POLYACHENKO **Yury**

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Education

Moscow Institute of Physics and Technology (National Research University) (MIPT) *Moscow, Russia*

B.S. IN APPLIED PHYSICS AND MATHEMATICS, SPECIALIZATION IN COMPUTATIONAL PHYSICS *Sep. 2017 - Present*

- **SPECIALIZATION:** Comp. condensed matter physics, Molecular dynamics, Practice of HPC, Soft-matter physics, Machine learning in condensed matter physics, Comp. solid-state physics, Comp. statistical mechanics, DFT (ongoing), Simulation of biomolecules (ongoing)
- **MATHEMATICS:** Real analysis and Calculus, Differential geometry, Harmonic analysis, Complex Analysis, Analytic geometry, Linear algebra, Differential Equations, Computational Mathematics, LPDE, Probability theory (ongoing)
- **PHYSICS:** General Physics (Mechanics, Thermodynamics and Molecular Physics, Electricity and Magnetism, Physical Optics), Theoretical Mechanics, Field Theory, Quantum Mechanics, Solid State Physics, Statistical physics (ongoing).
- **COMPUTER SCIENCE:** C/C++, UNIX-based systems and multithreading, Parallel computations via MPI and CUDA.
- **GPA 4.95/5 (9.11/10), top 3% of the class.**

Experience

MIPT, Laboratory of supercomputer methods in condensed matter physics *Moscow, Russia*

UNDERGRADUATE STUDENT *Sep. 2018 - Present*

- Reproduced an experiment of measuring the bulk modulus for the crystalline Lysozyme. 2020. Supervisor - Stegailov V.V.
- Investigated behavior of the **Lennard-Jones system** near the boiling points via space-time correlators. Delivered reports at **several conferences**. 2019. Supervisor - Norman G.E.. The project was supported by the Russian Science Foundation.
- Studied self-diffusion in Lennard-Jones systems using classical MD implemented in **LAMMPS**. Delivered a report on the obtained results at the MIPT conference. 2018. Supervisors - Timofeev A.V. and Norman G.E.
- Created from scratch an MD simulation engine (C/C++, CUDA, OpenMP, Python, Matlab). The package was used to test and improve Kinetic Molecular Theory equations. 2018.

École Polytechnique Fédérale de Lausanne (EPFL), Laboratory for Biomolecular Modeling ** Lausanne, Switzerland*

SUMMER RESEARCH PROGRAM INTERN, * REMOTE DUE TO COVID *Jul. - Aug. 2020*

- Suggested a method of defining an interface site for an unbound conformation using the MD trajectory of a bound complex.
- Benchmarked the MaSIF-site method on solvated protein conformations using the suggested method.

MIPT, Department of Computer Science *Moscow, Russia*

TEACHING ASSISTANT *Sep. - Dec. 2019*

- Worked as a mentor and as a teaching assistant on a Python CS freshmen course. Helped to design exercises for the course.

Innovative Oil & Gas Technologies (IOGT), *D. of methodological support for geophysical well logging* *Moscow, Russia*

PROGRAMMER *Feb. - May. 2019*

- Created 2 Matlab standalone GUI applications aimed at automatization and standardization of the process of interpretation of well-logging data.

MIPT, *Laboratory of Mechanical Systems and Processes Modeling* *Moscow, Russia*

INTERN *Aug. - Oct. 2018*

- Simulated elastic wave propagation using ray tracing (Matlab, C/C++, OpenMP).
- The project was used as a proof-of-concept model in the work «Development of methods of modeling processes in a human body upon application of intelligent systems of non-invasive surgery» supported by the Russian Science Foundation.

Conferences & Summer schools

63rd National Scientific MIPT Conference *Moscow, Russia*

POLYACHENKO Y. A., KONDRATYUK N. D., STEGAILOV V. V. «MOLECULAR-DYNAMICAL MODEL OF THE CRYSTALLINE LYSOZYME» // WORKS OF THE 63RD NATIONAL SCIENTIFIC MIPT CONFERENCE. FUNDAMENTAL AND APPLIED PHYSICS. 2020. *23–29 Nov. 2020*

Wolfram Summer School 2020 ** Boston, USA*

STUDENT, * REMOTE DUE TO COVID *Jun. 28 – Jul. 17 2020*

- Implemented solvent-excluded and solvent-accessible surfaces into wolfram language.
- Studied the interconnection between the Wolfram Language and the OS, the integration with the C language, creation of packages.

XXXV International Conference on Equations of State for Matter
Kabardino-Balkaria, Russia

POLYACHENKO Y. A., FLEITA D. IU., PISAREV V. V., NORMAN G. E. «EQUILIBRIUM – METASTABLE SINGULARITY IN THE LENNARD-JONES SYSTEM» // ABSTRACTS OF THE XXXV INTERNATIONAL CONFERENCE ON EQUATIONS OF STATE FOR MATTER. 2020. P. 247.
1–6 Mar. 2020

62nd National Scientific MIPT Conference, Specialization «Fundamental bases of multi-scale atomistic simulation and modeling»
Moscow, Russia

POLYACHENKO Y. A., FLEITA D. IU., PISAREV V. V., NORMAN G. E. «SINGULARITY AT THE POINT OF TRANSITION FROM EQUILIBRIUM TO METASTABLE STATES OF LENNARD-JONES VAPOR AND LIQUID» // WORKS OF THE 62ND NATIONAL SCIENTIFIC MIPT CONFERENCE. FUNDAMENTAL AND APPLIED PHYSICS. 2019. PP. 216-217.
18–23 Nov. 2019

16th Symposium FAMMS-2019 Foundations of Atomistic Multiscale Modeling and Simulation.
New Athos, Georgia

POLYACHENKO Y. A., FLEITA D. IU., PISAREV V. V., NORMAN G. E. «STUDY OF LENNARD-JONES SYSTEM NEAR THE BOILING POINT VIA SPACE-TIME CORRELATORS» // PROCEEDINGS OF 16TH RUSSIAN SYMPOSIUM FAMMS-2019 FOUNDATIONS OF ATOMISTIC MULTISCALE MODELING AND SIMULATION. P. 10.
15–26 Aug. 2019

Internship at the Russian national educational center Sirius in the scientific-technological projects program «Big Challenges»
Sochi, Russia

INTERN
30 Jun. – 26 Jul. 2019
- Helped senior-school students master Linux, Bash, Python, and LAMMPS
- Guided a group of senior school students in conducting research dedicated to studying collective motion in Lennard-Jones systems.

Summer School on Classical MD for Material Science, Nanotechnology and Biophysics, SISSA
Trieste, Italy

STUDENT
10–21 Jun. 2019
- Studied Dimension reduction, Umbrella sampling, Approaches to polymer and protein dynamics.

61st National Scientific MIPT Conference, Specialization «Fundamental bases of multi-scale atomistic simulation and modeling»
Moscow, Russia

POLYACHENKO Y.A., TIMOFEEV A.V. «DIFFUSION IN THE LENNARD-JONES SYSTEM». // WORKS OF THE 61ST NATIONAL SCIENTIFIC MIPT CONFERENCE. FUNDAMENTAL AND APPLIED PHYSICS. 2018. PP. 165-167.
19–25 Nov. 2018

Publications

1. V. Negodin, **Y. Polyachenko**, D. Fleita, V. Pisarev, G. Norman «Kinetic singularities at transition points from equilibrium to metastable states of the Lennard-Jones particle system», *J. of Molecular Liquids.* (Submitted)

Achievements

Jan.2019...	**Recipient**, Scholarship for excellence in studies	*MIPT*
Sep. 2020	**Certificate**, International Summer Supercomputing Academy (Python HPC track)	*MSU*
Feb. 2020	**Elected**, HZB summer student program (* canceled due to COVID)	** Berlin, Germany*
Feb. 2020	**Awardee**, National Physics Olympiad for Undergraduates «I am a professional»	*Moscow, Russia*
Aug. 2019	**Co-author**, Program «β-GeoGaz» registered in the Russian Federal Service for Intellectual Property	*Russia*
Aug. 2019	**Co-author**, Program «α-GeoGaz» registered in the Russian Federal Service for Intellectual Property	*Russia*
Aug. 2019	**100% final grade**, Stanford «Machine Learning» course on Coursera	
May 2019	**Elected**, CECAM School «Introduction to Biomolecular Simulation with GROMOS»	*Vienna, Austria*
Jan. 2019	**Awardee**, National Physics Olympiad for Undergraduates «I am a professional»	*Moscow, Russia*
Jan. 2019	**Awardee**, National Mathematics Olympiad for Undergraduates «I am a professional»	*Moscow, Russia*
Nov. 2018	**2nd place**, 61st National Scientific MIPT Conference	*Moscow, Russia*
Jun. 2018	**Top 10 of the class ($\sim$ 1100 people)**, Scientific project competition at MIPT.	*MIPT*
Aug. 2017	**Recipient**, President scholarship (for 4 and possibly 6 years), for multiple school achievements.	*Russia*
Apr. 2017	**29th place**, Russian National Physics Olympiad for high school students.	*Kazan, Russia*

Skills

Experienced	Python, C/C++, Matlab, Linux
In particular	**C/C++:** OpenMP, POSIX threads, MPI, CUDA, OpenGL, VCL/Firemonkey **Python:** Jupyter, scipy, numpy, matplotlib, sklearn, mdtraj, numba, MPI **Other:** Git, LAMMPS, GROMACS, Wolfram Mathematica, LaTeX, Origin, slurm
Languages	English (Advanced, 105 TOEFL IBT), Russian (Native), French (Elementary)