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*. 2020. (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)