Adeesh KOLLURU
PhD Student at Carnegie Mellon University

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Personal Website

Interests : Graph Neural Networks, Computational Catalysis

🎓 EDUCATION

| 2020-2025 | *PhD in Chemical Engineering*, **Carnegie Mellon University** ; Advisor : Zachary Ulissi |
| 2016-2020 | *B. Tech in Chemical Engineering*, **Indian Institute of Technology Delhi** |

💻 PROJECTS

ACCELERATED LEARNING OF QUANTUM SIMULATORS FOR GEOMETRIC OPTIMIZATIONS
Facebook AI Research and Carnegie Mellon University
Worked on developing a machine learning based hybrid approach for accelerating the process of geometric optimization. We first train a GNN to predict next state from a given state and then perform relaxations from trained force predicting model.

Geometric Optimization | Graph Neural Networks | Catalysts

TRANSFER LEARNING FOR CATALYTIC/MOLECULAR PREDICTIONS USING OC20
Carnegie Mellon University
Conducted fine tuning experiments with pre-trained models on OC20 dataset to get close to 15% improvement in performance on other small scale catalyst as well as molecular databases.

Transfer Learning | Graph Neural Networks | Catalysts | Small Molecules

MACHINE LEARNING BASED CONTROL OF AERATION RATE FOR MAMMALIAN CELLS IN A BIOREACTOR   AUGUST 2019 - MAY 2020
B.Tech Thesis, Indian Institute of Technology Delhi | Advisor : Anurag Rathore
Developed a machine learning based control model to optimize aeration rate for mammalian cell in a stirred tank reactor. It predicts Viable Cell Concentration (VCC) through a random forest model and the mass transfer coefficient from theoretical approach and combined them to determine the optimal aeration rate.

Machine Learning | Process Control | Reactor Modeling

🎓 AWARDS

2020	Merit Award : For being in the Top 7% of Chemical Engineering batch of IIT Delhi
2018	Distinctive performance in Overall Activities from Chemical Engineering Society, IIT Delhi
2018	Colors Award : For being a promising sportsperson of IIT Delhi
2016	KVPY fellowship : Awarded by Govt. of India for being in the Top 1% in math and science across the country
2016	National Science Talent Search Exam (NSTSE) : Awarded Gold Medal, Tablet for securing All India Rank 1

☰ SKILLS

Languages : Python (PyTorch, PyTorch Geometric, DGL, TensorFlow, Keras), C++   **Software :** Ansys, Fluent, Matlab, Gromacs

☰ PUBLICATIONS

> **Rotation Invariant Graph Neural Network using Spin Convolution**
  M.Shuaibi, **A. Kolluru**, A. Das, A. Grover, A. Sriram, Z. Ulissi, C.L. Zitnick
  Arxiv Link
> **Neurips 2021 Competition : Open Catalyst Challenge**
  A. Das, M. Shuaibi, S. Goyal, **A. Kolluru**, J. Lan, A. Palizhati, A. Sriram, B. Wood, A. Grover, D. Parikh, Z. Ulissi, C.L. Zitnick
  Accepted to **NeurIPS 2021**

☰ EXTRACURRICULAR ACTIVITIES

- Served as Sports Secretary of the Board for Sports Activities, IIT Delhi
- Conducted various National debating tournaments as Representative of Debating Club, IIT Delhi
- Represented IIT Delhi in Waterpolo and won Silver medal in 4x100 Medley Relay Aavhan Sports Meet 2018, IIT Bombay
- Won Best Waterpolo Player award twice consecutively in Intra-College competitions of IIT Delhi
- Breaking Adjudicator, Intra-IIT Parliamentary Debate'18   • Breaking Speaker, Intra-IIT Parliamentary Debate'19
- Volunteered for Humanity Foundation that works for the welfare of visually impaired students