

*Lomonosov Moscow State University,  
Faculty of Computational Mathematics and Cybernetics,  
Scientific Research Computing Center,  
Scientific Educational Center “Supercomputing Technologies”*

Interdisciplinary workshop

“HPC & Life Science”

*December 10, 2012,  
2-nd educational building, room 238*

Agenda

13.00 -13.30

**Ruhong Zhou**, *IBM Thomas Watson Research Center, Research Staff Scientist & Manager, Soft Matter Theory and Simulation, IBM Thomas Watson Research Center, Adjunct Professor, Department of Chemistry, Columbia University, New York*  
**Large Scale Biomolecular Modeling with IBM Blue Gene**

13.30 – 14.00

**Alessandro Curioni**, *IBM Zurich Research Lab, Department Manager, Mathematical & Computational Sciences, IBM Research Division*  
**Simulations for Life Science and Healthcare in the Blue Gene Era**

14.00-14.20

**R. Efremov**, *M.M. Shemyakin & Yu.A. Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences*  
**Recognition specificity of proteins and biomembranes: a computational view**

14.20 – 14.40

**D. Cherepanov**, *A.N. Frumkin Institute of Physical chemistry and Electrochemistry, Russian Academy of Science*

**Pharmacological properties of ionic mitochondrial antioxidants studied by molecular dynamics via supercomputer simulations**

14.40 – 15.00

**A. Nemukhin**, *Department of Chemistry, M.V. Lomonosov Moscow State University, and N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences*

**Development and Application of Quantum Mechanical – Molecular Mechanical (QM/MM) Methods: Enzymatic Catalysis and Fluorescent Proteins**

15.00 – 15.30 Break

15.30-15.50

**V. Sulimov**, *Scientific Research Computing Center, M.V. Lomonosov Moscow State University*

**Application of computer-aided molecular modeling for new drugs design**

15.50 -16.10

**A. Favorskiy, S.Mukhin, N.Sosnin, M.Abakumov, A.Bunicheva**, *Computational Mathematics and Cybernetics Faculty, M.V. Lomonosov Moscow State University*

**Mathematical modeling of blood circulation in the spatial graph of vessels**

16.10 -16.30

**A. Pankratov**, *Computational Mathematics and Cybernetics Faculty, M.V. Lomonosov Moscow State University*

**High-performance computing solutions for the problem of recognition of repeats in genomes**

16.30 - 16.50

**Y. Kiselev, M. Orlov**, *Computational Mathematics and Cybernetics Faculty, M.V. Lomonosov Moscow State University*

**Analytical and Numerical Investigation of Optimal Control Problems in Microbiology**

16.50 – 17.30 - **Discussions**

17.30 – 18.00 - **Tea, coffee**