BOLUTITO BABATUNDE

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EDUCATION

Carnegie Mellon University

Doctor of Philosophy in Mechanical Engineering Master of Science in Mechanical Engineering December 2022 Advisors: Dr. Rebecca E Taylor, Dr. Jonathan Cagan GPA: 3.96 / 4.0

Texas Tech University

Bachelor of Science in Mechanical Engineering Minor: Computer Science, Mathematics GPA: 3.90 / 4.0

SKILLS

Languages: Python, C++ (OpenGL), Git Frameworks: PyTorch, AWS, NumPy, Pandas, SciPy, Trimesh, Plotly, oxDNA MD Simulation, oxDNA-analysis-tools, Agarose Gel Electrophoresis, Atomic Force Microscopy, DNA Nanotechnology Software: ChimeraX, CaDNAno, Scadnano

PHD RESEARCH

Carnegie Mellon University THESIS

Investigating a flexible framework for automating multilayer DNA origami design

- Developing a computational casting technique to automate solid and hollow DNA origami designs by casting a long single-stranded DNA (ssDNA) around or within a triangular mesh leveraging generative optimization strategies (i.e shape annealing)
- Integrating an adjustable ssDNA axis orientation feature to enhance design capabilities, influence structural density, uniformity, and generating novel routing patterns
- Created custom Python algorithms to convert generated designs into formats compatible with standard bioinformatic tools, scadnano, caDNAno and oxDNA
- Developed a custom Python stapling algorithm to efficiently automate routing of hundreds of short oligonucleotides (or ssDNAs) to cinch long ssDNA routing patterns generated by computational casting technique
- Supervising an in-house lab technician to manufacture and characterize designs using gel-electrophoresis and collaborating with an Assistant Professor at University of Pittsburgh to ensure formation with transmission electron microscopy (TEM)
- Partnering with a PhD student to create new lab website and maintain Ubuntu 20.04 lab server and Amazon Web Services (AWS) Elastic Compute Cloud (EC2) instances for lab members

ACADEMIC PROJECTS

(LTI-11685) Introduction to Deep Learning

PROTEIN LANGUAGE MODELING: CODING LIFE'S CODE

- Teamed up with master's student to modify the PyTorch-based SPOT-1D-LM model by incorporating ProteinBERT embeddings and integrating additional ResNet layers for single sequence analysis to investigate protein structurefunction relationship
- Utilized modified SPOT-1D-LM to classify eight-state labels for protein secondary structure (SS8), achieving comparable accuracy, including on challenging Neff1-2020 set with no homologs (69.07%)
- Conducted an ablation study to eliminate overfitting by introducing weight decay and L1 regularization, leading to improved performance and validation loss stability from 5th epoch onward

(MEG-24787) Machine Learning and AI for Engineers

CLASSIFYING SCAFFOLD ROUTINGS OF DNA ORIGAMI DESIGNS

- Implemented a custom convolutional neural network (CNN) utilizing PyTorch for gap detection in cross-sectional view images of hollow designs produced by computational casting technique
- Partnered with PhD student to develop a custom CNN, achieving 73% accuracy for encapsulated ssDNA designs, outperforming VGG16 (86%) and ResNet50 (78%) showed increased loss after 20 epochs
- Improved accuracy to 92% by reclassifying dataset into three classes: large gap, small gap, and encapsulated

Pittsburgh, PA August 2024 (Expected)

> Lubbock, TX May 2019

Pittsburgh, PA

August 2019 - August 2024

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Pittsburgh, PA

August 2023 - December 2023

August 2022 - December 2022

Pittsburgh, PA

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ADDITIONAL RESEARCH EXPERIENCE

Los Alamos National Laboratory

ATHENA SCHOLAR GRADUATE INTERN

- Constructed a functional prototype of a temperature controller connected to a chamber for heating specimens using Programmable Logic Controller (PLC) programmed with LABVIEW (systems engineering software) for remote system operation
- Designed temperature controller parts for machining with Creo (3D modeling software)
- Leveraged Robotic Operating System (ROS) and Movelt to program a robotic arm to grab object for heating

Texas Tech University

UNDERGRADUATE RESEARCH INTERN

- Created a flexible, sensitive, and wearable strain sensor using a silver nanowire (AgNW) pattern etched between two layers of polydimethylsiloxane (PDMS) for monitoring biomedical disorders
- Developed a custom Arduino algorithm in C for data acquisition customized for detecting resistive strain .
- Characterized strain sensor by formulating and building a mechanical device to simulate stretch/release cycles in 1 cm increments and bending cycles in 10 degree increments

Los Alamos National Laboratory

FUTURE FEMALE LEADERS IN ENGINEERING UNDERGRADUATE INTERN

- Constructed a functional prototype of a temperature controller using Proportional-Integral-Derivative (PID) tuning connected to heating mantle for specimens requiring carefully regulated heating
- Optimized electrical wiring and designed detailed wiring diagram for temperature control system with 2 thermocouples to measure temperature of heated specimens
- Acquired data of temperature response with LABVIEW and designed temperature controller parts for machining with Creo

TEACHING ASSISTANT EXPERIENCE

Carnegie Mellon University

NANOSCALE MANUFACTURING USING STRUCTURAL DNA NANOTECHNOLOGY

- Conducting workshops to introduce 15 students to bioinformatics tools in DNA origami, including caDNAno. scadnano, and oxDNA MD simulation
- Managing user accounts and overseeing AWS EC2 instances for 15 students to host downloaded bioinformatic tools
- Conducting office hours to help students design complex DNA origami nanostructures with lengths of 1000+ bases

Carnegie Mellon University

FUNDAMENTALS OF MECHANICAL ENGINEERING

- Prepared homework, guizzes, and exam problems to introduce and facilitate learning of fundamental mechanical engineering topics to 100+ undergraduate students
- Coordinated efforts with 1 faculty member and 1 teaching assistant to design comprehensive assessments with corresponding rubric and solutions, ensuring alignment with learning objectives

PUBLICATIONS

- Babatunde, Bolutito; Cagan, Jonathan; Taylor, Rebecca E. (2024). "An Improved Shape Annealing Algorithm for the Generation of Coated Deoxyribonucleic Acid Origami Nanostructures." ASME Journal of Mechanical Design. 146, no. 5: 051708. https://doi.org/10.1115/1.4064242 (Special Issue of the ASME Journal of Mechanical Design featuring top papers from IDETC 2023)
- Babatunde, Bolutito; Arias, Sebastian D.; Cagan, Jonathan; Taylor, Rebecca E. (2021). "Generating DNA Origami Nanostructures through Shape Annealing." Applied Sciences. 11, no. 7: 2950. https://doi.org/10.3390/app11072950
 - This paper introduces a novel approach to DNA origami design, overcoming limitations of current automated tools that primarily adopt a top-down approach. The novel approach uses the shape annealing algorithm to create a language that defines the relationships between sections of a long DNA strand and drives the language towards a preferred configuration. This method increases design complexity and codes unique characteristics into structures.

CONFERENCES / PRESENTATIONS

Benjaminson, Emma; Babatunde, Bolutito; Cagan, Jonathan; Taylor, Rebecca E. (24-27 September 2023). "Towards a Graph Neural Network Capable of Realistically Predicting DNA Nanostructure Equilibrium Dynamics" 2nd IACM Mechanistic Machine Learning and Digital Engineering for Computational Science, Engineering and Technology Symposium (MMLDE-CSET), University of Texas at El Paso, El Paso, TX, USA

Los Alamos, NM

Lubbock, TX

May 2018 - August 2018

Pittsburgh, PA January 2024 - Present

Pittsburgh, PA

January 2022 - May 2022

Los Alamos, NM May 2019 - August 2019

January 2018 - May 2019

- Babatunde, Bolutito; Cagan, Jonathan; Taylor, Rebecca E. (20-23 August 2023). "An Improved Shape Annealing Algorithm for the Generation of Coated DNA Origami Nanostructures." International Design Engineering Technical Conferences and Computers and Information in Engineering Conference (IDETC/CIE 2023), Boston Park Plaza, Boston, MA, USA
- Babatunde, Bolutito; Cagan, Jonathan; Taylor, Rebecca E. (8-12 August 2022). "A Refined Shape Annealing Algorithm for the Optimal Generation of DNA Origami Designs." DNA28: The 28th International Conference on DNA Computing and Molecular Programming (Track C), University of New Mexico, Albuquerque, NM, USA
- Babatunde, Bolutito; Cagan, Jonathan; Taylor, Rebecca E. (4 March 2022). "A Formal Automated Approach for Controlling the Wall Thickness of Coated DNA Origami Designs." 2022 PhD Research Symposium, Carnegie Mellon University, Pittsburgh, PA, USA. (Best poster award in MicroNano Research)
- Babatunde, Bolutito; Arias, Sebastian D.; Cagan, Jonathan; Taylor, Rebecca E. (12-15 April 2021). "A Formal Approach for Automated Generation of DNA Origami Designs." FNANO 2021: 18th Annual Conference Foundations of Nanoscience (Computational Tools), Virtual

AWARDS AND HONORS

MEOS (Mechanical Engineering Outreach Stars) Award - Silver LevelJune 2022Department of Defense (DoD) National Defense and Engineering Graduation Fellowship Program (NDSEG)March 2021National Science Foundation (NSF) Graduate Research Fellowship Program (GRFP), Declined.March 2021National Consortium for Graduate Degrees for Minorities in Engineering and Science (GEM) FellowshipMarch 2021

VOLUNTEER EXPERIENCE

Mechanical Engineering Graduate Student Organization (MEGSO) Social Chair	July 2022 - May 2023
2023 National Biomechanics Day at Carnegie Mellon University, Pittsburgh, PA	March 2023
2022 National Biomechanics Day at Carnegie Mellon University, Pittsburgh, PA	March, April 2022
5 th Summer Physics Camp for Young Women (LANL), Virtual	June 2021
2021 National Biomechanics Day at Carnegie Mellon University, Pittsburgh, PA	March 2023
Gelfand Outreach Workshop – Nanoengineering with DNA, Pittsburgh, PA	November 2019
Carnegie Science Center Sci Tech Day – Nanoengineering with DNA, Pittsburgh, PA	November 2019

REFERENCES

Dr. Jonathan Cagan David and Susan Coulter Head of Mechanical Engineering George Tallman and Florence Barrett Ladd Professor Associate Director, Human+AI Design Initiative Carnegie Mellon University 5000 Forbes Avenue, Pittsburgh, PA 15213 <u>cagan@cmu.edu</u> Relationship: Academic Advisor

Dr. Rebecca Taylor

ANSYS Career Development Chair of Engineering Associate Professor in Mechanical Engineering Carnegie Mellon University 5000 Forbes Avenue, Pittsburgh, PA 15213 <u>bex@cmu.edu</u> Relationship: Academic Advisor

Dr. Philip LeDuc

William J. Brown Professor, Mechanical Engineering Director, Center for the Mechanics and Engineering of Cellular Systems Carnegie Mellon University 5000 Forbes Avenue, Pittsburgh, PA 15213 <u>prleduc@cmu.edu</u> Relationship: Committee Member