

CCP2013 Moscow

XXV IUPAP Conference on Computational Physics

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					
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 I	Parallel Sessions III	Parallel Sessions IV	
16.00- 16.30		Coffee	Coffee	Coffee	
16.30- 18.40	Registration & Welcome 17.30-21.00	Parallel Sessions II	Poster Session I	Poster Session II	
18.40		End of program	End of program	End of program	

List of Plenary Talks

Plenary Talk 1. August 21, 09.45–10.30, Dezso Horvath, *Search for the Higgs Boson: a Numerical Adventure of Exclusion and Discovery*

Plenary Talk 2. August 21, 11.00–11.45, Kurt Binder, *Simulations of Interfacial Phenomena in Soft Condensed Matter and Nanoscience*

Plenary Talk 3. August 21, 11.45–12.30, Vladimir E. Zakharov, *Numerical Modeling of Ocean Waves*

Plenary Talk 4. August 22, 09.00–09.45, Ali Alavi, *Quantum Monte Carlo approach to the ground state eigenvalue problem of many-electron systems*

Plenary Talk 5. August 22, 09.45–10.30, Ian T. Foster, *Preparing for the Computer Revolution*

Plenary Talk 6. August 22, 11.00–11.45, Wolfgang Paul, *Monte Carlo Simulations of Semi-flexible Polymers: From Single Chains to Nematic Melts*

Plenary Talk 7. August 22, 11.45–12.30, Isaak M. Khalatnikov, *Numerical Methods for Partial Differential Equations and Early Days of Computational Physics*

Plenary Talk 8. August 23, 09.00–09.45, Tomo-Hiko Watanabe, *Exploring phase space turbulence in magnetic fusion plasmas*

Plenary Talk 9. August 23, 09.45–10.30, Carlo Pierleoni, *First-principle calculations of high pressure hydrogen*

Plenary Talk 10. August 24, 09.00–09.45, Morten Hjorth-Jensen, *Living at the edge of stability, understanding the limits of the nuclear landscape: Computational and algorithmic challenges*

Plenary Talk 11. August 24, 09.45–10.30, Natalia Artemieva, *Airbursts – from Tunguska to Chelyabinsk*

Plenary Talk 12. August 24, 11.00–11.45, Stefan Gottloeber, *Formation of structure in the Universe*

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

SESSIONS II, August 21, 16:30–18:40

D.1 Molecular Dynamics	Red Hall
B.1 Differential Equations and Chaos	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, <i>Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage</i> (Invited Speaker)
A.1.2	14:20–14:45	Alexander Lyubartsev, <i>Systematic coarse-graining of molecular models by the Inverse Monte Carlo: Theory, practice and software</i>
A.1.3	14:45–15:10	Johannes Zierenberg, <i>Application of the parallel multicanonical method to lattice gas condensation</i>
A.1.4	15:10–15:35	Elmar Bittner, <i>Parallel-tempering cluster algorithm</i>
A.1.5	15:35–16:00	Ivanov Viktor Aleksandrovich, <i>Intramolecular structures in a single copolymer chain consisting of flexible and semiflexible blocks: Monte Carlo simulation of a lattice model</i>

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

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

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

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

A.3.5	15:30– 15:55	Khisamutdinov Alfred, <i>Imitation Monte Carlo methods for Boltzmann equation problems, parallelization of the algorithms with splitting</i>
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B.1. Differential equations and Chaos. August 21, Beige hall, 16:30–18:40.

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

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

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

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

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

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

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

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

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

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

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

3.1.1	13:50–14:10	Luca Baiotti, <i>Fully general-relativistic simulations of binary neutron-star mergers</i> (Invited Speaker)
3.1.2	14:10–14:35	Cristina Torres, <i>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</i>
3.1.3	14:35–15:00	Khoperskov Sergey, <i>Evolution of multi-component spiral disc galaxies: dynamics of gas, stars and dark matter</i>

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

4.1.1	15:20–15:40	Joan Adler, <i>I want to simulate problem X</i>
4.1.2	15:40–16:00	Salagaram Trisha, <i>Simplified pseudopotential problems for the classroom</i>

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

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, <i>Quantum time correlation functions via noisy Monte Carlo and classical trajectories</i> (Invited Speaker)
5.2.2	14:20–14:45	Fedorova Anotonina N., <i>Quantum Modeling: from Coarse Graining to a Tower of Scales</i>
5.2.3	14:45–15:10	Ryabushkin O.A., <i>Concept of equivalent temperature of the nonlinear-optical crystal interacting with nonuniform laser radiation</i>
5.2.4	15:10–15:35	Konyashkin A.V., <i>Novel method for identification of intrinsic vibration modes in piezoelectric crystals</i>
5.2.5	15:35–16:00	Baranov A.I., <i>The equivalent temperature model in process of nonlinear conversion of laser radiation</i>

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

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

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

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

6.2.1	13:50–14:15	Petrosyan Arakel, <i>Large eddy simulations of compressible magnetohydrodynamic turbulence in space plasma. Model developments and validations</i>
6.2.2	14:15–14:40	Shevelev Mark, <i>Numerical simulations of the Kelvin-Helmholtz instability development in a bounded supersonic plasma flow</i>
6.2.3	14:40–15:05	Morozov Igor Vladimirovich, <i>The method of Wave Packet Molecular Dynamics for warm dense matter and nonideal plasma simulations</i>
6.2.4	15:05–15:30	Viacheslav Belyi, <i>Model kinetic description for many-component plasma</i>

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

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

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 carbide*
- 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 in an 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 of spin 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. Russkov Alexander, *Analysis of cloud computing application in scientific centre*
- P1.23. Shul'man A. Ya., *Self-consistent mean-field approximation in the density functional theory of many-electron unbounded systems*
- P1.24. Vali Rashid, *Effects of the in-plane magnetization on the conductance properties of the topological insulator ferromagnet/insulator/superconductor junctions*
- 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 Gennagyeвна, *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 initio calculations*
- 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*

