Pratik Patil

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AI scientist | Computational Biophysicist | Scientific Machine Learning Researcher

Profile

PhD researcher in **computational protein biophysics**, **machine learning**, and **quantum-computing modelling**, currently in near completion of my doctoral thesis. My research develops **physics-grounded AI representations** for molecular systems, with applications in **protein dynamics**, **molecular simulation**, **drug discovery**, and **scientific computing**. I also bring prior industry experience as a full-stack software engineer for **cheminformatics**, **bioinformatics**, **retrosynthesis**, **sequence analysis**, and **production ML systems**. The current work in progress are described on abstract level, with further technical details available for discussion during interviews.
I aim to build **AI- and quantum-computing based hybrid drug discovery pipelines** that are **faster**, **cheaper**, and more **precise**, enabling better decisions across molecular design, simulation, optimisation, and therapeutic discovery.

Research Experience

In-silico R&D, PhD Scholar (Industry funded) 2023 – Present
Evotec Pharma *Abingdon, UK*

- Research in **AI-driven molecular modelling**, **computational protein biophysics**, and **quantum computing**
- Developing physics-grounded ML representations for studying **protein conformational ensemble**, residue interactions, solvent-mediated effects, and molecular state transitions (markov state models)
- Research direction: Physics informed neural networks for protein ensembles, scalable molecular dynamics post-processing, protein ensemble interpretation, druggable-state selection, and simulation-informed drug discovery workflows

Tech Skills

AI/ML: **PyTorch**, **JAX**, PyTorch Geometric, TensorFlow/Keras, scikit-learn, graph neural networks, transformers, representation learning (Data2Vec), information-theoretic analysis, group theory, manifolds, physics-informed neural networks
Computational Drug Discovery: **Protein conformation ensembles**, molecular dynamics analysis (MDAnalysis), sequence analysis, RDKit, Retrosynthesis
Quantum Computing: Qiskit, PennyLane, quantum state representation, quantum machine learning
Scientific Software: **Python**, C++, FastAPI, Flask, Dash, VueJS, Angular, **Docker (CI/CD)**, Celery, RabbitMQ, Redis, MongoDB, MySQL, Neo4J, Elasticsearch, AWS ECS/ECR, **Cloud Native applications**

Selected Research Projects

Protein modelling with Quantum Computing for Molecular State Analysis

- Developed a high-level research framework for representing proteins through **residue-level physical features**, interaction structure, and sampled state distributions
- Explored how quantum circuit sampling and thermodynamic reasoning can support interpretable views of **protein energy landscapes** and residue interaction network
- Presented related poster work at YMF-2025, MGMS conf., Oxford
- Won first prize for Poster presentation at the Research Day, University of Suffolk, 2026

High Performance Computing (HPC) library for calculating Protein solvation with JAX

- Studying how **solvation-aware molecular features** can improve interpretation of protein conformational ensembles and molecular dynamics trajectories
- This Python library employs Analytical and Numerical SASA algorithms with high parallelism optimisation enabled by JAX

GNN and Transformer-based manifold Learning for Protein Conformational Ensembles

- Built residue-level and atom-level graph representations for analysing protein conformational flexibility and ensemble behaviour
- Worked with molecular dynamics-derived data structures using Python, PyTorch/PyTorch Geometric, NumPy, SciPy, and MDAnalysis
- Presented research talks at Evotec on protein conformational ensembles and graph-based ML representations

Education

Doctor of Philosophy (Ph.D.) Feb 2023 – Present
Digital Futures Institute, University of Suffolk *Ipswich, UK*
- Thesis titled: Quantum Computing and AI methods for Protein Ensemble modelling
- Industry funded research fellowship by Evotec Pharma

Bachelor of Engineering in Computer Engineering August 2015 – May 2019
Savitribai Phule Pune University *Pune, India*
- Reinforcement Learning based AI agent for neon car racing
- Research project on NLP feature extraction
- Applied machine learning for health and societal applications

Software Engineering Experience

Software Engineer – Scientific Applications June 2019 – January 2023
e-Zest Solutions Limited *Pune, India*
- **Situation:** Scientific users needed usable web platforms for cheminformatics, bioinformatics, retrosynthesis, sequence analysis, and ML-assisted workflows
- **Task:** Translate research prototypes and domain-specific requirements into maintainable software services, interfaces, and deployment workflows
- **Action:** Built and integrated applications using **FastAPI**, Flask, VueJS, Angular, Docker, MongoDB, MySQL, RabbitMQ, Redis, Celery, RDKit, MarvinJS, TensorFlow/Keras, and AWS ECS/ECR
- **Result:** Helped move scientific ML and molecular informatics workflows from prototype stage toward user-facing, reproducible, and deployable software applications

Selected Industry Projects

Retrosynthesis and Chemical Informatics Platform May 2020 – April 2021
- Developed components for retrosynthesis route prediction, reaction-tree visualisation, molecular editing, and prediction serving
- Integrated **RDKit**, AiZynthFinder-style workflows, TensorFlow, Flask, Angular, MarvinJS, and Docker in a multi-container scientific application

Sequence Analysis and Clustering Platform April 2021 – October 2022
- Developed a web-based sequence analysis platform with distributed job execution for ML-driven clustering, alignment, and sequence-processing workflows
- Implemented backend services and job orchestration using **FastAPI**, Celery, RabbitMQ, Redis, MySQL, and VueJS

Applied ML Prototypes and Productionisation (Other projects) 2019 – 2023
- Built and deployed ML prototypes across computer vision, NLP, and recommendation workflows, strengthening practical experience in **model deployment**, APIs, containers, and production ML design

Publications

Patil, P., Bonde, B., Choubey, B. (2026). *A Quantum Circuit Framework for Protein Ensemble-Level Energetics.* arXiv, 2026. [Online]. Available: https://arxiv.org/abs/2608.0549

Patil, P., Bonde, B., Choubey, B. (2026). *JaxProtSASA: A High-Performance Computing library for computing Protein SASA using JAX.* (in press)

Patil, P., Bonde, B., Choubey, B. (2026). *Solvation informed AI model for Protein ensemble sampling.* (in press)

Bonde, B., **Patil, P.**, Choubey, B. (2024). *The Future of Drug Development with Quantum Computing.* In: Heifetz, A. (eds) High Performance Computing for Drug Discovery and Biomedicine. Methods in Molecular Biology, vol. 2716. Humana, New York, NY. Available: https://pubmed.ncbi.nlm.nih.gov/37702939/

Patil, P., Thealla, P., Bonde, B. (2024). *Harnessing AI for Enhanced Cybersecurity: Trends, Challenges, and Future Prospects.* In P. Thealla, V. Nadda, S. Dadwal, L. Oztosun, G. Cantafio (Eds.), Corporate Cybersecurity in the Aviation, Tourism, and Hospitality Sector (pp. 258-272). IGI Global Scientific Publishing. Available: https://doi.org/10.4018/979-8-3693-2715-9.ch014

Achievements

- Won **first prize** for presenting *Protein Encoding on Quantum Circuit for Ensemble Analysis* poster at the 3MT, UoS, 2026
- **Three-year PhD scholarship** by Evotec Pharma, 2023

Research Engagements

- Presented *Protein Encoding on Quantum Circuit* poster at Young Modellers' Forum, MGMS conference, Oxford, 2025
- Sponsored AMD–DiRAC HPC Hackathon/Conference, Birmingham 2025, to build and benchmark **Fragment Molecular Orbital (FMO)** based binding affinity calculations using **GAMESS (US)** on AMD Instinct MI300A Instinct accelerators
- Presented at **Quantum.Tech Conference, London 2024**

Training/Certifications

- **Production Machine Learning Systems** – Google Cloud, 2023
- **End-to-End Machine Learning with TensorFlow on GCP** – Google Cloud, 2022