Md Khayrul Islam

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EDUCATION

Lehigh University   Pennsylvania, USA
Ph.D. in Mechanical Engineering and Mechanics; GPA: 3.84/4.00   Jan 2021 − Current
- Awarded P.C. Rossin College of Engineering **fellowship**.

Lehigh University   Pennsylvania, USA
M.S. in Mechanical Engineering and Mechanics; GPA: 3.84/4.00   Jan 2021 − May 2023
Thesis Title: Predicting Drug Loading in Extracellular Vesicles through Coarse-Grained Molecular Dynamics Simulation got published on **PCCP**.

IBM   Online
Professional Certificate in Data Science   Aug 2024
- Mastered data science competencies including Python, machine learning, SQL, data visualization, and AI, culminating in a capstone project..

Bangladesh University Engineering and Technology   Dhaka, Bangladesh
B.Sc. in Industrial and Production Engineering; GPA: 3.55/4.00   Jun 2014 − Oct 2018
Thesis Title: Molecular dynamics simulation of the mechanical properties of CNT-polyoxymethylene composite with a reactive forcefield got published on **Molecular Simulation**
- Awarded SCEA- PTAK prize global case study competition **scholarship**

Programming: Python, C, MATLAB, Bash, SQL, HTML, CSS
ML and DSA: PyTorch, LangChain, Scikit-learn, LLM, Pandas, DSA, ML Algorithms
Simulation: LAMMPS, COMSOL, ANSYS, SolidWorks, EspressoMD
Miscellaneous: CUDA, AWS, Docker, Git, Parallel Computing

WORK AND RESEARCH EXPERIENCE

Lehigh University   Bethlehem, PA
Graduate Research Assistant   Jan 2021 - Present
- Collaborated in a multidisciplinary team to publish 11 Q1 journal papers in computational biology and machine learning, featured in prestigious journals including Nature Communications, ACS, and RSC series.
- Supervised 2 undergraduate and 1 master's students; led 5 multidisciplinary group projects involving students from Bioengineering, Computer Science, and Mechanical Engineering.
- Designed the official **website** and administered lab's **GitHub**, and Slack; managed computational resources including server setup, management, and resource allocation.

Lehigh University   Bethlehem, PA
High-Performance Computing Server Administrator   Jan 2023 - Present
- Administered a high-computing server valued at $500K, funded by **NSF**. Engineered initial setup, optimized for on-demand resource allocation, achieving production-readiness for multi-disciplinary research applications.

GMS Composite Knitting Ind. Ltd.   Dhaka, Bangladesh
Management Trainee   Feb 2019 - Aug 2019
- Developed an Excel VBA automated line balancing algorithm, improving line balancing efficiency by a factor of 15.
- Optimized floor efficiency via Excel VBA, achieving an 8-12% efficiency boost by maximizing total floor productivity with minimal machinery.

PROJECTS

Semi-Supervised Learning   Aug 2023 - Present
Developed and executed a comprehensive project plan, integrating autoencoder and Res-NET technologies with **PyTorch** for the automated clustering of immune cells, thereby enhancing microfluidic sorting processes.

Transformer Based Trajectory Prediction   Jan 2023 - Present
Constructed a Transformer-based machine learning model for predicting cell trajectories in microfluidics, aiding in the optimization of device designs such as DLD.

Multiplex-IML   Jan 2022 - Dec 2023
Developed Multiplex Image Machine Learning (MIML) framework that combines label-free cell images with biomechanical data, achieving 98.3% accuracy in cell classification with potential advancements in disease diagnostics. (Under review)

Bio-FEM   Dec 2022 - Jul 2023
Implemented the Finite Element Method and numerical modeling of biological systems; accepted by **Nature Communications**.

HSC-CNN   *Jul 2021 - Dec 2022*

Implemented deep learning-based predictive identification of functional subpopulations of hematopoietic stem cells with F1 score > 0.8. (Under review at Blood Advances) **Stem Cell Research & Therapy**

COVID-FVM   *Dec 2020 - Jul 2021*

Conducted a 6-month study on COVID-19 droplet dynamics using FVM, leading to safer healthcare practices through optimized surface wettability. Featured on the **Journal of Applied Physics** cover.

PUBLICATIONS

1. Yaling; Jagota Wu, Yue; **Khayrul Islam** ; Liu. Microdroplet resuspension off surfaces. *ACS Langmuir*, [Under review]

2. **Khayrul Islam**, Ratul Paul, Shen Wang, and Yaling Liu. Miml: Multiplex image machine learning for high precision cell classification via mechanical traits within microfluidic systems. *ACS Journal of Chemical Information and Modeling*, [Under review]

3. Mehedi Hasan, **Khayrul Islam**, and AKM Masud. Tailoring polyamide nanocomposites: The synergistic effects of swcnt chirality and maleic anhydride grafting. *ACS Applied Engineering Materials*, 2024

4. Yuwen Zhao, Yue Wu, **Khayrul Islam**, Ratul Paul, Yuyuan Zhou, Xiaochen Qin, Qiying Li, and Yaling Liu. Microphysiologically engineered vessel-tumor model to investigate vascular transport dynamics of immune cells. *ACS Applied Materials Interfaces*, 16(18):22839–22849, 2024

5. Shen Wang, Jianzhong Han, Jingru Huang, **Khayrul Islam**, Yuheng Shi, Yuyuan Zhou, Dongwook Kim, Jane Zhou, Zhaorui Lian, Yaling Liu, et al. Deep learning-based predictive classification of functional subpopulations of hematopoietic stem cells and multipotent progenitors. *Stem Cell Research Therapy*, 15(1):74, 2024

6. Yue Wu, Yuwen Zhao, **Khayrul Islam**, Yuyuan Zhou, Saeed Omidi, Yevgeny Berdichevsky, and Yaling Liu. Acoustofluidic engineering of functional vessel-on-a-chip. *ACS Biomaterials Science Engineering*, 9(11):6273–6281, 2023

7. Ratul Paul, Yuwen Zhao, Declan Coster, Xiaochen Qin, **Khayrul Islam**, Yue Wu, and Yaling Liu. Rapid prototyping of high-resolution large format microfluidic device through maskless image guided in-situ photopolymerization. *Nature Communications*, 14(1):4520, 2023

8. Anshu Raj, Sk Md Ahnaf Akif Alvi, **Khayrul Islam**, Mohammad Motalab, and Shuozhi Xu. An atomistic study of the tensile deformation of carbon nanotube–polymethylmethacrylate composites. *Polymers*, 15(13):2956, 2023

9. Yue Wu, Yuwen Zhao, Yuyuan Zhou, **Khayrul Islam**, and Yaling Liu. Microfluidic droplet-assisted fabrication of vessel-supported tumors for preclinical drug discovery. *ACS Applied Materials Interfaces*, 15(12):15152–15161, 2023

10. **Khayrul Islam**, Meghdad Razizadeh, and Yaling Liu. Coarse-grained molecular simulation of extracellular vesicle squeezing for drug loading. *Physical Chemistry Chemical Physics*, 25(17):12308–12321, 2023

11. Yue Wu, Yuyuan Zhou, Ratul Paul, Xiaochen Qin, **Khayrul Islam**, and Yaling Liu. Adaptable microfluidic vessel-on-a-chip platform for investigating tumor metastatic transport in bloodstream. *Analytical Chemistry*, 94(35):12159–12166, 2022

12. Mehdi Nikfar, Ratul Paul, **Khayrul Islam**, Meghdad Razizadeh, Anand Jagota, and Yaling Liu. Respiratory droplet resuspension near surfaces: Modeling and analysis. *Journal of Applied Physics*, 130(2), 2021

13. **Khayrul Islam**, Sourav Saha, and AKM Masud. Molecular dynamics simulation of the mechanical properties of cnt-polyoxymethylene composite with a reactive forcefield. *Molecular Simulation*, 46(5):380–387, 2020

CONFERENCE PRESENTATIONS

1. **Khayrul Islam**, Yuwen Zhao, Shen Wang, and Yaling Liu. Machine learning based classification of cells by mechanical properties in microfluidic device. *48th Annual Northeast Bioengineering Conference (NEBEC 2022) (April 2022), Columbia University, New York City, New York*, 2022

2. **Khayrul Islam**, Tahreen Nabila, and AKM Masud. Investigation of the mechanical properties of polypropylene /carbon nanotube composite by molecular dynamics simulation. *13th International Conference on Mechanical Engineering, Dhaka, Bangladesh*, 2019