Saurabh Sivakumar

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Interests: *Multi-scale quantum chemistry, Computational catalysis and materials modelling, Geometric deep learning, Fine-tuning ML models, High-performance computing and Automated workflow development*

Education

University of California — Davis, CA
Ph.D. in Chemical Engineering — *Sep 2021 – Present*

Carnegie Mellon University — Pittsburgh, PA
M.S in Chemical Engineering — *Aug 2019 – Dec 2020*

National Institute of Technology — Tiruchirappalli, India
B.Tech in Chemical Engineering, Minor in Economics — *Jul 2015 – May 2019*

Skills

- **Software/Frameworks:** VASP, ORCA, QuantumEspresso, LAMMPS, PLUMED, jDFTx, BerkeleyGW, Gaussian, COMSOL, OVITO, VMD, ChemCAD
- **Programming/Markup Languages:** Python (**Packages:** Pytorch, ASE, RDKit, MDanalysis, OpenMM, pySCF, CuPy, Numba, WandB, Parsl, Deap), R, C++, Bash, OpenACC, LaTeX

Research Experience

Graduate Student Researcher — Sep 2021 – Present
University of California (Advisor: ***Ambarish Kulkarni****)* — *Davis, CA*

- ML-accelerated design of novel thermal and electrocatalysts for sustainable energy applications.
- Developed graph and descriptor-based machine-learned potentials (MLPs) to describe surface-mediated adsorption, diffusion, and reaction phenomena; resulting MLPs are 1000x faster than the typical quantum chemistry methods.
- Led the MLP development efforts within the Kulkarni group; trained 4 graduate students and 3 undergrads in using benchmarking and benchmarking MLPs for dynamics (enhanced sampling) and property predictions.
- Combined several open source Python libraries to develop automated workflows for transition state search for metal catalysts; these tools are now being generalized to other materials
- Constructed computational workflows and curated datasets to enable large-scale screening of molecules and their properties for electrochemical oxygen separation.
- Participated in several large collaborative projects funded by DOE and industry for applications related to micro-kinetic modelling, catalyst deactivation, ML and electrochemical separations.

Graduate Researcher & Research Assistant — Jan 2020 – Jul 2021
Carnegie Mellon University (Advisor: ***Zachary Ulissi****)* — *Pittsburgh, PA*

- Applied machine learning and mathematical modelling to enhance the field of atomic-scale simulations
- Developed open source software and sampling strategies for an Active learning framework to accelerate Nudged Elastic Band calculations and Molecular Dynamics
- Built and tested workflows to identify lowest energy nanoclusters on a potential energy surface using a modified genetic algorithm enhanced with MLPs (Neural networks and Gaussian processes)
- Assisted a collaborative effort funded by ARPA-E working on surface segregation with Deep Reinforcement learning through dataset training and Bayesian optimization for hyperparameters

Undergraduate Thesis — Jan 2019 – May 2019
National Institute of Technology (Advisor: ***S Saravanan****)* — *Tiruchirappalli, India*

- Designed a chemical plant and associated equipment for manufacturing Trichloroethylene

Research Intern — May 2018 – Aug 2018
Singapore University of Technology and Design (Advisor: ***Arief S Budiman****)* — *Singapore*

- Worked with collaborators on projects related to optimizing lightweight solar PV modules with a poly-carbonate substitute

Publications

- Enabling robust offline active learning for machine learning potentials using simple physics-based priors
  - Muhammed Shuaibi, **Saurabh Sivakumar**, Rui Qi Chen and Zachary W Ulissi
  - [Paper Link]
- Cluster-MLP: An Active Learning Genetic Algorithm Framework for Accelerated Discovery of Global Minimum Configurations of Pure and Alloyed Nanoclusters
  - Rajesh K. Raju, **Saurabh Sivakumar**, Xiaoxiao Wang and Zachary W Ulissi
  - [Paper Link]
- Toward an ab Initio Description of Adsorbate Surface Dynamics
  - **Saurabh Sivakumar** and Ambarish Kulkarni
  - [Paper Link]
- An Automated Pynta-based Curriculum for ML-Accelerated Calculation of Transition States
  - Trevor Price, **Saurabh Sivakumar**, Matthew S. Johnson, Judit Zador and Ambarish Kulkarni
  - [Paper Link] (Under Review)

Selected Projects

Implementation of DOSTransformer Mar 2024 – Jun 2024

- Implemented Multi-Modal transformers to predict the density of states for crystalline structures based on existing code
- Modified the code to streamline training and improve functionality and obtained model metrics; Presented and evaluated cases for further improvement.

Classification of Musk Dataset from UC Irvine Mar 2022 – Jun 2022

- Implemented a neural network, k-NN, decision tree, and logistic regression classifiers with a prediction accuracy of at least 96% across all the classifiers.

Analysis of the COVID-19 dataset Jan 2022 – Mar 2022

- Exploratory analysis on the COVID-19 time-series dataset curated by the New York Times to showcase the effect of the COVID-19 pandemic across the USA.

Model predictions from the Abalone dataset from UC Irvine Sep 2021 – Dec 2021

- Performed Box-cox transformation, used a Greedy search strategy to implement a stepwise regression algorithm to find the best model according to AIC and BIC criterion. Implemented ridge regression on the dataset due to high multicollinearity as a comparison

Conferences & Posters/Talks

- AIChE Annual Meeting 2020 (Virtual). November 20 2020
  - An Active Learning Framework for Accelerating Saddle Point Searches
  - [Poster Abstract Link]
- Sandia & CERCAS Symposiums 2022
  - Developing an integrated experiment theory approach to provide new insights into heterogeneous catalysis
  - [Poster Link]
- NERSC AUG. Oct 23 2024
  - Optimizing Chebyshev Interaction Model with Parallel Programming: From OpenMP to GPU Acceleration

Other Experiences & Awards

- NSF ACCESS compute grant worth 8m credits (100k node hrs) (Oct 2021 - Present)
- Multiple NERSC compute grants totalling over 50k CPU and GPU node hrs (Nov 2021 - Present)
- Judge, UC Davis ChemE symposium (Sep 2023)
- Reviewer, Journal of Open Source Software (Feb 2024 - Present)
- Teaching Assistant, Chemical Reaction Engineering, 2023
- Head, Media Relations – Pragyan (NITT's Technical Organization)