

School Workshop  
«Supercomputers in scientific studies: horizons of atomistic modeling and effective  
supercomputer co-design»

Program of lectures and reports

JULY 26, WEDNESDAY

9-45 - School-workshop opening

10-00 - Alexander Semenov (JSC NICEVT)

Co-design of supercomputer applications, system software and architecture for high-speed interconnect Angara

10-30 - Maxim Gorshenin (JSC MCST)

Current status and development of the Elbrus computing platform

11-00 - Alexander Murashov (JSC T-Platforms)

Domestic hardware products for HPC market, their tuning and examples of deployment

11-30 - Vyacheslav Vecher (JIHT RAS)

Optimizing energy consumption in classical and quantum molecular dynamics calculations

11-50 - Vsevolod Nikolskii (HSE)

CPUs with ARM architecture for high performance computing

12-10 - Mikhail Khalilov (HSE)

Topology-aware placement of MPI processes for clusters with Angara communication network

12-30 - LUNCH

13-30 - Vladimir Stegailov (JIHT RAS/HSE)

Angara-based hybrid supercomputer for efficient acceleration of computational materials science studies

14-00 - Alexey Yanilkin (VNIIA)

Quantum mechanical calculations in computational materials science

14-30 - Pavel Levashov (JIHT RAS)

High-performance simulation of ultra-short laser pulses action on matter achievements and problems

15-00 - Alexey Rykounov (RFNC-VNIITF)

An equation of state for  $\text{CaCO}_3$  at high pressures and temperatures

15-30 - Mikhail Medvedev (INEOS RAS)

Supercomputer-rescued quantum chemical modeling

JULY 27, THURSDAY

10-00 - Roman Efremov (IBCh RAS/HSE)

Structural/functional adaptation of proteins to membrane environment

10-30 - Anton Polyansky (IBCh RAS)

Estimation of conformational entropy of biopolymers from molecular dynamics simulations

11-00 - Alexander Chertovich (MSU)

Statistical physics of polymers

11-30 - Kirill Smirnov (HSE)

Interactions of transmembrane peptides with lipid environment as probed by molecular dynamics simulations

11-50 - Mikhail Logunov (MIPT)

Nanocavitation during deformation of polyethylene with/without carbon nanotubes

12-10 - Ekaterina Dlinnova (HSE)

Statistical analysis of finite-difference scheme errors in molecular dynamics method

12-30 - LUNCH

13-30 - Maria Egorova (VNIIA)

Voronoi dynamic domain decomposition for load-balanced parallel simulations of materials in extremes with particle methods

14-00 - Ilnur Saitov (HSE)

Fluid-fluid phase transition in warm dense matter

14-30 - Alexey Karavaev (RFNC-VNIITF)

MD study of self-irradiation effects on dislocation dynamics in  $\delta$ -Pu

15-00 - Grigory Smirnov (JIHT RAS/HSE)

Pseudopotentials for first-principles calculations of uranium compounds

15-30 - School-workshop closing