SANGEETH BALAKRISHNAN, Ph.D.

○ sbalakri@umd.edu ○ (+1) 515 708 8021

RESEARCH FOCUS

Machine Learning, Generative AI, Physics Informed Machine Learning, Material and Drug Discovery

EDUCATION

2020 – May 2024	**University of Maryland, College Park, USA** Ph.D. in *Mechanical Engineering*, CGPA: 4.00/4.00
2018-2020	**Iowa State University, USA** M.S. (thesis) in *Mechanical Engineering*, CGPA: 4.00/4.00
2013-2015	**Indian Institute of Technology, Madras, India** M. Tech (thesis) in *Mechanical Engineering*, CGPA: 8.91/10
2009-2013	**University of Kerala, India** B. Tech in *Mechanical Engineering*, CGPA: 8.3/10

RESEARCH EXPERIENCE

1. Postdoc at University of Maryland [Sep24–Present]

Applying NLP, Transformers and Physics Informed ML approaches to address challenges in material science.

2. Graduate Research Assistant at University of Maryland [Jan20–May 2024]

Thesis title: Machine Learning under Scarce Data Regime for Design and Discovery of Materials

Worked on *graph-based VAE for joint embedding and constrained local optimization* of molecular data [1,3], objective *GAN's for optimization* [6], *Physics Informed Neural Networks* and *nonlinear time series analysis* embedding methods, *Gaussian Process* [2], *Graph Neural Network, Natural Language Processing, Bayesian Optimization* and variety of *ensemble models* at the intersection of machine learning and molecule discovery.

3. Graduate Research Assistant at Iowa State University [Aug18–Dec19]

Worked on applying *mutlifidelity CNN* and *Graph theory for imaging data* [4], Computer Vision, *RNN encoder decoder* for real-time series prediction [Github-1], *Dual attention RNN* for real time control and other interesting problems using *Double Deep Q-Reinforcement Learning* and *Rotationally Equivariant autoencoder* [Github-2, 3].

4. Design Engineer - Virtual Product Development Division at Caterpillar R&D-India [July15-July18]

Responsible for the development of advanced engineering data analysis software used for structural data analysis and visualization. Provided training, technical support and published technical documents in development and usage of Data Analysis Tool Kit.

5. Graduate Research Assistant at Indian Institute of Technology, Madras [Aug13–July15]

Worked on developing a *continuum electrochemical* model to simulate effects of mechanical degradation in lithium-ion batteries using COMSOL and Mathematica [5], developed *Finite Element Methods* for plane stress-strain-axisymmetric problems, *Weibull analysis* to predict endurance limit from Stress-Cycle curve.

ACHEIVEMENTS

- Outstanding Graduate Assistant Award from University of Maryland, USA.
- Graduate Dean Scholarship from Iowa State University.
- Engineering Data Analysis Software Quality Award from Caterpillar Virtual Products Division USA.
- MMM10 and GSCCM-ECS Travel Awards to present my work at MMM10 Conference in Baltimore, MD, USA, 2022, and at GSCCM ECS Symposium, Chicago, IL, USA, 2023.

TECHNICAL SKILLS

Languages: Python, MATLAB, Mathematica, PV-Wave

Deep Learning packages: PyTorch, TensorFlow, Keras, Scikit-Learn, OpenCV, Pandas, Google Cloud, Docker, FastAPI, Flask, tkinter, Cuda, Langchain, RDkit, LangGraph, Hugging Face, JAX, Code Deployment

PUBLICATIONS

1. **Sangeeth Balakrishnan**, et al. "Locally Optimizable Joint Embedding Framework to Design Nitrogen-rich Molecules that are Similar but Improved." Molecular Informatics 40, no. 7 (2021): 2100011.

2. **Sangeeth Balakrishnan**, et al. Machine learning for shock compression of solids using scarce data. Journal of Applied Physics 21 April 2023; 133 (15): 155902.

3. Hu Yong, Jennifer L. G, R Pesce-Rodriguez, Chi-Chin Wu, Scott D. W, Z Liu, **Sangeeth Balakrishnan** et al. "Releasing chemical energy in spatially programmed ferroelectrics." Nature Communications 13, no. 1 (2022): 6959.

4. Yang Chih-Hsuan, B S S Pokuri, X Y Lee, **Sangeeth Balakrishnan**, et al., "Multi-fidelity machine learning models for structure–property mapping of organic electronics." Computational Materials Science 213 (2022): 111599.

5. Swaminathan Narasimhan, **Sangeeth Balakrishnan**, Kiran George. "Elasticity and size effects on the electrochemical response of a graphite, li-ion battery electrode particle." Journal of The Electrochemical Society 163, no. 3 (2015): A488.

6. **Sangeeth Balakrishnan**, et al., "Material Mixture design using Interpretable ML." submitted to JANNAF.

7. **Sangeeth Balakrishnan**. "Data efficient assimilation of multi fidelity information.", Iowa State University, 2020.

8. **Sangeeth Balakrishnan** "Machine learning in scarce data regime for design and discovery of materials.", UMD.

9. **Sangeeth Balakrishnan**, et al. "Machine Learning of Equation of State for Non-Ideal Materials", submit for review

9. **Sangeeth Balakrishnan**, et al., "Physics Informed ML for Material Performance Prediction", to be submitted

CONFERENCES

1. **Sangeeth Balakrishnan**, et al., "Application of Machine Learning to Predict Shock Compression Response in Notional Unreacted Solids", 10th International Conference on Multiscale Materials Modeling, 2022.

2. **Sangeeth Balakrishnan**, et al., "Ameliorating synthesis and scarce data challenges through joint embedding for high energy molecule generation." Bulletin of the American Physical Society, 2022.

3. **Sangeeth Balakrishnan**, et al., "A Machine Learning Framework to Predict Unreacted Shock Compression Response of Solids Under Scarce Data", 23rd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, 2023.

4. Jesse Hearn, **Sangeeth Balakrishnan**, et al. "Jointly Embedded Machine Learning Approach for Polymer Combustion Properties. “Bulletin of the American Physical Society 67 (2022)