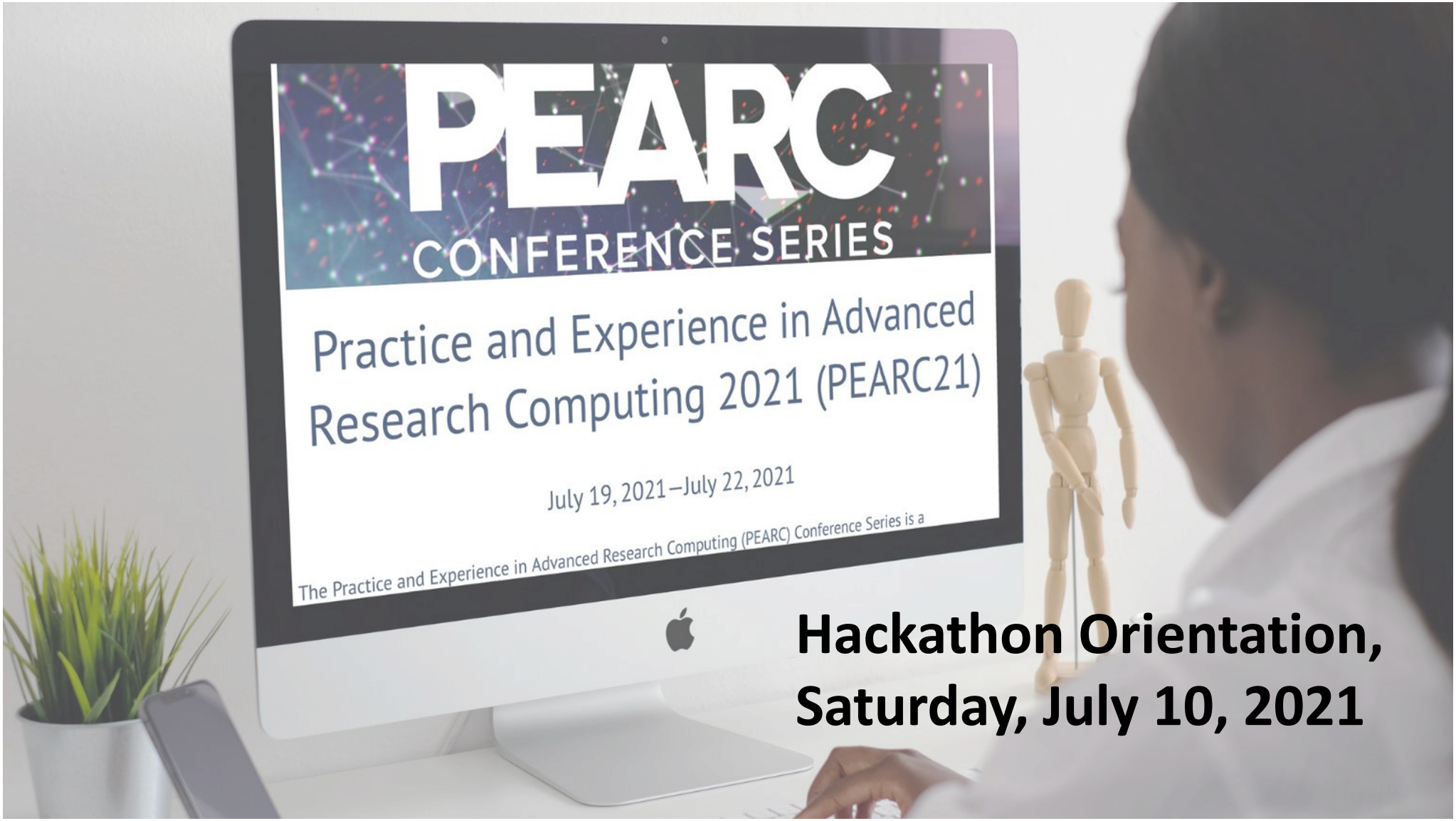


Hackathon Orientation, Saturday, July 10, 2021

PEARC21 Student Program

- Elizabeth Leake (STEM-Trek) and Alana Romanella (Virginia Tech)
- Is everyone registered for PEARC21? It's free, ask me!
- Have you also applied with the student program?
- Orientation Day: **Sunday, July 18**, 10 a.m. to 6 p.m. Pacific Time.
  - **Highlights:** Hour of CI, Hour of OSG, Internship Spotlight, Cybersecurity Careers Panel, Mentoring Program, Resume Clinic, PitchIT Workshop, and more!
  - Please monitor our Slack channel (everyone has been added).
- Details: https://pearc.acm.org/pearc21/student-program/
- Questions? Write to: PEARC21students@gmail.com

Christopher Sherald

University of Kansas Undergraduate Scholar;
NSF XSEDE EMPOWER Internship with
Dr. Hartwin Peelaers

The Condensed Matter Physics research internship involved the use of VASP code and the Atomic Simulation Environment Python package.

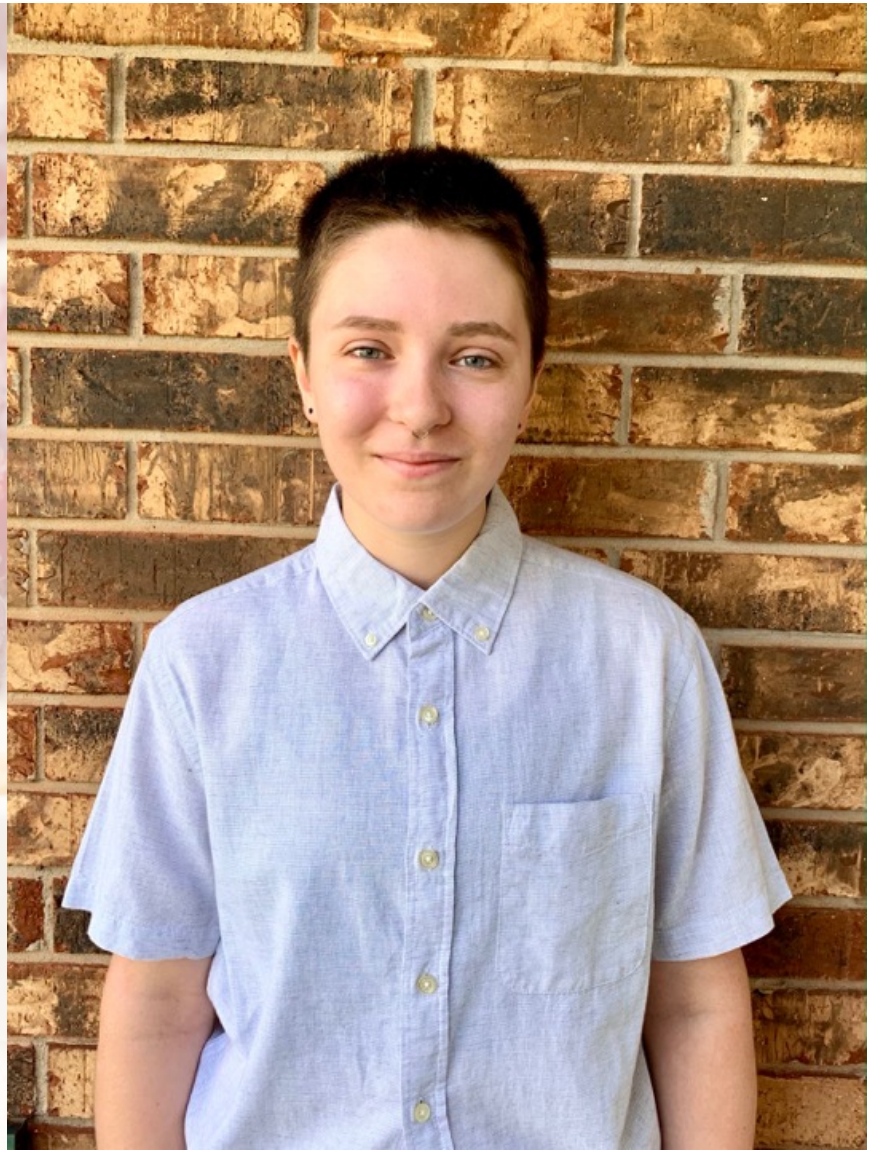
"During my internship, I used UK's high-performance computing resources which sped up the simulation process by about six times! I presented my research at the National Society of Black Physicists conference and was awarded Best Poster."

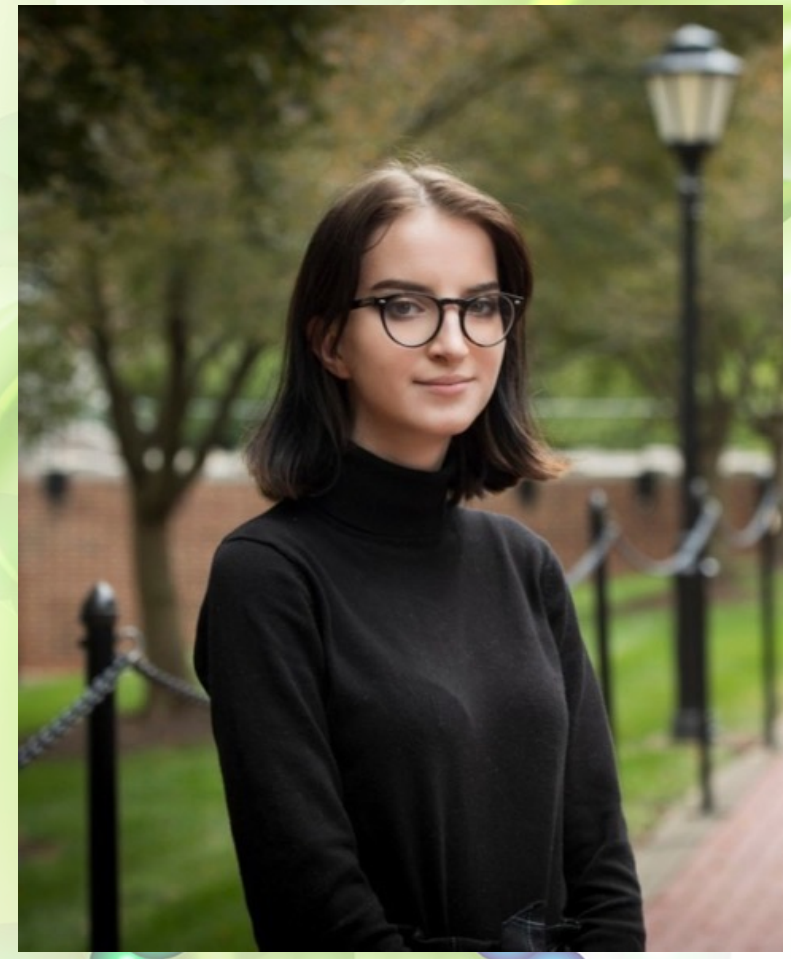
Arianna Martin

Southwest Oklahoma State University
NSF XSEDE Campus Champion and EMPOWER intern under SWOSU
Assistant Professor Jeremy Evert.

In preparation for the Oklahoma HPC Competition, Arianna and their team built Raspberry Pi clusters with shared file systems. Their team also tuned algorithms with MPI to solve the Traveling Salesperson challenge, and tested scaling efficiency.

Arianna's team won a division first place prize, and presented at multiple regional meetings.

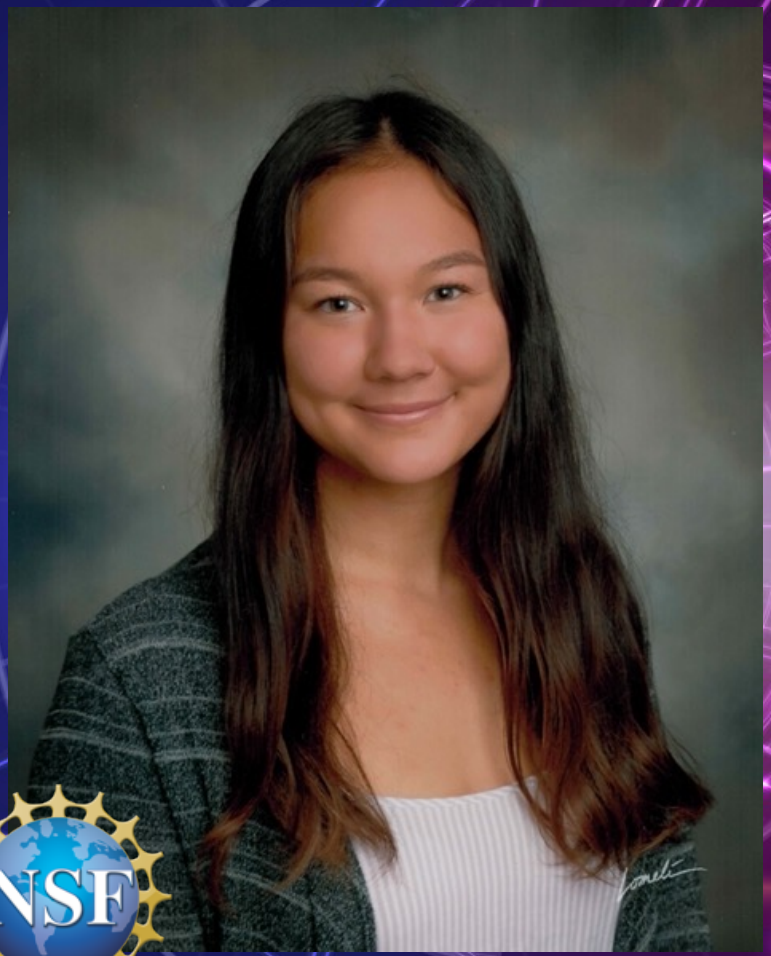




Tanya Nesterova

University of Delaware Undergraduate;
NSF XSEDE EMPOWER Biophysical Chemistry internship with Dr. Juan Perilla.

- With cryogenic electron microscopy specialists, developed algorithms that help define the morphology of HIV capsids exhibiting the missing wedge artifact in tomograms, and a pipeline for high throughput virtual screening of small molecules (potential HIV cofactors).
- Conducted electrostatics analysis on molecular dynamics simulations of the Ebola virus nucleocapsid, and learned how to submit parallelized jobs to run on the NSF Bridges HPC system at the Pittsburgh Supercomputing Center.
- Coauthored article in *The Journal of Chemical Physics.*



Christiana Marchese

Pomona College undergraduate; NSF XSEDE EMPOWER internship with Professor Xinlian Liu (Hood College).

Project: "*Location-Aware Community Characterization*," used deep learning models to predict mental health outcomes.

- Learned the basics of geospatial analysis with Pytorch, Sklearn and Geopandas.
- Used TACC's Stampede2 supercomputer.
- Developed neural networks and a linear regression model to assess the risk of suicide, by California county, using U.S. Census Bureau and Center for Disease Control data.
- Presenting a poster at PEARC21.

Emily Costa

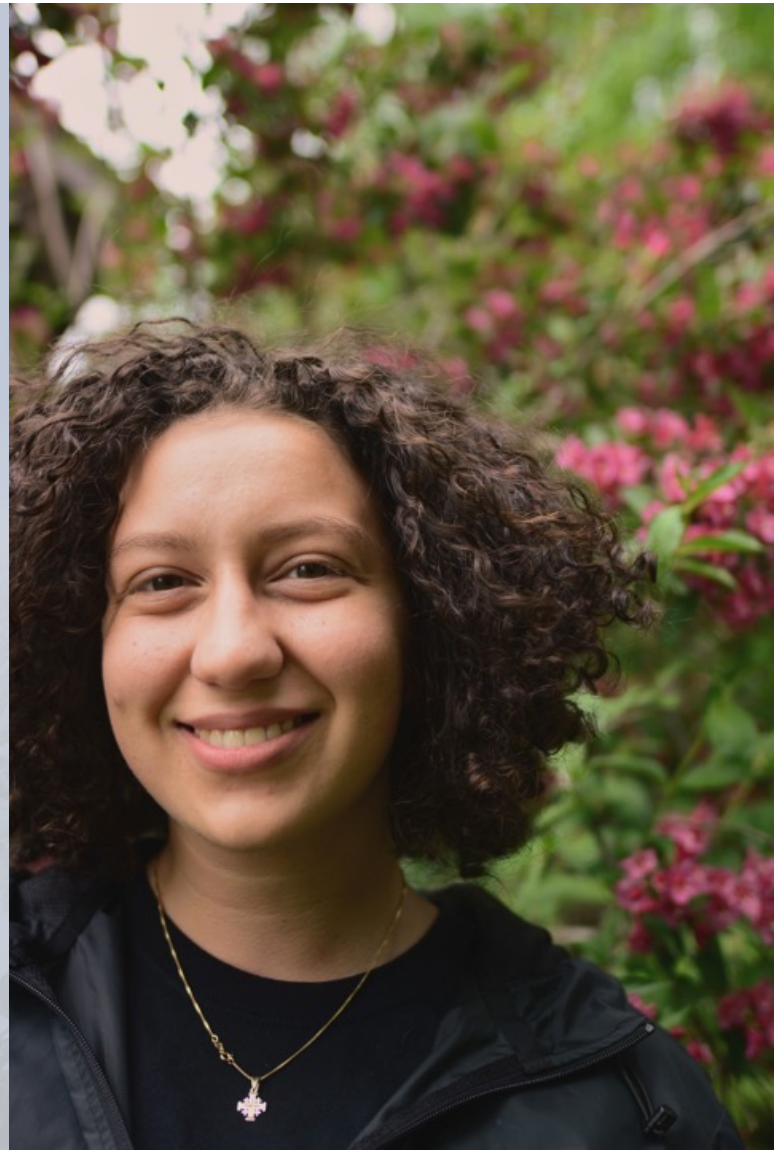
Northeastern University Computer Engineering PhD student

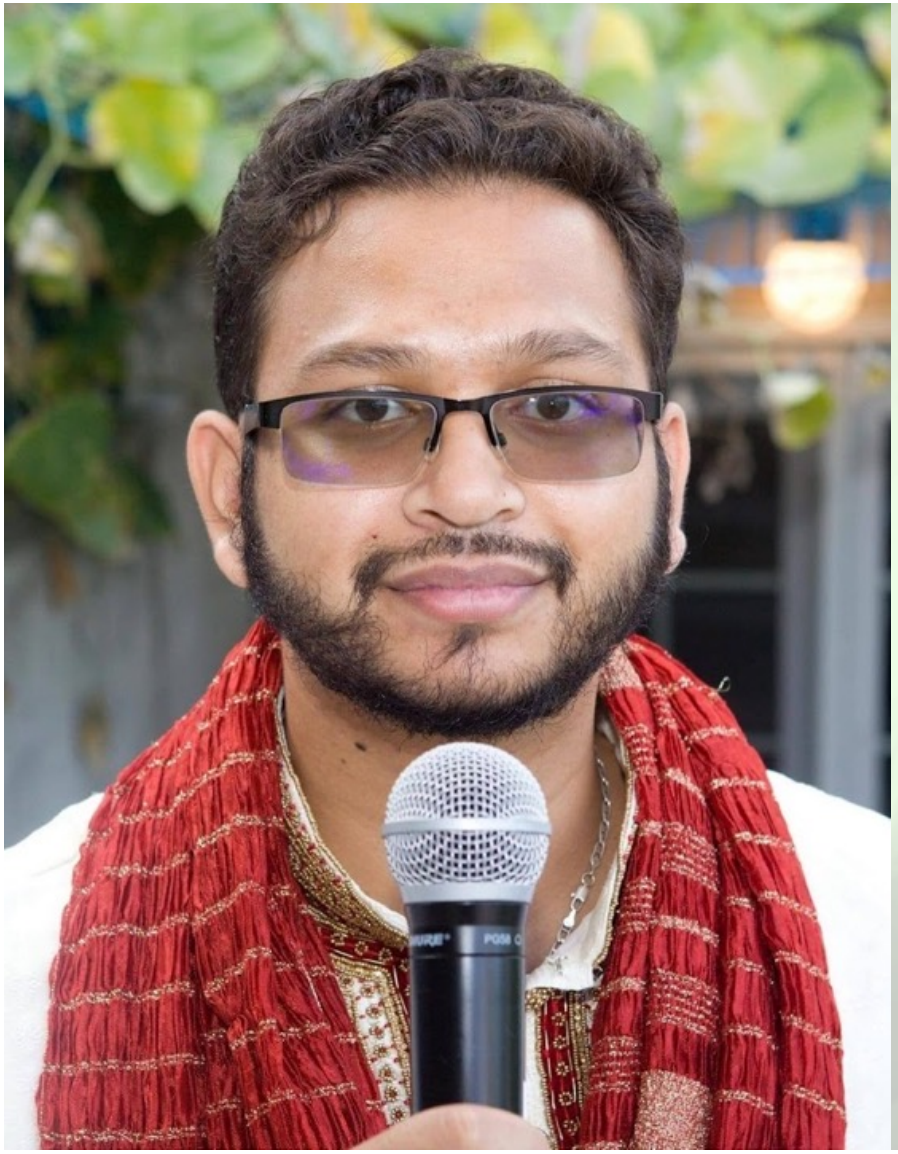
At Oak Ridge National Laboratory (ORNL), Emily is completing a “GEM” fellowship with Dr. Gina Tourassi. In 2019, she participated in the ORNL Pathways to Computing Internship Program under Dr. Suhas Somnath.

ORNL GEM Internship highlights:

- Contributed to a computational framework for scaling a Bayesian inference algorithm which integrated into open-source scientific Python packages, pyUSID and pycroscopy, to facilitate large-scale spectroscopic image processing and data storage.
- Built automated software tests that support continuous integration to reinforce package reliability and code quality.
- Used ORNL's high-performance computing resources and deployed code on *Summit*, the most powerful supercomputer at the time.

OAK RIDGE National Laboratory





Jamil Gafur

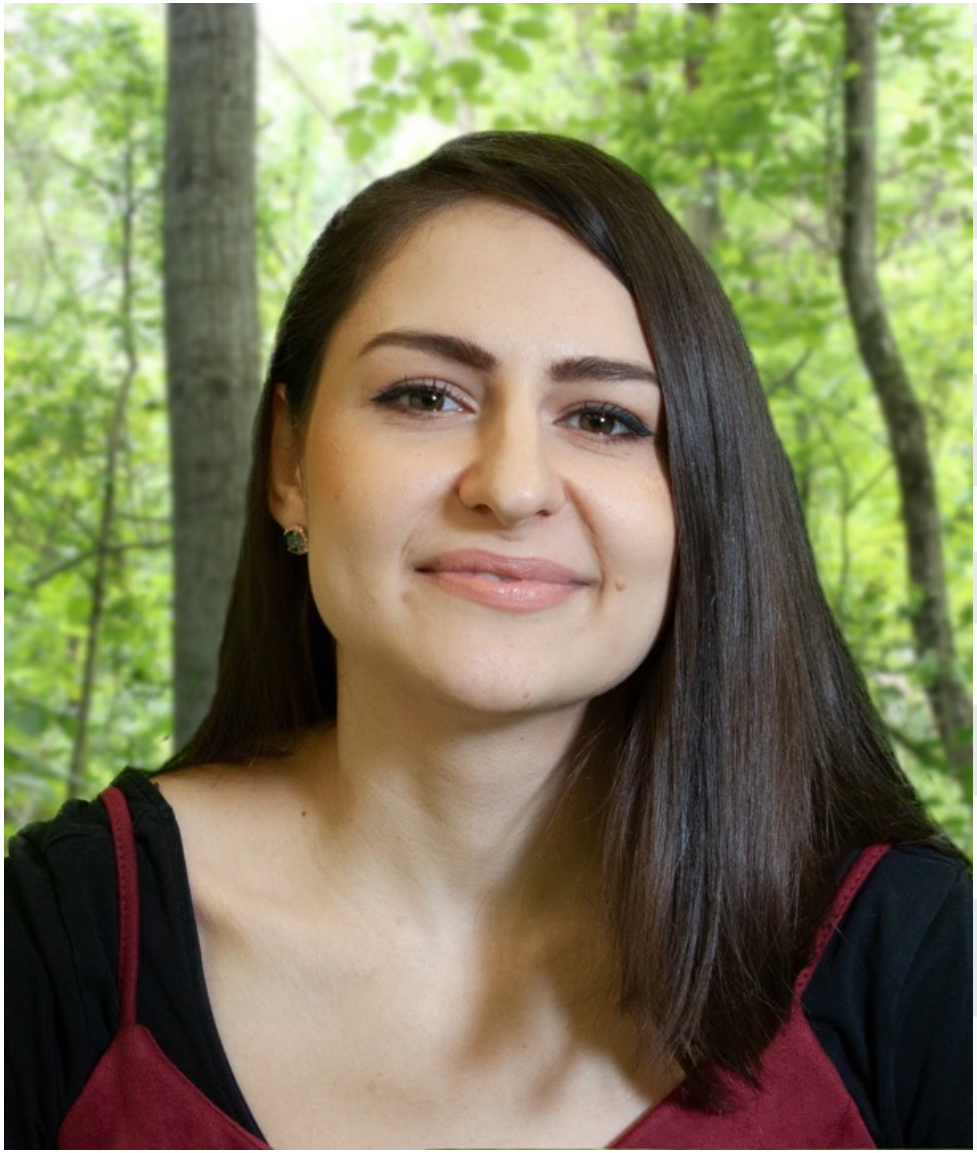
University of Iowa Computer Science PhD Student

Summer 2021 Fellowship with Drs. Michael Crowley and Lintao Bu at the Oak Ridge Institute for Science and Education, National Renewable Energy Lab's Renewable Resources and Enabling Science Center.

While much is known about polymer flows, there is no quantitative understanding of flow-induced weight migration (FIWM) of molecules.

"We're profiling and optimizing a Fortran codebase so that it will make more efficient use of compute nodes and therefore run faster on NREL's Eagle supercomputer."

NREL
Transforming ENERGY



Ina Murphy

Northern Illinois University
MFA candidate, 3D Animation and Video Game Design

Summer 2021 internship with Argonne's Visualization Lead Joe Insley where she is learning how to use production quality rendering tools for scientific visualization.

Ina's work will be featured in the PEARC21 Visualization Showcase.

Argonne NATIONAL LABORATORY