VLADIMIR LADYGIN, PHD

Computational Biologist | Atomistic Modeling | Generative AI
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Summary

- 8+ years of experience applying machine learning and high-performance computing to scientific problems.
- Proficient in Python and C++ for large-scale atomistic modeling; pipeline, and scientific software design.
- Blend scientific rigor with strong communication — working in multidisciplinary fields in the R&D field.
- Develop new methodologies for uncertainty quantification and active learning to reduce the amount of data required for model training and implementation of self-consistent loops.

Skills

Programming: Python (PyTorch, TensorFlow, scikit-learn, LangGraph), C/C++, Java, Bash, High Performance Computing (CPU/GPU)

Machine Learning: Equivariant GNN, DDPM, Flow Matching, Transformers (GPT), VAE/Autoregression, Gaussian Process, Deep Bayesian Networks

Computational Chemistry: DFT, CI/CC, QMC, MPS, Metadynamics, MD, Monte Carlo MD, ManyBody codes

Computational Biology: MSA, Folding/Docking with AlphaFold and Boltz2, Boltz2Affinity, Metadynamics Simulation of Protein/Aptamer complexes, VAMPnets

Experience

Grafron Bioscience — Location
Head of Computations — 05/2025 - Present

- Led computational research for cancer early detection and therapeutics.
- Architected platform for the de novo design of 100+ viable designs in 24 hours with validated nM binding affinity
- Implemented MLFF for charged systems based on MACE and OMol dataset, reaching chemical accuracy.
- Designed and implemented generative AI in silico pipelines, reducing simulation time by 90%.
- Performed a large-scale MLFF-MD simulation for binding energy calculation on antibody and aptamer complexes.

Caltech — Location
Visiting Scientist — 01/2025 - 07/2025

- Improved foundation models for materials design with tensor network techniques
- Used high-performance computing to perform ab initio calculations
- Implemented and trained machine learning models for the design of energy and semiconductor materials
- Implemented Many-Body quantum physics codes in Python for tractable materials simulation
- Performed and analyzed neutron scattering experiments
- Reduced computational time of MD trajectory analyses by 99% introducing efficient CPU+GPU communication

Skolkovo Inc — Location
Scientific Computing Researcher — 09/2018 - 01/2021

- Designed machine learning-based software for uncertainty quantification of phase diagrams as an alternative to the CALPHAD method with an active learning
- Applied deep Bayesian learning techniques for solving the curse of dimensionality problem in the description of multicomponent systems
- Performed large-scale MLFF simulations of phase coexistence simulations and benchmarking of machine learning interatomic potentials

VNIIA — Location
Nuclear Materials Computational Scientist — 09/2017 - 01/2021

- Validated Foundation models for Materials Design
- Applied machine learning for the modeling of nuclear material degradation
- Build high-performance computing pipelines to bridge DFT accuracy and atomistic simulation

Eduction

Caltech
PhD in Materials Science

Caltech
MS in Materials Science

Skolkovo
MS in Data Science and Scientific Computing

MIPT
MS in Computational Chemistry

MIPT
- Applied Physics and Mathematics
- Minor in Chemistry

Projects

Computational platform for de novo drug design applied to cancer treatment and therapeutics

Designed and led implementation of a drug discovery platform incorporating GenAI, sequence-structure predictions, MD, affinity, and physical gates gates

Bayesian learning of thermodynamic integration and numerical convergence for accurate phase diagrams
https://journals.aps.org/prb/abstract/10.1103/PhysRevB.104.104102

Implemented fully automated pipeline for phase diagram calculation and uncertainty quantification using Gaussian Processes