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: Machine learning in condensed matter physics DFT (ongoing), Simulation of biomolecules (ongoing)
 Comp. condensed matter physics, Molecular dynamics, Practice of HPC, Soft-matter physics, Comp. solid-state physics, Comp. statistical mechanics.
- MATHEMATICS: Computational Mathematics, LPDE, Probability theory (ongoing), etc.
- PHYSICS: Quantum Mechanics, Solid State Physics, Statistical physics (ongoing), etc.
- 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

- Mentored 4 first-year 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 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 Feb. - May. 2019

PROGRAMMER

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 Aug. - Oct. 2018

INTERN

- 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

POLYACHENKO YURY · CURRICULUM VITAE

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

30 Jun. – 26 Jul. 2019

INTERN

- · 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

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 & Patents _

- 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 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	* Berlin, Germany
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 Elected , CECAM School «Introduction to Biomolecular Simulation with GROMOS»	Vienna, Austria
Jan. 2019 Awardee , National Olympiads in Physics and Mathematics for Undergraduates «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 (\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	Pvthon.	C/C++.	Matlab.	Linux

C/C++: OpenMP, POSIX threads, MPI, CUDA, OpenGL, VCL/Firemonkey Python: Jupyter, scipy, numpy, matplotlib, sklearn, mdtraj, numba, MPI In particular

Other: Git, LAMMPS, GROMACS, Wolfram Mathematica, LATEX, Origin, slurm

Languages English (Advanced, 105 TOEFL IBT), Russian (Native), French (Elementary)