Asawari Pagare

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Education

University of North Carolina at Chapel Hill — Chapel Hill, USA
Ph.D. in Chemistry, Advisor: Prof. Zhiyue Lu — 2021–07/2025 (Expected)

Indian Institute of Science — Bangalore, India
M.Sc. in Chemistry — 2019–2020

Indian Institute of Science — Bangalore, India
B.S.(Research) in Chemistry — 2015–2019

Technical Skills

- **Coding:** Python, Julia, C

  (Libraries: PyTorch, PyTorch Geometric, TensorFlow, Pandas, Numpy, Scipy, SciKit, Matplotlib, mpl)
- **Softwares:** Matlab, Mathematica, LAMMPS, Blender, Adobe Illustrator
- **ML architectures:** GNN, GAN, GraphSage
- **Applied mathematical skills:** Information theory, Probability theory, Stochastic thermodynamics, Calculus, Complex Analysis, Differential Equations, Linear Algebra

Research and Teaching Experience

Graduate Research Assistant at the University of North Carolina at Chapel Hill
Lu Group, Department of Chemistry — 2021-Current

- **Information theory and machine learning classification of nonequilibrium biological sensors beyond steady states**[1]: This project focuses on uncovering the relationship between a sensor's graph and it's performance in temporal pattern recognition using information theory. I generated data using simulations that I then curated to classify using machine learning to classify sensors. This lead to uncovering a design principle that may be used in artificial sensors. This manuscript is currently under preparation and the codes are made available on GitHub.
- **Stochastic distinguishability of Markovian trajectories** [2]: A sensor responsible for sensing it's environment can be characterized by its ability to tell apart different time-dependent environments. Our formulation circumvents sampling difficulties to compute KL divergence and it explicitly connects trajectory KL divergence with individual transition events and their waiting time statistics.
- **Theoretical upper bound of multiplexing in biological sensory receptors** [3]: Using computational, probabilistic and information theoretical approach we had shown that a sensor can multiplex – sense multiple environmental information simultaneously. We came up with a theoretical upper bound of multiplexing and proposed rank-deficient maximum likelihood as a technique to obtain the upper bound for a receptor and identify it's accuracy and sensitivity in sensing different environmental variables. The codes used for this project are available on GitHub.

Teaching Assistant at the University of North Carolina at Chapel Hill
Quantitative Lab II (102L) in Spring 2022
Physical Chemistry lab (481L) in Fall 2021

Undergraduate Research Experiences

BS Thesis at the Indian Institute of Science Bangalore, India

Cherayil Group, Department of Inorganic and Physical Chemistry 2018-2019

- 'Stochastic thermodynamics of a harmonically trapped colloid in linear mixed flow[4]': A system of a harmonically trapped colloid subjected to linear mixed flow was successfully shown to satisfy various fluctuation theorems like the integral fluctuation theorem, Jarzynski relation, Bochkov-Kuzovlev relation and the detailed fluctuation theorem.

Summer Intern at the University at Buffalo Buffalo, USA

Errington Group, Department of Chemical and Biological Engineering Summer, 2018

- Studied the phase coexistence properties of an ionic liquid using Monte Carlo and Molecular simulations. Properties of a Room Temperature Ionic Liquid (RTIL) called 1,3-dimethylimidazolium tetrafluoroborate ($[C_1mim][BF_4]$) at a temperature higher than its thermal degradation temperature were calculated and the phase behaviour for a constant temperature of 1000K and varying densities was studied.

Summer Intern at the Indian Institute of Science Bangalore, India

Cherayil Group, Department of Inorganic and Physical Chemistry Summer, 2017

- 'Thermodynamics and work fluctuations of a closed quantum system with applications to interacting spin-1/2 particles': Characteristic function and work distribution of a system of spin 1/2 particles interacting via J coupling were derived. Local violations of the second law caused by the considerable thermal and quantum fluctuations were clearly observed.

Summer Intern at the Indian Institute of Science Bangalore, India

Cherayil Group, Department of Inorganic and Physical Chemistry Summer, 2016

- 'The different dimensions of dimensional analysis'[5]: Dimensional analysis and scaling properties were used to show scaling behaviour in the phenomenon of slowing down of magnets when dropped through a metallic pipe.

Publications and selected Presentations

[1] **A. Pagare** and Z. Lu, "Information benchmark for biological sensors beyond steady states – mpemba-like sensory withdrawal effect", *arXiv:2406.04304, 2024*,

[2] **A. Pagare**, Z. Zhang, J. Zheng, and Z. Lu, "Stochastic distinguishability of markovian trajectories", *arXiv preprint arXiv:2401.16544*, 2024.

[3] **A. Pagare**, S. H. Min, and Z. Lu, "Theoretical upper bound of multiplexing in biological sensory receptors", *Physical Review Research*, vol. 5, no. 2, p. 023 032, 2023.

[4] **A. Pagare** and B. J. Cherayil, "Stochastic thermodynamics of a harmonically trapped colloid in linear mixed flow", *Physical Review E*, vol. 100, no. 5, p. 052 124, 2019.

[5] **A. Pagare** and B. J. Cherayil, "The different dimensions of dimensional analysis", *Resonance*, vol. 23, no. 6, pp. 641–661, 2018.

- Oral presentation on '**Can a single ligand-receptor sense multiple channels of information?**' April 2023
  TriMolS Symposium 2023, Raleigh, NC
- Poster presentation on '**Theoretical upper bound of multiplexing in biological sensory receptors** May 2022
  The Workshop on Stochastic Thermodynamics III, WOST III 2022
- Oral presentation on '**Can a single ligand-receptor sense multiple channels of information?**' March 2022
  APS March Meeting 2022, Chicago, Illinois

Other Hobbies

- Jigsaw puzzles, traveling, cooking, reading and looking after my plants.