

International Conference on Computer Simulation in Physics and beyond

September 6-10, 2015, Moscow, Russia



ORGANIZED BY:

National Research University Higher School of Economics
Science Center in Chernogolovka
Landau Institute for Theoretical Physics



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

KEYNOTE SPEAKERS:

- Norbert Attig, Germany - *"Impacts of Current Hardware and Software Developments on Simulation Sciences"*
Bertrand Berche, France - *"Academic research groups: evaluation of their quality, quality of their evaluation"*
Alexander Bogdanov, Russia - *"Solution of Financial Mathematics Real-Time Problems by Virtual Supercomputer"*
Oleg Druzhinin, Russia - *"Numerical simulation of small-scale mixing processes in the upper ocean and atmospheric boundary layer"*
Hans Herrmann, Switzerland - *"Discontinuous Percolation"*
Chin-Kun Hu, Taiwan - *"Protein aggregation might not be related to protein misfolding"*
Nail Inogamov, Russia - *"Surface 3D nanostructuring by tightly focused laser pulse: lagrangian codes and molecular dynamics"*
Nobuyasu Ito, Japan - *"Social sciences with supercomputer"*
Wolfhard Janke, Germany - *"Computer Simulation Studies of Polymer Adsorption and Aggregation"*
Helmut Katzgraber, USA - *"Beyond Moore's Law? Seeking Quantum Speedup Through Spin Glasses"*
Ralph Kenna, United Kingdom - *"Maths Meets Myths - Quantitative Investigations of Ancient Narratives"*
Lin Hai-Qing, China - *"Study of Superconductivity in Polycyclic Aromatic Hydrocarbon"*
Yuri Lozovik, Russia - *"Puzzle of supersolid: history and current state"*
Mark Novotny, USA - *"Spanning Trees, Continents, and the Quantum/Classical Divide on D-Wave 2 machines"*
Igor Petrov, Russia - *"Computational problems in Arctic Research"*
Arkady Satanin, Russia - *"Generation of entangled microwave photons in superconducting circuits"*
Walter Selke, Germany - *"Classical and quantum anisotropic Heisenberg antiferromagnets"*
Vladimir Shchur, United Kingdom - *"On modern problems and methods for data analysis in human genomics"*
Sauro Succi, USA - *"Lattice Boltzmann simulations of flowing matter across scales: classical, quantum and relativistic"*
Martin Weigel, United Kingdom - *"Fragmentation of fractal random structures"*
Alexandre Zagoskin, United Kingdom - *"The grand challenge of quantum computing: bridging the capacity gap"*

TOPICS:

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

ADVISORY BOARD:

Tikhonov Alexander - academician of RAO, chair
Evtushenko Yuri - academician of RAS
Zelenyi Lev - academician of RAS
Ivannikov Viktor - academician of RAS
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PROGRAM COMMITTEE:

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VENUE:

Tallinskay ul. 34, Moscow

WEBSITE:

<http://csp2015.ac.ru/>

CONFERENCE CHAIR:

Lev Shchur



ФЕДЕРАЛЬНОЕ АГЕНТСТВО
НАУЧНЫХ ОРГАНИЗАЦИЙ



Российская Академия Наук



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

Conference Time Table

| Time | Sunday Sept, 6 | Monday Sept, 7 | Tuesday Sept, 8 | Wednesday Sept, 9 | Thursday Sept, 10 |
|-------------|---|------------------------------|------------------------------|------------------------------|----------------------|
| 08.30 | | Registration | Registration | Registration | |
| 09.00-09.15 | | Registration | Plenary Talk 4 | Plenary Talk 4 | Plenary Talk 12 |
| 09.15-09.45 | | Opening | | | |
| 09.45-10.30 | | Plenary Talk 1 | Plenary Talk 5 | Plenary Talk 9 | Plenary Talk 13 |
| 10.30-11.00 | | Coffee | Coffee | Coffee | Coffee |
| 11.00-11.45 | | Plenary Talk 2 | Plenary Talk 6 | Plenary Talk 10 | Plenary Talk 14 |
| 11.45-12.30 | | Plenary Talk 3 | Plenary Talk 7 | Plenary Talk 11 | Closing |
| 12.30-13.50 | | Lunch | Lunch | Lunch | End of program |
| 13.50-16.00 | | <u>Parallel Session S7-1</u> | <u>Parallel Session S8-1</u> | <u>Parallel Session S9-1</u> | |
| | | <u>Parallel Session S7-2</u> | <u>Parallel Session S8-2</u> | <u>Parallel Session S9-2</u> | |
| | | <u>Parallel Session S7-3</u> | <u>Parallel Session S8-3</u> | <u>Parallel Session S9-3</u> | |
| 16.00-16.30 | | Coffee | Coffee | Coffee | |
| 16.30-18.40 | Registration & Welcome 17.30-21.00 | <u>Parallel Session S7-4</u> | Poster Session | Social Program | |
| | | <u>Parallel Session S7-5</u> | | | |
| | | <u>Parallel Session S7-6</u> | | | |
| 18.40 | | End of program | End of program | End of program | |

List of Plenary Talks

Room N 504

Plenary Talk 1. September 07, 09.45-10.30, **Nail Inogamov**, *Surface 3D nanostructuring by tightly focused laser pulse: lagrangian codes and molecular dynamics*

Plenary Talk 2. September 07, 11.00-11.45, **Ralph Kenna**, *Maths Meets Myths - Quantitative Investigations of Ancient Narratives*

Plenary Talk 3. September 07, 11.45-12.30, **Hans Herrmann**, *Discontinuous Percolation*

Plenary Talk 4. September 08, 09.00-09.45, **Wolfhard Janke**, *Computer Simulation Studies of Polymer Adsorption and Aggregation*

Plenary Talk 5. September 08, 09.45-10.30, **Vladimir Shchur**, *On modern problems and methods for data analysis in human genomics*

Plenary Talk 6. September 08, 11.00-11.45, **Norbert Attig**, *Impacts of Current Hardware and Software Developments on Simulation Sciences*

Plenary Talk 7. September 08, 11.45-12.30, **Lin Hai-Qing**, *Study of Superconductivity in Polycyclic Aromatic Hydrocarbon*

Plenary Talk 8. September 09, 09.00-09.45, **Bertrand Berche**, *Academic research groups: evaluation of their quality, quality of their evaluation*

Plenary Talk 9. September 09, 09.45-10.30, **Mark Novotny**, *Spanning Trees, Continents, and the Quantum/Classical Divide on D-Wave 2 machines*

Plenary Talk 10. September 09, 11.00-11.45, **Yuri Lozovik**, *Puzzle of supersolid: history and current state*

Plenary Talk 11. September 09, 11.45-12.30, **Boris Chetverushkin**, *On the simulations in hydrodynamics and aerodynamics*

Plenary Talk 12. September 10, 09.00-09.45, **Alexandre Zagoskin**, *The grand challenge of quantum computing: bridging the capacity gap*

Plenary Talk 13. September 10, 09.45-10.30, **Helmut Katzgraber**, *Beyond Moore's Law? Seeking Quantum Speedup Through Spin Glasses*

Plenary Talk 14. September 10, 11.00-11.45, **Sauro Succi**, *Lattice Boltzmann simulations of flowing matter across scales: classical, quantum and relativistic*

Schedule for Parallel Sessions

Parallel Session S7-1

September 07, 13:50-16.00, Room N 504

| Time | Name | Title |
|-------------|-------------------------------------|---|
| 13.50-14.20 | Martin Weigel, (Invited Speaker) | Fragmentation of fractal random structures |
| 14.20-14.45 | Lev Barash | Effective conductivity of tessellations in the plane |
| 14.45-15.10 | Alexander Kolpakov | Numerical analysis in the problem of capacity of systems of densely placed bodies |
| 15.10-15.35 | Helen Popova | Dynamical systems for modeling the evolution of the magnetic field of stars |
| 15.35-16.00 | Ivan Popov | Non-equilibrium critical vortex dynamics of disordered 2D XY-model |

Parallel Session S7-2

07 September 2015, 13:50-16.00, Room N 304

| Time | Name | Title |
|-------------|-------------------|---|
| 13.50-14.20 | Sergey Aleshin | The spatially inhomogeneous structures in the solution of Fisher-Kolmogorov equation with delay |
| 14.20-14.45 | Anatoly Manita | On behavior of stochastic synchronization models |
| 14.45-15.10 | Vladimir Semyonov | Resonance phenomena in extended Mathieu equation: theory and simulation |
| 15.10-15.35 | Viacheslav Belyi | A new model kinetic collision operator |
| 15.35-16.00 | Igor Kulikov | The Numerical Hydrodynamic Modeling of Interacting Galaxies by means Hybrid Supercomputer on base Intel Xeon Phi accelerators |

Parallel Session S7-3

07 September 2015, 13:50-16.00, Room N 214

| Time | Name | Title |
|-------------|-------------------------------------|--|
| 13.50-14.20 | Oleg Druzhinin (Invited Speaker) | Numerical simulation of small-scale mixing processes in the upper ocean and atmospheric boundary layer |
| 14.20-14.45 | Mark Shevelev | Kelvin-Helmholtz instability development in presence of the magnetic field shear and the density profile |
| 14.45-15.10 | Marina Boronina | Implicit scheme for the Maxwell equations solution in case of flat 3D domains |
| 15.10-15.35 | Dmitry Kachulin | New Compact Equation for Numerical Simulation of 1D and 2D Freak-Waves on Deep Water |
| 15.35-16.00 | Yuri Tarasevich | Desiccation of sessile particle-laden droplets: beyond 'coffee-ring effect' |

Parallel Session S7-4

07 September 2015, 16:30-18.40, Room N 504

| Time | Name | Title |
|-------------|------------------------------------|--|
| 16.30-17.00 | Igor Petrov (Invited Speaker) | Computational problems in Arctic Research |
| 17.00-17.25 | Alexey Poyda | Data-intensive multispectral remote sensing of the nighttime Earth for environmental monitoring and emergency response |
| 17.25-17.50 | Vladislav Sidorenko | Natural Oil Reservoirs: Computer Simulation of the Sedimentary Architecture |
| 17.50-18.15 | Arakel Petrosyan | Numerical modeling of complex geophysical flows in shallow water approximation |
| 18.15-18.40 | Dmitry Petrov, Nikolay Khokhlov | Computer simulation of Arctic problems by grid-characteristic method |

Parallel Session S7-5

07 September 2015, 16:30-18.40, Room N 210

| Time | Name | Title |
|-------------|-------------------|--|
| 16.30-17.00 | Grigory Smirnov | Application of atomistic simulation for modeling of gas hydrates |
| 17.00-17.25 | Nataliia Atamas | Influence of hydrophobic properties of dissolved substance to the local structure of the ionic liquid dmim ⁺ /Cl ⁻ at 400K |
| 17.25-17.50 | Pavel Dyshlovenko | Computer simulation of charge stabilized colloidal crystals |
| 17.50-18.15 | Vadim Kretov | Mathematical modeling of emission in small-size cathode |
| 18.15-18.40 | Sergey Lebedev | Computer Simulation of Thin Stripper Target Behaviour Under Bombardment of Intense Pulsed Ions |

Parallel Session S7-6

07 September 2015, 16:30-18.40, Room N 214

| Time | Name | Title |
|-------------|------------------|---|
| 16.30-17.00 | Valery Kovalev | Simulation of catalytic properties of thermal barrier coatings for space vehicles in dissociated air |
| 17.00-17.25 | Sergei Balakirev | Computer simulation of GaAs/GaAs(001) epitaxial growth considering V/III flux ratio |
| 17.25-17.50 | Sergey Lepeshkin | Structure and electronic spectra of silicon nanoclusters passivated by hydrogen and oxygen: evolutionary algorithm and first-principles study |
| 17.50-18.15 | Anatoly Antipov | Numerical studies of fundamental principles of ion transport in electrochemical systems based on autocatalytic redox-mediator mechanism |
| 18.15-18.40 | Andrey Prokhorov | The use of fuzzy modelling for predicting the values of the classic potential barrier of the reaction phenyl radical with hydrocarbons |

Parallel Session S8-1

08 September 2015, 13:50-16.00, Room N 504

| Time | Name | Title |
|-------------|----------------------------------|---|
| 13.50-14.20 | Chin-Kun Hu (Invited Speaker) | Protein aggregation might not be related to protein misfolding |
| 14.20-14.45 | Yuri Tarasevich | Some generalized models of random sequential adsorption of linear k-mers on a square lattice: jamming and percolation |
| 14.45-15.10 | Franco Ferrari | Heavily parallelized codes for the energy minimization and Monte Carlo simulation of polymer knots |
| 15.10-15.35 | Nikita Orekhov | Graphite melting: atomistic kinetics resolves longstanding controversy |
| 15.35-16.00 | Elena Sheka | Open-shell molecule: Problems of computer simulation and the reality of spin contamination of the molecule ground state |

Parallel Session S8-2

08 September 2015, 13:50-16.00, Room N 210

| Time | Name | Title |
|-------------|---|--|
| 13.50-14.20 | Alexander Bogdanov (Invited Speaker) | Solution of Financial Mathematics Real-Time Problems by Virtual Supercomputer |
| 14.20-14.45 | Laura Hernandez | Quantifying the differences between the auction and the negotiated market: the role of the structure of interactions |
| 14.45-15.10 | Laura Hernandez | Multilayer network model of mutualistic ecosystems: network structure and biodiversity |
| 15.10-15.35 | Yuri Tarasevich | Virtual network as excitable medium |
| 15.35-16.00 | Larisa Manita | Optimization problems for WSNs: trade-off between synchronization errors and energy consumption |

Parallel Session S8-3

08 September 2015, 13:50-16.00, Room N 214

| Time | Name | Title |
|-------------|--|---|
| 13.50-14.20 | Andrey Demichev, Alexander Kryukov | Open marketplace for simulation software on the basis of a web platform |
| 14.20-14.45 | Dmitry Gudovskikh, Sboev Alexander, Rybka Roman and Moloshnikov Ivan | Method of assessment of textual emotiveness with use of psycholinguistic markers on base of morphological features for analysis of social processes in networks and blogs |
| 14.45-15.10 | Alexandr Sboev, Roman Rybka, Dmitry Gudovskikh and Ivan Moloshnikov | Syntactic parsing sentences in Russian language based on selected set of parameters and neural networks |
| 15.10-15.35 | Alexandr Sboev, Ivan Moloshnikov, Dmitry Gudovskikh and Roman Rybka | A probabilistic-entropy approach of finding thematically similar documents with creating context-semantic graph for investigating evolution of society opinion |
| 15.35-16.00 | Alexandr Sboev, Danila Vlasov, Alexey Serenko and Roman Rybka | A comparison of learning abilities of spiking networks with different spike timing-dependent plasticity forms |

Parallel Session S9-1

09 September 2015, 13:50-16.00, Room N 504

| Time | Name | Title |
|-------------|---------------------|---|
| 13.50-14.20 | Nikolay Izmailyan | Ising model on plane: numerical solution |
| 14.20-14.45 | Dmitriy Pilipenko | Computational investigation of stable formation condition for Fe _x Ni _{1-x} alloy films on paramagnetic substrate |
| 14.45-15.10 | Ivan Belov | Monte Carlo-based bond switching method for generation of the SiC/SiO ₂ interface |
| 15.10-15.35 | Dmitriy Romanovskiy | Monte Carlo simulation of magnetic multilayered structures with giant magnetoresistance effects |
| 15.35-16.00 | Nikolai Usov | The universal behavior of dense clusters of magnetic nanoparticles |

Parallel Session S9-2

09 September 2015, 13:50-16.00, Room N 210

| Time | Name | Title |
|-------------|---|--|
| 13.50-14.20 | Pavel Lebedev | Integrating GPGPU computations with CPU coroutines in C++ |
| 14.20-14.45 | Vsevolod Nikolskiy, Vladimir Stegailov | Efficiency of ARM processors for classical molecular dynamics calculations |
| 14.45-15.10 | Alexander Belov | Improving the efficiency of solving discrete optimization problems (by the example of VRP) |
| 15.10-15.35 | Alexander Nozik | The DataForge framework for data acquisition and analysis |
| 15.35-16.00 | Vladimir Mironov | Adaptation of the Hartree-Fock method in GAMESS (US) to Intel Xeon Phi architecture |

Parallel Session S9-3

09 September 2015, 13:50-16.00, Room N 214

| Time | Name | Title |
|-------------|-------------------------------------|---|
| 13.50-14.20 | Arkady Satanin (Invited Speaker) | Generation of entangled microwave photons in superconducting circuits |
| 14.20-14.45 | Alexander Vasiliev | Quantum Hashing via ϵ -Universal Hashing Constructions |
| 14.45-15.10 | Vasili Kosiantchouk | Free-molecular gas flow through the oscillating membrane |
| 15.10-15.35 | Evgeny Pospelov | Ageing and memory effects in non-equilibrium critical behavior of 3D diluted Ising model with low-temperature initial state |
| 15.35-16.00 | Stepan Konakov | 3D simulation and analytical model of chemical heating during silicon wet etching in microchannels |

Schedule for Poster Session

08 September 2015, 16:30-18.40, Room N

- P1. Maria Stogova, Marina Mamonova and Vladimir Prudnikov** (Omsk F. M. Dostoevsky State University), *Computer calculations of energy and magnetic characteristics of substitutional adsorption of the monolayer iron film in depend of surface face orientation.*
- P2. Anna P. Soldusova, Pavel V. Prudnikov and Maria A. Medvedeva** (Omsk State University), *Monte-Carlo simulation of ultrathin magnetic films critical behavior.*
- P3. Yanina Parshakova and Andrey Ivantsov** (Institute of continuous media mechanics UB RAS), *Modeling of stratified flows in the problem of the morphological behavior of a sandpit.*
- P4. Andrey Ivantsov and Tatyana Lyubimova** (Institute of Continuous Media Mechanics UB RAS), *Settling of a liquid drop in a porous medium saturated by another liquid.*
- P5. Tatyana Lyubimova and Nadezhda Zubova** (Institute of Continuous Media Mechanics UB RAS), *Vibrational convection of ternary mixture in a closed cavity in zero gravity conditions.*
- P6. Kamal Khizriev, Akai Murtazaev and Taa Taaev** (Amirkhanov Institute of Physics, Daghestan Scientific Center of the Russian Academy of Sciences), *Investigation of phase transition of the model magnetic hard/soft bilayer by the Monte Carlo method.*
- P7. Andrew Shcherbakov and Marat Biktimirov** (National Research University "Higher School of Economics", Moscow Institute of Electronics and Mathematics), *Personal assistant with components of artificial intellect.*
- P8. Svetlana Shikota** (Science Center in Chernogolovka), *Transformation of IT infrastructure of science centre and data intensive processing.*
- P9. Yanina Parshakova and Andrey Ivantsov** (Institute of continuous media mechanics UB RAS), *Numerical investigation directional solidification of binary alloys under the action of rotational vibrations.*
- P10. Marina Kashina** (Perm State University) **and Aleksey Alabuzhev** (Institute of Continuous Media Mechanics UB RAS), *The oscillations of cylindrical drop under influence of nonuniform alternating electric field.*
- P11. Mariya Kaysina** (Perm State University) **and Aleksey Alabuzhev** (Institute of Continuous Media Mechanics UB RAS), *Influence of contact line motion on translation vibrations of a cylindrical bubble.*
- P12. Julia Dubenskaya, Alexander Kryukov, Andrey Demichev** (SINP MSU, Moscow) **and Nikolay Prikhodko** (NovSU, Veliky Novgorod), *New security infrastructure model for distributed computing systems.*
- P13. Anastasia Batanova and Pavel Dyshlovenko** (Ulyanovsk State Technical University), *Elastic constants of charge stabilized colloidal crystal with body-centered cubic lattice.*

- P14. Alexander Vasiliev** (Kazan Federal University), *A Model of Quantum Communication Device for Quantum Hashing.*
- P15. Denis Goldobin and Anastasiya Pimenova** (Institute of Continuous Media Mechanics UB RAS), *Coherence of noisy oscillators with delayed feedback inducing multistability.*
- P16. Nikolay Prikhodko, Viktor Abramovsky, Natalia Abramovskaya** (NovSU, Veliky Novgorod), **Andrey Demichev, Alexander Kryukov** (SINP MSU, Moscow) **and Stanislav Polyakov** (NovSU, Veliky Novgorod), *A Web Tools for Research in Nonlinear Optics.*
- P17. Anastasiya Pimenova and Denis Goldobin** (Institute of Continuous Media Mechanics UB RAS), *Boiling of oil fields by lava intrusions.*
- P18. Lev Barash** (Landau Institute for Theoretical Physics) **and Alexander Tchekhovskoy** (UC Berkeley), *High accuracy relativistic magnetohydrodynamics with OpenACC and MPI.*
- P19. Alexander Chernyshev and Alexander Schmidt** (Ioffe Institute), *Impact of gas diffusion on bubbly flow pattern.*
- P20. Sergei Mariin** (ITMO University), *Preselecting resources to improve scientific workflows scheduling efficiency in cloud environments.*
- P21. Liliia Ziganurova** (Higher School of Economics) **and Lev Shchur** (Science Center in Chernogolovka), *Virtual Time Profile Modeling in Parallel Discrete Event Simulation.*
- P22. Dmitry Glyzin, Vyacheslav Golubenets and Daniil Frolov** (P.G. Demidov Yaroslavl State University), *Software Toolkit for Interactive Simulations of Reaction-Diffusion Problems on HPC Clusters.*
- P23. Maria Guskova** (National Research University Higher School of Economics), **Lev Shchur and Lev Barash** (Science Center in Chernogolovka), *RNGAVXLIB: Program library for random number generation, AVX realization.*
- P24. Boris Korneev** (Moscow Institute of Physics and Technology) **and Vadim Levchenko** (Keldysh Institute of Applied Mathematics). *Detailed numerical simulation of shock-body interaction in 3D multicomponent flow.*
- P25. Dmitry Zendrikov** (Moscow Institute of Physics and Technology) **and Alexander Paraskevov** (National Research Centre "Kurchatov Institute"). *Autowaves of spiking activity synchronization in a model neuronal network with relaxational synaptic plasticity.*
- P26. Tatiana Savelieva, Sergey Model and Victor Loschenov** (GPI RAS), *Numerical modelling of light transport in human ocular fundus for photodynamic therapy planning.*

Social Program

09 September 2015, 16.30 -18.40

Address of directorate

Krymsky Val Ulitsa, 9, Moscow, 119049

Nearest Metro stations

- Park Kul'tury (circle line)
- Oktyabr'skaya
- Leninsky Prospekt
- Vorob'evy Gory



The central entrance can be accessed via the 'Garden Ring' road (*Sadovoye Koltso*). Entrances can also be accessed via Leninsky Avenue (*Leninsky Prospekt*), and via Neskuchny Garden and Vorob'evy Gory.

