V S Dhruthi Boddapati

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Research Summary

My master's research focused on molecular dynamics and multiscale modeling, where I co-developed **ChemXDyn**, a dynamics-based framework for accurately identifying species and reactions from MD trajectories (*ab initio* methods, reactive force fields (ReaxFF), and machine-learned interatomic potentials). The extracted reaction mechanisms and rate constants were validated against experimental data and further assessed at the continuum scale through predictions of ignition delay times and flame speeds. My broader research interests include molecular dynamics, multiscale modeling, scientific computing, and machine learning.

Education

Indian Institute of Science (IISc), Bengaluru — CGPA: 8.90/10
M.Tech, Computational and Data Sciences, ***Advisor: Dr. Konduri Aditya*** *(website)* — *Aug. 2023 – May 2025*

Andhra University College of Engineering (AUCE), Andhra University — CGPA: 9.28/10
B.Tech, Chemical Engineering — *Aug. 2019 – Jun. 2023*

Projects

ChemXDyn: A dynamics-based trajectory analyzer for atomistic simulations

- Developed a **novel dynamics-based trajectory analysis framework** compatible with *ab initio*, reactive force fields (ReaxFF) and machine learning interatomic potentials (MLIPs).
- Implemented **forward and backward time windowing** for robust differentiation between persistent chemical bonds and transient collisional contacts.
- Designed **parallelized core modules** in Python for time-resolved interatomic distance analysis, enabling quantification of species lifetimes and occurrence frequencies.

Multiscale modeling of fuel oxidation using reactive MD and machine-learned potentials

- Performed detailed **bond order analysis** and dynamic analysis techniques such as **Fast Fourier Transform (FFT), power spectrum (PS) analysis, and vibrational energy** profiling to distinguish bonded and non-bonded interactions.
- Used **ChemXDyn** to validate ReaxFF-based MD of hydrogen, multi-valent nitrogen chemistry in ammonia, and **neural-network molecular dynamics** (NNMD) simulations of methane combustion against experimental data.
- Proposed a **multiscale modeling** framework to investigate chemical kinetics at the molecular scale and validate the resulting mechanisms at the continuum scale through **flame speeds and ignition delay times** (IDT).
- These works culminated in my master's thesis, "A reactive molecular dynamics framework to obtain chemical kinetic models for fuel oxidation."

Study of NO_x formation pathways from atomistic simulations

- Benchmarked ChemXDyn against state-of-the-art trajectory analyzers (ChemTrYzer, ReacNetGenerator), demonstrating **higher accuracy** and a **significant reduction in spurious species and reactions**.
- Identified key reaction intermediates such as $\mathbf{N_2H}$ and critical reactions, elucidated their role in NO_x pathways.

Deep learning–based image classification for structural vulnerability assessment

- Developed a complete image-processing pipeline using SIFT and CLAHE for robust feature extraction.
- Trained and benchmarked multiple deep learning models, including ResNet-50/152, InceptionV3, Xception, and EfficientNet, alongside classical ML methods such as Random Forests and Support Vector Machines.

Publications

1. Raj, M., **Dhruthi, B.**, Arunan, E., Phani, M., Konduri, A. "ChemXDyn: Unraveling species and reactions from reactive molecular dynamics through dynamics-based interatomic distance analysis." *(Under review, Proceedings of the National Academy of Sciences (PNAS), 2025).*
2. **Dhruthi, B.**, Raj, M., Phani, M., Konduri, A. "Extracting NO_x pathways from atomistic simulations of ammonia combustion." *(Manuscript in preparation).*

3. Tadikonda, S.S., Raj, M., **Dhruthi, B.**, Phani, M., Konduri, A. "Quantitative assessment of dynamics-based kinetic parameter extraction using ChemXDyn." *(Under review, 41st International Symposium on Combustion (2026), Paper ID: 1302).*
4. Deepti, S., Raj, M., **Dhruthi, B.**, Phani, M., Konduri, A. "Dynamics-based detection of aromatic species and soot nucleation pathways using reactive molecular dynamics." *(Under review, 41st International Symposium on Combustion (2026), Paper ID: 1394).*

Presentations

Indo-German Workshop on Hardware-Aware Scientific Computing (IGHASC) Nov. 26 - 30, 2024
Poster *Heidelberg, Germany*

Raj, M., **Dhruthi, B.**, Phani, M., Konduri, A. "Novel multiscale modeling methodology for chemical kinetic modeling of fuel oxidation using atomistic calculations."
(Best poster award).

Work Experience

Sr. Data Scientist at Lam Research, Bangalore, India July 2025 - present

- Part of AI Hub within Global Business Intelligence Solutions (GBIS), focusing on developing AI-powered tools for LamBots.
- Built and integrated multiple solutions, such as an image-generation module and an Outlook mail and calender connector into existing enterprise applications.
- Responsible for end-to-end integration of these tools across backend and frontend systems, using Azure ML Studio and MongoDB.

Technical Trainee at Visakhapatnam Steel Plant (RINL - VSP) Dec 2021 - Jan 2022

- Worked in Coke Oven & Coal Chemicals Plant (CO & CCP), gaining exposure to large-scale industrial processes.
- Evaluated the performance of the cooling towers and heat-exchangers at the Mechanical, Biological, and Chemical (MBC) treatment plant to improve efficiency in continuous wastewater treatment.
- Assessed temperature-control mechanisms essential for sustaining biological treatment and proposed steps for system optimization.

Skills

Programming Languages: C, C++, Java, Python, MATLAB
Libraries: NumPy, pandas, Scikit-learn, TorchANI, Matplotlib, SciPy, Open Babel, RDKit
Tools/Frameworks: Git, OpenMP, MPI, SLURM, Jupyter, Azure ML, LaTeX, PyTorch, Keras/TensorFlow
Simulation/Modeling: LAMMPS, Packmol, DeePMD-kit, Ovito, VMD, CP2K

Courses

Introduction to Molecular Simulations
Introduction to Scalable Systems
Machine Learning for Cyber-physical Systems
Numerical Linear Algebra
Numerical Optimization
Introduction to Data Science
Numerical Solution of Differential Equations
HPC for Quantum Modeling of Materials
Scientific Computing with Quantum Algorithms
Applied Combustion

Academic Awards & Achievements

- Recipient of Ministry of Education (MoE), Government of India fellowship (2023 - 2025).
- Recipient of undergraduate merit award, NSF scholarship (2019 - 2023).
- Secured first rank in the school in AISSCE (CBSE) - 2019 examination.
- Awarded for the highest score in Science in the ICSE - 2017 examination at school.

Extracurricular Activities & Interests

- Vice-President of The Communicons English Club, an official club of Andhra University.
- Trained in classical dance forms (Bharatnatyam and Kuchipudi), recognized in Indian Book of Records, Limca Book of Records for Bharatnatyam group performances.
- Secured first place in the Women's Cricket Championship during Thorite (90th Department Day Celebrations, Department of Chemical Engg., AU, 2023).