

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:** ML in Condensed Matter Physics, DFT, Simulation of Biomolecules, Practice of HPC, Comp. Condensed Matter Physics, Molecular Dynamics, Soft-Matter Physics, Comp. Solid-State Physics, Comp. Statistical Mechanics.
- **MATHEMATICS:** Computational Mathematics, LPDE, Probability Theory, etc.
- **PHYSICS:** Quantum Mechanics, Solid State Physics, Statistical Physics, ED of continuous media, etc.
- **COMPUTER SCIENCE:** Parallel Computations via MPI and CUDA, C/C++, UNIX-based Systems and Multithreading.
- GPA 4.95/5 (9.15/10), top 3% of the class.

Experience

MIPT, Laboratory of supercomputer methods in condensed matter physics

Moscow, Russia

UNDERGRADUATE STUDENT

Sep. 2018 - Present

- Mentored 4 undergraduates in their voluntary individual projects. 09.2020 – present
- Computationally reproduced an experiment of measuring the bulk modulus for the **crystalline Lysozyme**. Supervisor - Stegailov V.V. 2020.
- Investigated behavior of the **Lennard-Jones system** near the boiling points via space-time correlators. Delivered reports at **several conferences**. The project was supported by the Russian Science Foundation. Supervisor - Norman G.E.. 2019.
- Studied self-diffusion in Lennard-Jones system using classical MD implemented in **LAMMPS**. Delivered a report on the obtained results at the MIPT conference. Supervisors - Timofeev A.V. and Norman G.E. 2018.
- Created from scratch an MD simulation engine (C/C++, CUDA, OpenMP, Python, Matlab). The package was used to test and improve Kinetic Theory of Gases. 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

Sep. 2017 - Present

- I participate in developing and supporting a number of subroutines for interpreting well-logging data. Supervisor – Babkin I.V.

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 supported by the Russian Science Foundation. Supervisor – Beklemysheva K. A.

Conferences & Summer schools

XXXVI International Conference on Interaction of Intense Energy Fluxes with Matter

Kabardino-Balkaria,
Russia

POLYACHENKO Y. A., KONDRATYUK N. D., STEGAILOV V. V. «MOLECULAR-DYNAMICAL MODEL OF CRYSTALLINE LYSOZYME» // ABSTRACTS OF THE XXXVI INTERNATIONAL CONFERENCE ON INTERACTION OF INTENSE ENERGY FLUXES WITH MATTER. 2021.

1–6 Mar. 2021

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. PP. 498. (IN RUSSIAN)

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 in 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.

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.

18–23 Nov. 2019

FUNDAMENTAL AND APPLIED PHYSICS. 2019. PP. 216-217. (IN RUSSIAN)

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

15–26 Aug. 2019

MODELING AND SIMULATION. 2019. P. 10. (IN RUSSIAN)

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. (IN RUSSIAN)

19–25 Nov. 2018

Publications

2. 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*. doi:10.1016/j.molliq.2020.114954. 2020.
1. Co-author of programs « α -GeoGaz» and « β -GeoGaz» registered in the Russian Federal Service for Intellectual Property. 2019.

Achievements

Jan.2019 – –Jul.2021	Recipient , Scholarship for excellence in studies	MIPT, Russia
Jan. 2021	Ph.D. offers , Princeton, PME UChicago, NYU	
Sep. 2020	Certificate , International Summer Supercomputing Academy (Python HPC track)	MSU, Russia
Feb. 2020	Awardee , National Physics Olympiad for Undergraduates «I am a professional»	Moscow, Russia
Aug. 2019	100% final grade , Stanford «Machine Learning» course on Coursera	
May 2019	Accepted , CECAM School «Introduction to Biomolecular Simulation with GROMOS»	Vienna, Austria
Jan. 2019	Awardee , National undergraduates olympiads in physics and mathematics «I am a professional»	Moscow, Russia
Nov. 2018	2nd place , 61 st National Scientific MIPT Conference	Moscow, Russia
Jun. 2018	Top 10 of the class (~ 1100 people) , Scientific project competition at MIPT.	MIPT, Russia
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++: STL, OpenMP, POSIX threads, MPI, CUDA, OpenGL, VCL/Firemonkey Python: Jupyter, scipy, numpy, matplotlib, sklearn, mdtraj, numba, MPI Other: Git, slurm, LAMMPS, GROMACS, Chimera, Pymol, Wolfram Mathematica, \LaTeX , Origin
Languages	English (Advanced, 105 TOEFL IBT), Russian (Native), French (Elementary)