

# 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. 2 students delivered oral reports on obtained results. 09.2020 – ...
- 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

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

### 63<sup>rd</sup> National Scientific MIPT Conference

Moscow, Russia

POLYACHENKO Y. A., KONDRATYUK N. D., STEGAILOV V. V. «MOLECULAR-DYNAMICAL MODEL OF THE CRYSTALLINE LYSOZYME» // WORKS OF

23–29 Nov. 2020

THE 63<sup>RD</sup> NATIONAL SCIENTIFIC MIPT CONFERENCE. FUNDAMENTAL AND APPLIED PHYSICS. 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. I., PISAREV V. V., NORMAN G. E. «EQUILIBRIUM – METASTABLE SINGULARITY IN THE LENNARD-JONES

1–6 Mar. 2020

SYSTEM» // ABSTRACTS OF THE XXXV INTERNATIONAL CONFERENCE ON EQUATIONS OF STATE FOR MATTER. 2020. P. 247.

## 62<sup>nd</sup> 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 62<sup>ND</sup> NATIONAL SCIENTIFIC MIPT CONFERENCE. FUNDAMENTAL AND APPLIED PHYSICS. 2019. PP. 216-217.

18–23 Nov. 2019

## 16<sup>th</sup> 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 16<sup>TH</sup> 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.

## 61<sup>st</sup> 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 61<sup>ST</sup> 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 « $\alpha$ -GeoGaz» and « $\beta$ -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 **2<sup>nd</sup> place**, 61<sup>st</sup> National Scientific MIPT Conference

Moscow, Russia

Jun. 2018 **Top 10 of the class (~ 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 **29<sup>th</sup> 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,  $\text{\LaTeX}$ , Origin, slurm

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