Saurabh Sivakumar

sausiva@ucdavis.edu | linkedin.com/in/saurabhsivakumar | github.com/saurabhsivakumar

Education

University of California — Davis, CA
PhD 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

- Computational Catalysis
- Data science applications in Engineering
- Deep Learning and Active Learning
- Renewable Energy
- Mathematical modelling and optimization techniques

Skills

- **Software & Frameworks:** COMSOL, GAMS, MATLAB, ChemCAD, VASP, LAMMPS, Ovito
- **Languages:** Python, C/C++, LaTeX, Markdown, SQL
- **Libraries:** Numpy, Scipy, Matplotlib, Pandas, scikit-learn, PyTorch, Dask, Deap, ASE

Research Experience

Graduate Researcher & Research Assistant — Jan 2020 – Jul 2021
Carnegie Mellon University — *Pittsburgh, PA*

- Focused on applying machine learning and mathematical modelling to the field of atomic scale simulations on projects with the Ulissi Group in the department of Chemical Engineering
- Developed and applied an Active learning framework for accelerating Nudged Elastic Band calculations to reduce required ab-initio force calls
- Built and tested a program to identify lowest energy nanoclusters on a potential energy surface using a modified genetic algorithm
- Implemented a genetic algorithm with inbuilt active learning methods (Neural networks and Gaussian processes) to reduce the computational time required for identifying the optimal shape of nanoclusters
- Assisted the team working on surface segregation with Deep Reinforcement learning with dataset training and bayesian parameter optimization

Undergraduate Thesis — Jan 2019 – May 2019
National Institute of Technology — *Tiruchirappalli, India*

- Designed a chemical plant and associated equipment for manufacturing Trichloroethylene with a teammate, under the guidance of Dr. Saravanan
- 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 — *Singapore*

- Guided by Dr. Arief Budiman, worked with his group on projects related to optimizing lightweight solar PV modules with a polycarbonate substitute
- Conducted experiments to check feasibility of the Polycarbonate Ethylene Vinyl Acetate as a substitute for glass in a PV module using a Delaminator

Publications

- Enabling robust offline active learning for machine learning potentials using simple physics-based priors
  - Developed a framework using active learning that trains a NN based on the differences between the energy and force values calculated using ab-initio calls and morse potentials. This significantly minimized the time required for computation
  - [ArXiv Link]

Selected Projects

Classification of Musk Dataset from UC Irvine Mar 2020 – May 2020

- Performed principal component analysis and tested classification algorithms on a large dataset
- Implemented a neural network, k-NN, decision tree and logistic regression classifiers
- Presented results including decision boundaries and errors for the classifiers

Modelling for ventilation system to reduce airborne infection Mar 2020 – May 2020

- Conducted simulations on COMSOL to determine the ideal location of vents to increase the efficiency of removal of airborne bacteria

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

- Performed optimisation to an industrial scheduling problem(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 and presented a case for further improvement (recommended adding further uncertainty in certain parameters)

Production and Supply Chain Optimisation Sep 2019 – Dec 2019

- Analysed and reproduced the trend in results of the publication 'Comparison of formulations for the two-level uncapacitated facility location problem with single assignment constraints' (Mixed interger linear problem) using code written on GAMS working as a team of three
- Compared and presented the key results(optimisation solver times) obtained with those of the paper and analysed the reasons for any difference

Conferences & Posters

- AIChE Annual Meeting 2020 (Virtual). November 20 2020
  - An Active Learning Framework for Accelerating Saddle Point Searches
  - [Poster Link]

Leadership experience and Organizations

- Head, Media Relations – Pragyan (NITT's Technical Organization)
- Member – Marine Technological Society of NITT (Oct 2017 – May 2019)
- Member, Organising/Marketing – Alchemy (NITT Chemical Engineering Symposium)
- Member, AIChE (Oct 2019 - Present)