Egor KOLESNIKOV
Theoretical biophysicist

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I have strong background in computational biophysics and physics. Experienced in molecular dynamics simulations of biomolecules. Six years of experience investigating ion-DNA and protein-DNA interactions at atomistic level. Developed models for atomistic and coarse-grained simulation of chromatin and its components. Took part in development of implicit solvation algorithms for atomistic modeling, implemented in AMBER program package. Worked part-time as a scientific journalist.

EDUCATION

2023-ongoing *PhD student.*, Virginia Tech, Physics Department.
2021-2023 *PhD student.*, Moscow Institute of Physics and Technology, DGAP.
2019-2021 *Master of Science*, Moscow Institute of Physics and Technology, DGAP.
2015 – 2019 *Bachelor*, Moscow Institute of Physics and Technology, DGAP
VT PhD GPA : 3.67/4

PUBLICATIONS

2021 Kolesnikov, E. S., Gushchin, I. Y., Zhilyaev, P. A., Onufriev, A. V. Similarities and Differences between Na+ and K+ Distributions around DNA Obtained with Three Popular Water Models. *Journal of Chemical Theory and Computation.* https://doi.org/10.1021/acs.jctc.1c00332.

2023 Kolesnikov, Y. S., Gushchin, I. Y., Zhilyaev, P. A., Onufriev, A. V. Why Na^+ has higher propensity than K^+ to condense DNA in a crowded environment. *The Journal of Chemical Physics* https://doi.org/10.1101/2023.05.15.540899

2024 Kolesnikov E. S., Xiong Y., Onufriev A. V. Implicit Solvent with Explicit Ions Generalized Born Model in Molecular Dynamics : Application to DNA. *Journal of Chemical Theory and Computation* https://doi.org/10.1021/acs.jctc.4c00833

WORK IN UNEVERSITIES

Sep 2023 – Ongoing
Theoretical biophysicist, LABORATORY FOR THEORETICAL AND COMPUTATIONAL MOLECULAR BIOPHYSICS COMPUTER SCIENCE AND PHYSICS (VIRGINIA TECH, COMPUTER SCIENCE DEPARTMENT),
Study of DNA compaction mechanisms using MD simulations
PhD program :
- Refinement of the ion parameters for implicit solvent/explicit ions simulations of the nucleosome
- Developement of a protocol of nucleosome simulations for generation of a representative ensemble of hustone tails conformations
- Finding the optimal solvent model for H4-tail simulations

AMBER | LAMMPS | Python | NumPy | Curves+ | PyMol | VMD | CHIMERA | LaTeX | Academic writing

Jul 2019 – Dec 2022
Theoretical biophysicist, LABORATORY OF STRUCTURAL ANALYSIS AND ENGINEERING OF MEMBRANE SYSTEMS (MIPT),
Study of DNA compaction mechanisms using MD simulations
Master program :
- Simulation of DNA in the presence of sodium and potassium using different solvent models, analysis of trajectories. Finding optimal water model for DNA simulations.
- Explanation why Na^+ has higher propensity than K^+ to condense DNA in a crowded environment.
- Finding optimal parameters for model of explicit ions in implicit water.

PhD program :
- Investigation of chromatin dynamics using coarse-grained MD simulations

Jan 2018 – Jun 2019
Molecular biologist, LABORATORY FOR STRUCTURAL BIOLOGY OF GPCRS,
Examination of the biophysical properties of GPCR receptors embedded into lipid nanodiscs
- Synthesis of A2A protein and its examination in different types of nanodiscs.

Molecular biology | PCR | Protein expression | Protein purification

Jan 2024 – May 2025 | Teaching assistant, Virginia Tech Physics Department,
- Teaching laboratory works
- Checking students' lab reports

Sep 2022 – Dec 2022 | Teaching assistant, Extramural Physical and Technical School (MIPT),
- Checking students' homework

Skills

Programming language	Python
MD program packages	AMBER, LAMMPS
Frameworks, tools, libraries	Linux, Conda, GitHub, VMD, CHIMERA, PyMol, LaTeX, NumPy, SciPy, Matplotlib