Pallab Dutta

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https://pallab-dutta.github.io github.com/Pallab-Dutta

Current Position

Since 2020 **Research Scholar, IISER Kolkata, India**
Working at the interface of computational chemistry and machine learning #ML4Science.

Education

2015 – 2020 **Integrated BsMs, IISER Kolkata, India**
Major: Biological Sciences, Minor: Physical Sciences
Thesis title: *Expectation Maximization for Rare Event Sampling: Isomerization of Proline.*
Advisor: Prof. Neelanjana Sengupta

Publications

Research Articles

1. H. Chatterjee, P. Dutta, M. Zacharias, and N. Sengupta, "Learning transition path and membrane topological signatures in the folding pathway of bacteriorhodopsin (br) fragment with artificial intelligence," *The Journal of Chemical Physics*, vol. 162, no. 10, 2025. DOI: https://doi.org/10.1063/5.0250082.
2. P. Dutta, A. Kshirsagar, P. Bibekar, and N. Sengupta, "Conformational ensemble of the nsp1 ctd in sars-cov-2: Perspectives from the free energy landscape," *Biophysical Journal*, vol. 122, no. 14, pp. 2948–2959, 2023. DOI: https://doi.org/10.1016/j.bpj.2023.02.010.
3. P. Dutta and N. Sengupta, "Efficient interrogation of the kinetic barriers demarcating catalytic states of a tyrosine kinase with optimal physical descriptors and mixture models," *ChemPhysChem*, vol. 24, no. 6, e202200595, 2023. DOI: https://doi.org/10.1002/cphc.202200595.
4. P. Dutta and N. Sengupta, "Expectation maximized molecular dynamics: Toward efficient learning of rarely sampled features in free energy surfaces from unbiased simulations," *The Journal of Chemical Physics*, vol. 153, no. 15, 2020. DOI: https://doi.org/10.1063/5.0021910.

Review Article & Book Chapter

1. P. Dutta, H. Chaterjee, and N. Sengupta, *Entropy in biomolecular conformation, recognition and aggregation, Comprehensive Biophysics, 2nd Ed.* Elsevier, 2025. DOI: just-accepted.
2. P. Dutta, P. Roy, and N. Sengupta, *Effects of external perturbations on protein systems: a microscopic view.* ACS Publications, 2022, vol. 7, pp. 44 556–44 572. DOI: https://doi.org/10.1021/acsomega.2c06199.

Conference Proceedings

1. N. Sengupta, P. Dutta, A. Kshirsagar, and P. Bibekar, "Expectation maximised molecular dynamics: An unsupervised machine learning approach toward rapid estimation of biomolecular transition barriers," 3, vol. 123, Elsevier, 2024, 43a.
2. D. Das, A. Vaze, H. Rai, *et al.*, "Bacman: A probiotic bacterial batman to protect the citizens of gotham from arsenic poisoning.," Oct. 2018.

Teaching

Autumn Semester 2019-2020 — **Teaching Assistant, IISER Kolkata, India**
Introduction to Computer Programming

Spring Semester 2019-2020 — **Teaching Assistant, IISER Kolkata, India**
Introduction to Computing

Autumn Semester 2020-2021 — **Teaching Assistant, IISER Kolkata, India**
Biology Laboratory III (Biophysics Computational Laboratory)

Spring Semester 2020-2021 — **Teaching Assistant, IISER Kolkata, India**
Biostatistics

Skills

Languages	English, Hindi, Bengali
Coding	Python, HTML, CSS, JavaScript, LaTeX, bash, WSL2
Computational Tools	Cloud computing at AWS, High Performance Computing, NAMD, Amber, Gromacs, OpenMM
Machine Learning	TensorFlow, Pytorch
Animation	Blender, Molecular Nodes

Miscellaneous Experience

Awards and Achievements

2018 — **Gold Medalist**, iGEM 2018
I along with my team, worked on developing probiotic bacteria to treat arsenic poisoning. I had explicitly worked on the supporting mathematical model. We presented the results as a conference paper in the International Genetically Engineered Machine (iGEM) 2018 meet.

2021 — **Winner of National HPC Hackathon**, AWS and Intel.

2023 — Selected for ML4Science Visiting Scholar Program at IIIT-Hyderabad.

DST INSPIRE Senior Research Fellowship.

Certification

2020 — **Machine Learning, Coursera**.
I completed two introductory courses on deep learning taught by Prof. Andrew Ng.

Extracurricular Activities / Interests

Coding	I like creative coding and developing applications including chatbots that help keep track of my research activities/progress.
Art	I am interested in media designing, animation, and science communication through these mediums.
Literature	I am interested in the History of Sciences, Philosophy, and Mythology. I love both to read and write poetry in Bengali