Saurabh Sivakumar

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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*

Interests

- Multi-scale atomistic simulations
- Data science applications in Engineering
- Deep Learning and Active Learning
- High-performance computing and automated workflow development

Skills

- **Software/Frameworks:** VASP, QuantumEspresso, LAMMPS,ORCA, COMSOL, GAMS, OVITO, ChemCAD
- **Programming/Markup Languages:** Python (**Packages:** ASE, Pytorch, scikit-learn, Numpy, Scipy, RDKit, MDanalysis, Seaborn, Matplotlib, Plotly, Pandas, WandB, Deap), R, Bash, LaTeX, C/C++, Markdown,SQL

Research Experience

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

- ML-accelerated design of novel thermal and electrocatalysts for sustainable energy applications.
- Developed 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 2 undergrads in using MLPs.
- 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
- Participated in several large collaborative projects funded by DOE and industry for applications related to catalyst deactivation and electrochemical separations.

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

- Applied machine learning and mathematical modeling 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
- 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 (Adviser: S Saravanan) — *Tiruchirappalli, India*

- Designed a chemical plant and associated equipment for manufacturing Trichloroethylene
- Formulated a theoretical design with focus on cost analysis and safety using ChemCAD

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

- Worked with collaborators on projects related to optimizing lightweight solar PV modules with a poly-carbonate substitute
- Conducted multiple experiments to test the bonding strengths of these poly-carbonates on PV cells

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]
- Quantifying surface diffusion of adsorbates on transition metal surfaces with machine-learned potentials
  - **Saurabh Sivakumar** and Ambarish Kulkarni
  - Manuscript in preparation (Working title)

Selected Projects

Classification of Musk Dataset from UC Irvine Mar 2022 – June 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.
- Studied the effect of varying kernel types for SVM and different optimizers for NN and performed feature extraction with PCA
- Presented key results such as decision boundaries and errors for the classifiers

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

- Exploratory analysis on the COVID-19 dataset curated by the New York Times to showcase the effect of the COVID-19 pandemic across the USA.
- Visualized the number of cases/mortalities to each county and state in the USA using plotly and Chloropleth plots.
- Analyzed the trends in certain states and counties by plotting the time series over 2 years with a weekly moving average to gain useful insights into the effect of vaccination rates.

Linear regression with the Abalone dataset from UC Irvine Sep 2021 – Dec 2021

- Found the best linear regression model to predict the age of abalone using a four-step methodology with R
- 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

Optimal Scheduling of Copper concentrate operations under uncertainty Jan 2020 – May 2020

- Optimized an industrial scheduling problem with uncertainty (Mixed Integer Nonlinear problem) for a copper plant using code written in GAMS
- Corroborated the results of the publication on which the project was based; presented and assessed cases for further improvement.

Conferences & Posters

- 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 using atomically dispersed materials
  - [Poster Link]

Other Experiences & Awards

- ACCESS compute grant worth 750k credits (500k core hrs) (Oct 2021 - Present)
- Multiple NERSC compute grants totalling over 20k CPU and GPU node hrs (Nov 2021 - Present)
- Judge, UC Davis ChemE symposium (Sep 2023)
- Member, AIChE (Oct 2019 - Present)
- Member, ACS (Feb 2021 - Present)
- Teaching Assistant, Chemical Reaction Engineering, 2023
- Head, Media Relations – Pragyan (NITT's Technical Organization)