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Koushik Naskar

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Objective

Machine Learning and Data Science enthusiast with a Ph.D. in Computational Chemistry (awaiting defense), experienced in Python, C, Fortran, and high-performance computing, seeking quantitative researcher or data scientist opportunities.

Education

2018 - 2024	**Ph.D.** in Theoretical & Computational Chemistry at *Indian Association for the Cultivation of Science, Kolkata* (Thesis submitted) Expected date of degree: June 2024	
2015 - 2017	**Master of Science (Physics)** at *Indian Institute of Technology, Guwahati*	(8.32/10.0)
2012 - 2015	**Bachelor of Science (Physics)** at *Presidency University, Kolkata*	(7.33/10.0)
2012	**Higher Secondary** at *Howrah Zilla School* (Affiliated to WBCHSE)	(84.40%)

Skills

Numerical Programming	Python (NumPy, SciPy, Pandas, Matplotlib etc.), C, C++, Fortran
High-Performance Computing	OpenMP, MPI, CUDA (GPU), Job Scheduler (PBS, Slurm)
Machine Learning	Scikit-Learn, PyTorch, Neural Network, Deep learning, Natural Language Processing, Time Series Analysis
Web Development	HTML, CSS, Javascript, React JS, NodeJS, Django, Flask, Dash-Plotly
Database	SQLite, PostgreSQL, MongoDB
Software Development	Electron JS, Flutter
Miscellaneous	Big Data, Git, Shell scripting, MS Excel, LaTeX, CI/CD

Experience

Doctoral Research Scholar, IACS, Kolkata, India

- Created "*ADT*", a software package using Python and Fortran to construct diabatic potential energy surfaces both numerically and analytically. Implemented OpenMP parallelization and HDF5 file I/O, achieving a ∼6x reduction in computation time. (Published in *J. Chem. Theory Comput.*). *https://github.com/AdhikariLAB/ADT-Program*
- Developed a highly parallelized software package using Fortran and C to perform quantum dynamics simulation of elementary chemical reactions. Discovered novel ways to parallelize using OpenMP and MPI schemes across hundreds of cores and nodes of computing cluster/supercomputer, enhancing efficiency by up to 4x. (Manuscript in preparation)
- Designed a parallel Python package that substantially simplifies and improves the efficiency of constructing global potential energy, achieving a 10x performance boost. *https://github.com/Koushikphy/PESMan*

Data Science Projects

- Developed an end-to-end pipeline for exploring, analyzing, and predicting customer churn risk at a bank using a Random Forest classifier, achieving an accuracy of 86%.
- Implementated SVM, Random Forest, and KNN for multi-class classification to predict obesity risk, attaining a top accuracy score of 90%.
- Utilized a CNN model with transfer learning for classifying paddy diseases with an accuracy rate of 96%.
- Applied the ARIMA model for time series analysis, successfully forecasting trends and patterns with high accuracy.

Master's Student, IIT Guwahati

- Developed efficient parallel codes in Python and Fortran for simulating and visualizing the formation and dissociation of Hydrogen bonds in water in the presence of ions, using Molecular Dynamics.

Other Projects

- *Interactive Data Editor*: Designed a novel graphical approach for easy refinement and removal of irregularities from data. Built with Node JS and Electron JS. Deployed CI/CD pipelines on GitHub Actions for building software binaries for different OS/platforms. *https://github.com/Koushikphy/Interactive_Data_Editor*
- *TeleJobReminder*: Developed a Telegram bot using Python Flask, PostgreSQL and Telegram API that keeps track of computer jobs and sends notification when the job finishes/fails. Deployed on the cloud. *https://github.com/Koushikphy/TeleJobReminder*
- Created a Django web server for efficiently managing multiple Workstations/Clusters through a dashboard. *https://github.com/Koushikphy/System-Status-Checker*
- *kbib*: Crafted a Python tool that generates academic references from DOIs or PDFs in various formats by utilizing the CrossRef REST API. Deployed it on PyPI for easy access. *https://github.com/Koushikphy/kbib*

Research Publications

13. K. Naskar, S. Mukherjee, S. Ghosh and S. Adhikari, *J. Phys. Chem. A*, **128**, 1438 (2024)
12. S. Mukherjee†, K. Naskar†, S. Hazra, M. K. Sah and S. Adhikari, *J. Phys. Conf. Ser.*, **2769**, 012012, (2024)
11. M. K. Sah, S. Mukherjee, K. Naskar, S. Hazra and S. Adhikari, *Int. J. Quantum Chem.*, **123**, e27212 (2023)
10. M. K. Sah, S. Mukherjee, S. Saha, K. Naskar, and S. Adhikari,*J. Chem. Phys.*, **159**, 244116 (2023)
9. K. Naskar, S. Ghosh, S. Adhikari, M. Baer and N. Sathyamurthy,*J. Chem. Phys.*, **159**, 034302, (2023)
8. K. Naskar, S. Ravi, S. Adhikari, M. Baer and N. Sathyamurthy,*J. Phys. Chem. A*, **127**, 3832, (2023)
7. J. Dutta, K. Naskar, S. Adhikari, J. Meyer and M. Somers,*J. Chem. Phys.*, **157**, 194112 (2022)
6. K. Naskar, S. Ghosh and S. Adhikari, *J. Phys. Chem. A*, **126**, 3311 (2022)
5. S. Mukherjee, S. Ravi, K. Naskar, S. Sardar and S. Adhikari*J. Chem. Phys.*, **154**, 094306 (2021)
4. J. Dutta, S. Mukherjee, K. Naskar, S. Ghosh, B. Mukherjee, S. Ravi and S. Adhikari,*Phys. Chem. Chem. Phys.*, **22**, 27496 (2020).
3. B. Mukherjee†, K. Naskar†, S. Mukherjee, S. Ravi, K. R. Shamsundar, D. Mukhopadhyay and S. Adhikari, *J. Chem. Phys.*, **153**, 174301/1-20 (2020)
2. K. Naskar†, S. Mukherjee†, B. Mukherjee, S. Ravi, S. Mukherjee, S. Sardar and S. Adhikari, *J. Chem. Theory Comput.*, **16**, 1666-1680 (2020).
1. K. Naskar, S. Mukherjee, S. Ghosh, T. Sahoo and S. Adhikari,*Int. Rev. Phys. Chem.*, **38**, 287 (2019).

(†indicates equal contribution)

Awards and Scholarships

2020	CSIR-NET Senior Research Fellowship
2017	Graduate Aptitude Test in Engineering (GATE)
2015 & 2016	CSIR-NET Junior Research Fellowship
2015	Joint Admission to MSc (JAM)
2012	DST-INSPIRE Scholarship for Higher Education (SHE)
2010 & 2011	DST-INSPIRE SEATS Award & Internship

Certificates

- PyTorch for Deep Learning with Python Bootcamp
- Python for Data Science and Machine Learning Bootcamp
- Django 3 - Full Stack Websites with Python Web Development