ODYSSEAS VAVOURAKIS

ML for Biomolecular Structure — DPhil (PhD) Student, University of Oxford

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EDUCATION

SABS R^3 EPSRC CDT - DPhil (PhD) Programme

Balliol College, University of Oxford, UK

Sep 2023 – present

- first-year student, currently on rotation projects
- prior coursework in software engineering, mathematical modelling, structural drug discovery, data science, and scientific computing

M.Sc. Computational Biology & Bioinformatics

ETH Zürich, Switzerland

Sep 2020 – Aug 2023

- graduated **with distinction**; **GPA 5.9 / 6.0** ($= \mu + 1.75\sigma$); UK 1st class equivalent
- **top grade** for **thesis project** (on right)
- total of **151 / 120 ECTS credits**; additional coursework on RL & probabilistic ML, NLP, computational quantum chemistry and physics, game theory
- jointly awarded with Universities of Zurich and Basel

B.Sc. Biochemistry

Heidelberg University, Germany

Sep 2015 – Aug 2018

- **GPA 1.5** (UK 1st class equivalent; best possible: 1.0)
- additional coursework on programming foundations and computational methods

PUBLICATIONS

Exact tunneling splittings from symmetrized path integrals

G. Trenins, L. Meuser, H. Bertschi, O. Vavourakis, R. Flütsch, and J. O. Richardson

2023 | Journal of Chemical Physics

- https://doi.org/10.1063/5.0158879
- a new path-integral molecular dynamics simulation technique to calculate exact ground-state tunnelling splitting patterns in small molecules without wavefunctions

INTERESTS

Geometric DL | Generative Models | Comp. Protein Design | Biomolecular ML | Comp. Biophys. | Bayesian ML | Phylogenetic Inference | Evolutionary & Learning Dynamics | Physical Chemistry

RESEARCH EXPERIENCE

Rotation Project

***De Novo* Generative Antibody Design**

Mar 2024-present | OPIG, University of Oxford

- *in silico* antibody design with generative AI
- advised by Prof C. Deane, Prof M. Bronstein; F. Dreyer & D. Cutting (Exscientia)

Master's Thesis Project

Boost-SE: Wide-Spectrum Enzyme-Substrate Interactions from Multi-Task Recommendations using Protein Language Models

7 months (2023) | ETH AI Center, ETH Zürich

- recommendation system to propose likely-interacting enzyme-substrate pairs given a set of MACCS fingerprints + enzyme sequences
- enables inductive enzyme and compound discovery
- trained on binary, positive/unlabelled metabolic pathway data + auxiliary targets
- uses fine-tuned pLM sequence embeddings
- advised by Prof A. Krause, J. Rothfuss, M. Mutný

Rotation Project

Calculating Tunnelling Splittings with Path-Integral Molecular Dynamics

3.5 months (2022) | D-CHAB, ETH Zurich

- helped develop the mathematical method, implemented and validated the sampling scheme and estimator
- built path-integral molecular dynamics simulation package from scratch
- see publication on left
- advised by Prof J. Richardson; Dr G. Trenins

Bachelor's Thesis Project

Spectrin-Repeat Mechanical Unfolding with Atomistic Force-Probe MD

3.5 months (2018) | HITS, Heidelberg

- studied rupture force and sequence determinants of unfolding behaviour of spectrin repeat domains under mechanical tension with force-probe molecular dynamics (GROMACS)
- advised by Prof F. Gräter; Dr C. Daday

CO-CURRICULARS

Cooperativeness in Graph-Based Systems

Summer Game Theory Course Project

Summer 2021 — ETH Zurich

- studied collective phase changes in cooperative behaviour in agents facing iterated prisoner's dilemma interactions while interconnected in a dynamic random graph structure
- three-person group project; won best presentation

Information Theory & Evolution

Summer School/Academic Retreat

Summer 2016 — Ftan, Switzerland

- two-week workshop on information-theoretic approaches to the evolution of intelligence
- gave introductory presentation on information theory
- co-wrote agent-based simulation framework to model emergence of intelligence (three-person group project)

WORK EXPERIENCE

Sergeant (NATO OR-5; Military Service)

Hellenic Air Force

Nov 2018 - Nov 2019 — Athens, Greece

- **Clinical Biochem – General Air Force Hospital**
  - photometric/spectroscopic sample analysis, clinical assessment and reporting; responsible for ER samples; technical maintenance
- **Fuel Chemist – Eleusis Air Base**
  - scanning electron microscopy of engine micro-debris for predictive maintenance
  - aircraft fuel and engine lubricant quality control and contamination assessment (i.a. optical emission spectroscopy)

LABORATORY EXPERIENCE

Degree-Associated Practicals

Heidelberg University

2015 - 2017 — Heidelberg, Germany

- **Biochemistry:** experience in lipidomics; lipid click chemistry; FACS; CRISPR knockouts; immunoprecipitation (ChIP/qPCR); HPTLC; fluorescence microscopy; retroviral transduction; cloning; protein interaction & kinetic assays; protein purification; primer design
- **(In)Organic Chemistry:** AAS, IR, Raman, EI MS, 1D & 2D NMR; small molecule crystallography & theory; multi-stage organic and inorganic synthesis; classical quantitative analysis (potentiometry, conductometry, electrogravimetry etc.);
  non-spectroscopic inorganic analysis

DISTINCTIONS

Oxford University **Clarendon Scholar**
Oxford University **Scatcherd European Scholar**
Balliol College **John Henry Jones Scholar**

2023-2028

Scholar at **Studienstiftung des deutschen Volkes** (Germany's single most prestigious scholarship)

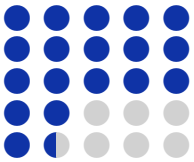
2015-2018 and 2020-2023 (B.Sc. and M.Sc.)

SKILLS

Python & PyTorch
R
C++
Other
Git, Shell & UNIX, Docker, LaTeX

LANGUAGES

English
German
Modern Greek
Spanish
Latin



LEISURE

- online lectures/courses
- seminar talks, podcasts, non-fiction
- language learning, linguistics