HEMI

HOPKINS EXTREME
MATERIALS INSTITUTE

Student Research Internships and Apprenticeships

Summer 2020

JOHNS HOPKINS
UNIVERSITY

From the HEMI Director

Each summer, the Hopkins Extreme Materials Institute (HEMI) at Johns Hopkins University offers a number of opportunities for high school, undergraduate, and graduate students to conduct research both within HEMI as well as at our partner institutions. Despite COVID-19, the summer of 2020 was no different. The internships we offer are competitive, and I am always impressed by the quality of our applicants. These exciting internships provide the students experience with state-of-the-art research techniques and provide the opportunity for individual mentorship. Students gain valuable insights into university-led research, which we hope will inspire them to pursue a future career in a STEM-related field.

Given the pandemic, all of our internships had to be conducted completely remotely this year. I am extremely proud of the students and the research activities they accomplished under these constrained circumstances! I am also grateful to the faculty hosts, mentors, and administrative personnel who ensured the students had the resources and received the guidance needed for a rich and rewarding experience. HEMI would like to acknowledge the following organizations who made these opportunities possible: the Army Educational Outreach Program, the CCDC Army Research Laboratory and Army Research Office, the National Endowment for the Arts, the Maryland Institute College of Art, and The Whiting School of Engineering at Johns Hopkins University. The summaries included herein (written entirely by the students) provide a glimpse of the hard work they accomplished within a short period of time. I hope this encourages students to apply in 2021!

Sincerely,

KT Ramesh
Director
Alonzo G. Decker Chair Jr. Professor of Science and Engineering

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HEMI Administration Supporting these Programs

Lori Graham-Brady
Associate Director

Victor Nakano
Executive Prog. Dir.

Bess Bieluczyk
Sr. Admin. Coord.

Jess Ader
Sr. Comm. Specialist

Research and Engineering Apprenticeship Program (REAP)

REAP is a summer STEM program that places talented high school students, from groups historically under-represented and underserved in STEM, in research apprenticeships at JHU. REAP apprentices work under the direct supervision of a mentor on a hands-on research project. REAP apprentices are exposed to the real world of research, gain valuable mentorship, and learn about education and career opportunities in STEM. REAP apprenticeships are 5-8 weeks in length (minimum of 200 hours) and apprentices receive a stipend.

Program Goals

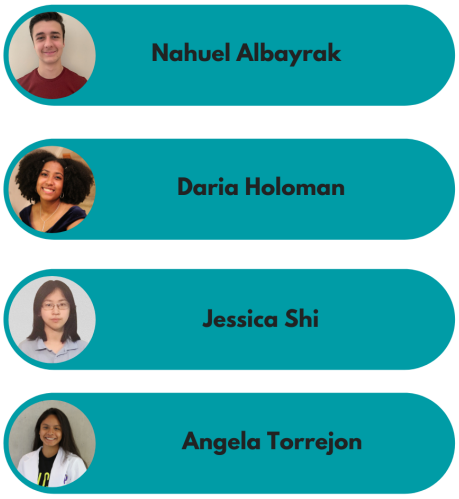
- To provide high-school students from groups historically under-represented and underserved in STEM, including alumni of the AEOP's UNITE program, with an authentic science and engineering research experience;
- To introduce students to the Army's interest in science and engineering research and the associated opportunities offered through the AEOP;
- To provide participants with mentorship from a scientist or engineer for professional and academic development purposes; and
- To develop participants' skills to prepare them for competitive entry into science and engineering undergraduate programs.

Funding Sponsor

Army Educational Outreach Program, administered by the Rochester Institute of Technology

Website Information

https://www.usaeop.com/program/reap/



2020 REAP Students

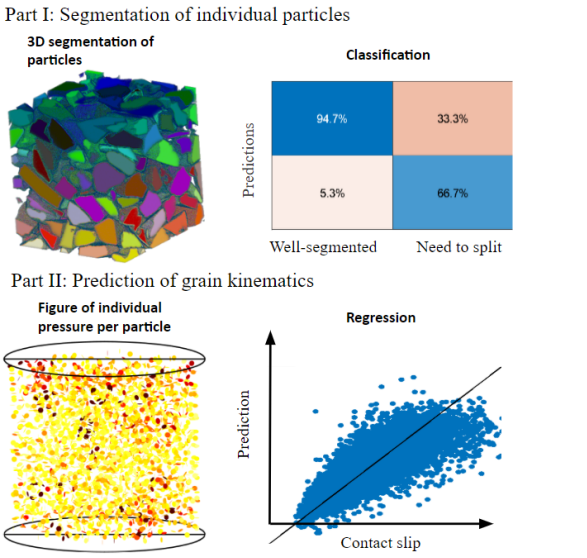
Nahuel Albayrak

Chesapeake Science Point High School, Hanover, Maryland
Mentor: Chongpu Zhai
Faculty Host: Professor Ryan Hurley
Department of Mechanical Engineering
Johns Hopkins University

Project Title: Application of Machine Learning in Granular Material

Machine learning was employed to investigate particle micromechanics of granular materials. Training data used in this study was extracted from X-Ray Computed Tomography (XRCT) and 3D X-ray diffraction (3DXRD) tests by Hurley's group in synchrotron facilities, for a range of stressed granular packing. In Part I of this REAP program, classification models were

implemented for improving segmentation in XRCT images of angular quartz packing. Particle segmentation is essential in characterizing packing structure and particle kinematics in tested samples. Classification models were used to identify particles needed to be split or merged in pre-segmented XRCT images with water-shed method. Wrongly segmented particles were manually labelled as training outputs and features extracted from local voxel values in XRCT images were used as training inputs. For implemented models, the prediction accuracy of K-nearest Neighbor was 94.7 % for particles needed to be merged and 66.7% for particles to be split. In Part II, X-ray measurements of three packing of ruby spheres with different levels of lateral confinement were considered. Regression models were used to predict local particle rearrangement represented by inter-particle slip, which was calculated based on X-ray measurements. Training input included 135 variables in previous loading steps including relative particle locations, particle fabric, particle-resolved stress, particle translation and rotation. Among different models, median-Gaussian Support Vector Machine yielded a prediction with the coefficient of determination of 0.73.



Daria Holoman

Springbrook High School, Silver Spring, Maryland
Mentor: Dylan Madisetti
Faculty Host: Professor Jaafar El-Awady
Department of Mechanical Engineering
Johns Hopkins University

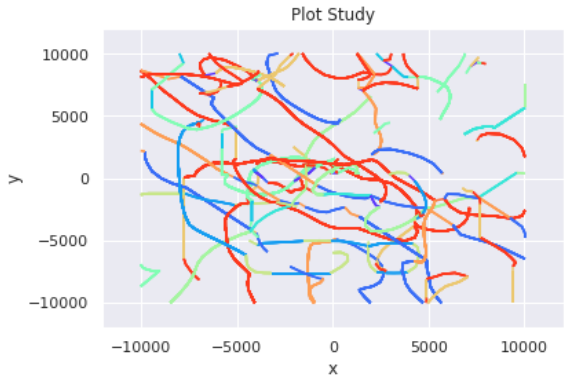
Project Title: Plotting for Discrete Dislocation Dynamics

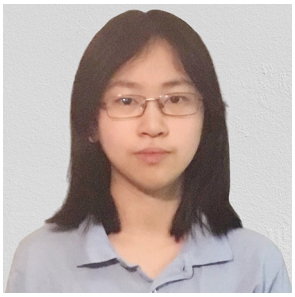
Dislocations are a defect in the crystal structure that can move around on a slip plane. Over time, as the dislocations grow and move around, it weakens the material. So, it is important to track these dislocations so that engineers are able to predict the stability of the different materials over time. While tracking discrete dislocations, the data was being exported into Paraview, a separate program used to visualize data. This process was time consuming and made it difficult to view the dislocations and data at the same time, because they are in two different programs.

For this project, the goal was to create a program that allows the dislocations to be viewed directly in Jupyter, an online platform where code can be developed and shared. Two classes were created using Python, the Graph class and the Plotter class. The Graph class uses Depth First Search (DFS) to traverse the dislocation information and collect dislocation lines. Depth First Search also assigns colors to the dislocations based

off of their slip planes. The Plotter class plots in 2D and 3D based on the timestep(s) given. The library Ipyvolume is used to create the 3D plots, and the library Matplotlib is used to create the 2D plots.

Over the course of this internship I was able to successfully develop a program that plots the dislocations directly in Jupyter in 2D and 3D. Opening the data in Paraview takes a total of 30 seconds, while using Jupyter takes 15 seconds. By plotting directly in Jupyter, it saves time and is more efficient than having to export the data into Paraview. The next step for working on this project would be to be able to export a movie file directly in Jupyter that shows the dislocations growing over the different timesteps.





Jessica Shi

Thomas S. Wootton High School, Rockville, Maryland
Mentor: Marco Galvani
Faculty Host: Professor Mark Robbins
Department of Physics and Astronomy
Johns Hopkins University

Project Title: Molecular Dynamic Simulations to Measure Pressure and Rate Dependence of a Simple Hydrocarbon Fluid

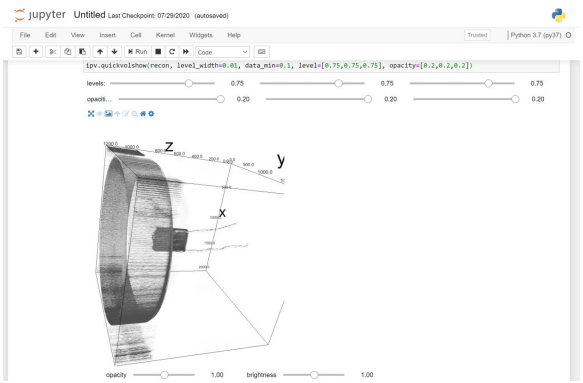
The viscous properties of lubricant fluids are important for determining the amount of heat dissipation during lubrication. In the elastohydrodynamic lubrication regime, the dominating contribution comes from the pressure dependence of the Newtonian viscosity. Recent work in the literature has focused on measuring this dependence with both experimental and computational techniques for different fluids. While molecular dynamics (MD) simulations cannot presently reach the Newtonian regime of viscosity at high pressures, it is possible to measure viscosity at high rates and extrapolate to the Newtonian regime using a model of shear thinning. We use MD simulations to measure the pressure and rate dependence of a simple hydrocarbon fluid (2,2,4-trimethylhexane) using a potential parameterized for high-pressure simulations. Our simulations are able to reproduce previously reported results and the literature and could be extended to other hydrocarbon fluids.

Angela Torrejon

Connelly School of the Holy Child, Potomac, Maryland
Mentor: Lucas Pressley
Faculty Host: Professor Tyrel McQueen
Department of Chemistry
Johns Hopkins University

Project Title: Micro-CT Reconstruction in the Jupyter notebook

The study of solid-state materials and their properties is done to understand the interactions within quantum materials and to find possible uses for such materials in today's world. This study is best done with single crystals as high-quality single crystals allows for detailed investigation. These crystals are formed with a flux growth, which is a method that obtains crystals by cooling a hot molten liquid of the desired compound dissolved in a solvent. One problem is that flux could be incorporated into the sample which can interfere with analysis of the crystal. However, you can use Micro-ct to detect such flux. Micro-ct is a nondestructive, powerful method used to characterize objects in three dimensions which allows the user to view the full sample. Mico-ct is a useful technique used to look at defects in crystals. It involves three parts: the sample, the source, and detector. The source is shot through the sample and measured on the detector. Mico-ct data is collected rotating the sample relative to the source and the detector and taking many snapshots from many different angles. Each snapshot measures the absorption of the x rays of the sample. One is able to take a large series of 2-dimensional series from a range of angles, back out and reconstruct the dimensional version of the data. However, such data is typically reliant on a commercially licensed software which takes up a lot of storage. To solve this, a Jupyter notebook was designed through Sciserver to be able to reconstruct acquired Micro-ct data, visualize and calculate parameters from the data. This allows users to use this open source and access data in a facilitated manner without using up storage. Some future goals to work on would be to further calculate parameters from the data, add on to the code for more options for visualizing three-dimensional data, and to ultimately use the Jupyter notebook as a tool to examine single crystals.



Undergraduate Research and Apprenticeship Program (URAP)

URAP provides undergraduate students with an authentic science and engineering research experience alongside university researchers sponsored by the Army Research Office. Through this commuter program, students will develop skills in Army critical science and engineering research areas in a university lab setting to prepare them for the next steps of their educational and professional career.

The US Army established the Center for Materials in Extreme Dynamic Environments (CMEDE) to design, develop and test improved soldier protection materials. JHU leads the CMEDE collaborative research alliance, which includes university and research institutions across the United States, the United Kingdom, Switzerland, and Germany. Together these partners, in close collaboration with the CCDC Army Research Laboratory, serve a vital role as a materials-by-design capability for the US Army. URAP opportunities within CMEDE are available at universities performing research on this program.

Students receive an educational stipend and contribute to the Army's research in the laboratory while learning research methods, using advanced research equipment and becoming a part of an active research group. This authentic experience provides exposure to science and engineering research careers.

Program Goals

- Provide authentic science and engineering research experience to undergraduate students pursuing science and engineering majors;
- Introduce students to the Army's interest and investment in science and engineering research and the associated educational opportunities available through the AEOP and DoD;
- Provide participants with experience in developing and presenting scientific research;
- Provide participants with experience to develop an independent research program in preparation for research fellowships, graduate school, and careers in science and engineering research;
- Benefit from the expertise of a scientist or engineer as a mentor for professional and academic development purposes; and
- Develop students' skills and background to prepare them for professional and academic development purposes.

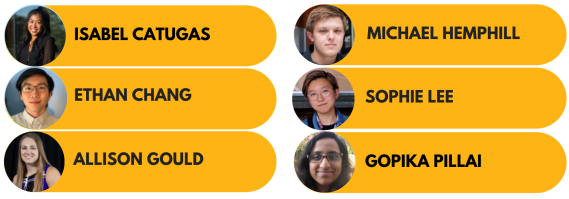
Funding Sponsor

Army Research Office through the Army Educational Outreach Program and the Center for Materials in Extreme Dynamic Environments

Website Information

URAP - https://www.usaeop.com/program/urap/

CMEDE - https://hemi.jhu.edu/cmede/



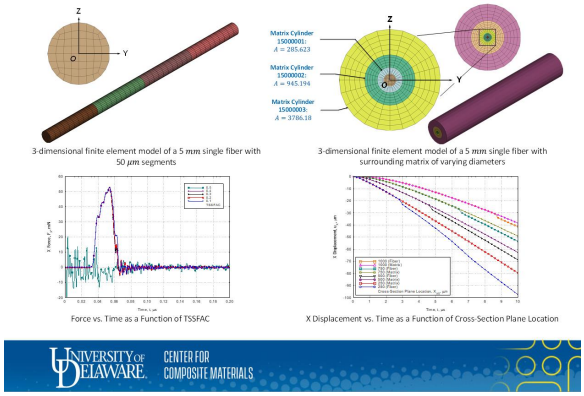
2020 URAP Students

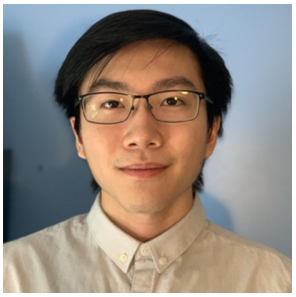
Isabel Catugas

University of Delaware, Newark, Delaware
Faculty Host& Mentor: Professor Bazle Haque
Department of Mechanical Engineering and
Center for Composite Materials
University of Delaware

Project Title: Micromechanical Modeling of Axial Tension Behavior of Unidirectional Composites

This research studies the behavior of two single fiber finite element models and a 5 mm multi-fiber unidirectional composite under axial tension. Two micromechanical finite element models of a 5 mm single fiber with and without surrounding matrix have been developed to validate the fiber fracture and fiber-matrix interface fracture behavior. A time step study is also performed to determine an appropriate time step scale factor for use in future simulations. The single fiber model is implemented into the 5 mm multi-fiber unidirectional composite after the fracture behaviors are validated and additional axial tension simulations will be conducted.





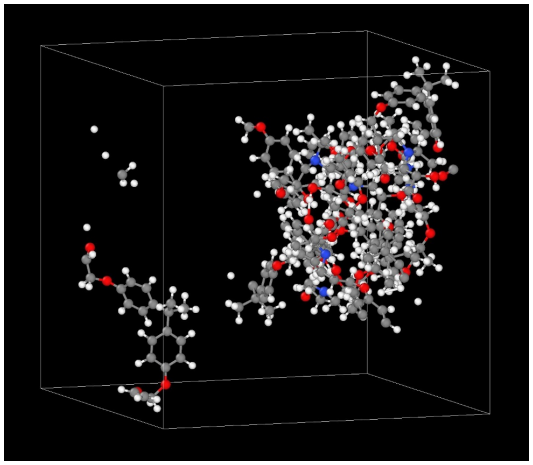
Ethan Chang

University of Delaware, Newark, Delaware
Mentor: Dr. Sanjib Chowdhury
Faculty Host: Professor John Gillespie
Department of Mechanical Engineering and
Center for Composite Materials
University of Delaware

Project Title: Developing Accelerated ReaxFF Framework for Epoxy Curing Reaction within LAMMPS

Epoxide-amine curing reactions affect the properties of thermoset epoxy resins as well as their composite materials. Molecule Dynamics (MD) simulation is a more viable way to simulate these reactions to understand the reaction kinetics and structure-properties relationship of epoxy resins. Commercial software such as Software for Chemistry & Materials (SCM) exist, but they are expensive and not always easily accessible. Therefore, we are developing an accessible reactive MD framework using open source LAMMPS that can run simulations for testing epoxy-amine reactions. In the accelerated ReaxFF procedure that we are implementing, we initially identify the reacting carbon and oxygen on the epoxide group and the reacting nitrogen and hydrogen of the amine group. Then, utilizing the LAMMPS-Python library, we 'bond boost' the reacting atoms by applying a restraint energy when they are

within a certain distance of one another. This method is incredibly efficient and decreases the time it takes to cure.



Allison Gould

Rutgers University, Piscataway, New Jersey
Faculty Host & Mentor: Professor Richard Haber
Department of Materials Science & Engineering
Rutgers University

Project Title: The Development of Photocurable Resin

Initially, material formulation, processing and characterization techniques were learnt and applied on metal inks for Additive Manufacturing. In the lab, safety protocols were followed. Then, COVID-19 caused a hindrance to in-person lab work and forced us to work remotely. This was disappointing to hear at first, however, the benefits of a remote experience were made clear. Scientific literature was read and summarized so that the average person could understand the process and the materials used in photopolymerization printing. In addition, formulation and testing criteria of photopolymer slurries were explored. Also, professional-looking graphs that communicated data in a visually compelling way were created. These 115 graphs were compiled and analyzed in a 75-slide report. Lastly, communication, teamwork, collaboration, and presentation skills were gained.

Michael Hemphill

University of Delaware, Newark, Delaware
Mentor: Dr. Sanjib Chowdhury
Faculty Host: Professor John Gillespie
Department of Mechanical Engineering and
Center for Composite Materials
University of Delaware

Project Title: The Effect of Surface Roughness on Glass-Silane-Epoxy Interphases

In this study, the interaction of epoxy resin with the glass fiber (silica) surface in the presence of monolayer glycidoxypropyltrimethoxy silane (GPS) is studied using molecular dynamics (MD) simulations while accounting for realistic surface roughness. Previous studies have studied these same interactions, but did so with perfectly flat, small glass surface using periodic boundaries. Previous simulation results indicate that the presence of silane in the fiber-epoxy interphase significantly improves composites performances. In the absence of silane, fiber-epoxy non-bonded (i.e., no direct chemical bond) interaction is very weak, and failure is at the fiber surface. However, presence of silane increases the covalent bonding interactions in the fiber-epoxy interphase. As a result, composite strength and energy absorption capability improves significantly by increasing the number of bond sites at the fiber surface and promoting progressive failure through multiple damage modes. In this study, real-world data of a glass fiber surface was gathered from AFM experiment, and this surface was replicated in the atomistic model. This realistic surface was than altered to allow it to be used periodically. At this point monolayer GPS was added to the surface in several concentrations and the model was further prepared using general AMBER force field. Moving forward, the composite model will be loaded in tension (Mode-I), shear (Mode-II) and mixed-mode with the reactive force field ReaxFF to investigate the effects of surface roughness on interphase properties. This rough surface will also be used to investigate the effects of hydrostatic pressure and friction in Mode-II loading.

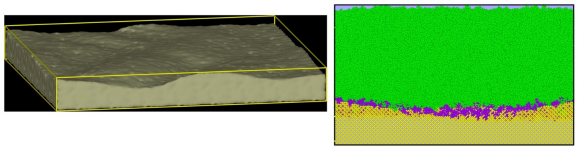


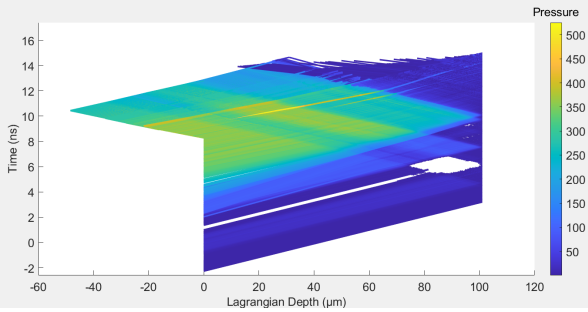
Figure: Rough fiber surface (left) and atomistic fiber-matrix interphase model (right).

Sophie Lee

Johns Hopkins University, Baltimore, Maryland
Faculty Hosts: Professor June Wicks
Department of Earth and Planetary Sciences
Johns Hopkins University
and
Professor Todd Hufnagel
Department of Materials Science and Engineering
Johns Hopkins University

Project Title: Pressure history in ramp-compressed Fe using the method of characteristics

Ramp compression experiments were carried out on thin FeSi targets, utilizing diamond windows; however, only free surface pressure profile data can be collected during these experiments. This project aimed to create or alter a code to map the pressure history of ramp compression experiments using the method of characteristics, a method that is able to plot intersections of "wavelets" in ramp compression by using pressure profile data collected during the experiment and equation of state (EOS) data of the material(s). In this context, ramp compression is defined as gradual quasi-isentropic compression, and can be discretized into wavelets. These wavelets travel at increasing sound speeds as they propagate through the sample. Existent matlab code that was able to calculate the characteristics of wavelets and plot the pressure history of example free surface and EOS data was used in order to understand how the method of characteristics solved for the intersections of wavelets. This code was altered to be able to intake data collected during a ramp compression experiment. This altered code was able to incorporate free surface ramp compression data and map the approximated pressure history for a model sample stack. By being able to map pressure history, this code will give a more accurate calculation of pressure for ramp compression experiments.



Gopika Pillai

University of Houston, Houston, Texas
Mentor: Connor Bradfield
Faculty Host: Professor KT Ramesh
Department of Mechanical Engineering
Johns Hopkins University

Project Title: Creating Axons for the Mesoscale Brain Model & Analyzing Progression of Traumatic Brain Injury on a Mesoscale

Current research treats brain tissue homogenously when analyzing deformation and mechanics of Traumatic Axonal Injury at the continuum level. This is problematic since injury initiates at the cellular level. More sophisticated modeling techniques are required to determine the distribution of axonal strains at smaller length scales where structural heterogeneity is more pronounced. My research consisted of two objectives: (1) develop MATLAB code to generate idealized axon geometries for future computational models and (2) conduct literature reviews of potential brain injury mechanisms that occur at smaller length scales (i.e. the mesoscale and microscale). For my first research objective, I developed automated code to create cylindrical-like axons such that their random path stays within the white matter's curved boundaries in a mouse brain. However, even one axon varies in width and composition throughout

its length, hence the axonal response to TBI could potentially differ in distinct areas of the brain. This idea supports research of the axonal lipid bilayer membrane revealing that the membrane develops instantaneous pores in response to TBI (Montanino et al., 2020). Additionally, recent research has demonstrated that neuronal, but not glial cells, developed significant pores in its membrane six hours post-TBI, suggesting that neurons possess a unique signaling mechanism over the evolution of injury (Hernandez et al., 2020). The blood-brain barrier (BBB) is also significantly affected by different TBI models, as signaling between pericytes and endothelial cells lining the BBB is down-regulated. Consequently, BBB integrity is compromised, decreasing protein expression along the basement membrane, creating pores such that blood serum proteins leak into the BBB, and neuronal and glial cell markers leak into the blood. Interestingly, the BBB and neuronal membranes have specific resealing periods. The neuronal membrane indicated resealing properties one-week post-injury. However, pericyte-endothelium signaling was shown to increase at 12 hours post-injury, implying that the BBB might be retightening itself (Bhowmick et al., 2019).

This heterogeneity of brain structures can project to a larger scale, hence for future computational mesoscale models, TBI should be viewed as a progression of multiple pathways, involving signal cascades of neurons, glia, vasculature, as well as axonal deformation.

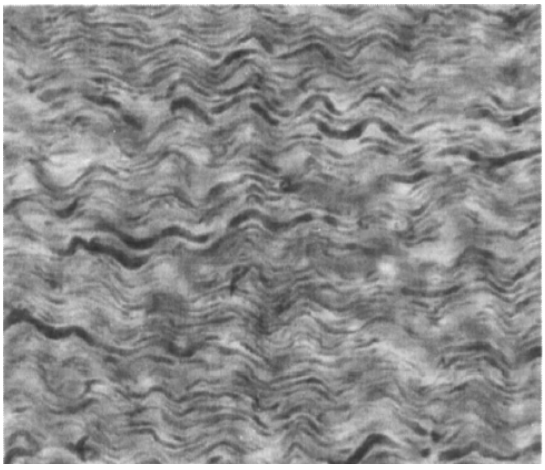


Figure (a) Undulated appearance of axonal microstructure in the guinea pig optic nerve (Bain et al., 2003).

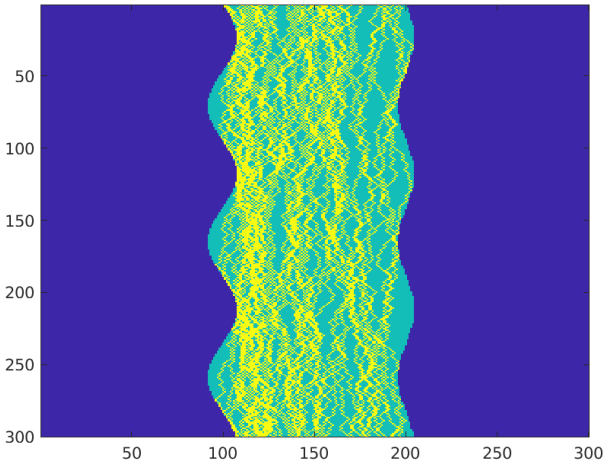


Figure (b) 2-D view of 50 axons taking randomized paths within the curvature of the white matter (cyan), separated from the gray matter (purple). This was generated in MATLAB and is useful for future computational brain models.

Extreme Science Internships (ESI)

ESI provides opportunities for Morgan State University (MSU) students to participate in both internal and external internships associated with the Center for Materials in Extreme Dynamic Environments (CMEDE). ESI are STEM-focused with a particular emphasis on providing research opportunities related to MEDE, a basic research program focused on designing, developing and testing improved soldier protection materials.

ESI is open to undergraduate and graduate students in MSU's School of Computer, Mathematical, and Natural Sciences and the School of Engineering.

Internal ESI are hosted by MSU faculty on the campus of Morgan State University. External ESI are conducted at one of the CMEDE university and research institutions located across the United States, the United Kingdom, Switzerland, and Germany. ESI are paid internships in accordance with MSU policies and regulations.

Program Benefits

- Opportunities for undergraduate/graduate students to gain a research experience, and to present the findings of their research;
- Opportunities for students to meet colleagues at majority institutions to develop research collaborations;
- Engage representatives from majority academic institutions to explore opportunities to pursue graduate degrees; and
- Expand their professional networks and further position students for future job opportunities.

Funding Sponsor

CCDC Army Research Laboratory through the Center for Materials in Extreme Dynamic Environments

Website Information

Morgan State University ESI

https://www.morgan.edu/school_of_computer_mathematical_and_natural_sciences/student_programs/internships_and_fellowships/extreme_science_internships.html

CMEDE

https://hemi.jhu.edu/cmede/

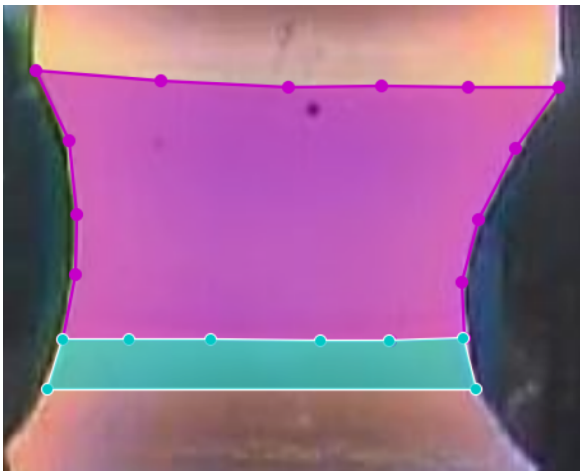
Deidre Grogan

Morgan State University, Baltimore, Maryland
Mentor & Faculty Host: Mr. David Elbert
Hopkins Extreme Materials Institute
Johns Hopkins University

Project Title: Building Open Training Stacks for Image Segmentation of Boron Carbide Experiments

Recent synthesis of large, single crystals of boron carbide (B4C) in a laser diode floating zone furnace (LDFZ) produced high purity single crystals ideal for characterization and development of advanced protection materials. The LDFZ method is challenging due to the complexity and breadth of tunable parameters. To improve LDFZ operational

efficiency and outcome quality, image segmentation is being developed using the Mask R-CNN framework. A new, more precise and broader training set of >900 image has been produced to facilitate retraining the image-segmentation learner and advance application of ML in the LDFZ.



HEMI/MICA Extreme Arts Summer Projects/Internships

Extreme Arts is a joint program between HEMI at Johns Hopkins University and the Maryland Institute College of Art (MICA). The program brings faculty and students from both institutions together to explore unique perspectives on extreme events. The program aims to encourage collaboration among artists and researchers to examine data, interpret outcomes, and translate results from extreme events in new ways. It is our hope that this dialog will create a stronger community through a shared sense of curiosity and exploration.

MARYLAND INSTITUTE COLLEGE OF ART

The Extreme Arts summer projects/internships provides an opportunity for MICA students to spend a summer within HEMI. Students receive a stipend during the internship, which is co-advised by MICA and HEMI faculty members.

Program Goals

- To provide an opportunity for meaningful engagement among engineers, scientists, artists and designers that sparks a creative dialog and leads to new outcomes;
- To explore systems of communication that translate ideas and provide platforms for engineers, scientists, artists and designers to discuss concepts and develop a common understanding;
- To create programming between JHU researchers and MICA faculty/students that examines new approaches to HEMI-related materials research and data visualization; and
- To design a framework that serves as a model for sustained, long-term partnership between JHU and MICA.

Funding Sponsors

National Endowment for the Arts,
The Whiting School of Engineering at JHU, and MICA

Website Information

https://hemi.jhu.edu/academic-programs/hemimica-extreme-arts-program/hemi-micasummerinternship/

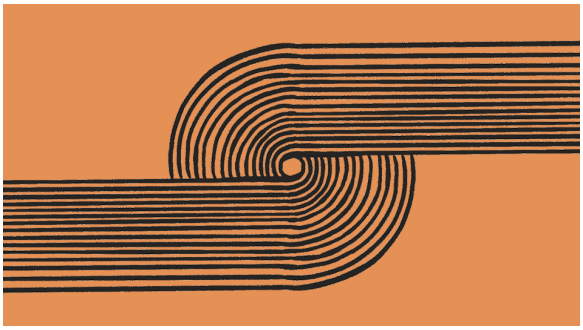
Chelsea Conrad Danielle Duplain

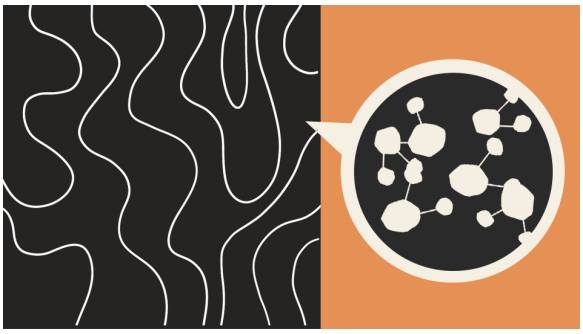
Chelsea Conrad

Focus Area: Illustration
MICA Advisor: Rebecca Bradley, Illustration
HEMI Advisor: Professor Sarah Hörst
Department of Earth and Planetary Sciences
Johns Hopkins University

Project Title: Our Past and Titan's Future

Studying Planetary Science feels a little bit like waking up from a very disorienting nap with a blindfold on. Are we at the beginning of the day? At the end? Where is everyone else? Are they outside? Upstairs? Were they here already? Have they not come yet?
Of all the stars, planets, and galaxies we've discovered, we have yet to find life.
But maybe we just haven't found life yet, and it's actually happening right before our eyes. Titan, Saturn's largest moon, is an incredibly Earth-like place. There are processes happening there now that seem to be just like the processes that we think created life on Earth. Watching that story unfold has a lot to teach us.



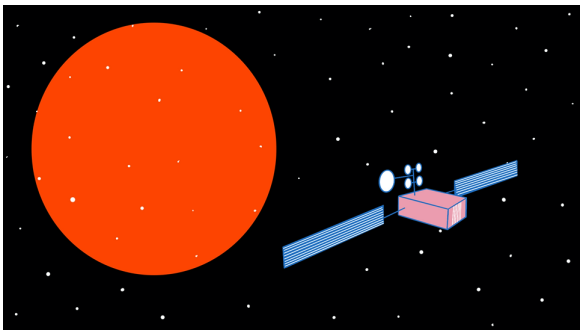


Danielle Duplain

Focus Area: Illustration
MICA Advisor: Rebecca Bradley, Illustration
HEMI Advisor: Professor Stavros Gaitanaros
Department of Civil and Systems Engineering
Johns Hopkins University

Project Title: Optics: Architected Materials

For my summer project with HEMI I worked with Stavros and his team to create an animated infographic video summarizing their work constructing architected materials in the lab. I was inspired by the innovation and willingness to explore new solutions at the heart of their research and wanted to make the philosophy behind this work approachable and understandable.



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