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 — 2021–2025 (Expected)

Indian Institute of Science (#1 ranked university in India) — Bangalore, India
B.S.(Research) - MSc in Chemistry — 2015–2020

Technical Skills

- **Coding:** Python, Julia (Python libraries: PyTorch, PyTorch Geometric, Pandas, RDKit, Numpy, Scipy, SciKit, Matplotlib, mpl, nglview, MDAnalysis)
- **Softwares:** Matlab, Mathematica, Pdb2pqr, Meeko, Blender, Adobe Illustrator
- **ML architectures:** GNN, GAN, GraphSage, Knowledge Graphs
- **Applied mathematical skills:** Information theory, Probability theory, Stochastic thermodynamics, Calculus, Complex Analysis, Differential Equations, Linear Algebra
- **Relevant courses:** Computational Medicinal Chemistry school (Upcoming in Oct 2024 in Boston), Computer-Aided Drug Design, Crash course on molecular docking in Python, Machine learning with graphs

Research and Teaching Experience

Graduate Research Assistant at the University of North Carolina at Chapel Hill
Lu Group, Department of Chemistry — 2020-Current

- **Information theory and machine learning classification of nonequilibrium biological sensors beyond steady states**[1]: Demostrated (using information theory and machine learning) that a ligand-receptor sensor with more unbound states in its state transition graph may show enhanced performance in recognizing a concentration up-shift while it is away from steady states. These results may be used to system specific studies in tweaking the best drug efficacy in target based therapies.[1]
- **Stochastic distinguishability of Markovian trajectories**: Derived (using probability theory, Markov model and linear algebra) a general formula for the distinguishability of different temporal environments by an arbitrary sensor in non-equlibrium using KL divergence that circumvents sampling difficulties. It explicitly connects trajectory KL divergence with individual transition events and their waiting time statistics allowing for an computationally cheap formulation and novel insights into temporal pattern recognition by biological and artificial sensors.[2]
- **Theoretical upper bound of multiplexing in biological sensory receptors**: Demostrated (using computation, probability and information theory) that a ligand-receptor sensor can multiplex – sense multiple environmental information simultaneously. A theoretical upper bound of multiplexing was obtained and a mathematical technique called the rank-deficient maximum likelihood was proposed to obtain the upper bound for a receptor and identify it's accuracy and sensitivity in sensing different environmental variables. This result motivates controlling other environmental factors in target-based therapies to enhance desired results.[3]

Teaching Assistant at the University of North Carolina at Chapel Hill
Quantitative Lab II (102L) in Summer II 2024 and Spring 2022
Physical Chemistry lab (481L) in Fall 2021
– Mentored, managed and lead students to run experiments, analyze and interpret data

Undergraduate Research Experiences

BS Thesis and MSc Thesis at the Indian Institute of Science Bangalore, India
Cherayil Group, Department of Inorganic and Physical Chemistry 2018-2020

- MSc Thesis – 'Stochastic thermodynamics of a polymer in linear mixed flow': Demonstrated (through analytical calculations) fluctuation theorems – integral fluctuation theorem, Jarzynski relation, Bochkov-Kuzovlev relation and the detailed fluctuation theorem – to be satisfied by a polymer in linear mixed flow.
- BS Thesis – 'Stochastic thermodynamics of a harmonically trapped colloid in linear mixed flow': Demonstrated (using analytical calculations) that a harmonically trapped colloid in linear mixed flow satisfies various fluctuation theorems.[4]

Summer Intern at the University at Buffalo Buffalo, USA
Errington Group, Department of Chemical and Biological Engineering Summer, 2018

- 'Monte Carlo and Molecular Dynamics simulations to study the phase coexistence properties of a Room Temperature Ionic Liquid (RTIL)'

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'

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", *J Chem Phys.*, vol. 160, no. 171101, 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.

- Poster presentation on '**Information theory classification of biological sensors** June 2024
  American Conference on Theoretical Chemistry 2024, Chapel Hill, NC.
- 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.

Awards

- Kishore Vigyanik Prothsahan Yojana (KVPY) Fellowship 2015–2020
  Awarded by the Dept. of Science and Technology, Govt. of India. Awarded to the top 250 (less than 0.001%) students in India for demonstrated abilities in science and technology.