

# International Conference

## "Computer Simulation in Physics and beyond"

October 9-12, 2017, 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 where senior scientists and students may have opportunity to speak each other and exchange ideas and views on the developments in the area of high-performance computing in most sciences.

Program of the conference is concentrated on the analysis and discussion of research and activity in supercomputer simulations that generally lie on the boundary of scientific branches, i.e. which are multidisciplinary research.

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

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

### KEYNOTE SPEAKERS:

**Gregory Goltsman**, HSE Tikhonov Moscow Institute of Electronics and Mathematics, Russia - *"Superconducting Nanowire Single-Photon Detector as a Key Element for Quantum Photonic Integrated Circuits"*

**Wolfhard Janke**, Universitat Leipzig, Germany - *"From Particle Condensation to Polymer Aggregation"*

**Erik Luijten**, Northwestern University, USA - *"Dynamic Computation of Dielectric Effects in Self-Assembly and Active Matter"*

**Jonathan Machta**, University of Massachusetts, USA

**Eugene Tyrtyshnikov**, Institute of Numerical Mathematics, Russia - *"Advances in Theory and Practice of Tensor Decompositions Using Low Rank Matrices"*

**Oleg V. Vasilyev**, Scoltech, Russia - *"Hierarchical Numerical Simulation of Turbulence"*

**Martin Weigel**, Coventry University, United Kingdom - *"Monte Carlo methods for massively parallel architectures"*

**Riccardo Zecchina**, Bocconi University, Italy - *"The out-of-equilibrium landscape of neural networks learning algorithms: from driven stochastic processes to quantum annealing"*

**Ruiqin Zhang**, City University of Hong Kong, Hong Kong - *"Electron tunneling lifetime in atomic systems, a projected Green's function method"*

### TOPICS:

- Simulations in Statistical Physics
- Physics and mechanics of polymers
- Space research: simulations and big data
- Methods and software for simulations in research and engineering (hydrodynamics, aerodynamics, etc.)
- Simulation of brain activity
- Bioinformatics, methods and algorithms in genome research
- Methods and algorithms in drug development
- Simulations in material science
- Simulation and analysis of social networks
- Simulation and analysis of technical networks (roads, urban transportation, data networks, etc.)
- Algorithms, methods, and tools with properties of scalability and enhanced parallel simulations
- Informatics and education

### VENUE:

Tallinskay ul. 34, Moscow

### WEBSITE:

<http://csp2017.ac.ru/>

### PROGRAM COMMITTEE:

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CONFERENCE CHAIR: Lev Shchur



# International Conference on Computer Simulation in Physics and beyond

**October 9-12, 2017, Moscow, Russia**

## Conference Time Table

<b>Time</b>	<b>Monday October, 9</b>	<b>Tuesday October, 10</b>	<b>Wednesday October, 11</b>	<b>Thursday October, 12</b>
<b>08.30</b>	<b>Registration</b>	<b>Registration</b>	<b>Registration</b>	
<b>09.00- 09.15</b>	<b>Registration</b>	<b>Plenary Talk 4</b>	<b>Plenary Talk 8</b>	<b>Plenary Talk 12</b>
<b>09.15- 09.45</b>	<b>Opening</b>			
<b>09.45- 10.30</b>	<b>Plenary Talk 1</b>	<b>Plenary Talk 5</b>	<b>Plenary Talk 9</b>	<b>Plenary Talk 13</b>
<b>10.30- 11.00</b>	Coffee	Coffee	Coffee	Coffee
<b>11.00- 11.45</b>	<b>Plenary Talk 2</b>	<b>Plenary Talk 6</b>	<b>Plenary Talk 10</b>	<b>Closing</b>
<b>11.45- 12.30</b>	<b>Plenary Talk 3</b>	<b>Plenary Talk 7</b>	<b>Plenary Talk 11</b>	
<b>12.30- 13.50</b>	Lunch	Lunch	Lunch	End of program
<b>13.50- 16.00</b>	<u>Parallel Session S9-1</u>	<u>Parallel Session S10-1</u>	<u>Parallel Session S11-1</u>	
	<u>Parallel Session S9-2</u>	<u>Parallel Session S10-2</u>	<u>Parallel Session S11-2</u>	
	<u>Parallel Session S9-3</u>	<u>Parallel Session S10-3</u>	<u>Parallel Session S11-3</u>	
<b>16.00- 16.30</b>	Coffee	Coffee	Coffee	
<b>16.30- 18.40</b>	<u>Parallel Session S9-4</u>	Social Session	Poster Program	
	<u>Parallel Session S9-5</u>			
	<u>Parallel Session S9-6</u>			
<b>18.40</b>	End of program	End of program	End of program	

## List of Plenary Talks

**Plenary Talk 1.** October 09, 09.45-10.30, **Wolfhard Janke**, *From Particle Condensation to Polymer Aggregation*

**Plenary Talk 2.** October 09, 11.00-11.45, **Lev Barash**, *Transport in drying sessile droplets*

**Plenary Talk 3.** October 09, 11.45-12.30, **Erik Luijten**, *Dynamic Computation of Dielectric Effects in Self-Assembly and Active Matter*

**Plenary Talk 4.** October 10, 09.00-09.45, **Oleg Druzhinin**, *The study of the effects of sea-spray drops on the marine atmospheric boundary layer by direct numerical simulation*

**Plenary Talk 5.** October 10, 09.45-10.30, **Eugene Tyrtyshnikov**, *Advances in Theory and Practice of Tensor Decompositions Using Low Rank Matrices*

**Plenary Talk 6.** October 10, 11.00-11.45, **Martin Weigel**, *Monte Carlo methods for massively parallel architectures*

**Plenary Talk 7.** October 10, 11.45-12.30, **Oleg Vasilyev**, *Hierarchical Numerical Simulation of Turbulence*

**Plenary Talk 8.** October 11, 09.00-09.45, **Riccardo Zecchina**, *The out-of-equilibrium landscape of neural networks learning algorithms: from driven stochastic processes to quantum annealing*

**Plenary Talk 9.** October 11, 09.45-10.30, **Nail Inogamov**, *Simulation of the diffraction limited gaussian and vortex illuminations of supported metallic films*

**Plenary Talk 10.** October 11, 11.00-11.45, **Ruiqin Zhang**, *Electron tunneling lifetime in atomic systems, a projected Green's function method*

**Plenary Talk 11.** October 11, 11.45-12.30, **Gregory Goltsman**, *Superconducting Nanowire Single-Photon Detector as a Key Element for Quantum Photonic Integrated Circuits*

**Plenary Talk 12.** October 12, 09.00-09.45, **Sergey Moiseenko**, *Operator-difference method for astrophysical MHD problems*

**Plenary Talk 13.** October 12, 09.45-10.30, **Eugeniy Burovski**, *Phase transitions in evolutionary space games*

## Schedule for Parallel Sessions

### Parallel Session S9-1

October 09, 13:50-16.00, Room N 403

*Chair: A. Belov*

Time	Name	Title
13.50-14.20	Sergey Glyzin	Relaxation Oscillations of the Repressilator Model
14.20-14.45	Anatoly Manita	Distributed time synchronization algorithms and opinion dynamic
14.45-15.10	Aleksandr Belov	Method for detecting data synchronization errors in distributed information systems
15.10-15.35	Sergey Aleshin	Computational aspects of the wave distribution problem in the logistic equation with spatial deviation
15.35-16.00	Suemi Rodriguez Romo	Electromagnetic simulation of thread Peano antennas created by Context-free Grammar language

### Parallel Session S9-2

October 09, 13:50-16.00, Room N 404

*Chair:*

Time	Name	Title
13.50-14.20	Dmitry Petrov	Application of grid-characteristic method to some seismic exploration problems in the arctic
14.20-14.45	Sergei Starikov	Multiscale simulation of point defects behavior in nuclear fuels: uranium dioxide and uranium nitride
14.45-15.10	Mariia Korneva	The investigation of the recrystallization process in the Zr-Nb alloys using atomistic simulations
15.10-15.35	Andrey Kalinichev	Computational Molecular Modeling of Aqueous Interfaces for Environmental and Materials Science Applications
15.35-16.00	Mikhail Posypkin	Numerical Simulation of 2D-crystals Structures with Optimization Methods

### Parallel Session S9-3

October 09, 13:50-16.00, Room N 405

Chair: *A. Menshutin*

Time	Name	Title
13.50-14.20	Arkady Satanin	Stabilization of driven quantum systems moving under the influence of dissipation and noise
14.20-14.45		
14.45-15.10		
15.10-15.35	Anton Menshutin	Efficient algorithm for DLA problem in multiple dimensions
15.35-16.00	Suman Majumder	Universal Scaling Laws for Clusters Growth and Aging During Collapse of a Polymer

### Parallel Session S9-4

October 09, 16:30-18.40, Room N 403

Chair: *L. Barash*

Time	Name	Title
16.30-17.00	Lev Barash	Population annealing algorithm, its GPU implementation and its analysis
17.00-17.25	Minh Duc Nguyen	A framework to monitor activities of satellite data processing in real-time
17.25-17.50	Evgenii Tsymbalov	Compact high-order difference approximations for rod lateral vibrations equation
17.50-18.15		
18.15-18.40		

## Parallel Session S9-5

October 09, 16:30-18.40, Room N 404

Chair:

Time	Name	Title
16.30-17.00	Iliia Kuznetsov	Investigation of lunar dusty exosphere with future Russian lunar missions: Simulation Approach and Measurements Control
17.00-17.25	Olga Krivonosova	Nonlinear Interaction of Waves in Rotating Spherical Layers
17.25-17.50	Vladimir Vinnikov	Numerical Simulation for Meteoroid Dark Flight
17.50-18.15	Leonid Zotov	Analysis of the Chandler wobble of the Earth
18.15-18.40	Dmitriy Zhilenko	The Different Types of Turbulence in Rotating Spherical Layers
18.40-19.05	Elena Zhukova	Acceleration and Particle Transport in Collisionless Plasma in the Process of Dipolarization and Nonstationary Turbulence

## Parallel Session S9-6

October 09, 16:30-18.40, Room N 405

Chair: *L. Manita*

Time	Name	Title
16.30-17.00		
17.00-17.25	Pavel Dyshlovenko	Modelling of charge stabilized colloidal crystals
17.25-17.50	Aleksandr Zlotnik	Numerical methods with discrete transparent boundary conditions for solving the time-dependent Schrodinger equation in unbounded domains
17.50-18.15	Alexander Shemendyuk	Boundary Conditions that Imitate Cauchy Problem for Finite-Difference Approximations of Basic Mathematical Physics Equations
18.15-18.40	Mariya Ronzhina, Larisa Manita	Singular solutions for vibration control problems

## Parallel Session S10-1

October 10, 13:50-16.00, Room N 403

Chair: *S. Slastnikov*

Time	Name	Title
13.50-14.20	Farid Ablayev	Quantum Hash Functions Realization in the model of Quantum Branching Programs
14.20-14.45	Andrej Vnukov	The development of efficient algorithms for multi-threaded parallel. Processing in the module scaling digital images
14.45-15.10	Stanislav Polyakov	Heavily parallelized codes for the energy minimization and Monte Carlo simulation of polymer knots
15.10-15.35	Sergey Slastnikov	Applying swarm intelligence algorithms for NP-hard problems
15.35-16.00	Liliya Ziganurova	The analysis of conservative and optimistic parallel discrete event simulation algorithms on small-world networks

## Parallel Session S10-2

October 10, 13:50-16.00, Room N 404

Chair: *Yu. Lozovik*

Time	Name	Title
13.50-14.20	Sergey Belousov	A subcell technique for numerical analysis of optical properties of 2D metamaterials with the finite-difference time -domain method
14.20-14.45	Tokuei Sako	Electron wave packet dynamics for spin dependent tunneling current induced in one-dimensional nanostructure
14.45-15.10	Dariya Smirnova	Development of atomistic description for Zr-Nb
15.10-15.35	Xian-hu Zha	Theoretical investigations on the physical properties and fabrication mechanisms of Mxenes
15.35-16.00	Carlos Vega de las Heras	On the time required to freeze water

## Parallel Session S10-3

October 10, 13:50-16.00, Room N 405

Chair:

Time	Name	Title
13.50-14.20		
14.20-14.45	Aleksandr Kazakov	Grid-characteristic method on unstructured meshes: problems and applications
14.45-15.10	Roman Karpichev	Effective Path Planning via Diffusion of Kill/Death Ratio on Tactical Path Finding Graph based on Voronoi Navigational Mesh
15.10-15.35	Nikolay Khokhlov	Numerical simulation of the dome of an atomic reactor destruction due to the earthquakes
15.35-16.00	Alexander Bogdanov	On porting of applications to new heterogeneous systems

## Parallel Session S11-1

October 11, 13:50-16.00, Room N 403

Chair: *Yu. Tarasevich*

Time	Name	Title
13.50-14.20	Alexander Vulfson	An integral model of the convective jet including the pressure effect and the forms of the vertical fluxes in the turbulent surface layer of the atmosphere
14.20-14.45	Vladimir Aristov	Nonclassical nonequilibrium transport on the basis of numerical solving the boltzmann kinetic equation
14.45-15.10		
15.10-15.35	Eugeni Soroko	How the methods of natural sciences can help in the studies of ethnically mixed families?
15.35-16.00	Yuri Tarasevich	2D composites with rod-like fillers: Computer simulation of electrical conductivities



## Parallel Session S11-2

October 11, 13:50-16.00, Room N 404

Chair: A. Favorskaya

Time	Name	Title
13.50-14.20	Giuliano Orso	Anderson transitions of matter waves in laser speckle potentials
14.20-14.45	Andrey Tolstykh	Multioperators strategy for constructing arbitrary high-order approximations and schemes for PDE's with applications to fluid dynamics
14.45-15.10	Alena Favorskaya	Elastic migration based on the Born approximation
15.10-15.35	Kamal Kumar Choudhary	Enhancement in specific heat by nano-crystallization: softening of phonon frequencies mechanism
15.35-16.00	Victor Chetverikov	Properties of the Tent map for decimal fractions with fixed precision

## Parallel Session S11-3

October 11, 13:50-16.00, Room N 405

Chair: A. Teslyuk

Time	Name	Title
13.50-14.20	Sergey Bozhko	DFT simulations of Sb(111) surface states
14.20-14.45	Anton Teslyuk	New approach for structure reconstruction with machine learning methods in XFEL and Cryo-EM experiments
14.45-15.10	Vasily Tseplyaev	Evaluation of dislocation mobility and plastic properties of molybdenum using molecular dynamics
15.10-15.35	Alexey Chernov	Optimal vaccine allocation in two SIR centers with migration fluxes
15.35-16.00		

## **Schedule for Poster Session**

**October 11, 16:30-18.40, Hall, 4<sup>th</sup> floor**

- P1. Atamas N. (National Taras Shevchenko University of Kyiv),** *Diffusion mechanisms in systems ionic liquid - aromatic hydrocarbons by molecular dynamics simulation.*
- P2. Batanova A. (Ulyanovsk State Technical University),** *Modeling of charge-stabilized colloidal crystals with bcc crystal lattice.*
- P3. Blinov A. (NRU HSE),** *Simulation System for Making Political and Macroeconomical Decisions and Its Development.*
- P4. Bogolubsky I. (JINR),** *Lattice study of effective gluon mass at various boundary conditions.*
- P5. Bondarev A. (Voronezh State Technical University),** *Monte Carlo Simulation of Random-Anisotropy Amorphous Magnets.*
- P6. Burtyka F. (Southern Federal University),** *Algorithms for solvents of unilateral matrix polynomials over prime finite fields.*
- P7. Chau S.W. (National Taiwan University),** *Modeling of Fiber Orientation in a Twin-Screw Extrusion Process.*
- P8. Dosaev A. (Institute of Applied Physics of the Russian Academy of Sciences),** *Numerical simulation of solitary waves on deep water with constant vorticity.*
- P9. Fadeeva M. (NRU HSE, Science Center in Chernogolovka),** *Analytical structure of transition matrix in Wang-Landau algorithm.*
- P10. Gladskikh D. (NNSTU n.a. R.E.Alekseev, IAP RAS),** *Numerical modeling of thermal regime in inland water bodies with field measurement data.*
- P11. Glyzin D. (Yaroslavl State University; Science Center in Chernogolovka),** *Toolkit for Interactive Simulations of Distributed Delay Differential Problems on HPC Clusters.*
- P12. Goryunov V. (Yaroslavl State University; Science Center in Chernogolovka),** *Invariant numerical characteristics of diffusion chaos in the problem of Belousov reaction simulating.*
- P13. Guskova M. (NRU HSE, Science Center in Chernogolovka),** *Modern random number generators using AVX512 instruction set.*
- P14. Ivanovsky L. (Yaroslavl State University; Science Center in Chernogolovka),** *Bifurcation of spatially nonuniform regimes in one boundary- value problem with deflection.*
- P15. Kashina M. (Perm State University),** *The oscillations of oblate drop between heterogeneous plates under uniform electric field.*
- P16. Kaurav N. (Government Holkar Science College, India),** *Exponential Heat Capacity in Natural Nickel Nanolattice: A Quantum Size Effect.*
- P17. Khomutov E. (NRU HSE, Science Center in Chernogolovka),** *Analysis of the optimistic algorithm in the method of parallel simulation of discrete events.*
- P18. Klimenkova O. (NRU HSE, Science Center in Chernogolovka),** *Sensitivity of the hitting probability to the finite size of the random walk.*
- P19. Klimin S. (Institute of Spectroscopy RAS),** *Ab initio simulation of phonon and electronic properties of BaGa<sub>2</sub>GeS<sub>6</sub> crystal with disordering in Ga-Ge sublattice.*
- P20. Klimin S. (Institute of Spectroscopy RAS),** *Ab initio study of vibrational spectra of multiferroic CuCrO<sub>2</sub>.*
- P21. Kolotev S. (NRU HSE, Science Center in Chernogolovka),** *Algorithms for research critical parameters of Prisoner's Dilemma.*
- P22. Kosyanchuk V. (Lomonosov Moscow State University),** *Hybrid method for*

*modeling slow gas mixture flows in devices with micro- and macro- space scales.*

**P23. Kuznetsova A. (NRU HSE),** *Regional model based on adapted WAVEWATCH III and WRF models for the prediction of surface wind waves on the reservoir and wind.*

**P24. Malutin A. (NRU HSE, Science Center in Chernogolovka),** *Dynamics of Spatial Evolutionary Game.*

**P25. Nagatkin A. (Ulyanovsk State Technical University),** *Modeling of monolayer charge-stabilized colloidal crystals.*

**P26. Okulich E. (Lobachevsky University),** *Molecular-dynamic simulation of atomic process under filament formation in memristive structure based on silicon oxide.*

**P27. Orlova E. (NRU HSE),** *Generative Adversarial Networks in particle physics simulations.*

**P28. Parshakova Y. (Institute of Continuous Media Mechanics UB RAS),** *Computer modeling of technogenic thermal pollution zones in large water objects.*

**P29. Preobrazhenskaia M. (Yaroslavl State University; Science Center in Chernogolovka),** *Asymptotics of  $N$ -dimensional tori in the generalized Korteweg - de Vries equation.*

**P30. Ryazanova A. (Technological Institute for Superhard and Novel Carbon Materials, Moscow Institute of Physics and Technology),** *Simulation of hydrogen and oxygen atoms interaction with the point defects on the hydrogenated diamond surface.*

**P31. Sirotin D. (Yaroslavl State University; Science Center in Chernogolovka),** *Buckling beam driven oscillations.*

**P32. Soustova I. (Institute of Applied Physics, Russian Academy of Sciences),** *The model of turbulent transfer and dynamics of small-scale turbulence in the stratified fluid.*

**P33. Stepovich M. (Tsiolkovsky Kaluga State University, Ivanovo State University),** *On one peculiarity of the model describing the interaction of the electron beam with the semiconductor surface.*

**P34. Stepovich M. (Tsiolkovsky Kaluga State University, Ivanovo State University),** *On the possibility of using the galerkin projection method to simulate the two-dimensional diffusion of excitons generated by an electron beam in a semiconductor material.*

**P35. Tan Ch.L (National Taiwan University),** *Modeling of Fiber Orientation in a Twin-Screw Extrusion Process.*

**P36. Tarasevich Yu. (Astrakhan State University),** *Identification of current carrying part of a random resistor network: electrical approaches vs graph theory algorithms.*

**P37. Tarasevich Yu. (Astrakhan State University),** *Science and ethics meet: a mathematical view on one kind of violation of publication ethics.*

**P38. Terentyev A. (Kazan Federal University)** *Modeling and simulation of a programmable quantum processing device*

**P39. Trubochkina N. (NRU HSE),** *Fractal tomography and its application in 3d vision.*

**P40. Trubochkina N. (NRU HSE),** *Transitional circuitry for studying the properties of DNA.*

**P41. Tokareva S. (University of Zurich),** *Staggered grid residual distribution scheme for Lagrangian hydrodynamics.*

**P42. Tsymbalov E. (Skolkovo Institute of Science and Technology),** *Surrogate modelling of Si and Ge electronic properties under elastic strain.*

**P43. Vasiliyev A. (Kazan Federal University),** *Quantum Hashing and Small-biased Sets.*

## Social Program

10 October 2017, 16.30 -18.40

**Information at the conference desk**



ФЕДЕРАЛЬНОЕ АГЕНТСТВО  
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