Frank Fu

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Summary

I solve problems in biology/chemistry using machine learning and molecular dynamics.

Education

Ph.D. Computational Chemistry – The University of Queensland	Jul 2023 - Present
MSc. Biological Sciences – The University of Auckland	Mar 2023
BSc. Biological Sciences – The University of Auckland	Mar 2021

Experience

- **Research Intern** QDX, Melbourne   Feb - Jun 2025
  - Implemented novel machine learning framework for automatic recognition and deployment of collective variables in proprietary molecular dynamics software
  - 4x speedup compared to tradition enhanced sampling workflows, in addition to requiring minimal prior knowledge of the system under study

- **Lab Demonstrator** The University of Auckland   Mar 2021 - May 2023
  - *BIOSCI 107: Biology for Biomedical Science* – microbiology lab techniques such as culturing, microscopy, and gel electrophoresis
  - *BIOSCI 220: Quantitative Biology* – statistical modelling/analysis using the R programming language
  - *BIOSCI 355: Genomics* – bioinformatics techniques such as sequence alignment, structure prediction, and phylogenetics

- **Research Assistant** The University of Auckland   Dec 2021 - Mar 2022
  - Performed experimental evolution of genetically modified *S. cerevisiae* to observe evolutionary dynamics between competing populations
  - Experiment results were used to contribute to a successful grant application

Skills

Programming C/C++, Python, R
Machine learning Supervised learning with PyTorch/libtorch, scikit-learn, DGL
Molecular dynamics *classical*: GROMACS, PLUMED, OpenMM | *quantum*: xTB

Publications

- Fu, Y., & Takeuchi, N. (2024). Evolution of the division of labour between templates and catalysts in spatial replicator models. *Journal of Evolutionary Biology, 37(10*, 1158-1169.
- Fu, Y., Stroet, M., & O'Mara, M. L. (2025). A graph-based machine learning framework to assign empirical interaction parameters for novel molecules. In review.

Awards

The University of Queensland Industry Placement Scholarship	2025
The University of Queensland Earmarked PhD Scholarship	2023
Best Poster, The Association of Molecular Modellers of Australasia Conference	2023

Conference presentations

Selected talk at The Association of Molecular Modellers of Australasia Conference	2025
Selected talk at QUIBIC Symposium	2025
Selected talk at the Annual Conference of the Australian Society for Biophysics	2023