electron by at least three Gaussians results in the ground state energy for H and He to be within 1% error compared to the exact values.

The main feature of SWPMD is the ability to study electron dynamics taking into account the wave function branching. As a test case we consider tunnel ionization of simple atoms in a short laser pulse. It is shown that the SWPMD results are in a good agreement with more accurate quantum-mechanical calculation methods. Other dynamical events such as electron-ion scattering and propagation of and electron in the nonideal plasma are considered [5].

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MODEL KINETIC DESCRIPTION FOR MANY-COMPONENT PLASMA

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The most widely used kinetic model equation especially in the discrete simulation of plasma and gas dynamics is Bhatnagar, Gross & Krook (BGK) model [1]. The advantage of the BGK model is that the solution of the kinetic equation reduces to that of a system of algebraic equations. A weak point is that the model implies that the Prandtl number equals 1. A graver situation arises in the case of many-component systems [2, 3]. A new form of the collision operator for a Coulomb plasma is derived. One-component and many-component systems are considered. The proposed collision operator properly takes into account the relaxation of the first 13 hydrodynamic moments. Besides this, it accounts for the non-diagonal component contribution in the quadratic approximation in the expansion of the linearized collision operator with respect to the complete system of Hermite polynomials. It is shown that for a system of charged particles with the Coulomb interaction potential, these contributions are essential and lead to Spitzer corrections to the transport coefficients [4]. A consistent derivation of the model linearized collision operator for a many-component system is presented. In these results an ambiguity in the choice of coefficients is eliminated, in contrast to the BGK type models [2, 3]. A technique for reconstruction of the non-linear model collision integral form based on a known expression for the model linearized operator is proposed [5]. It is shown that the model collision integral in the local (not complete) equilibrium approximation does not contain a complicated exponential, that is common for the BGK type integrals. Boltzmann's H-theorem is proved for our model.

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Supercomputing Center of Moscow State University: Computational Factory and Education

Vl.V.Voevodin

Today high performance computing technologies make the key development trend in many countries. This is more important in view of the fact that today computation sciences come to the fore practically in all economic spheres from researches to industry and business. In view of significance of development and practical application of high performance computing technologies the system of higher education faces the most important task of operative and mass training of specialists in computational sciences, parallel computing, high performance computing. This task cannot be accomplished by simply putting some new courses and disciplines into the study programs. It requires a serious systematic approach. It requires serious changes in foundations of higher education. This is important today but this will be extremely important for the exascale era. This is vital for exascale. In the talk basic principles of proposed changes will be discussed as well as the main results of the national presidential project "Supercomputing Education" will be presented to illustrate current changes in Russia for the last three years.

Development of software for managing network resources based on the approach of software-configurable network

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Creating a scalable industrial automation systems that stores and processes large amounts of data and works on consumers demand as services (for example, for the design of complex products, decision support, planning and resource optimization, image processing and pattern recognition with non-destructive testing, etc.) requires new approaches to computer networks, because service work is carried out in an environment where neither the number of orders for the process nor the number of pre-existing resources cannot be known beforehand, and even dynamically change during computation.

One promising new approach involves the creation of distributed multiserver applications based on software-configurable networks, both once the tasks originally configurable and modifiable during operation of the system "on the fly" in real time, for example, depending on the characteristics of the input task flow.

To create intelligent software-configurable networks with a controlled distribution of the load on the network is proposed to use multi-agent technology, which allows to introduce elements of self-organization in the operation of considered networks for a rapid, flexible and effective response to emerging challenges in the service system, or the failure of any network resources for example, channels or computational elements. Created methods and tools will allow the automating of the process of adaptive dynamic load balancing on the network, while reconfiguring the network at the software level if necessary.

A mathematical model of the system includes a plurality of interconnected resources - computing power (servers) that are designed for different tasks, with different capacities, all of which are linked by a network relationships (count channels) data. At random times, tasks are coming into the system and each server creates a queue of tasks to perform. Each task has its value, as well as each server and the data transmission channel have their rates. Tasks characterized by computing features or data storage requirements, data volumes required computational power, etc., some of these characteristics may not be known until the end of the job. Each task and each computing resource in the network have an agent who control plan for the task and workload on its resource. Resource agent is primarily assesses the task ability of their performance on their site. If it is impossible - asks the neighboring agents of resources for assistance in solving the problem. As a result, the agents of servers talking to each other and the task-agents, knowing the requirements and deadlines for implementation, during which the current construction plan specifying the placement of tasks on servers that adapts as the arrival of new tasks, new servers-nodes connection or disable existing ones (with this can be considered a variable performance). Agents estimate the channel capacity of the chosen directions of transmission and build the most appropriate route. Negotiations are going to redistribute load in the network. Most free server "attract" a load from the other servers, and eventually, the load is evenly distributed over the network. With a corrupted server, if that happens, the problem "spill over" to other servers.

The implementation process includes the development of mathematical models for reconfigurable networks, classes of agents for their modeling, algorithms and operation logic of decision making by the agents on the distribution of resources in the network, protocols in the event of their negotiations and conflict resolution.

A Communication Algorithm for the Patch-based Multiblock Structured Mesh Applications

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Multiblock structured mesh allows to handle complex configurations which are widely existed in computational physics applications. A Patch-based data structure is always used in applications with multiblock structured mesh to get satisfying parallel performance. However, such Patch-based data structure seriously challenges the block to block data communications. This talk presents an algorithm for such communication and introduces its integration to JASMIN infrastructure to support the peta-scale simulations while tens of thousands of processors are used. Performance results show its robustness.

Patch-based Computing for Large Scale Unstructured Mesh Applications

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ABSTRACT A patch-based data structure is presented here for large scale unstructured mesh simulations. According to the data structure, computational domain is divided into some groups of patches, and each group is assigned to one processor. Based on the data structure, two-level parallelism using MPI and OpenMP can be implemented easily. Further, the communication pattern for neighboring patches is presented. The programming interface of the data structure is designed so that application experts can easily develop programs which can run on thousands of cores efficiently. Numerical results show that such data structure is well suitable for unstructured mesh simulation on multi-core parallel computer, and it can support the design of object-oriented unstructured mesh infrastructure.

Supercomputing Infrastructures in Europe

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Abstract

In the past decade a number of very successful endeavours have been launched and brought into operation by the EU in the field of High Performance Computing (HPC) infrastructures. The first major infrastructure was DEISA, the Distributed European Infrastructure for Supercomputing Applications, which was a consortium of leading national Supercomputing centres that aimed at fostering the pan-European world-leading computational science research. DEISA was funded through several EU projects in the period 2004 to 2011 and finally handed over its services to PRACE.

The mission of PRACE (Partnership for Advanced Computing in Europe) is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. PRACE seeks to realize this mission by offering world class computing and data management resources and services through a peer review process. PRACE currently (June 2013) has 25 member countries and offers peer reviewed access to 6 Tier-0 HPC systems with a total capability of 15 PFlop/s. These systems are provided by 4 PRACE members (BSC/Spain, CINECA/Italy, GCS/Germany, and GENCI/France) who committed HPC-resources worth of €400 million for the period 2010-2015. Since its creation in mid 2010, PRACE has provided 5.5 billion CPU-cores hours to hundreds of projects from all scientific disciplines. PRACE is established as an international not-for-profit association (aisbl) with seat in Brussels. It is complemented by several projects. The PRACE project partners receive EC funding since 2007 under the PRACE Preparatory and Implementation Phase Projects for a total of €67 million complemented by the consortium budget of over €43 million.

Further European HPC infrastructures are dedicated to specific regions, like HP-SEE to South-Eastern Europe or LinkSCEEM to the Eastern Mediterranean.

In the presentation all these infrastructures will be introduced briefly, followed by a detailed description of PRACE, the most important HPC infrastructure in Europe. In some detail organisation, hardware, HPC access, peer review process, scientific case, scientific successes, education and training and relations to industry will be discussed.

Automatic code generation for scientific computing

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We present our recent work on implementing Domain Specific Language for use in Monte-Carlo simulations. The language, called QIRAL, is designed to be as close to scientific representation of the problem as possible. The higher level representation is done in LaTeX and comprises of the part describing the Lagrangian and the part describing iterative solution method. The QIRAL then produces C code along with OpenMP pragmas to be linked together with appropriate low-leve primitives library. The performance is comparable to the vanilla hand-written code but allows for experimentation with various data layouts, potentially improving the performance on novel architectures.

Building Parallel SPH Programs with a Unified Infrastructure

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Abstract

Smoothed particle hydrodynamics (SPH) method has gain popularity because of its ability on dealing with problems with large deformation. SPH simulations with high accuracy often demand large amount of computation, which requires parallel computing. Although it is relatively easy to develop a serial SPH program, it is hard to develop a parallel SPH program running efficiently on thousands of CPU cores.

There are two fundamental and common problems in developing parallel SPH programs:
(1) SPH particle data structure;
(2) SPH particle communication.
Furthermore, load balancing, resilience, parallel IO and visualization analysis are also important for large scale simulations.

This report presents our current work:
(1) a data structure with “block-cell” compact storage for SPH particles;
(2) a particle communication component including migrating particles and filling ghost particles;
(3) a load balancing component supporting various load modeling methods and load balancing methods;
(4) a parallel IO library, a resilience library and a visualization analysis software.
This work has been implemented in a unified infrastructure called JASMIN. SPH program developers can build parallel SPH programs by integrating their serial programs with the above components.

Several parallel SPH programs have been built on JASMIN infrastructure, including incompressible flow simulation program, high velocity impaction program, etc. A simulation of three dimensional aluminum sphere impacting aluminum sheet with 300 million SPH particles has been run on 4608 CPU cores on TianHe-1A supercomputer, achieving a parallel efficiency of 45% comparing to 9 CPU cores.

Experimental research automation system

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Abstract

A software system, intended for automation of a small scale research, has been developed. The software allows one to control equipment, acquire and process data by means of simple scripts. The main purpose of that development is increase experiment automation easiness, thus significantly reducing experimental setup automation efforts. In particular, minimal programming skills are required and supervisors have no reviewing troubles.

Interactions between scripts and equipment are managed automatically, thus allowing to run multiple scripts simultaneously. Unlike well-known data acquisition commercial software systems, the control is preformed by an imperative scripting language. This approach eases complex control and data acquisition algorithms implementation.

A modular interface library performs interaction with external interfaces. While most widely used interfaces are already implemented, a simple framework is developed for fast implementations of new software and hardware interfaces.

While the software is constantly development with new features being implemented, it is already used in our laboratory for automation of a helium-3 cryostat control and data acquisition. The software is opensource and distributed under Gnu Public License.

RSC scalable and energy efficient HPC solutions: applications in solving computational physics problems

A. Moskovsky

RSC Group specializes in high-density liquid cooling design for HPC, “RSC Tornado” architecture based on commodity components. The existing “RSC Tornado” can deliver up to 200 TFlops per 80cm 80 cm 42U rack or 156 TFLOPS/m3, with the newest Intel Xeon Phi coprocessor 7120X, de-facto record density for x86-based systems. RSC has proven it’s technology in a track record of projects, including Europe’s largest Xeon Phi based computer at Russian Academy of Sciences.

The RSC projectы include (but not limited to):

- MVS-10P supercomputer at Joint Supercomputing Centre of Russian Academy of Sciences. The machine holds 72nd position in the Top 500 list of the most powerful supercomputers. The MVS-10P is the most energy efficient supercomputer in Russia according to the Green 500 list.
- RSC Tornado machine at South Ural State University, that has more than 700 compute nodes with direct liquid cooling.
- Roshydromet, Russian weather monitoring agency, which uses RSC computer for weather forecast and climate research.

The talk will describe example of complex physics problems that are solved with the help of RSC machines in the field of molecular simulations, weather forecast and engineering problems.

A detailed Numerical Analysis for High-T_c Superconductivity Phase Diagram Based on the Slave-Boson Representation of *t-J* Hamiltonian

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One of the major theoretical challenges in high-T_c superconductivity is to reproduce the observed phase diagrams which display the monotonously decreasing pseudgap temperature and the dome shaped superconducting transition temperature in the plane of temperature vs. hole concentration. Earlier Lee and Salk reported a successful reproduction of the phase diagram by introducing a realistic slave-boson approach to the Heisenberg term in the *t-J* Hamiltonian [1]. More recently, Shin et.al. present temperature and doping dependencies of magnetic susceptibility and spin pairing correlations involved with spin dynamics in high-T_c superconductivity. [2].

We perform a detailed numerical analysis of phase diagrams in the high-T_c superconductivity using U(1) slave-boson representations of the *t-J* Hamiltonian. For different values of J/t such as 3, 5, 7 and on the various lattice sizes such as 20x20, 30x30, 50x50, we see if calculated T_c values converge to the observed T_c value in high-T_c superconductivity phase diagram.

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PRAND: GPU accelerated parallel random number generation library

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The library PRAND for pseudorandom number generation for modern CPUs and GPUs is presented. It contains both single-threaded and multi-threaded realizations of a number of modern and most reliable generators recently proposed and studied in [1,2,3,4,5] and the efficient SIMD realizations proposed in [6,7]. One of the useful features for using PRAND in parallel simulations is the ability to initialize up to 10^{19} independent streams. Using massive parallelism of modern GPUs and SIMD parallelism of modern CPUs substantially improves performance of the generators.

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Kinetic Growth Random Walks

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Random walks are investigated since the 1950's and there
are quite a number of different models for them e.g.
the self-avoiding walk and the kinetic growth walk.
Here the kinetic growth walk is investigated in comparison
to existing and up to date knowledge and results for the self
avoiding walk. These comparisons were done on regular lattices
as well as on diluted lattices up to percolation clusters
yielding results that clearly support the distinction of
both models in all the cases stated above.

Radiation damage thin coating of silicon carbid

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General physical and physico-chemical problems of ion implantation and radiation physics of solid body related with physical problems of inert gases ions implantation in crystal lattice are considered in computer experiments. This models are focused on research of radiation-thermal modification of properties of materials. Kinetic equations of Kolmogorov–Feller and Einstein–Smoluchowski had been formulated in general. The radiation damaging are able to be described in terms of probability density of distribution defects into lattice and this approach is applied to description of initial stage of first-order phase transition. The equations in partial derivative are solved using Stochastic Simulation Method /SSM/(original method which is similar to molecular dynamics but different from the approach of imitation real particles of lattice). We have used set of stochastic differential equations equivalent to kinetic equations in partial derivatives. Gaseous defects (pores) appear as a result of penetration into lattice of inert gas ions of high energy (about several keV). This model is used for prediction of radiation damage (in case of cover silicon carbide). The same model is considered for creation of new materials using radiation stimulated structures of porosity. Method of stochastic analogue[1] is based on theory according to which the kinetic equations of parabolic type are uniquely linked with stochastic differential equations /SDE/ Ito and with the density of transition probabilities of Markov random process, the solution of SDE's Ito can be interpreted as the distribution function /DF/of the corresponding kinetic equation[1, 3-5]. Coefficients of the kinetic equations depend on probability density defects distribution namely the thermodynamic potential of nucleation[3,4] (or Gibbs energy) and long-range potentials of indirect elastic interaction of lattice defects each with other (occurs through the perturbation of acoustic phonons lattice defects and Friedel oscillations of electrons density). Diffusion in the phase space of defects sizes {G} and diffusion in phase space {R} of crystalline lattices are accounted also as coefficients depended on DF. So, Brownian motion of radiation defects in thin layers of silicon carbide occurs under the influence of long-range forces. Stable solution of linear SDE's Ito-Stratonovich [2] is modified on a case quasilinear equations of model as stable numerical method the second order of accuracy with infinite area of sustainability (according to the new definitions and theorems of [2]) on a regular grid of time (without the limitations on the time step). Calculations have shown, that the porosity formation in a layer of silicon carbide depends on its thickness, doses, temperature and degree of discrepancy of parameters lattices layer of the coating and the substrate. Elastic stress from defects in the layers of mkm- thickness can reach value of stress corresponding discrepancy between lattice parameters of layers «coating-substrate» during of initial stage of nucleation (~ms). Study of the mechanisms of phase transition which are non-equilibrium at short time (about 10 mks) carry out by meance SSM. Calculations are important in fusion reactor materials science, electrical propulsion engines of the spacecraft, and also in the creation of porous semiconducting and dielectric materials [7].

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Numerical analysis and forecasting nonlinear dynamics of chaotic systems using a chaos theory methods (application to neurophysiology and econophysics)

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Nonlinear modeling of chaotic processes is based on the concept of a compact geometric attractor, which evolve with measurements. We present an advanced approach to analysis and forecasting nonlinear dynamics of chaotic systems, based on conceptions of chaos and recurrence plots method. As example, a few geophysical systems are studied. Since the orbit is continuously rolled on itself due to the action of dissipative forces and the nonlinear part of the dynamics can be found in the neighborhood of any point of the orbit y (n) other points of the orbit yr(n), r = 1, 2, ..., N, that arrive neighborhood y (n) in a completely different times than n. Then you can build different types of interpolation functions that take into account all the neighborhoods of the phase space, and explain how these neighborhoods evolve from y (n) to a whole family of points about y(n+1). Use of the information about the phase space in the simulation of the evolution of the physical process in time can be considered as a major innovation in the modeling of chaotic processes. This concept can be achieved by constructing a parameterized non-linear function F (x, a), which transform y (n) to y(n+1) = F[y(n),a], and then use different criteria for determining the parameters a . Further, since there is the notion of local neighborhoods, we can create a model of the process occurring in the neighborhood, at the neighborhood and by combining together these local models to construct a global non-linear model to describe most of the structure of the attractor. In finding the coefficients of a there is a possible encounter a few problems, which at first glance seem to be purely technical, but are related to the nonlinear properties of the system. If the low-dimensional chaotic system, the data that can be used for fitting, normally cover any available locally dimension, but only a certain subspace. Therefore, the linear system of equations to be solved by fitting is “ill-conditioned”. However, if the system noise is present, the equations formally are not ill-conditioned, but part of the decision relating to the "direction" of noise points to the future, is not having a sense. As an application we employ a variety of techniques (in versions [1-3]) for characterizing dynamics of the nonlinear econophysical and neuro-physiological systems identifying the presence of chaotic elements. As example, let us underline that an ability to provide interaction between the different areas of the brain by using a multichannel electro- entselophalogrmams helps determine the location of the foci of abnormal activity in brain of patients with epilepsy. Many diseases of the brain, including epilepsy, Parkinson's disease, are associated with abnormal synchronization large groups of neurons in the brain. Particular attention is paid to a non-linear signals as obvious is a typicality of a chaotic behavior of nonlinear systems. To analyze measured time histories of the neuro-physiological system responses with the use of the recurrence plots method the phase space of these systems was reconstructed by delay embedding. The mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov exponent’s analysis, and surrogate data method are used for comprehensive characterization. The correlation dimension method provided a low fractal-dimensional attractor thus suggesting a possibility of the existence of chaotic behaviour. Statistical significance of the results was confirmed by testing for a surrogate data. We also present the concrete numerical results regarding the ensembles fluctuations of spontaneous Parkinsonian tremor of a few patients.

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Monte Carlo simulation of correlated electronic liquid crystalline phases

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Strongly correlated electronic systems especially those in two dimensions exhibit some of the most intriguing phenomena in condensed matter physics. Strong interactions can drive such systems into novel electronic quantum phases that cannot be described by standard paradigms. Understanding how novel quantum phases stabilize and simulating their properties is one of the biggest challenges in condensed matter physics. Therefore, computational studies of novel unconventional correlated quantum phases of electrons are a topic of great interest. In this work we present Monte Carlo simulation results for strongly correlated electronic liquid crystalline phases observed at certain even-denominator filling factors of quantum Hall liquid states. The anisotropic electronic liquid crystalline phases are described by a broken rotational symmetry wave function. Monte Carlo energy simulations of systems of electrons in disk geometry indicate that such an exotic anisotropic liquid crystalline quantum Hall phase with broken rotational symmetry is more energetically favored than an isotropic one depending on the nature of the effective interaction potential.

Nanoring bilayer

Ricardo Lopes da Silva

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Abstract

Magnetic nanoring structures have been the focus of recent research interest due to their attractiveness for technological applications such as non-volatile solid-state memory and magnetic logic circuits. Due to their topological characteristics magnetic nanorings can exhibit multiple stable remanent states (onion state in addition to two vortex, or flux state), controlled by external magnetic field or currents. Logic gates have also been engineered to perform Boolean operations. For device applications, it is essential for the magnetic elements to have a reproducible and controllable magnetic switching mechanism. Modifications to the rings, such as altering the ellipticity, creating notches, off-centering the hole, the ring geometry, and introducing sharp corners, as well as the use the exchange bias, have been effective in changing the reversal mechanism and, in particular, modifying the chirality of the vortex state. The majority of reversal process observed in ring structures involve the nucleation and annihilation of the vortex state. In this work we are using the Monte Carlo method to investigate the mechanism of inversion of magnetization in nanorings composed of two coupled layers (a ferromagnetic layer overlaid by an antiferromagnetic layer). Our system is modeled by the distribution of magnetic particles over a three-dimensional lattice and represented by the Hamiltonian:

$$\begin{aligned} H = & -J_F \sum_{<i,j>} \vec{S}_{1i} \cdot \vec{S}_{1j} - J_{AF} \sum_{<i,j>} \vec{S}_{2i} \cdot \vec{S}_{2j} - J_I \sum_{<k,l>} \vec{S}_{1k} \cdot \vec{S}_{2l} \\ & - D_z \sum_i (S_{1i}^z)^2 - D_{xy} \sum_i ((S_{2i}^x)^2 + (S_{2i}^y)^2) - \sum_i \vec{H}_i \cdot \vec{S}_i \\ & + D \sum_{\substack{<i,j> \\ i \neq j}} \frac{\vec{S}_i \cdot \vec{S}_j - 3(\vec{S}_i \cdot \hat{e}_{ij})(\vec{S}_j \cdot \hat{e}_{ij})}{e_{ij}^3} \end{aligned} \tag{1}$$

where the first term is the ferromagnetic layer, and $\vec{S}_{1i}$ the magnetic moments of this layer and $J_F > 0$ a exchange interaction strength between nearest neighbors. The second term is the antiferromagnetic layer with magnetic moments $\vec{S}_{2i}$ and exchange interaction strength $J_{AF} < 0$. The third term is the interaction between the layers where $J_I > 0$ or $J_I < 0$ and the vectors $\vec{S}_{1k}$ and $\vec{S}_{1l}$ are the magnetic moments belonging to the interface antiferro-ferromagnetic. The fourth term represents the easy axis anisotropy of the FM layer (Fe [001]), and D_z anisotropy constant and S_{1i}^z component of the magnetic moment in direction of preferred orientation, in this model, $+\hat{z}$. The fifth term is the easy-plan anisotropy that represents the preferred direction of magnetization in the AFM layer (NiO

or CoO [110]), where S_{2i}^{x} and S_{2i}^{y} are the components of the magnetic moment in the plane xy and D_{xy} anisotropy constant. The sixth term is the Zeeman energy is $\vec{H}_i$ the vector magnetic field. The last term is the dipolar interaction, where D is the dipole strength and $\hat{e}_{ij}$ the distance between two magnetic moments located at sites i and j. The vector $\vec{S}_i$ in the last two terms represent the magnetic moment at site i in all layers. Here we use the approach to classical spins, where the magnetic moments satisfy the condition $|\vec{S}_i| = 1$.

Sync and anti-sync in a system of coupled oscillators

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The dynamics of similar, self-sustained oscillators coupled by a common platform exhibits fascinating collective behavior. Experiments performed with pendulum clocks [1,2] and metronomes [3,4] reported both the absence of synchronization, in-phase synchronization, anti-phase synchronization, beat-death phenomenon, or even chaotic dynamics. Here we present a numerical study on two self-sustained oscillators placed on a common movable platform. As order parameter for synchronization we use the Pearson correlation coefficient between the oscillators coordinates. As a function of the relevant physical parameters of this system we reproduce all the experimentally reported dynamics. We provide conditions for obtaining stable and emergent in-phase or anti-phase synchronization.

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A Lattice Model for Malaria Transmission: mean-field approach and simulation

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We study a simple lattice model for the transmission of malaria in a population. Our model is based on Ross' model with the inclusion of diffusion by mosquitoes. The transmission of the disease to humans occurs through contact with an infected mosquito, while a healthy mosquito can become infected through contact with an infected human. Recovered individuals are susceptible to re-infection. The mosquitoes diffuse through the lattice, spreading the disease. We obtain the evolution equations for the densities of infected humans and mosquitoes using mean-field theory (MFT), via cluster approximation at site level. We show that our model is equivalent to Ross' model if we use independent probabilities or in the limit of high diffusion rate. We also determine the basic reproduction number. An estimation of the covariance for having two infected individuals at the same site stresses the importance of the correlation among the system components, mainly for low diffusion rates. A high mosquito diffusion provokes a mixture of the system components, therefore, diminishing the correlation between the populations. As a result, the probabilities are independent, explaining the mean-field behavior in this limit. We show preliminary results of Monte Carlo simulation.

Fluctuation Relations and Crystallization

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Hard spheres undergo a fluid to solid phase transition if the packing fraction is larger than approx. 0.5. The nucleation process and forming structures are still under investigation. A new approach is to correlate forming structure and dissipation. Fluctuation relations are the method of choice. Increasing the pressure with time results in thermodynamic work, linked by the first law of thermodynamics to dissipation.
Studying fluctuation relations of structural phase transition and even slow dynamics is important. A new kind of fluctuation enters the dynamics that is macroscopic instead of microscopic based on thermal fluctuations.

Numerical simulation of turbulent flow in Taylor-Green vortex decay

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In large eddy simulation (LES) methods the quality of the numerical solution strongly depends on the properties of the subgrid dissipation. Here we present the results of numerical simulation of Taylor-Green vortex decay for low-Reynolds turbulent case. Simulation is based on quasi, or regularized gas dynamic (QGD) equation system, that generalizes the Navier-Stokes system and differs from it by additional nonlinear dissipative τ- terms, e.g. [1]. This mathematical model can be regarded as a nice alternative to existing filter models for LES methods and can be used for unified simulations of both laminar and low-Reynolds turbulent flows. In turbulent flow simulation τ-terms play the role of subgrid dissipation, in laminar flow calculations they stabilize the numerical solution, e.g. [2].

Figures below show the vorticity contours in numerical simulation of the Green-Taylor vortex flow decay for Reynolds numbers Re = 1600 for time t=0 and t=15. In the last figure the comparison of the kinetic energy (E) dissipation rate $\varepsilon = -\frac{dE}{dt}$ with the etalon data from [3] are demonstrated for Re = 1600 and 280. Here Mach number is equal to 0.1, computational grid is 65^3, working gas is nitrogen in normal conditions.

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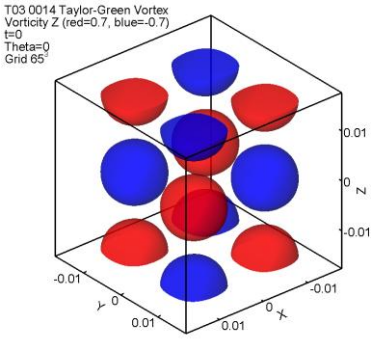

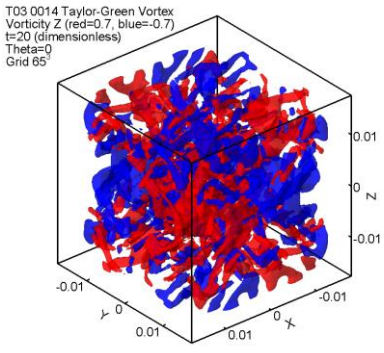

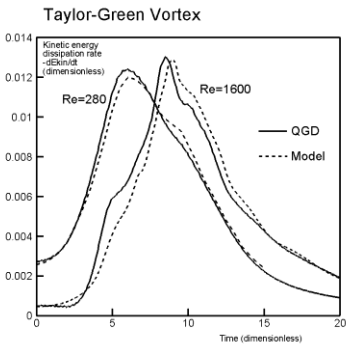

First principles study of properties of the oxidized Cu(100) and Cu(110) Surfaces

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The study of oxidation of single crystal metal surfaces is important in understanding the corrosive and catalytic processes associated with thin film metal oxides. Copper oxides have also attracted much attention in the area of renewable energy research. The process by which oxide layers are formed on metal surfaces, however, is still not well understood. The structures formed on the oxidized transition metal surfaces vary from simple adlayers of chemisorbed oxygen to more complex structures which result from the diffusion of oxygen into subsurface regions. In this work, an *ab-initio* investigation of the stability and associated physical and electronic properties of the Cu(100) missing row reconstructed surface and the added row reconstructed Cu(110) surface at various oxygen coverages is presented using density functional theory (DFT). Changes in the electron work function, adsorbate binding energy, surface dipole moment, surface energy, deformation electron density, density of states, and band structure of both surfaces with oxygen coverage have been explored and discussed. Calculations include both on-surface and mixed on- and sub-surface sites for oxygen. The studied mixed structures are all found to be energetically more favorable as compared to structures formed by pure on-surface oxygen adsorption. Calculations of electronic properties from first principles have been also performed for the (100) and (110) surfaces of Cu_2O to use for comparison. The first-principles calculations in this work have been performed on the basis of the Density Functional Theory (DFT) and using DMOl3 code. The obtained theoretical results have been compared with available experimental data.

This work was supported in part by the National Science Foundation Grant # DMR-0907679.

Quasi Long Range Order of Defects in Frustrated Antiferromagnetic Ising Models on Spatially Anisotropic Triangular Lattices

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We study a novel phase in an antiferromagnetic Ising model on an anisotropic triangular lattice using a Monte Carlo method. It is known that there is no phase transition down to zero temperature in the model with only nearest-neighbor interactions, in which the exchange coupling of one direction is equal to or stronger than those of other two directions. In the presence of the anisotropy, i.e., the coupling of one direction being stronger than the others, the low-temperature physics is governed by domain-wall excitations (defects) residing on bonds of the strong-coupling direction. In this presentation, we show that an additional small attractive interaction between defects (introduced by adding a ferromagnetic next-nearest-neighbor interaction in the weak-coupling direction) leads to a Berezinskii-Kosterlitz-Thouless (BKT) transition at a finite temperature. The BKT phase can be viewed as the phase with a quasi long-range order of defects. We numerically determine the phase diagram in a wide parameter regime, and also argue the phase structure from statistical-mechanics and field-theory viewpoints.

Numerical modeling of atomic and nuclear systems in an intense laser field and resonance phenomena in heavy ions collisions

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We present new numrical approach for studying interaction of the finite Fermi systems (atoms, nuclei) with an intense external fields (electric and laser fields). It is the combined relativistic operator perturbation theory (OPT) and energy formalism [1]. The OPT formalism includes a new quantization procedures of states for finite Fermi-systems in a strong field. The zeroth order Hamiltonian H of this PT possesses stationary bound and scattering states. To overcome formal difficulties, the zeroth order Hamiltonian was defined by the set of the orthogonal eigen values and eigen functions without specifying the explicit form of the 0th potential. The special computer code is carried out (PC complex "Superatom"). New data on the DC, AC strong field Stark resonances, multi-photon and autoionization resonances, ionization profiles for several few-body atomic (H, He, Li etc) and heavy atomic (Tm, Gd) systems are presented and compared with some other known theories (c.f.[1]). It has been discovered a significant broadening effect of the autoionization resonances in a sufficiently weak electric (laser) field for uranium atom.We present the results on the AC Stark shifts of single proton states in the nuclei ^{16}O, ^{168}Er and compared these data with known results by Keitel et al [3]. New data are also listed for the ^{57}Fe,^{171}Yb nuclei. Shifts of several keV are reached at intensities of roughly 10^{34} W/cm^2 for O and 10^{32} W/cm^2 for heavier nuclei. Lower excitations of even parity are possible in the two- or higher-order photon processes, and their energies are still more than 20 keV above the ground state energy.

Further a new unified quantum approach (OPT formalism, energy approach) [1] is used for numerical modeling the electron-positron pair production (EPPP) in the heavy nuclei collisions and treating a compound nucleus in an extreme electric field. Heavy ions collisions near the Coulomb barrier are surrounded by existence of narrow e+ line in a positron spectra [1,2]. The positron spectrum narrow peaks as a spectrum of the resonance states of compound super heavy nucleus are treated. The nuclear and electron subsystems are considered as two parts of the complicated system, interacting with each other through the model potential. The nuclear system dynamics is treated within the Dirac equation with an effective potential. All the spontaneous decay or the new particle (particles) production processes are excluded in the 0th order. The calculation results for cross-sections at different collision energies for ^{238}U+^{238}U, ^{232}Th+^{250}Cf systems are presented.

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Electron spectrum of a double-wall carbon nanotube within the frame of the nonlinear Schrödinger equation

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Keywords: nonlinear Schrödinger equation, carbon nanotubes, electron spectrum

Abstract text The electron spectra of single and double wall carbon metallic nanotubes are analyzed. The interaction of a free electron with atomic ions and bound electrons is approximated by an attractive delta-function potential in the single-particle Schrödinger equation written in the cylindrical coordinates. The interaction of an electron with other free electrons is presented by the Gross-Pitaevskii nonlinear repulsive potential.

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Effect of nitrogen impurity on the structural, mechanical and phonon properties of diamond from first-principle study

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Using a density functional approximation we investigated the structural, mechanical and phonon properties of the diamond doped with nitrogen and compared them with the properties of pure diamond. The calculated results for the pure diamond are in good agreement with experimental data and other ab-initio calculations.

First-principles calculations were performed in the plane wave basis approximation, using the ABINIT package. The pseudopotentials with GGA exchange-correlation functional were used in the structural and elastic calculations and LDA pseudopotentials in the Raman and IR calculations. The structure of the nitrogen-doped diamond was represented by 64-atom cubic supercell (the 2x2x2 repetition of 8-atom elementary diamond cell, where one carbon atom was replaced by nitrogen (NC_{63} cell)) that was relaxed with respect to the atom positions and lattice constants. For the calculating of elastic constants we used the method of small strains imposed to the equilibrium structure. For the computation of phonon density of states we used the direct method of calculating interatomic force constants. The Raman and IR intensities were calculated using the QUANTUM ESPRESSO package.

After the relaxation the lattice constant of nitrogen-doped diamond slightly increases, the elastic constants and moduli reduces. From the radial and bond angle distributions we can conclude that the substitutional nitrogen atom in diamond brought only local distortions in the diamond lattice. In nitrogen-doped diamond the elastic anisotropy decreases, the crystal becomes less brittle. The investigation of elastic anisotropy has shown that isotropic approximation is nonsufficient for the study of elastic properties in both pure and nitrogen-doped diamond. The hardness of nitrogen-doped diamond decreases. The calculated hardness anisotropy of diamond confirmed the experimental data that the hardness of the face (111) is much higher than the hardness of the face (100). The nitrogen doping tends to reduce the hardness anisotropy.

The phonon DOS bands of diamond are shifted down at nitrogen doping that testifies to weakening of interatomic interaction in nitrogen-doped diamond. The study of partial PDOS has shown that the nitrogen contribution is seen only within the PDOS of pure diamond that causes an appearance of resonant localized modes. The modes with the greatest nitrogen participation are more localized in comparison with the majority modes. The maximum at 1220 cm^{-1} in PDOS is due to the carbon atoms contribution, but the carbon atom, which is removed from the nitrogen atom and has three short bonds with nearest carbon atoms, forms the band at 1329 cm^{-1}.Unlike pure diamond the Raman tensor component α_{zz} is not equal to zero. The crossed component α_{xz}, as expected, is largest for modes near 1329 cm^{-1}.

Our calculations are consistent with the following experimental data: a C_{3v} local symmetry of nitrogen site in diamond, a lattice expansion in nitrogen-doped diamond, the frequencies of localized modes of carbons near nitrogen have the highest value in comparison to other modes, the noticeable contribution of nitrogen in IR intensity near 1100 cm^{-1}, the calculated elastic constants in diamond, hardness of the (111) face in diamond is higher than that of the (100) face.

Results of the carried-out calculations showed that, as masses of nitrogen and carbon differ a little, local modes of nitrogen have a resonant character, they are strongly hybridized with the diamond modes and they become poorly localized. On the other hand, a lattice distortion by nitrogen has the local character in nitrogen-doped diamond.

Pressure induced structural phase transition and lattice dynamics in thallium-V compounds

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Abstract: Most of the III–V type semiconductor materials have been subjected to intensive theoretical and experimental studies for many years. This is mainly due to their interesting electronic properties, their use in semiconductor devices and the relative ease with which such compounds can be synthesized. In the present study, an effective interionic interaction potential (EIOP) is developed to investigate the pressure induced phase transitions and lattice dynamics of the Zincblende thallium-V compounds: TlAs, TlP and TlN. The long range Coulomb, van der Waals (vdW) interaction and the short-range repulsive interaction up to second-neighbor ions within the Hafemeister and Flygare approach with modified ionic charge are properly incorporated in the EIOP. The vdW coefficients are computed following the Slater-Kirkwood variational method, as both the ions are polarizable. The estimated value of the phase transition pressure (Pt) and the magnitude of the discontinuity in volume at the transition pressure are consistent as compared to the reported data. The vast volume discontinuity in pressure volume phase diagram identifies the structural phase transition from Zincblende (B3) to NaCl (B1) structure. Phonon dispersion spectra are derived using EIOP and compare with the previous report.

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Numerical simulation of spin distribution evolution for super-paramagnetic materials

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There are several ways to simulate magnetic materials. One of them is modeling the distribution function. It is convenient to use computational fluid dynamics methods in order to obtain numerical solution of kinetic equations. In our opinion modeling of spin distribution is of the most interest thus we chose Brown model that describes only the evolution of the spin distribution for the superparamagnetics system [1].
For this problem triangular mesh on sphere was constructed. It is based on dodecahedron. Recursive subdivision was applied to adjust cells scale. In our simulation we used DG framework and Runge-Kutta time integration [2]. It is worth to mention that our mesh consists of spherical triangles instead of planar ones. On such cells one should use special basis functions. In this work we took spherical Bezier-Bernstein polynomials [3]. The last part of numerical method reconstruction procedure is hierarchical WENO type [4]. A few tests on known problems were carried out. Our method produced rather good results and it proved to be second order.

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Validity of Molecular Dynamics Simulations for Soft Matter

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In this work, we analytically examine the validity of molecular dynamics for a soft potential system by considering a simple one-dimensional system with a piecewise continuous linear repulsive potential wall having a constant slope a. We derive an explicit analytical expression for an inevitable relative energy change ΔE due to the discreteness, which is dependent on just two parameters: 1) α, which is a fraction of time step τ immediately after the collision with the potential wall, and 2) $\mu \equiv \frac{a\tau}{p_0}$, where p_0 is the momentum immediately before the collision. The whole space made by the two parameters α and μ can be divided into an infinite number of regions, where each region creates a positive or negative energy change ΔE. On the boundaries of these regions, energy does not change, *i.e*, $\Delta E = 0$. The maximal envelope of $|\Delta E|$ *vs.* μ shows a power law behavior $|\Delta E| \propto \mu^{\beta}$, with the exponent $\beta \approx 0.95$. This implies that the round-off error in energy introduced by the discreteness is nearly proportional to the discrete time step τ.

Scaling in the Diffusion Limited Aggregation Model: towards ultimate growth probability.

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Nowdays the field of statistical physics of equilibrium critical phenomena is clearly understood [1]. Critical exponents which characterize the behavior of a system near a critical point could be derived with the help of various well-established theories. These theories also explain why various systems behave very similarly near a critical point. From this standpoint, the universality concept is a rather well-grounded notion supported by numerous experiments and theoretical predictions.

In contrast, understanding nonequilibrium critical phenomena is still an open problem. In systems that belong to a self-organized criticality class [2] there is no control parameter that determine proximity to the critical point. Instead such systems exhibit fractal and scaling behavior in a very wide range of system properties. In 1981 Witten and Sander introduced a new model, called the diffusion limited aggregation (DLA) model [3], which describes pattern formation by a series of simple rules. These rules are essentially a Brownian random walk of single particle which wanders around an aggregate until it sticks to it after a collision. The repetition of these trivial rules leads to the formation of a very complex fractal object. Although the DLA model does not have any direct control parameter, like the percolation probability, it still has the main features of criticality: it exhibits fractal and scaling properties.

It is a long standing question wheather DLA model exibits universality. Numerous studies searched for evidence of universality by calculating the fractal dimension on different latices. Recent research [4] shows that there is no such universality in this model: the fractal dimension of on-lattice clusters approaches 3/2, while off-lattice clusters have a dimension close to 1.71.

Nevertheless, there are some indications of universality of different nature: several different models such as DLA, dielectric breakdown model, viscous fingering [5], and Laplacian growth have similar fractal dimension. But in

contrast to ordinary systems like Ising and Potts models, where typicaly two critical exponents coincide, here seems to be only one critical exponent (namely fractal dimension) that corresponds to DLA model.

In this work we address the following important question. Since the convergence of the DLA model is very slow there is some uncertainty about the actual value of the fractal dimension of the DLA cluster. To address this question we suggest a simple but complete picture of DLA growth based on analyzing the probability density function $P(r, N)$ for the next particle to be attached at a distance r from the origin. We propose a scale-invariant form for the function $P(r, N)$

$$P(r, N) = \frac{1}{R_{\text{dep}}} f\Big(\frac{r}{R_{\text{dep}}(N)}\Big).$$

and check our assumptions numerically. It immediately follows [7] from our theory that there is only one scaling exponent D and there is no multiscaling in an asymptotically large DLA cluster.

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Frustrations and phase transitions in the Ising model on square lattice

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The problem of frustrations and phase transitions in Ising model on 2D square lattice is explored in a great many works, but the overwhelming majority of investigations [1,2] consider one particular case.

In this work, we studied the problem of frustration origination and of phase transition suppression in Ising model on 2D square lattice with account of interactions between the nearest and the second neighbors in an external magnetic field. We considered more general cases, when the interactions between the nearest and the second neighbors change both in a value and in a sign.

The Hamiltonian of antiferromagnetic Ising model on the square lattice can be written as

$$\mathrm{H} = -J_{NN}\sum_{\langle i,j\rangle}(S_i \cdot S_j) - J_{NNN}\sum_{\langle i,j\rangle}(S_i \cdot S_j) - h\sum_i s_i\,, \qquad (1)$$

where $S_{i,j}=\pm 1$ is the Ising spin. The first term in the Equation (1) accounts for the exchange interaction of nearest neighbors by the value of $J_{NN}<0$, and the second term considers second nearest neighbors by $J_{NNN}<0$, h is the external magnetic field.

We used highly effective replete exchange algorithm of the Monte-Carlo method. A detail description of the replete exchange algorithm was reported in previous work [3].

The points and lines of frustrations, at which the phase transitions disappeared, were detected depending on signs and relative values of interactions and magnetic fields. The heat capacity, at that, lost a lambda-wise feature. The dependences of phase transition points on the relative values of interactions and magnetic field were obtained.

A new effect – the heat capacity splitting near the frustration points – was found. Also we found new magnetic structures and a new type of ordering, namely, the ordering in one direction and lack of ordering in other direction [4].

It was shown that passage through any frustration point (both with magnetic field and without it) causes a fundamental change in the structure.

The lack of interaction between nearest neighbors produced a frustrated field, and the presence of these interactions split this field on two; when increasing the external magnetic field the magnetic structure underwent a transformation twice and, except initial Neel and finite ferromagnetic structure, here appeared an intermediate structure.

Since the external magnetic field tended to order the spins ferromagnetically, it competed with antiferromagnetic interactions, which resulted appearance of new points frustrated depended on the value of exchange parameters and magnetic field.

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Analysis of cloud computing application in scientific centre

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As cloud computing continues to experience more widespread adoption and executives who have adopted the technology have become more comfortable and are now looking for new methods of optimizing the solutions, organizations in some of the most highly regulated sectors have been slower to adopt the technology, and might be putting themselves at a competitive disadvantage.

Seemingly it is due to complexity of cloud technologies itself, including variety of different products, jointed together. Joining of these products gives synergy effect and lets obtain also complex, but very tunable and scalable system. Cloud computing include different services: identity service, image service, messaging service, compute service, block storage service, network service.

Lets discuss these services concerning application in scientific centrum. Scientific centrum has specific requirements: organization of network services for scientific network (routing, proxy for access to different resources, library services, file storage, site hosting), administration of cluster. Consider cloud technologies for that sake on the example of OpenStack --- opensource platform. Cloud technologies gives opportunity to launch many different instances as virtual machines (VM). The principal question is question of network topology of VMs. Sole VM is connected to network via physical network of host. It is attained using network bridge. In cloud computing VMs are connected in subnets, it is implemented using different services --- quantum and Open vSwitch. Open vSwitch implements bridges, quantum implements virtual routing and network management. VMs are connected to global network via number of bridges and virtual router. It has detrimental influence on network connectivity. So network services should be located on usual hosts as native or VM, but not in the cloud. VMs in cloud could be used for educational purposes, e.g. for students. Also they could be used for scalable calculations.

Scalability of cloud computing has detrimental effect on network connectivity. Unfortunately, they should be used only if scalability of resources in time is the main factor.

Literature.

1. Web-resource http://openstack.org

2. Web-resource http://www.alcf.anl.gov/magellan

3. Web-resource http://aws.amazon.com/ec2/

Self-consistent mean-field approximation in the density functional theory of many-electron unbounded systems

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The density functional approach is based on the minimal property of the ground-state energy of finite N-electron system relative to the electron density variations. Evidently, this formulation does not make sense in the case of an unbounded electron system. Nevertheless, the set of 'Self-Consistent Equations Including Exchange and Correlation Effects' derived by Kohn and Sham with making use of an variational procedure is widely applied to infinite electron systems. As noted in [1], at that two new difficulties arise: the normalization problem of the continuous-spectrum eigenfunctions of the single-particle Hamiltonian, and unstable convergence (or divergence at all) of the iterative solution of these equations while achieving self-consistency. The workaround of these difficulties was achieved by introducing of a countable Hilbert space with Hamiltonian eigenfunctions as complete basis and by conversion of the Hartree term in the electrostatic energy functional in order to provide due account of boundary problem for Poisson equation [1]. The stable iterative solution of Kohn-Sham equations was obtained using these means for several inhomogeneous unbounded many-electron systems [2].

In this report the further development of the density functional theory for unbounded systems is presented. It is shown that the countable Hilbert space is strictly equivalent to Gelfand's rigged Hilbert space (Gelfand triplet [3]) in the form $\mathcal{S} \subset \mathcal{H}(L_2) \subset \mathcal{S}'$, where $\mathcal{S}$ is the Schwartz space of the ground functions. It allows one to define computationally convenient scalar productions for any pair of slowly growing distributions in the $\mathcal{S}'$-space, including continuous-spectrum eigenfunctions which are normalized to δ-function.

For the density functional to be extended to include unbounded systems, the Hartree energy term of the usual density functional was rearranged in the following manner

$$V_H \equiv 2\pi \iint_{all\ space} d^3\mathbf{r} d^3\mathbf{r}' \rho(\mathbf{r}) G_0(\left|\mathbf{r}-\mathbf{r}'\right|)\rho(\mathbf{r}') \to \int_{system\ subspace} d^3 r \left[\rho(\mathbf{r})u(\mathbf{r}) + \frac{1}{8\pi} u(\mathbf{r})\Delta u(\mathbf{r})\right],$$

which describes the Coulomb interaction of selected part of the unbounded system both with itself and the rest of the environment via non-variable boundary conditions. Here $\rho(\mathbf{r}) = n_+(\mathbf{r}) - n(\mathbf{r})$ is the mean charge density, u is the mean electrostatic potential, $G_0 = (4\pi\left|\mathbf{r}-\mathbf{r}'\right|)^{-1}$ is the Green function of Laplace operator $\hat{L} = -\Delta$ in the free space. The Poisson equation results now from the variational equality $\delta V_H/\delta u = 0$ with predetermined boundary values of u. These boundary conditions are changing the inverse Laplace operator $\hat{L}^{-1} \equiv G \neq G_0$ and, therefore, interelectron interaction in the system. The derivation of the expression for V_H has shown that the exact mean electrostatic energy is the sum of electrostatic energy of the mean density and the density fluctuations

$$\langle V_{ee}\rangle = V_H + 2\pi \iint_{system\ subspace} d\mathbf{r} d\mathbf{r}' \left[G(\mathbf{r},\mathbf{r}')\left\langle \delta\hat{n}(\mathbf{r})\delta\hat{n}(\mathbf{r}')\right\rangle - G_0(0_+)n(\mathbf{r})\delta\left(\mathbf{r}-\mathbf{r}'\right)\right],$$

where the exchange-correlation energy is presented as the electrostatic energy of the density fluctuations and the self-interaction is removed. The fluctuation-dissipation theorem allows the density-density correlation function to be expressed in terms the linear response function accounting for the mean field reaction (screening effect). In the independent-particle approximation, the total density matrix is replaced by the production of the single-particle density matrices $\hat{f}$, the $\langle\delta\hat{n}(\mathbf{r})\delta\hat{n}(\mathbf{r}')\rangle$ correlation function can be explicitly expressed in terms of eigenfunctions ϕ_λ of the $\hat{f}$ (natural orbitals), and we obtain the energy functional as the functional of eigenfunctions ϕ_λ and the mean potential u. The variations of this functional over ϕ_λ and u lead to the set of the self-consistent mean-field (SCMF) equations with the interaction energy of density fluctuations partly accounted for and self-interaction removed. The further simplifications allows one to derive from the SCMF functional several semi-empirical approximations such as Fermi-Amaldi correction to the Thomas-Fermi equations for many-electron atoms, exact exchange and screened-exchange generalizations of Kohn-Sham method [4].

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Effects of the in-plane magnetization on the conductance properties of the topological insulator ferromagnet/insulator/superconductor junctions

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We investigate theoretically the effects of the in-plane magnetization on the tunneling conductance of a ferromagnet/insulator/superconductor (F/I/SC) junction formed on the surface of a three dimensional topological insulator. The in-plane magnetization shifts the electron and hole Fermi surfaces in ferromagnetic layer and thus influences the Andreev reflection and tunneling conductance. The shifts of electron and hole Fermi surfaces are in opposite directions and thus the Andreev reflection, and consequently the tunneling conductance, decreases with increase of the in-plane magnetization. We also investigate the effect of the in-plane magnetization on the barrier strength dependence of the tunneling conductance. We find that the tunneling conductance as a function of barrier strength displays a π periodic oscillatory behavior, whose mean value and amplitude depend on the in-plane magnetization in addition to the bias voltage.

Computer Simulations of Self-Assembled Mesocrystals formed by Iron Oxide Nanocubes

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Monte Carlo simulations of the packing and thermodynamic properties of iron oxide nanoparticles in the shape of truncated cubes have been performed. Attractive Van-der-Waals interaction in Hamaker approximation and dipolar interaction between particles were considered. A parallel Monte-Carlo algorithm for modeling of self-assembly of nanoparticles was implemented in the computer program. The algorithm include anisotropic simulation shell fluctuations treated within Wang-Landau entropic sampling approach, as well as realistically described interaction between the nanoparticles taking into account their shapes.

The influences of the vacancies in the magnetic skyrmion lattice

Ricardo Lopes da Silva

March 7, 2013

Abstract

Recently the real space measurements of the two dimension Skyrmion structure has been made a low temperature in films of $Fe_{0.5}Co_{0.5}Si$ and close to room temperature in $FeGe$. These compounds share the same $B20$ structure with chiral cubic symmetry, and commonly show the helimagnetic ground state. When a magnetic field is applied normal to the plate, a $2D$ skyrmion lattice is observed. In this metallic compounds, the electric current can drag the skyrmion via a spin transfer torque, while the motion of the skyrmion generates a transverse electromotive force as the emergent electric field. Such electric controllability, as well as its particle-like nature with nanometric size, highlights skyrmion as a unique magnetic object with potential applications in spintronics and high-density magnetic storage devices. The skyrmion-like phase has been studied through the theoretical model and direct real-space observation as an excited state or spontaneous ground state. Even though these and many other issues should be investigated for a better comprehension of such configurations, it is noteworthy that even in the purest samples, structural defects are present, generally randomly distributed throughout the material. This defects can induce and control skyrmion motion, playing a crucial role in disrupting order in solids. The purpose of this work is to discuss the effects due to lattice defects such as nonmagnetic impurities in the formation of skyrmion lattice. In this work we are using the Monte Carlo method to investigate the formation of skyrmion in the presence of the impurities. Our system is modeled by the distribution of magnetic particles over a bi-dimensional lattice and represented by the Hamiltonian:

$$H = -J \sum_{<i,j>} \vec{\mu}_i \cdot \vec{\mu}_j - \vec{D} \cdot \sum_{<i,j>} (\vec{\mu}_i \times \vec{\mu}_j) - \sum_i \vec{h}_i \cdot \vec{\mu}_i. \qquad (1)$$

Here $\vec{\mu}_i = \mu_i^x \hat{x} + \mu_i^y \hat{y} + \mu_i^z \hat{z}$ is the unit spins vector at position i and the first sum $< i, j >$ is over nearest-neighbor spins with exchange interaction strength $J > 0$. The second term is the Dzyaloshinskii-Moriya (DM) interaction, where the vector product $(\vec{\mu}_i \times \vec{\mu}_j)$ favour canted spin structures and enforces a unique rotational sense such that the vector product is parallel to $\vec{D}$. From symmetry considerations the directions of $\vec{D}$ can be determined, and it is predominantly in plane surfaces, in this work we consider only DM interaction between nearest neighbours. The last term considers the effects of an external magnetic field $\vec{h}$.

Regularized shallow-water equations as a model for a solitary wave generation

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Among wave motions in seas and oceans, the birth and behavior of large-amplitude solitary waves (called in the literature extreme, or giant, waves) are of great interest. According to modern concepts and observational experience, in some cases, these waves can be generated by wind and act as a solitary wave or a group of solitons [1,2]. The mechanism of generation of wave–wind solitons has not been fully understood because this study in the real world is very difficult. Some aspects of this phenomenon was observed and investigated experimentally in a wind-water annular tunnel in, e.g. [3].

In this study, we show the results of direct numerical simulation of the evolution of an isolated wind–wave soliton. Numerical modeling is done on the basis of the regularized shallow-water equations [4]. These equations can be regarded as a generalization of the classical Saint-Venant system, that is accomplished by strongly non-linear additional terms with a small parameter as a coefficient. The corresponding numerical solutions correctly reflect the main characteristics of the generation and behavior of solitary waves observed in the experiment [3]. The wind strength and friction forces are taken into account. The example of soliton formation in the wind-water tunnel of the 6m length is shown on the figures below. The last figure shows the resulting solitary wave.

In the full presentation the form of regularized shallow-water equations will be shown together with the numerical algorithm, details of computational results and comparisons with theoretical investigations of the problem based on the analytical solution of Saint-Venant system.

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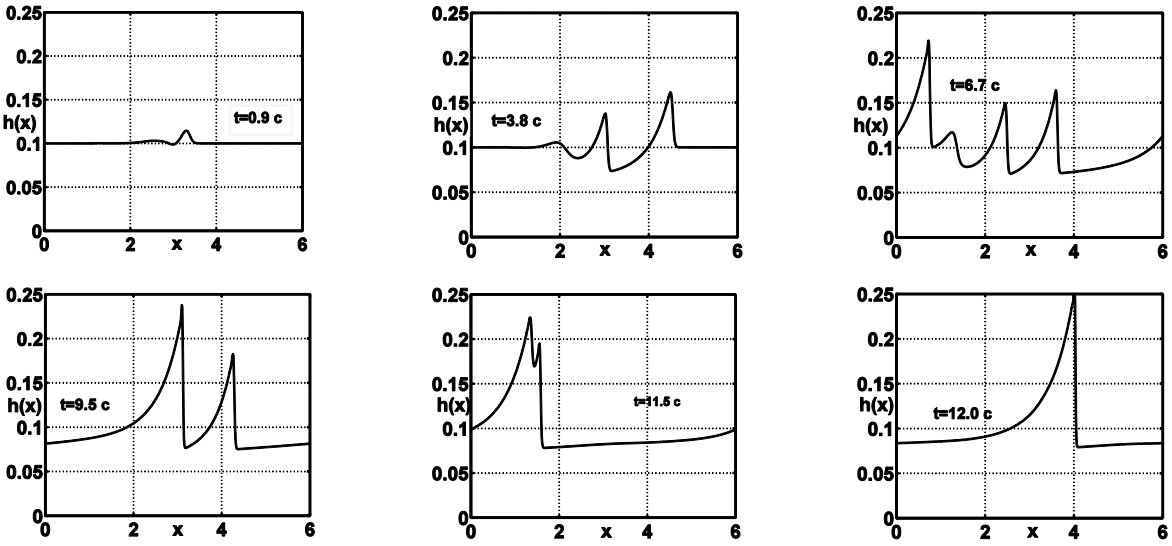

About the energy levels of GaAs

Kulpash Iskakova, Rif Akhmaltdinov

Computer simulation of the properties of the crystal lattice gives to use up to $10^{10} \div 10^{12}$ atoms. Using the described technique can be obtained from any of these atomic systems, as well as changes in the radii of coordination spheres at various distances. Simultaneously, you can get a number of nearby neighbors, the location of atoms on the coordination sphere.

We can develop an algorithm for constructing the structure of compound semiconductor-type A^3B^5, based on this principle. For example, to the type of A^3B^5 of semiconductor compounds it is used compound GaAs.

The case of uniform distribution of electrons in the space of interaction between them becomes energetically unfavorable. There is a possibility of an orderly configurations of the electrons in space. One more subtlety of crystal structure in calculating properties of the crystal related to the fact that the radii of the spheres accrue uniformly covering to a certain radius (for example, GaAs structure up to 498), then this is a violation of uniformity. Next violation of uniformity arises after a group of 918 atoms. Figures 1 and 2 are a group of atoms and their arrangement.

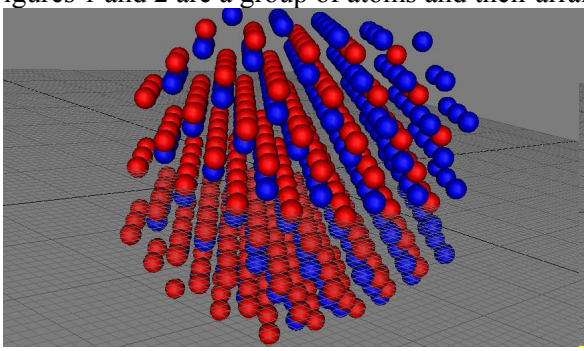

Fig. 1. The grid with a radius of coverage 5. where there are 498 atomic cores.

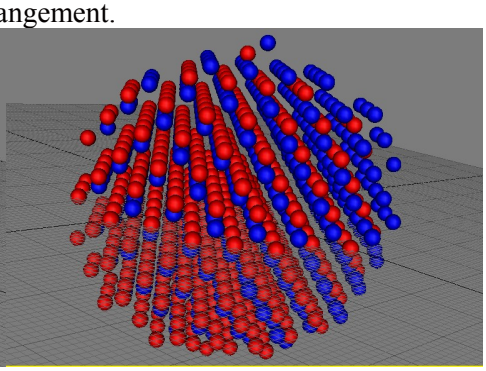

Fig. 2. The As atoms and Ga for the radius of coverage 6. Red marked atoms As, in blue denote atoms Ga. Central atom is As.

But in fact, such a violation of uniformity means that it is impossible to carry out "and self-evident and obvious" extrapolation of the results and methods of calculation for the "normal covered by the scope" on large radii, which is doing traditionally.

Links between the structural units play a dominant role. Coulomb attraction between electrons and nuclei combined into a solid unit. But again arise the question of the relationship of the spatial arrangement of the free electron gas with atomic nuclei in the crystal lattice. Contact in turn, arise from the nature of the electron distribution in space. In the existing models are impermeable ions crystal spherical. According to to the Pauli principle [1] and the theory of closed shells follows that atom is characterized by a stable electronic configuration. When crystal formation by being socialization electron leaving atomic orbital forms a defect in an electronic configuration resulting in an increase width of the unfilled valence [2-4]. In the crystal, when approaching to each other ions because of their impenetrability is broken quantum-mechanical effects. The main contribution to the total energy contributes strongly repulsive inter-ion Coulomb interaction. Much of the energy amounts electron-electron interaction in the calculation, which by existing methods there are big difficulties. The motion of the ions is inextricably linked with the movement of valence electrons [4, 5]. The total energy of the crystal depends on the location not only of ions and the electrons.

Therefore, in the calculation of the energy spectrum, it is necessary to consider the interaction of the electron and the probe with the cores and intercores. Oscillations are tightened to the centers of the cores and increase their amplitude with increasing levels of energy. This is explained the combined effects of strong impact of all cores and intercores on the test electron in the higher energy states. In the even states (2nd and 4th) are clearly visible the envelopes of the plane wave. In these states, the geometry of the crystal increases the total contribution of all the cores and the intercores in the amplitude of the envelope wave (the core and intercore lattice acts as a amplitude resonator). The energy

levels obtained in the space of wave vectors are periodic functions:

$$E_j(k_x+g) = E_j(k_x),$$

where g is a reciprocal lattice vector. The periodic dependence of the energy $E_j(x, k_x)$ from the one-dimensional wave vector k_x with a period $2k_x/a_0$ (where a_0 is the lattice period) throughout the entire crystal is obtained without regard the periodicity conditions.

Figures 3 and 4 shows the plots of the energy $E_j(x, k_x)$ of the coordinates of x and the wave vector k_x for a group of 498 atoms with an energy of 3.12 eV and 913 –2.93 eV.

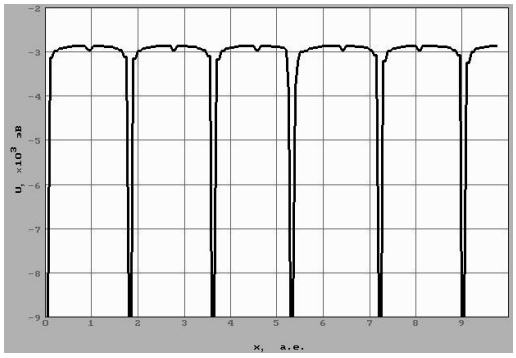

Fig. 3. The grid with a radius of coverage 5, where there are 498 atomic cores with an energy of 3.12 eV.

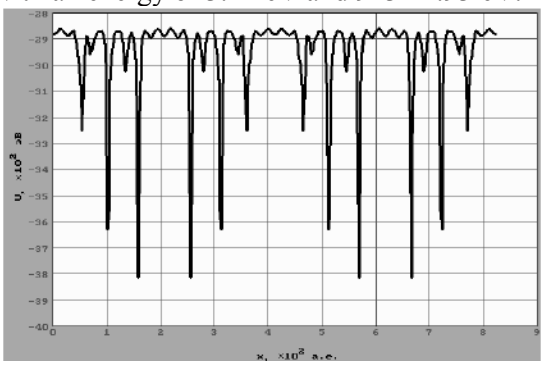

Fig. 4. The As atoms and Ga for the radius of coverage 6, where there are 913 atomic cores with an energy of 2.93 eV.

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Polymer Adsorption onto a Stripe-Patterned Surface

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05.06.2013

In recent years, polymer systems have received a great deal of attention from both, the experimental and the theoretical perspectives. However, a complete description of the properties of these materials does not currently exist. Therefore, further research is needed. This particular study is part of an ongoing effort to try to understand these systems and is focused on the adsorption of single polymer chains. Previous theoretical studies have provided phase diagrams that lay the foundations for a better understanding of the basic mechanisms of polymer adsorption. This particular study focuses on a single polymer chain in a confined volume and its adsorption onto a stripe-patterned surface.

A minimalistic simple-cubic lattice model was used where the chain is represented by an interacting self-avoiding walk (ISAW) and was confined between an attractive patterned wall and a steric wall with no interaction whatsoever. The pattern consisted of parallel stripes of defined width and separation. Besides the pattern parameters, three energy scales determine the phase diagram of the system: chain-surface attraction, chain-pattern attraction and chain self-attraction.

Chains of lengths up to $N = 19$ monomers were studied using the method of exact enumeration. The influence of the energy scales and pattern parameters on the system was analysed with the help of temperature vs. chain-pattern attraction phase diagrams. These diagrams were constructed by means of both canonical and microcanonical analysis of the enumeration data.

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Pressure-induced semiconducting behavior of calcium from *ab initio* calculations

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Pressure-induced dielectrization (full or partial) of fcc alkaline-earth metals Ca and Sr, as well as chemically similar to them rare-earth element Yb, has long attracted attention of both theoretical and experimental physicists. The resistivity measurements demonstrate that in a certain pressure range, each of these elements exhibits a semiconducting (or, perhaps, semimetallic) behavior, most pronounced in case of Yb (see [1] and references therein). In addition, at these pressures a thermopower anomaly is observed [2, 3]. Upon further compression, a re-entrance of metallic conductivity occurs, as the fcc→bcc structural transition takes place. Theoretically, the electronic spectrum of fcc alkaline-earth elements calculated within density functional theory (DFT) [4] is characterized by a hybridization gap which develops into a real gap upon compression and closes at the transition to a metallic bcc phase [5].

However, there are quantitative discrepancies between theory and experiment regarding both the width of energy gap and the pressure interval where it opens. On the one hand, the discrepancies can be attributed to inaccuracies in the transport measurements under pressure. On the other hand, this situation is certainly related to the well-known problem — incorrect estimation of band gaps within DFT. In order to obtain more accurate electron excitation spectra of semiconductors and insulators, the quasiparticle GW approximation is usually employed [6]. However, this method is notoriously complicated and computationally expensive. An alternative approach is to use hybrid functionals [7] that are superior to the DFT in reproducing the experimental gap values, at the same time allowing one to considerably reduce the computational cost as compared to the GW method.

We present *ab initio* calculations of the electronic structure of calcium in the pressure range up to ~20 GPa, where the fcc phase is stable. The initial calculations were done within DFT and then the GW method was applied. The comparison of obtained results demonstrates that with the GW method, the gap is wider and the pressure interval where it exists is smaller than in our DFT calculations. We also checked the applicability of the hybrid functional approach in the situation of variable compression. A value of mixing parameter α at various pressures was determined from comparison with our GW results. The obtained electronic spectra are relatively insensitive to small variations in α value.

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How to make large computer simulation user friendly: one practical example

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Modern research requires a lot of different pieces of technology and methodology to be combined into a single system. The field of computaional physics is not an exception. Computer simulations require knowledge of hardware and software, of modern computing libraries, methods of parallel programming, techniques of visualization and data analysis. Development of such a complex system from the very beginning is usually a difficult task and requires a lot of effort.

One possible solution to the outlined problem is to develop some middleware which can hide the complexity of the underlying system providing an interface to different services, starting from data and task management, parallel execution of tasks and ending with visualization and data analysis. Such combination of hardware and correspoinding middleware is called a platform and is a basic part of cloud computing technology. Since computational physics simulations are usually very complex and are based on the combination of a large number of elements, cloud computer systems that provide complete set of services are still in emergent stage. The most advanced and popular cloud computing system nanohub.org is based on Hubzero [1] platform developed at Purdue university.

In this paper we present our experience with the Hubzero platform [2], describe our own software for diffusion-limited-model simulation [3] adapted for Hubzero platform and also present modifications to the platform that are already implemented. We also propose some new ideas that should make cloud computing software more user-friendly and more popular in the area of computational physics.

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The Fluctuation-Dissipation Theorem of Topological Defect Colloidal Particles's energy on 2D Periodic Substrates: A Monte Carlo Study of thermal noise-like fluctuation and diffusion-like Brownian motion

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By Monte Carlo simulations, we have calculated mean-square fluctuations in statistical mechanics, such as those for colloids energy configuration are set on square 2D periodic substrates interacting via a long range screened Coulomb potential on any specific and fixed substrate when the system is in thermal equilibrium . These random fluctuations with small deviations from the state of thermodynamic equilibrium arise from the granular structure of them and appear as thermal diffusion with Gaussian distribution structure, are showing linear form of the Fluctuation-Dissipation Theorem on energy of particles constitutive a canonical ensemble. The noise-like variation of the energy per particle and order parameter versus the Brownian displacement of sum of large number of random steps of particles at low temperatures phase are presenting a markovian process on colloidal particles as well too.

Automatic post processing algorithm for passive seismic monitoring data

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Abstract. The problem of monitoring of different types of seismic events - geoacoustic precursors of earthquakes, industrial and field explosions, places fragments fall of separating parts of rockets-carriers, etc. is one of the key in the modern ecology of the environment. The peculiarity of this kind of monitoring is that it is mobile seismic groups, which should be based in the proposed area of occurrence of events [Avrorov, 2010].

One of the most important steps for solving the problems connected with the detection and identification of recorded data from passive sensors in mobile seismic array (MSA). The task of determining the nature of the source and its' coordinates lies in the basis of direction, referred to as the geoacoustic location. Using a new approach (not by location) by neural classification we will demonstrate usability of algorithm which based on quantitative parameters of signal.

Main idea. The increase on the demand for Passive Seismic especially in the domains of exploration and production has most recently become a challenging field of opportunity. The method based on uncontrolled sources, requires an understanding and analysis of what we call passive events in a careful manner, so as not to be misinterpreted leading to a possible damage of its credibility [Kapotas et al., 2006]. The problem of earthquake occurrence in platform territories, in spite of numerous examples of such seismic events, remains still unsolved in many aspects. This problem is particularly important for densely populated southern European Russia [Ulomov, 2007]. Another objective of seismic monitoring is to detect and locate underground nuclear explosions agreed with Comprehensive Nuclear-Test-Ban Treaty (CTBT) verification regime.

Modern seismological monitoring of the EEP is carried out by the Geophysical Survey of Russian Academy of Sciences (GS RAS) in close contact with different regional organizations, including academic and university research units. The objective of this presentation is to look at one of the methodologies that benefit from passive sources, and justify its use with case studies from MSA "Mikhnevo". The targets of MSA are the low-magnitude events (M > 1.5-4.5). The data of the Mikhnevo 3-C station from the GEOFON network are added to these observations for some earthquakes. MSA "Mikhnevo" is situated in a quiet area which is located about 80 km to the south of Moscow [Sanina et al., 2011].

Reviewing datasets we can observe some different seismic events. They could have nature from: natural hazard (landslides, earthquakes etc.) or anthropogenic activity (mining exploration, munitions disposal etc.). We need to produce an automatic algorithm which can indicate a seismic event nature. After this procedure operator will use results for next processing (such seismic event location). There are few programs in the world, but our interest is to create this algorithm for MSA "Mikhnevo", because we should consider territorial features (depth of the sediment layers, body wave velocities etc.). The seismic channel of MSA "Mikhnevo" is based on a SM3-KV short-period seismometer, widely used. The low-frequency acoustic/seismic background noise (between 0.5-10 Hz), which is actively emitted by the earth, lies near the central frequency of wanted signal (4-8 Hz – P-waves, 2-3 Hz – S-waves, 0.5-0.8 Hz – Surface waves). This is of particular importance in passive seismic systems where STA/LTA algorithms require an input signal. Typical casing failure events have large relative amplitude, a P/S ratio close to unity. Then we estimate P/S ratios, Hilbert transform, signal lasting and Fourrier spectra – these are waveform "portraits".

We provide an application *CASE (Classification Algorithm for Seismic Events)* employing Matlab 6.1. *CASE* can make solutions like an expert system providing an interpretator choice. Neural algorithms are the most powerful for classification and identification. The complex database includes waveform "portraits" (2004-2013 years) is used for network training.

I would like to thank IDG RAS for collected data and my academic tutor Sanina I.A.

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CALCULATIONS OF THE DIRECT AND COMPOUND REACTIONS OF NEUTRONS WITH NUCLEI

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Abstract

We elaborated Fortran program for neutron elastic and inelastic scattering calculations in coupled channels optical model with excitation low levels even-even deformed nuclei. Collective states of nuclei are considered in the rigid axial and non-axial rotator model.

Characteristics of reactions running through the compound nucleus can be calculated using this program with or without accounting for the influence of the direct reactions on their.

Results of some calculations are compared with experiments. They clearly demonstrate the capabilities of the program.

Models and solutions of quasi 2D turbulence with chemical reactions.

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Two models for quasi 2D turbulence with chemical reactions are used: a) the model of decaying turbulence; b) the model of forced turbulence. The paper presents the results of mathematical modeling of forced quasi 2D turbulence with chemical reactions. This model leads to new phenomena as compared to the case without chemical reactions. The KLB (Kraichnan-Leith-Batchelor) theory of 2D turbulence predicts the existence of two inertial ranges. The influence of chemical reactions both on forward enstrophy and inverse cascades is investigated. The characteristics of cascades for various parameters were obtained. The physical mechanism is corrected via data by generated numerical-analytical simulations.

Non-equilibrium critical dynamics of pure and diluted 2D XY model

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The study of systems characterized by slow dynamics is attracting considerable interest from both theoretical and experimental point of view [1]. This is due to the predicted and observed aging in slow evolution from non-equilibrium initial state and violation of the fluctuation-dissipation theorem [2]. The two-dimensional XY-model refers to systems that demonstrate an abnormally slow dynamics, and the main distinguishing feature is that the two-dimensional XY-model shows an anomalous behavior is not only near the phase transition temperature Berezinskii-Kosterlitz-Thouless T_{BKT}, but for all low-temperature phase. The aging is unusual phenomenon of the growth of the relaxation time of the system with the increasing of the "age" of the material. "Age" is the time elapsed since the sample preparation [3].

Relevance of the study of two-dimensional XY-model is due to a wide range of physical systems whose behavior can be described. Examples of such systems include [4-7]: Co and Ni films; important class of planar magnets; two-dimensional crystals; surface superconductors; superconducting thin film; Bose liquid film; superfluid liquid He; Josephson junction array; array of superconductor-ferromagnet-superconductor contacts; behavior of birds flocks; behavior mycetozes fungus-like organism; the behavior of some colonies of bacteria.

In this work a comprehensive study of the aging and the violation of the fluctuation-dissipation theorem in a pure and structurally disordered two-dimensional XY-model were carried out. The effects of coarsening and the temperature dependence of the rigidity in the low-temperature phase were discovered. It was obtained the dependence of the critical temperature on the defects concentration.

The reported study was supported by the Supercomputing Center of Lomonosov Moscow State University and Joint Supercomputer Center of the Russian Academy of Sciences.

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True self-consistent solution of Kohn-Sham equations for infinite systems with inhomogeneous electron gas

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The density functional approach in the Kohn-Sham approximation is widely used to study properties of many-electron systems. Due to the nonlinearity of the Kohn-Sham equations, the general self-consistence searching method involves iterations with alternate solving of the Poisson and Schrödinger equations. One of problems of such an approach is that the charge distribution renewed by means of the Schrödinger equation solution may be incompatible with boundary conditions on Poisson equation for Coulomb potential, as it has long been known since the articles of Bardeen [1] and Lang and Kohn [2]. The resulting instability or even divergence of iterations manifests itself most appreciably in the case of infinitely extended systems because the corresponding boundary-value problem becomes singular. The published attempts to deal with this problem were shown to be reduced in fact to abandoning the iterative method initially declared and replacing it with some approximate calculation scheme [3]. In general, these schemes are usually semi-empirical and do not permit to evaluate the extent of deviation from the exact solution. In [3] the iterative algorithm of solving the Kohn-Sham equations for unbounded systems with inhomogeneous electron gas has been formulated, which is based on eliminating the long-range character of Coulomb interaction as the cause of tight coupling between charge distribution and boundary conditions. This algorithm was implemented to the semi-infinite degenerate electron gas bounded by infinitely high potential wall or self-consistent potential barrier [4]. The work function and surface energy of simple metals in the jellium model have been calculated and successfully compared with the published experimental and computational results [5, 6].

Here we present the results of applying our algorithm to the calculation of the energy spectrum of quasi-two-dimensional (2D) electron gas in accumulation layer on the semiconductor surface. In such a structure, the states electrons are occupied belong both discrete and continuous parts of the energy spectrum. As a result, there are the high density of electrons bound close to the surface and the degenerate electron gas in the bulk of semiconductor. The stable convergence of iteration is obtained even in that case. To evaluate the adequacy of the method for the real structures, we calculated the energy spectrum of the quasi-2D electron gas in the case of the accumulation layer on the surface of n-InAs. This semiconductor has narrow band gap and appreciably non-parabolic conduction band that has to be taken into account. The computed energy levels correspond well to experimental data measured by the angle-resolved photoelectron spectroscopy method [7, 8]. Also, the difference between self-consistent solutions in the Hartree approximation and those with taking into account the exchange-correlation interaction is analyzed. This allows one to assess when the calculations can be restricted to the more simple case.

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Computational modelling dynamics of quantum and laser systems and backward-wave tubes with elements of a chaos

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We numerically study nonlinear optics and dynamics of some quantum (atomic), laser systems and backward-wave tube in order to detect a chaos elements (quantum chaos). Many systems in a modern quantum physics and electronics manifest the elements of the deterministic chaos and hyperchaos in its dynamics. Chaos theory establishes that apparently complex irregular behaviour could be the outcome of a simple deterministic system with a few dominant nonlinear interdependent variables. Here we present the results of studying the dynamical chaos regime in generation of a laser with absorbing cell and chaotic self-oscillations in the backward-wave tube on the basis of numerical analysis by means a complex of advanced methods and algorithms (in versions [1,2]). In ref.[3] there have been presented the temporal dependences of the output signal amplitude, phase portraits, statistical quantifiers for a weak chaos arising via period-doubling cascade of self-modulation and for developed chaos at large values of the dimensionless length parameter. Our analysis techniques includes a multi-fractal approach, methods of correlation integral, false nearest neighbour, Lyapunov exponent's, surrogate data, memory matrix formalism [1,2]. In table 1 we present the data on the Lyapunov exponents' for two self-oscillations regimes in the backward-wave tube: i). the weak chaos (normalized length: L=4.24); ii) developed chaos (L=6.1). The correlations dimensions are respectively as 2.9 and 6.2. Our analysis confirms a conclusion about realization of the chaotic features in dynamics of the backward-wave tube. The same program is realized for detecting the chaos regime in generation of a laser with absorbing cell and multi-electron atoms in a microwave field.

Table 1. Numerical parameters of the chaotic self-oscillations in the backward-wave tube: λ_1–λ_6 are the Lyapunov exponents in descending order, K is the Kolmogorov entropy (our calculation results)

Regime	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	K
Weak chaos L=4.24	0.261	0.0001	–0.0004	–0.528	–	–	0.261
Hyperchaos L=6.1	0.514	0.228	0.0000	–0.0002	–0.084	–0.396	0.742

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Measurement of Radon Concentration of Air Samples and Estimating Radiation Dose from Radon in SARI Province

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Abstract: Radon is a radioactive material. This gas is colorless, tasteless, odorless, and its main source element radioactive uranium-238 (^{238}U) .It has been recognized that the source of half the human dose, radon gas is present in the environment. Radon is a radioactive substance is carcinogenic and should always be careful and it worked perfectly.Since this element is emitting alpha particles also it is very dangerous to inhale a mist of decomposition products formed easily into the air and stick to lung tissue It is hard to focus on one part of it.In this study to measure radon in homes in the province of Sari dosimeters DOSEman SARAD GmbH company in Germany that are sensitive to alpha particles were used. Population of the city of Sari 495,369 people, and the urban population of the village of forty to sixty is the degree of concentration of 116.5 people per square kilometer., A percentage of the total household population of Sari in areas geographically different samples are selected (2600 times according to the latest population census sample data Sari city).Measuring radon in four different seasons in a year at home for sampling was done. Sensors 60-minute room bedroom or living at an altitude of 50 to 90 cm from the floor, away from windows and sunlight placed Howe dose rate and radon gas in homes has been measured. The amount of radon in your home in Spring 28.615Bq m^{-3}, in summer Bq m^{-3} 27.20, in the autumn 27.07Bq m^{-3} in winter Bq m^{-3} 36.95 measure . Both dose levels in spring .0032 μSv, in the summer 0.026 μSv, in the autumn 0.037μSv in winter 0.056 μSv is measured. Annual dose equivalent to approximately 0.0151μSv / year .Radon measurement results show that the average radon concentration is higher in winter than other seasons. The same dose in the winter than the other seasons. This difference could be due to lack of air movement and stillness, and the dose of radon indoors in the winter.

Keywords: Natural Radioactivity, Radon, Lung Cancer, Radiation Dose, SARI province

Angular correlation and genuine- and conjugate-Fermi holes in two-electron atomic systems

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Abstract. The ground and low-lying singly-excited states of He and He-like atomic ions have been studied by the full configuration method focusing on the angular correlation between the two electrons in the studied systems. The two-electron angle density distributions show distinct trends between the ground and excited states and between the singlet-triplet pair of states for different nuclear charge Z_n. The probability density distribution of the ground state has a strong dependence on the two-electron angle ϕ_- for small values of Z_n, such as $Z_n = 2$ and 3, which diminishes to zero as Z_n increases towards infinite. On the other hand, the probability density distributions of the singlet-triple pair of states of the (1s)(2p) configuration show a very weak dependence on ϕ_- for the small values of Z_n but a strong dependence for increasing Z_n, that represents peaks at $\phi_- = 0, \pm\pi$ and $\pm\pi/2$ for the singlet and triplet states, respectively. The origin of these angular dependences is rationalized on the basis of the structure of the genuine and conjugate Fermi holes.

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Calculation of optical properties of semiconductor nanocrystals in the framework of density functional theory using GPU parallel programming

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At the present time silicon nanocrystals form the basis of modern microelectronics and they are widely used for the diagnosis of biological objects. The problem of modeling at the atomic level is relevant for the design of silicon nanoparticles, which play an important role in creating active optical elements - quantum dots - doped silicon nanocrystals, the optical properties are essentially the next generation of optical storage, optical communication devices, etc [1]. There is a large class of situations where the nanocrystals with high quantum states of electrons population are subjected to the strong driving laser field.

In the present work an effective parallel algorithm is proposed for calculating optical properties of many-electron systems based on the dynamic density functional method [2]. The starting point of the time dependent density functional theory is a system coupled Schrödinger equations for the electron orbitals $\varphi_j(\vec{r},t)$: $i\frac{\partial}{\partial t}\varphi_j(\vec{r},t)=\left[-\frac{\nabla^2}{2m}+\upsilon_{KS}(\vec{r},t)\right]\varphi_j(\vec{r},t)$, где $\upsilon_{KS}(\vec{r},t)=\upsilon(\vec{r},t)+\int d^3\vec{r}\,'\frac{n(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|}+\upsilon_{xc}(\vec{r},t)$, is the sum of an external potential $\upsilon(\vec{r},t)$, the Hartree potential and the exchange-correlation potential $\upsilon_{xc}(\vec{r},t)$. In this work adiabatic approximation of the local density is used for $\upsilon_{xc}(\vec{r},t)$. The electron density of the interacting system $n(\vec{r},t)=\sum_{j=1}^{N}\left|\varphi_j(\vec{r},t)\right|^2$ can be defined as the sum of squares of the moduli of the single-particle orbitals filled with N electrons.

As a test for the solutions of the dynamic Kohn-Sham equations, the behavior of the interaction electrons in a spherical quantum dot is investigated. The result of the numerical solution is the Fourier transform of the dipole moment $<e\cdot\vec{r}>=\int e\cdot n(\vec{r},t)\cdot\vec{r}d^3\vec{r}$ of the system, which characterizes the excitation spectrum of interacting electrons in a quantum dot.

It was found that the most effective method for solving dynamic equations is the explicit Runge-Kutta 4th order. The main advantage of this algorithm is that the calculation of the wave function at each grid point can be performed independently, and therefore simultaneously. The Runge-Kutta method requires O (N) operations. After that requires a transfer of values of the wave function at the boundary nodes for systems with distributed memory and at only extension of the blocks on the boundary nodes for a system with shared memory. The developed algorithm has been realized on a GPU cluster. Testing of the algorithm was performed on the device with the maximum number of nodes produced by 30464 graphics cores.

The developed software component showed good scalability in the case of proportional resizing of the problem being solved. It is shown that the most effective solutions for the Schrodinger equation is a temporary method of Runge-Kutta method. The possibility of scaling data circuits on distributed memory systems and describes the implementation of the algorithm on the GPU. It has been demonstrated that the algorithm can be used to determine the spectra of both isolated and interacting silicon nanocrystals (quantum dots).

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Optimal Paths in Random Resistor Networks

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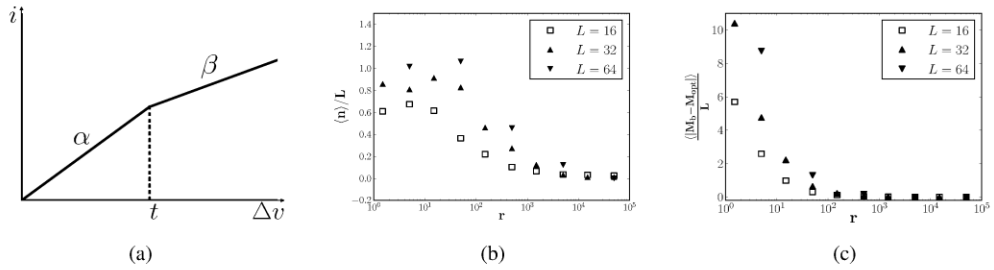
Abstract

Random resistor networks are often used to model transport in disordered systems, including more complex phenomena such as brittle fracture [1] and the flow of fluids with complex rheologies [2]. This is done by mapping the electrical properties of the individual conductive elements to those of elasto-plastic bars or fluid flow in channels.

A random resistor network is a network of conducting bonds with a piecewise linear characteristic (Fig. 1(a)). As the voltage drop over the bond increase, so does the current, until a threshold is reached. Each bond in the network has a random threshold drawn from a probability distribution, which introduce disorder in the system. This can in turn affect the macroscopic properties of the system. As the voltage drop over the entire network increase, more bonds reach their threshold, and a spanning path of broken bonds eventually forms.

When a spanning path forms, the macroscopic properties of the network change. In the case of fracture, the spanning path is a crack which disconnects the network, while for a Bingham fluid in a porous medium, the fluid flows through the medium along the spanning path. It is of interest where the spanning path forms [2]. It is already known [3] that the spanning path follows the optimal path for a perfect plastic behaviour ($\beta = 0$), where the optimal spanning path is the one which minimize the sum of the thresholds along the path.

We have studied where the spanning paths form in the network in the regime where $0 < \beta < \alpha$ (defined in the figure), and its relation to the optimal spanning path through the system [4]. Using a hierarchial model, we show that the formation of the spanning path is dependent on the ratio of the slopes in the characteristic, $r = \alpha/\beta$. The path should then be identical for different values of α and β, but a constant r, in a given network. As $r \to \infty$, the spanning path should follow the optimal path, both for $\beta = 0$ and $\alpha \to \infty$ with $\beta > 0$. Numerical results support this, and as r increase, the spanning path is more likely to follow the optimal path (Fig. 1(b)). At the same time, the mass of the spanning path decrease towards that of the optimal path (Fig. 1(c)), and the conducting elements of the network act as perfect plastics.



(a) (b) (c)

Figure 1: (a) Current-voltage characteristic of a conducting element with a threshold t. α and β denote the slopes of the linear elements. (b) Overlap between optimal path and backbone of spanning path for different r. n denotes the number of bond in the optimal path which are not in the backbone. (c) Difference in the mass of the backbone of the spanning path and the mass of the optimal path for different values of r.

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Nonlocal correlation functions and an integral model for nanomechanical properties of nanostructural complexes

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The mechanical properties of nanostructural materials is often considerably different in comparison with properties of isotropic medium with similar mechanical parameters. This fact caused extensive studies of computational methods for modeling nanomaterials and nature of its integral properties formation. Even for particular case of rheological properties modeling there is a long list of such computational methods, as lattice-Boltzmann, dissipative particle dynamics, Langevin dynamics and some continual assumption. All of these methods are proposed for using in so called multiscale models with molecular mechanics (MM) computational methods, frequently molecular dynamics or Monte-Carlo molecular simulation. The subject of theoretical interest here is finding such general set of parameters measured with molecular mechanics methods and allowed more accurately estimation of integral properties of the material. This issue has not been resolved for today.

Measurements of the same parameters for micro-scale and molecular-scale levels, as Young's modulus and the like are quite obvious and often used way. This method is associated with so-called "representative volume element (RVE)" which unfortunately usually turns out too big for MM simulation. For example, for the polymer matrix with 100nm length nanotube inclusion RVE will be about $1\mu m^3$.

In this research one new, more suitable and effective way of multiscale nanomaterials modeling is considered. In our model integral formulation of elasticity problem is used. It doesn't contain any integral parameters of media, which all described by integral core functions. The last are solutions of Kelvin-Somilyany, can be both estimate analytically, and measured directly with molecular dynamics method. From the point of view of statistical mechanics, integral core functions are just space and time-dependent correlation function for values of local deformation and mass velocity. Reduced requirement for volume of MM simulation and statistical-vested method of MM measurements are main advantages of this molecular- to micro-scale bridge.

We considered rheological properties of polymer nanocomposite material with inclusion of carbon nanotube. At micro-scale level, considered system was represented as continual polymer matrix with included nanotubes modeled as continual 1D objects. We also assume tube slipping relative to the polymer matrix. All necessary properties of medium were measured with MD simulation method.

For the control the quality and universality of suggested model, we also consider a problem about nanotube flow. This problem is well studied, simple in formulation and most similar for testing of nanomechanical models. Poisson equation for problem of stationary flow in cylindrical tube could be written in integral formulation by the same way. The grin functions of Poisson equation were considered as a space correlation function for liquid velocity in different points of real space. At the center of tube measured correlation function was similar to well-known analytical form, but near the wall considerably difference was found. However, just measured correlation function gave velocity profile similar to given directly by MD simulation.

Therefore, integral formulation of nanomechanical problem turns out not only more suitable, but also more general model. Integral formulation of tube flow problem, for example, allows correctly slip boundary condition describing, which is impossible in a differential model.

Title: Reference system for scanning probe tip fingerprinting

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Knowledge of the chemical structure of the tip asperity in Non-Contact Atomic Force Microscopy (NC-AFM) is crucial as controlled manipulation of atoms and/or molecules on surfaces can only be performed if this information is available. However, a simple and robust protocol for ensuring a specific tip termination has not yet been developed. We propose a procedure for chemical tip finger printing and an example of a reference system, the oxygen-terminated Cu(110) surface, that enables one to ensure a specific tip termination with Si, Cu, or O atoms. To follow this up and unambiguously determine tip types, we performed a theoretical DFT study of the line scans with the tip models in question and found that the tip characterization made based on experimental results (Cu/O-terminated tip imaging Cu/O atoms) is in fact incorrect and the opposite is true (Cu/O-terminated tip imaging O/Cu atoms). This protocol allows the tip asperity's chemical structure to be verified and established both before as well as at any stage of the manipulation experiment when numerous tip changes may take place.

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Monte Carlo renormalization group of dilute 3D Ising dynamics

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A computer simulations by the Monte-Carlo method of the critical dynamics of the diluted 3D Ising model are considered for samples with spin concentrations p_s=0.95, 0.8, 0.6 and 0.5. There is reason to believe that the influence of quenched impurities on the critical dynamics will be seen more clearly than in the equilibrium state, because of the specific conservation laws.

The disordered Ising model is specified by a system of spins $S_i = \pm 1$ with concentration p, which are associated with $N=pL^d$ sites of a d-dimensional lattice (L is length scale of the lattice). This gives $p2^N$ possible configurations $\{S\}$, with energy $E=-J\sum p_i\, p_j\, S_iS_j$, where the sum runs over nearest neighbours only, J represents spin interaction energy, and p_i are quenched site disorder variables. We consider a ferromagnetic system with $J<0$.

The use of the Metropolis kinetics makes it possible to immediately realize the dynamics of the Ising model with a relaxation of magnetization $m(t)= \sum_i^N S_i/N$ to the equilibrium value determined by the thermostat temperature T. In the simulation of the critical dynamics the initial state of the system is chosen with all spins parallel ($m(0)=1$) and with a temperature equal to the critical temperature. The critical temperature T_c for dilute magnetic materials is a function of the sin concentration p_s. It decreases with increasing p and vanishes at the threshold concentration p_c. For cubic lattice of Ising spins we would have $p_c \approx 0.3117$ and $T_c(0.95) \approx 4.26267$, $T_c(0.8) \approx 3.49948$, $T_c(0.6) \approx 2.42413$, $T_c(0.5) \approx 1.84509$ in units of J/k [1]. To determine the dynamical exponent z, which characterizes the critical slowing of the relaxation time of the system, $t_c \sim |T-T_c|^{-z\nu}$, we have used here the Monte-Carlo method, combined with the dynamical renormalization-group method. For this, the system was partitioned into blocks, where a block b^d of neighboring spins was replaced by a single spin whose direction is determined by the direction of most spins in the block. The redefined spin system forms a new lattice with magnetization m_b. We assume that the magnetization of the initial lattice relax to some value m_1, over a time t_b. Then by using two systems with block size b and b' and determining the relaxation times t_b and $t_{b'}$ of the block magnetization m_b and $m_{b'}$ reach to the same value m_1, the dynamic exponent z can be determined from the relation $t_b/t_{b'} = (b/b')^z$ or $z=\ln(t_b/t_{b'})/\ln(b/b')$ in the limit of sufficient large b and $b' \to \infty$.

We applied this algorithm to impure systems with dimensions of 144^3 and impurity concentrations presented above. The size of the system made it possible to partition into blocks with sizes $b=2, 3, 4, 6, 8, 9, 12, 16, 18, 24, 36$. The procedure of blocks partitioning of the initial spin and impurity configurations was implemented on the basis of the criterion of spin connectivity [2]. A relaxation simulating procedure consisting of 10000 Monte Carlo steps per spin was perfomed for each with 1000 runs with different impurity configurations over which the function $m_b(t)$ was averaged.

We obtained the sets of the exponent z_b values corresponding to the different b. The revealed dependence of z on b made extrapolation to the case $b \to \infty$ possible, assuming that $z_b = z_{b=\infty} + \text{const}\, b^{-\Omega}$. The resulted values of the dynamic exponent $z = z_{b=\infty}$ are z(0.95)=2.18 ± 0.03, z(0.8)=2.24 ± 0.03, z(0.6)=2.70 ± 0.05 and z(0.5)=2.78 ± 0.08. These values of the dynamic exponent confirm the steps-like universality law, for diluted 3D magnetic materials which was suggested at first in paper [2]. According to it, the critical behaviour of slightly and strong disordered systems divided by threshold of impurity percolation belongs to different classes of critical universality with different sets of exponents.

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Effects of the perpendicular magnetization on the nonlocal transport properties of the topological insulator ferromagnet/insulator/superconductor/insulator/ferromagnet junction

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We investigate theoretically the effects of the perpendicular magnetization on the electron elastic cotunneling (CT) and crossed Andreev reflection (CAR) in a ferromagnet/insulator/superconductor/insulator/ferromagnet (F/I/SC/I/F) junction formed on the surface of a three dimensional topological insulator. The perpendicular magnetization induces an energy gap in the linear spectra of the Dirac fermions on the surface of the topological insulator. We find that in the parallel magnetization configuration the conductance resulting from cotunneling G_{CT} is larger than the conductance resulting from crossed Andreev reflection G_{CAR}. While, for the antiparallel magnetization configuration the contrary is true and the nonlocal conductance $G_C = G_{CAR} - G_{CT}$ increases with increase of the magnetization. We also investigate the effect of the magnetically induced gap on the barrier strength dependence of the nonlocal conductance. We find that both the electron elastic cotunneling and the crossed Andreev reflection, as a function of barrier strength, show a $\pi/2$ periodic oscillatory behavior with mean value and amplitude which depend on the magnetically induced gap.

Numerical Integration of Quantum Dynamics in the Floating Multiple Gaussians Basis

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The Floating Multiple Gaussians Basis [1] is an effective basis for expansion of the trial wave function for the numerical quantum dynamics. For example, in the Split Wave Packets Molecular Dynamics method [2] single electron wave functions are expanded in a set of Gaussian wave packets (WP) ϕ_k. The Gaussians are called floating because their parameters (positions, momenta, etc.) are treated as dynamical variables. A trial many-body wave function is then constructed depending on the quantum approximation for electron spins, for example in the simplest Hartree case it reads: $\Psi_h(\{\mathbf{x}_k\},t) = \prod_k \phi_k(\mathbf{x}_k,t)$.

The trial wave function is substituted into the time dependent Schroedinger equation and the resulting equations of motion follow from the variational principle [3]:

$$\frac{dq_i}{dt} = \sum_j (\mathbf{N}^{-1})_{ij} \frac{\partial H}{\partial q_j}, \tag{1}$$

where **q** is the complete set of all dynamical variables of all WPs, $N_{ij} = -2\hbar \,\mathrm{Im}\left\langle \frac{\partial \Psi}{\partial q_i} \middle| \frac{\partial \Psi}{\partial q_j} \right\rangle$ is the norm matrix and *H* is the quantum expectation value of the energy for a given trial wave function. For the Gaussian basis the elements of the norm matrix may be obtained analytically, however inversion of the matrix is required at every time step of the numerical integration.

Numerical solution of equations (1) requires special consideration because the norm matrix may become degenerate. This degeneracy is a consequence of the general overcompleteness of the Gaussian basis, so even starting from the initial state with a nondegenerate norm matrix, the degeneracy may appear in the course of the system dynamics. We show that these degeneracy states are attractive for the dynamical system and thus constitute a serious problem when solving the dynamics numerically. Physically the degeneracy in the norm matrix is an indication of the linear dependence in the parameter set in a specific system state.

In the present work a method of dynamical treatment of the Gaussain degenerate states is proposed. The method is based on reducing the dimension of the parameter set representing the many body wave function when the norm matrix is close to degeneracy. The reduction of the parameter set is achieved by analyzing eigenspectrum of the norm matrix and introducing additional constraints to the system dynamics, which correspond to the eigenvectors with small eigen numbers. The constraints are introduced temporarily and conserve the total energy and the wave function norm. The method of dynamical constraints is applied together with the variable time stepping procedure to control the application and release of the constraints.

In this contribution we describe the method of dynamical constraints and its application to the Split WPMD simulations in detail. We implement the constrained norm matrix method within the variable time stepping scheme for the fourth order Runge-Kutta integrator. We analyze the effect of the constraints on the solution of the dynamical quantum systems. We show that the parameters of the method may be chosen so that the constraints do not influence the physical characteristics of the system such as quantum expectation values of particle coordinates, energies and quantum state populations.

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Numerical modeling and forecasting the geophysical (atmospheric and hydroecological) systems dynamics by using the non-linear prediction and chaos theory methods

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It is known that a chaos is alternative of randomness and occurs in very simple deterministic systems. Although chaos theory places fundamental limitations for long-rage prediction, it can be used for short-range prediction since ex facte random data can contain simple deterministic relationships with only a few degrees of freedom. Many studies in various fields of science have appeared, where chaos theory was applied to a great number of dynamical systems. The studies concerning non-linear behaviour in the time series of atmospheric constituent concentrations are sparse, and their outcomes are ambiguous. Our paper concerns results of the research into dynamics of variations atmospheric (atmospheric pollutants concentrations) and hydroecological (nitrates and sulphates concentrations in the river's water reservoirs) systems in the definite region by using the non-linear prediction approaches and a chaos theory methods (in versions [1-3]). A chaotic behaviour in the nitrogen dioxide and sulphurous anhydride concentration time series at a group of the sites in Odessa, Kiev, Donetsk, Alchevsk regions numerically investigated. To analyze measured time histories of the considered system responses with the use of the Recurrence Plots, the phase space of these systems was reconstructed by delay embedding. To reconstruct the corresponding attractor, the time delay and embedding dimension are needed. The former is determined by the methods of autocorrelation function and average mutual information, and the latter is calculated by means of correlation dimension method and algorithm of false nearest neighbours. It's shown that low-dimensional chaos exists in the time series under investigation. The spectrum of Lyapunov exponents (LE) is reconstructed as well as both Kaplan-Yorke dimension and Kolmogorov entropy that inversely proportional to the predictability limit are calculated.

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NUMERICAL SIMULATION OF DARK FLIGHT TRAJECTORY AND DISPERSION ELLIPSE FOR METEORITES

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Meteorite-producing fireballs pass the Earth's atmosphere in two consequent stages: hypervelocity entry of causing fireball meteoroid and decelerated terminal dark flight. Initial bright part of the trajectory can be considered linear (Gritsevich, 2008), however as the projectile descents into the lower heights, the aerodynamic drag becomes major factor in reducing velocity down to subsonic values. Dark flight estimations are crucial in determining the search area on the ground, since no reliable instrumental means of detection are available at present to follow the survived fragments at this part of the trajectory. The numerical simulation becomes the most robust tool to specify the terminal part of the trajectory.

For the problem of dark flight we consider the model of projectile dynamics, where ballistic objects are called particles and modeled as homogenous spheres with a given bulk density. The motion of a single particle in a gas is governed by the system of ODEs in Lagrange variables. External forces, acting on a particle, are the total drag, Magnus force and gravity. The drag coefficient is defined by Henderson formula. The air properties for Mach and Reynolds numbers can be computed from one of the atmosphere models, e.g. 1976 U.S. Standard Atmosphere.

During the descent each particle presenting meteorite fragment can shatter into smaller pieces if a threshold is met for impact pressure (a difference between stagnation and static pressure for isentropically decelerated compressible flow). Such fragmentation event introduces new particles to the computation. Underlying mathematical model neglects direct inter-particle collisions; however discrete trajectory method is not suitable, since we simulate transverse repulsive forces arising in separation dynamics of two fragments (Passey and Melosh, 1980) and use discrete element method. The corresponding force coefficient is defined according to (Artemieva and Shuvalov, 1996). Each particle is scattered by the sum of repulsive forces from all other particles within effective distance. The ordinary differential equations governing projectile dynamics are integrated by the second order Runge-Kutta scheme, which is sufficient in the presence of input data uncertainties. Since the particles do not interact with each other directly, we implemented parallel computations. The integration of each trajectory is carried out down to the surface, which can be either considered as zero height for the spherical or elliptical Earth model or can be realistically implemented as overlay of digital elevation model on reference ellipsoid WGS84 via one of the GIS, which effectively yields estimation for dispersion ellipse.

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Simulation of small quantum systems by Path Integral Numerical Methods

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We propose a new approach in obtaining the partition function of a system of several interacting particles (fermions) in external field within path integral Monte Carlo method based on direct averaging of exchange contributions over the positive weight determined by non-closed trajectories. This way the complete partition function is obtained at finite temperatures down to their low values. The new approach allows us to reach observably lower temperatures, compared to the previously proposed path-integral Monte Carlo method [1,2], thus permitting significantly to reduce the sign problem. The proposed approach yields an independent way to treat thermal properties of quantum systems, so the good agreement with previous data [1,2] allows us to test and state the validity of both approaches. The presented approach allows one to carry out calculations for low temperatures that make it possible to estimate the ground-state energy and low-temperature thermodynamics. A quantum dot model of several interacting electrons confined in a harmonic oscillator field was simulated. The interaction with environment (phonons, plasmons) was accounted for within harmonic heat bath approximation [3].

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