Curriculum Vitae

Debarshi Banerjee

Publications

1. Prasun Sarkar, **Debarshi Banerjee,** Shibashis Paul, Deb Shankar Ray - “Method for direct analytic solution of the nonlinear Langevin equation using multiple timescale analysis: Mean-square displacement” - *Phys. Rev. E 106, 024203*, **2022**

Research Interests

- Unsupervised Learning and Deep Neural Networks (applied to biological systems of interest)
- Excited-State and Non-Adiabatic Dynamics of Proteins
- Protein Folding and “Mis-folding”
- Causality Inference
- The molecular processes behind neurodegenerative diseases
- The origin of homochirality in proteins and sugars

Education

- **PhD fellow in Physics at ICTP and SISSA, Trieste, Italy (Oct 2022 - present)**
  - Supervisor: Prof. Ali Hassanali, ICTP
  - Affiliation: ICTP - Condensed Matter and Statistical Physics (CMSP)
  - Department: SISSA - Molecular and Statistical Biophysics (SBP)
  - Designation: UNESCO Predoctoral Research Fellow at ICTP
  - ERC Funded Fellowship on Hydrogen-bond Networks as Optical Probes (HyBOP)
  - Courses -
    - Statistical Mechanics
    - Molecular Dynamics
    - Polymer Physics
    - Unsupervised Learning
    - Biochemistry
    - Physical Chemistry
    - Enhanced Sampling
    - RNA Structure Prediction
    - Machine Learning for Materials Science

- **Master of High-Performance Computing at ICTP and SISSA, Trieste, Italy (Sep 2021 - Dec 2022)**
  - Graduated “summa cum laude”.
  - ICTP Scholarship recipient.
  - Master’s Thesis (Supervisors: Prof. Edgar Roldan, Prof. Ali Hassanali, Prof. Ivan Girotto) - “Development of a computational toolbox to analyse first-passage times and diffusion coefficients in heterogeneous soft-matter systems”.
  - Courses -
    - Advanced Programming with C, Fortran, C++, Python
    - Parallel Programming - MPI, OpenMP, CUDA (GPU)
    - Numerical Methods and Analysis
    - Numerical Linear Algebra
    - Linux HPC Cluster Management
    - Unsupervised Machine Learning
    - Supervised Machine Learning
    - Reinforcement Learning
    - Deep Learning
    - Natural Language Processing (NLP)

- Molecular Dynamics
- Electronic Structure Theory
- Advanced Optimization Techniques (for Intel CPUs)
- Parallel Fast Fourier Transform
- Approximation and Interpolation of Functions

❖ **Bachelor of Science (with Honours) (July 2016 - June 2019)**
- ➢ College: St. Xavier's College, University of Calcutta
- ➢ Division: First Division with Honours
- ➢ CGPA: 8.41 out of 10.0
- ➢ Rank: 4th
- ➢ Subjects: Chemistry, Physics, Mathematics
- ➢ Bachelor's Thesis (Supervisors: Dr. Rahul Sharma, Prof. Deb Shankar Ray) - "Application of classical perturbation methods in nonlinear dynamics and stochastic differential equations".

❖ **Grade XII - All India Senior School Certificate Examination of C.B.S.E. (2016)**
- ➢ Marks: 93.2%
- ➢ Subjects: Physics (95), Computer Science (92), Maths (95), Chemistry (96), English (88).
- ➢ School: Delhi Public School, Ruby Park, Kolkata
- ➢ Board: Central Board of Secondary Education

❖ **Grade X - Madhyamik Examinations of W.B.B.S.E. (2014)**
- ➢ Marks: 90.1%
- ➢ Subjects: Physical Sciences (100), Mathematics (100), Life Science (98), Geography (98), History (80), English (82), Bengali (74).
- ➢ School: Ramakrishna Mission Vidyalaya, Narendrapur, Kolkata
- ➢ Board: West Bengal Board of Secondary Education

Internships and Projects

❖ **Master's Thesis with Prof. Edgar Roldan, Prof. Ali Hassanali, Prof. Ivan Girotto at ICTP, Trieste:**
- ➢ Thesis Title: "Development of a computational toolbox to analyse first-passage times and diffusion coefficients in heterogeneous soft-matter systems"
- ➢ Duration: May 2022 - Oct 2022
- ➢ Worked on developing a high-performance, user-friendly software suite in Python (parallelised using "Dask") that can process molecular dynamics trajectories and infer the first-passage times and space-dependent diffusion coefficients. Originally, we reproduced results from prior publications, and then we applied this technique to obtain novel results that are now being prepared for publication.

❖ **Chemical Physics project with Prof. Deb Shankar Ray at IACS, Kolkata:**
- ➢ Research internship: "Non-Equilibrium Statistical Mechanics and Stochastic Differential Equations"
- ➢ Duration: 25/04/2019 - 31/08/2019
- ➢ Worked on a general method to solve Nonlinear Langevin Equations without using the Fokker-Planck formalisation, instead making use of Blekhman Perturbation Scheme. Wrote programs in Fortran-95 and Python, alongside the analytical results, to numerically simulate the system and compare corresponding analytical and numerical results.
- ➢ Collaborated with a postdoctoral student on a project using Renormalization Group approach to solve a Rayleigh type oscillator for both 2D and 3D models. The latter also involved dealing with the incidence of chaos in a system, and all codes, for numerical simulation as well as for measuring Lyapunov Exponent for the chaotic system, were written by me in Python.

❖ **Bachelor's Thesis with Dr Rahul Sharma at St. Xavier's College, Kolkata:**
- ➢ Thesis Title: "Perturbation Methods in Nonlinear Dynamics"
- ➢ Duration: 01/09/2018 - 30/03/2019
- ➢ Worked on solving a fluctuating barrier crossing problem using Lindstedt-Poincare method and

its comparison with Regular Perturbation Theory. Following this, analytical and numerical results were compared, and RMSD was found to be extremely low between the two.
- ➢ Wrote programs in Fortran-95, C++ to simulate stochastic systems, using Gaussian White Noise. Programmed various numerical methods to solve ODEs and PDEs which were necessary for numerical simulations.

- ❖ **Chemical Physics project with Prof. Deb Shankar Ray at IACS, Kolkata:**
  - ➢ Research internship: "Nonlinear Dynamics and Perturbation Theory"
  - ➢ Duration: 30/04/2018 - 31/08/2018
  - ➢ Learned the major perturbation methods: Lindstedt-Poincare, Krylov-Bogoliubov, Multiple Time Scale.
  - ➢ Learned the standard ways to solve stochastic differential equations from Van Kampen's review of the same. Explored potential applications of stochastic methods in chemical systems.
  - ➢ Applied these concepts to certain well-established chemical problems (such as Glycolytic Oscillation) and obtained promising results which seemed to match reasonably well.
  - ➢ Programs were written in Fortran-95 and Python. Some Bash scripting was also done.

- ❖ **Computational Chemistry project with Dr Rahul Sharma at St. Xavier's College, Kolkata:**
  - ➢ Research Internship: "Chemical Graph Theory"
  - ➢ Duration: 01/08/2017 - 10/11/2017
  - ➢ Wrote various programs in Python to create a system that relates graph-theoretical concepts to chemical structures and properties. The generated data was later used to train neural networks to predict chemical properties from their corresponding graph-based chemical structures.
  - ➢ It was not a successful project, but as it was my first internship, I learnt a lot about doing literature review, machine learning, neural networks, application of computational methods in chemical/biological problems, and the scientific method to approach novel research problems.

Skills

- ❖ Programming Languages - C, C++, Python, Fortran, Julia, Bash.
- ❖ Parallel programming using MPI and OpenMP.
- ❖ GPU computing using OpenACC and CUDA.
- ❖ Numerical Linear Algebra libraries - MKL, BLAS, LAPACK, SCALAPACK, PLASMA, MAGMA, SLATE.
- ❖ Technical Skills: Latex, Linux, Git.
- ❖ Primary subjects of interest - Biophysics, Molecular Dynamics, Unsupervised Learning, Deep Learning and Neural Networks, Neurodegenerative Diseases, Quantum Chemistry.
- ❖ Additional topics I am fascinated by: QSAR, QSPR, Nonequilibrium Statistical Mechanics, Information Theory, Stochastic Processes, Nonlinear Dynamics, Chaotic Systems, Quantum Computing.

Workshops and Conferences

- ❖ ICTP workshop on "Frontiers in Excited State Electronic Structure Methods: from Spectroscopy to Photochemistry", 2023
- ❖ ICTP workshop on "Computational Physics: Total Energy and Force Methods", 2023.
- ❖ ICTP workshop on "Non-Markovian Dynamics Far from Equilibrium", 2022.
- ❖ EPFL-CECAM workshop on "Multiscale Molecular Dynamics with MiMiC", 2022.
- ❖ Nobel Prize colloquium by Prof. Giorgio Parisi - ICTP, 2021.
- ❖ National colloquium - Modern Research Trends in Chemistry (MRTC), 2019.
- ❖ National colloquium - Modern Trends in Microbiology (MTIM), 2018.
- ❖ National colloquium - Facets of Chemistry in Materials and Biology (FOCMB), 2018.
- ❖ Data Innovation Labs workshop - "Data Science and Machine Learning", 2018.
- ❖ International colloquium - Facets of Chemistry in Biology (FOCB - II), 2017.
- ❖ National colloquium - Modern Trends in Microbiology (MTIM), 2017.
- ❖ National colloquium - Modern Trends in Microbiology (MTIM), 2016.

Posters Presented

- ❖ "Barrier Fluctuation and Stochastic Differential Equations", Modern Research Trends in Chemistry (MRTC), 2019.

- “Protein Folding - A Nonlinear Dynamics Perspective”, Modern Trends in Microbiology (MTIM), 2018 - 2nd Prize.
- “Molecular Machines - Its Applications in Molecular Computers and Disulphide Bond Formation”, Facets of Chemistry in Materials and Biology (FOCMB), 2018 - 1st Prize.

Communication and Interpersonal Skills

- Native Languages: Bengali, English, Hindi.
- English: IELTS Academic score - 8.5 (C2).
- Organiser of the ICTP Table Tennis Tournament, 2022.
- Member of the Core Committee for organising departmental seminars in 2018, 2019
- Member and Head of Editorial Committee for departmental seminars in 2018, 2019.

Community Service

- Presently a volunteer for an NGO called Padakshep which helps underprivileged students continue their education. My duties include, among other things, being the co-mentor and direct point of contact for an individual student. I help them academically and ensure that sufficient funds from Padakshep reach them in a timely manner. My Padakshep email is - debarshi.banerjee@padakshep.org
- Volunteered for the NSS (National Service Scheme) during my undergraduate days. I have gone to various villages to teach basic maths, language to children (aged 6-10) as part of this.
- Volunteered for “Hope Foundation” efforts to help vulnerable children.
- Member of the organising committee of various blood donation camps in the college.
- Participant in cleanliness drives organised by NSS.

Sports

- 1st place in ICTP Table Tennis Tournament, 2022, Singles.
- 2nd place in ICTP Table Tennis Tournament, 2022, Doubles.
- 1st place in SISSA Games - Table Tennis Cup, 2022, Doubles.

Hobbies

- Member of debate society during both school and undergraduate days.
- I play the Violin, Keyboard, and Tabla.
- I enjoy playing Chess and Table Tennis.
- I am an avid follower of various sports, in particular - Chess, Football, Formula 1, and Tennis.
- I am a voracious reader, mostly indulging in non-fiction.