

Egor Marin

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WORK EXPERIENCE

Machine Learning Scientist

ENPICOM B.V.

May 2024 — Present

Den Bosch, Netherlands

- full-cycle ML model development: from literature survey and data collection to reproducible training and deployment
- working with both generative and predictive models for various tasks in the antibody development field

Open-source software engineer

MDAnalysis via Google Summer of Code

May 2023 — September 2023

Remote

- wrote backward-compatible parallelization for molecular dynamics trajectory analysis

PhD Researcher

University of Groningen

June 2021 — Dec 2023

Groningen, Netherlands

- full-cycle membrane protein biochemistry: protein expression, purification, nanodisc reconstitution or crystallization
- processed cryoEM data (80 CryoSPARC projects), set up cryoEM data processing & management infrastructure
- supervised a project as a corresponding author: [“Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking”](#)

Junior Research Associate

Moscow Institute of Physics and Technology

March 2017 — September 2021

Moscow, Russia

- last-mile protein crystallography service: crystal harvesting, data management, synchrotron and XFEL data collection
- refined, analysed and deposited protein structures to PDB (38 structures as of September 2025)
- coordinated data analysis and manuscript preparation

Scientific Journalist

Moscow Institute of Physics and Technology

Jun 2022 — Aug 2022

Moscow, Russia

- wrote press-releases on published papers
- communicated with scientists & media.

EDUCATION

University of Groningen

PhD

2019 — 2023

Groningen, Netherlands

- thesis ‘On the methods of studying protein-ligand interaction dynamics’“
- methods: cryoEM, X-ray crystallography, protein biochemistry, protein biophysics
- publications in JACS, Crystal Growth & Design, Journal of Cheminformatics & Modelling

Computer Science Center

Full-time extracurricular educational program in computer science

2020 — 2022

St. Petersburg, Russia

- relevant coursework: Python, C++, Algorithms and data structures, Data science, Intro to Linux systems, Rust

Moscow Institute of Physics and Technology

MSc in applied mathematics and physics

2017 — 2019

Moscow, Russia

- managed bachelor and master students, created a course on modern protein crystallography
- publications in Science, Nature Communications, Science Advances, Scientific Data
- graduated *summa cum laude*

Moscow Institute of Physics and Technology

BSc in applied mathematics and physics

2017 — 2019

Moscow, Russia

- graduated *magna cum laude*
- related coursework: Calculus I-IV, Linear Algebra I-II, Complex Analysis, Differential Equations I-II, Analytical Mechanics I-II, Thermodynamics.

PUBLICATIONS

Maintainer, Hyperschedule (hyperschedule.io)

Nov 2023 — Present

- Maintain open-source scheduler used by 7000+ users at the Claremont Consortium with TypeScript, React and MongoDB

- Manage PR reviews, bug fixes, and coordinate with college for releasing scheduling data and over \$1500 of yearly funding
- Ensure 99.99% uptime during peak loads of 1M daily requests during course registration through redundant servers

SKILLS

- **Programming Languages:** Python, bash, Rust, C++, Typescript
- **Python:** uv/ruff/ty🔥, pytest, hypothesis, pydantic, dask
- **Data Science:** polars🐘, huggingface😊, pandas, numpy, sklearn, skrub
- **Deep Learning:** pytorch, lightning, jax, mlflow
- **ML in biology:** protein language models, diffusion/discrete diffusion/flow matching, Alphafold/Openfold/Boltz
- **Technologies:** AWS, Docker, SLURM, Modal, Airflow, Github actions
- **Cheminformatics:** RDKit, polaris, molecular docking, structural bioinformatics (MDAnalysis/mdtraj/biotite)

EXTRACURRICULAR ACTIVITIES

Open-source contributions

Jan 2021 — Present

- Founder of Les Amateurs (amateurs.team), currently ranked #4 US, #33 global on CTFTIME (2023: #4 US, #42 global)

MDAnalysis Core Developer

Jan 2021 — Present

- Founder of Les Amateurs (amateurs.team), currently ranked #4 US, #33 global on CTFTIME (2023: #4 US, #42 global)

Self-hosting

Jan 2021 — Present

Data Science Competitions

- Founder of Les Amateurs (amateurs.team), currently ranked #4 US, #33 global on CTFTIME (2023: #4 US, #42 global)