



NATIONAL
LABORATORY
OF THE ROCKIES

Building a Workforce in Advanced Computing through National Laboratory Internships

Presenters: Morgan Fong (University of
Texas at Austin) and Michael Martin (NLR)
Contributors: Hilary Egan, Marc Day, and
Kristi Potter (NLR)

The Need

Progress in science and technology increasingly depends on computational science and engineering (CSE) skills:

- Modeling and simulation (mod/sim).
- Data science.
- Machine learning and artificial intelligence (ML/AI).

CSE skills become even more powerful when combined with

- Domain science expertise.
- Ability to use High Performance Computing (HPC).

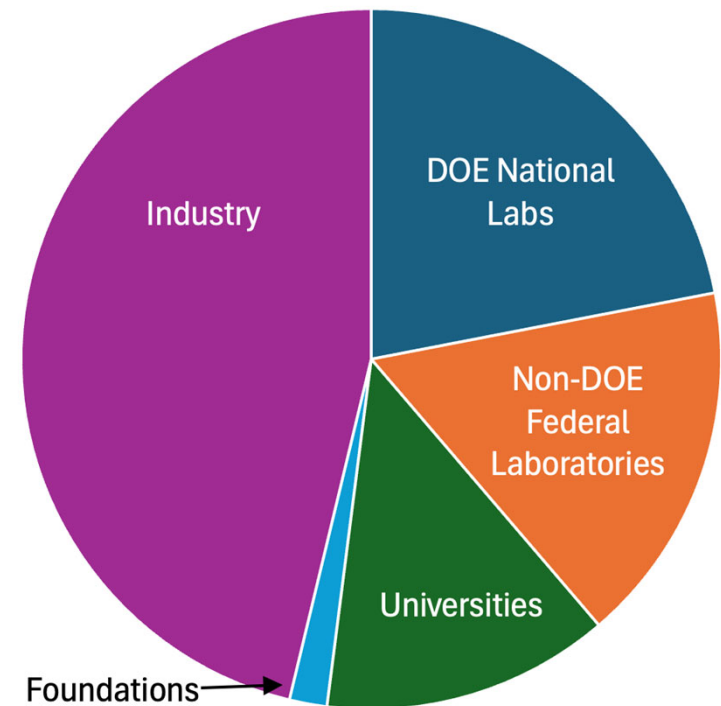
These skills are needed in **academic research, industry, and federal science.**

The Challenge

Obstacles to building these skills in universities:

- Lack of access to advanced hardware.
- Lack of faculty involved in HPC-based research.
- Challenges balancing computational science and domain science.

Is there a role for national laboratories to contribute to workforce development?



How the 137 Top-500 systems are divided across institutions.

Another path: Internships

NLR hosts internships sponsored through *project funds* focused on meeting project needs and *federally-funded internship/fellowships* focus on skill development while contributing to project needs.

NLR has hosted CSE undergraduate, postbacc, and graduate interns through

- Computational Science Graduate Fellowship (CSGF).
- Science Undergraduate Laboratory Internship (SULI).
- CMEI High Performance Computing for Energy Innovation Internship program (HPC4EI).
- National Nuclear Security Administration's IMPACT Internship (NNSA-IMPACT).
- National Science Foundation Mathematical Science Graduate Internship (NSF-MSGI).

Survey Design

Developed question themes with internship coordinators/mentors:

- **Computational Skills (e.g., using HPC)**
- **Familiarity with Energy Efficiency Topics (e.g., materials usage)**
- Research Skills (e.g., authoring research publications)
- Professional Skills (e.g., discussing findings with a technical audience)
- **Career Interests (e.g., interest in the National Lab system)**

Questions answered on 4-point scale comparing pre/post-internship experience

Participants & Data Analysis

~40% response rate, ~25 participants:

- DOE CSGF / SULI, CMEI HPC4EI, NSF MSGI
- Primarily early-stage PhD students
- Broad range of majors

Converted responses to 0-4 numeric scale

Performed t-test to check for improvements from internship or pre- to post-internship i.e., checked for $p < 0.05$

Computational Skills

General-purpose
Programming

Scientific
Programming

Distributed/Parallel
Programming

Collaborative Software
Development

Data Visualization
& Analysis

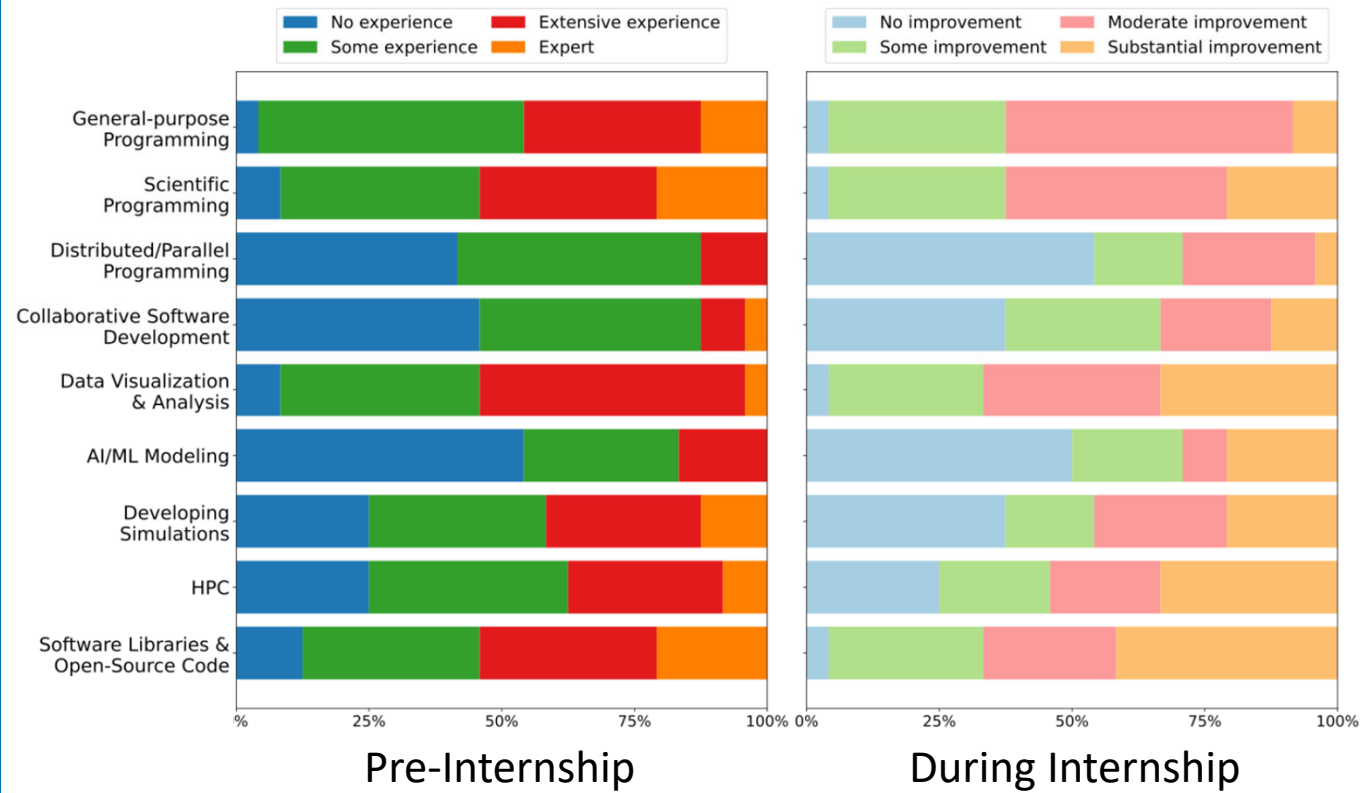
AI/ML Modeling

Developing
Simulations

HPC

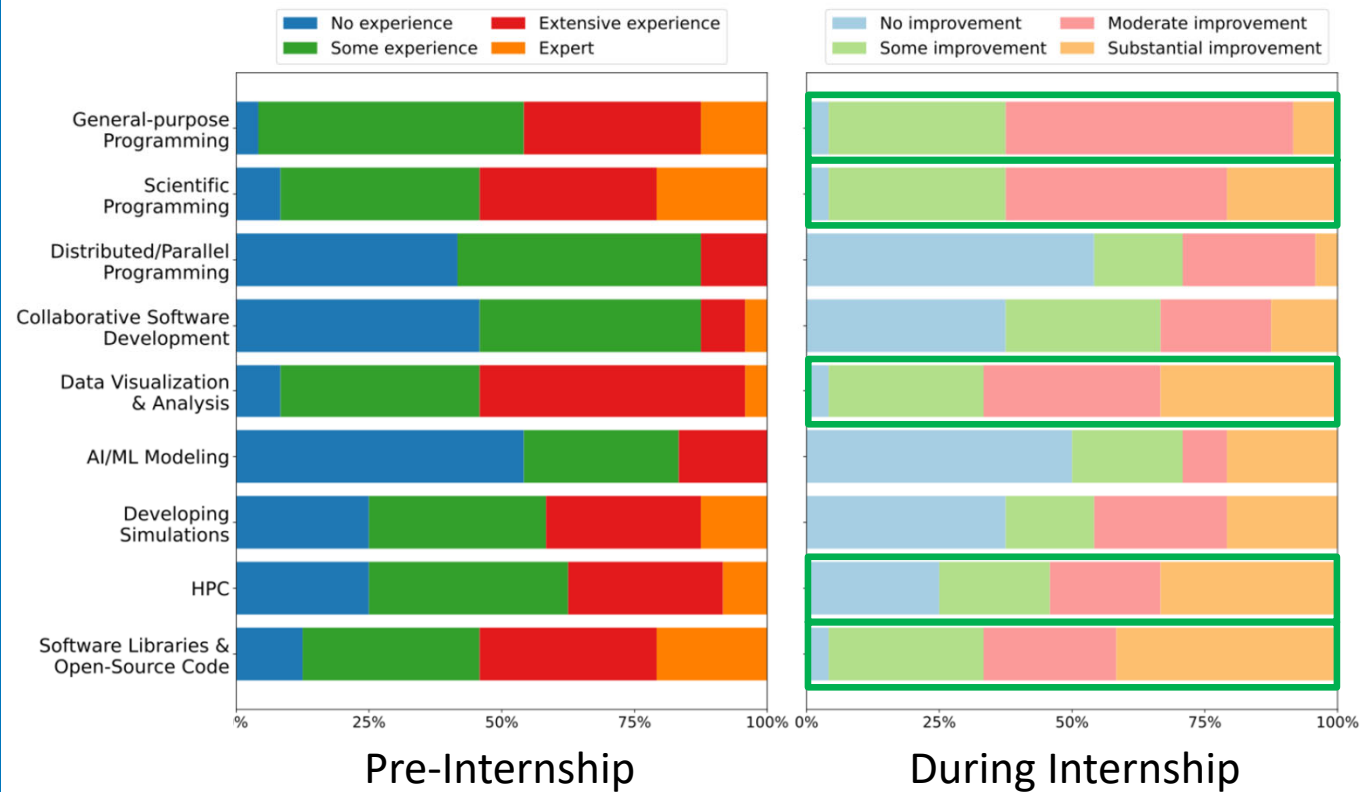
Software Libraries &
Open-Source Code

Computational Skills



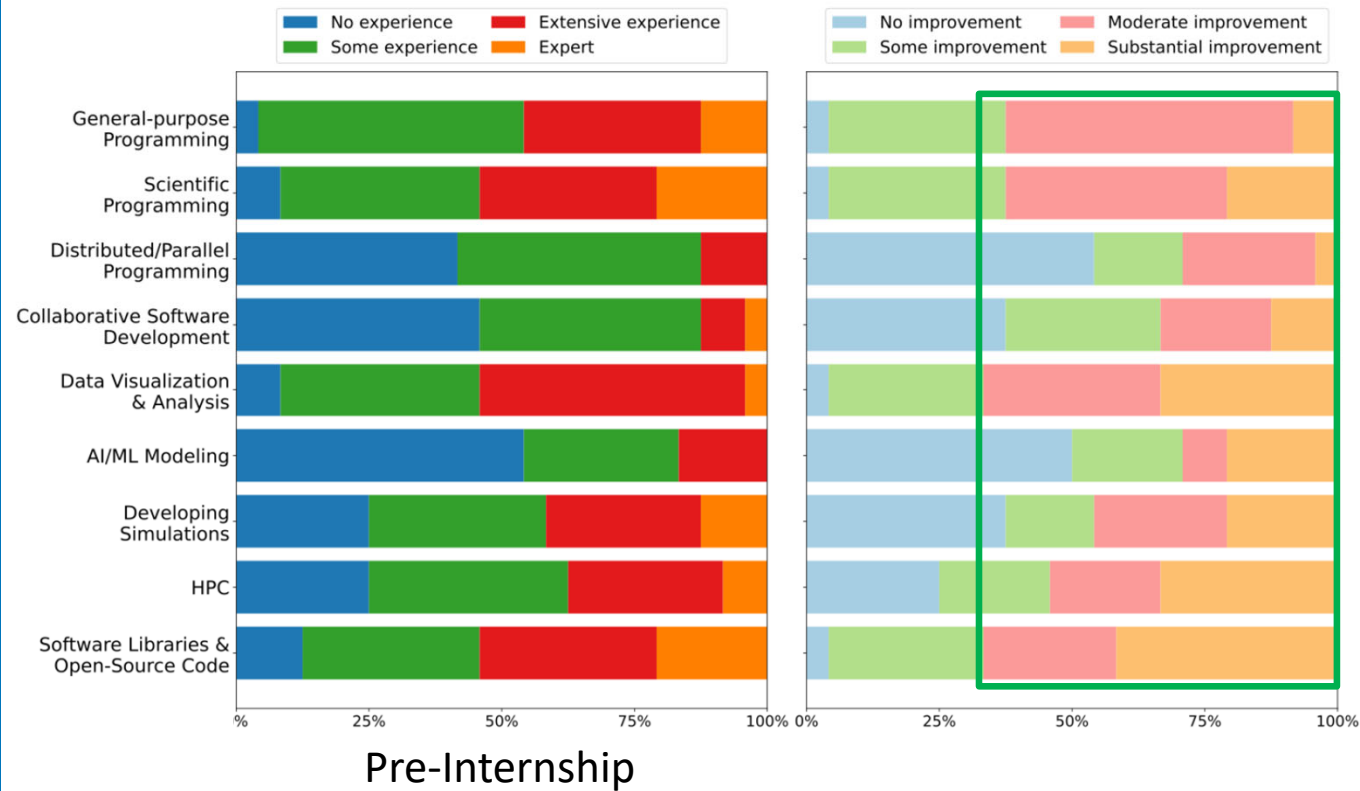
Computational Skills

- Some improvement or more across 5 skills



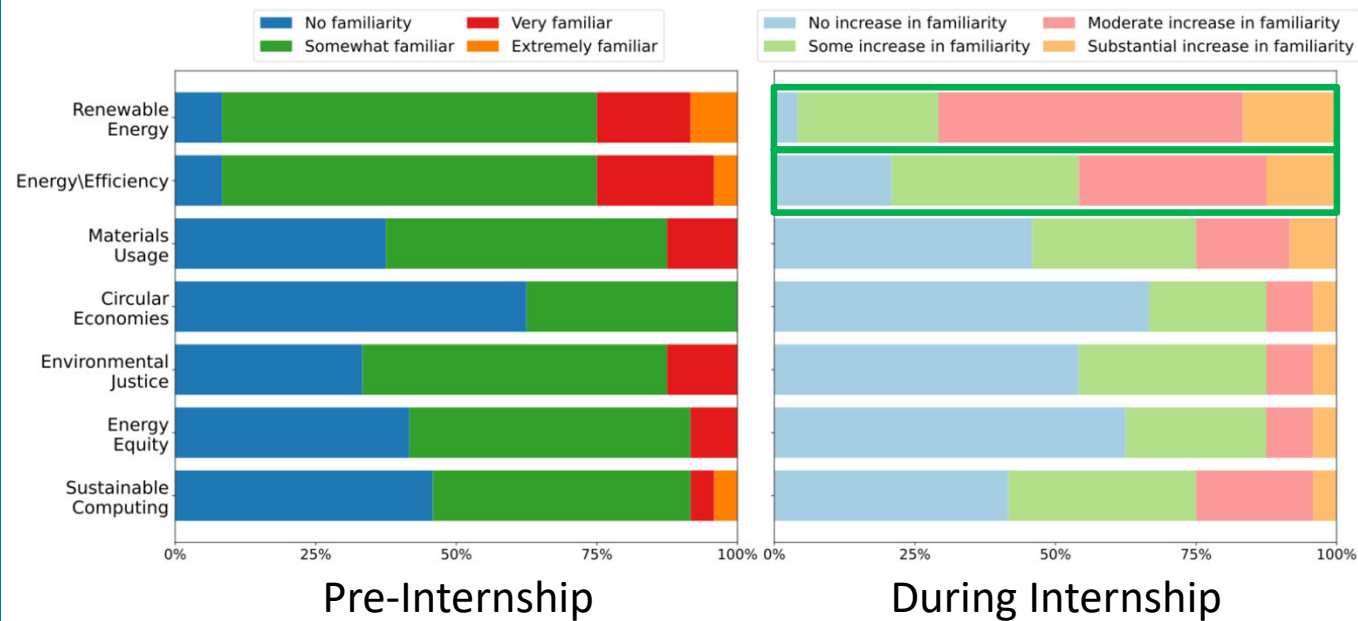
Computational Skills

- Some improvement or more across 5 skills
- 21 participants reported moderate to substantial improvement in 2+ skills



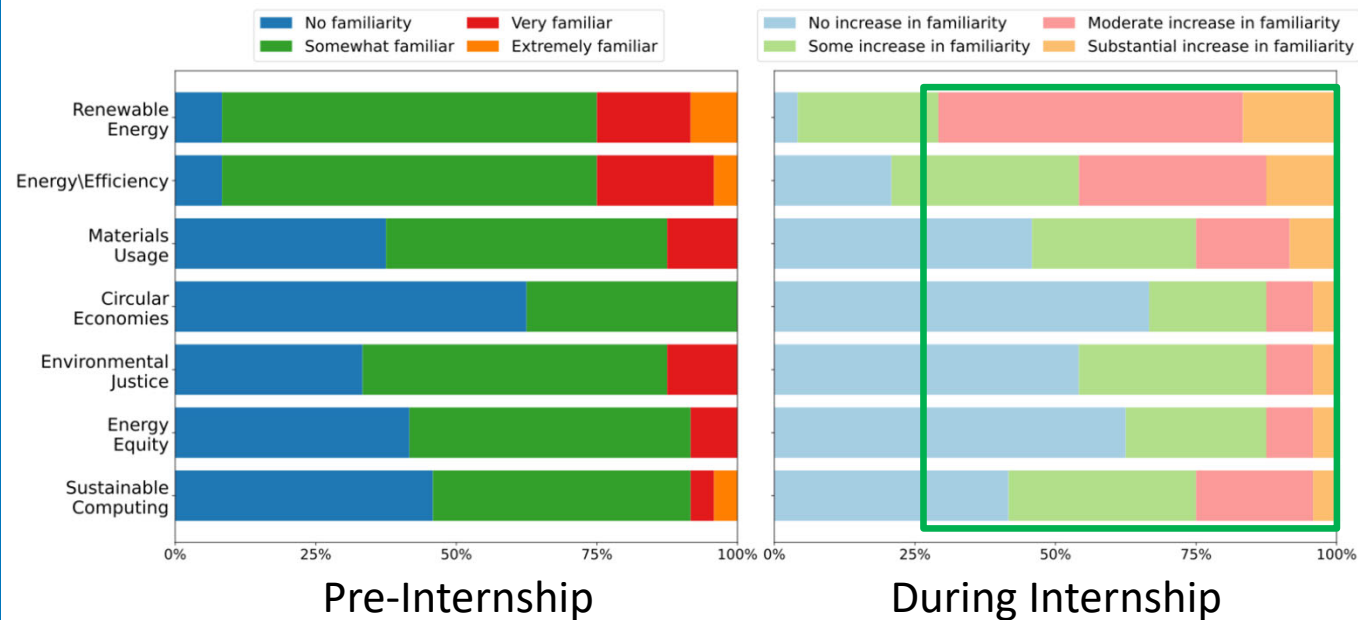
Familiarity with Energy Efficiency Topics

- Some improvement or more across 2 topics



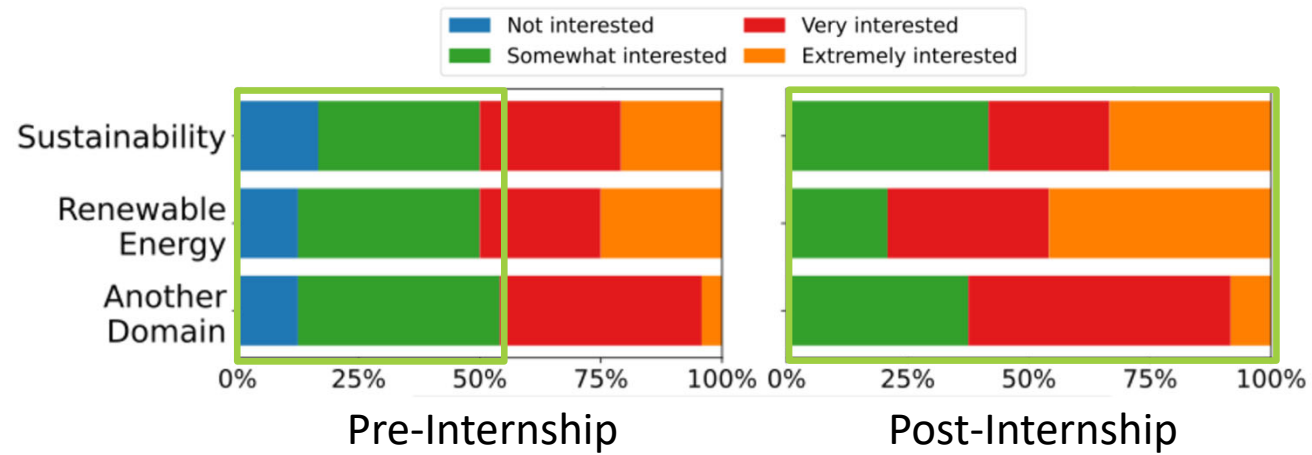
Familiarity with Energy Efficiency Topics

- Some improvement or more across 2 topics
- 19 participants reported moderate to substantial increase in familiarity in 1+ topics



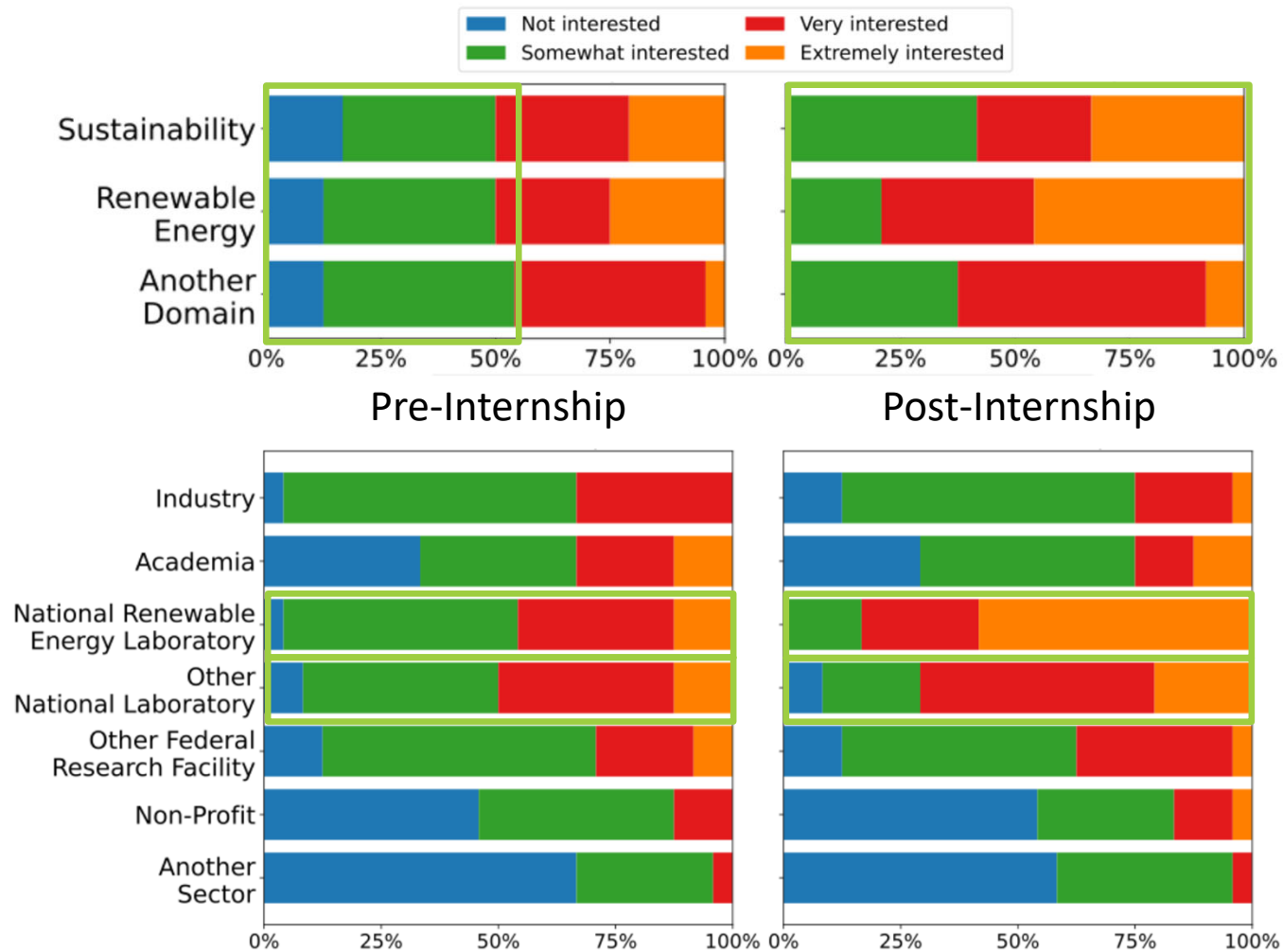
Career Interests

- Interest in domains increased



Career Interests

- Interest in domains increased
- Interest in careers at National Labs increased



Results Summary

From internship experiences participants report:

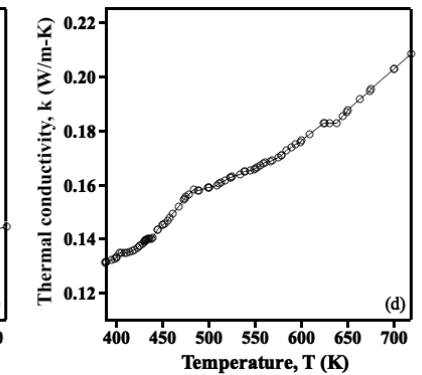
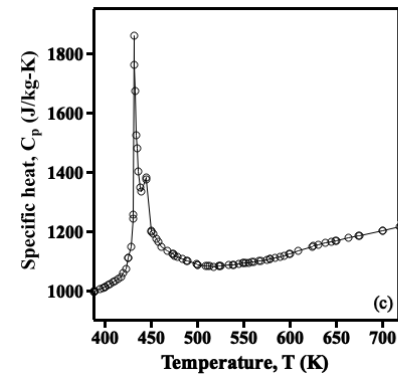
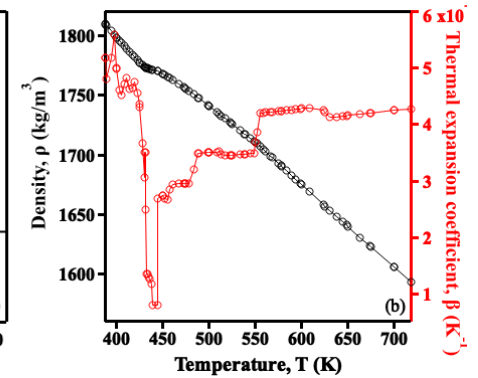
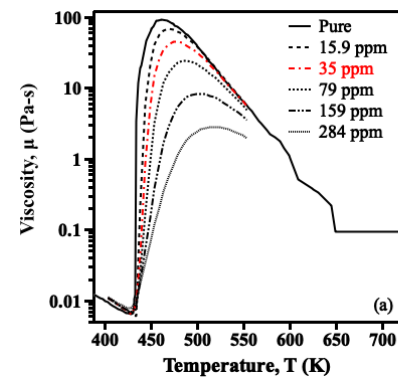
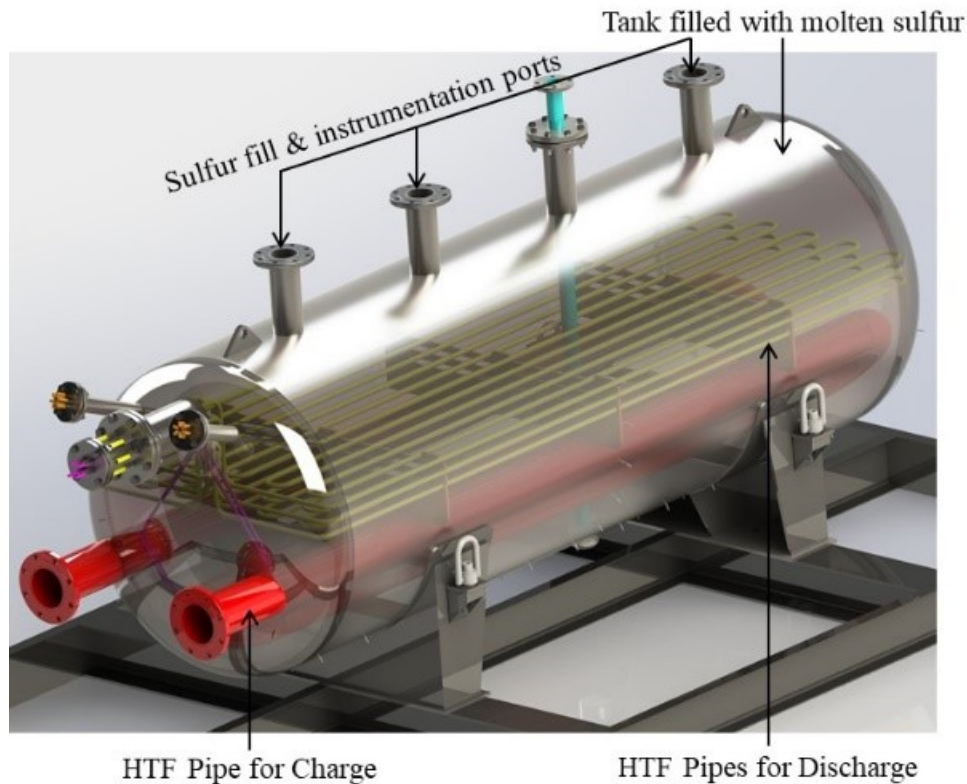
- Improvements in computational skills
- Greater familiarity with energy efficiency topics
- Greater interest in working at National Labs

After internships, participants report:

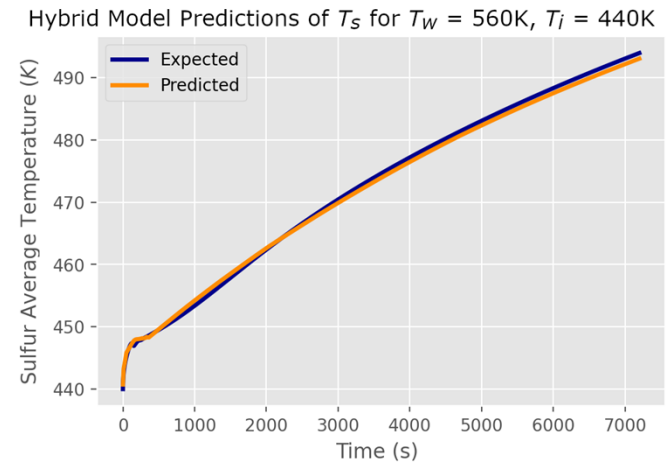
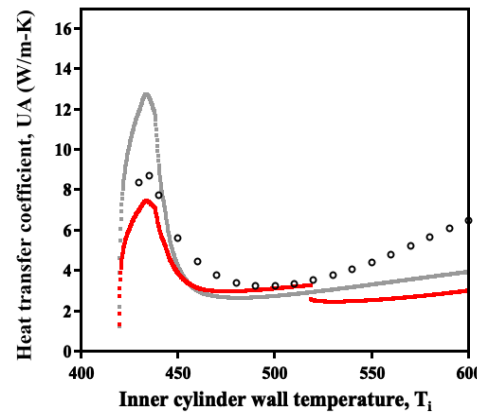
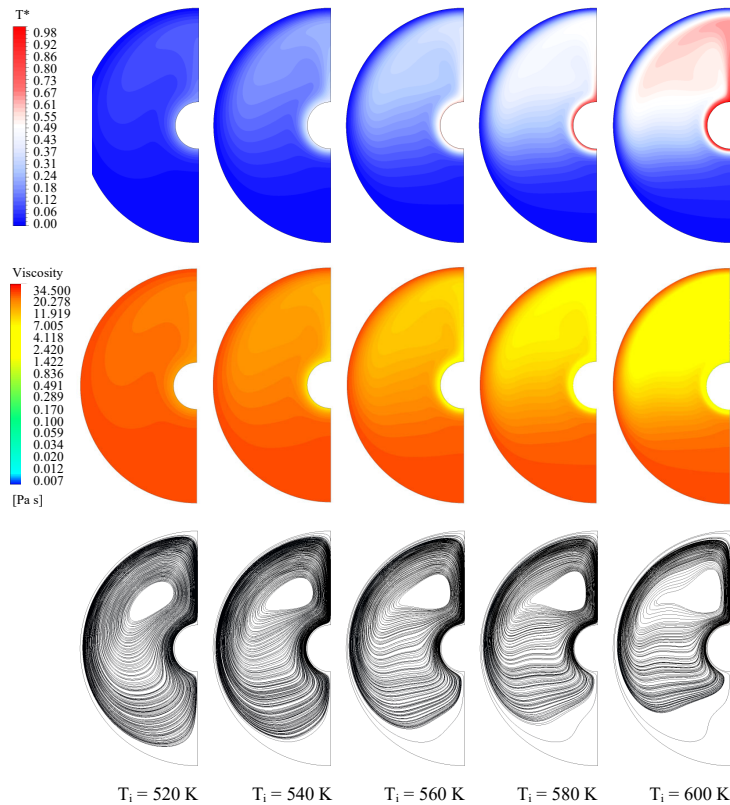
- Working At National Labs, industry, academia, government
- Using skills from internship in future job applications / positions

Previous Host Project: Element 16

NLR/Element 16 project on thermal energy storage in liquid sulfur.



Previous Host Project: Element 16



Variable properties “break” correlations used for design, but machine learning allows modeling of transient system performance.

Student Outcomes



Madeleine Oliver

Chemical Engineering PhD candidate, University of Oklahoma

Internship Goal: Gaining knowledge and skills beyond PhD dissertation to prepare for future career.

Internship project: CFD simulations of “model” geometry.



Kevin Menear

Computer Science MS student, Georgia Tech/K-12 Computer Science, Robotics, and Engineering Instructor.

Internship Goal: Explore National Laboratory system while expanding technical expertise.

Internship project: Evaluating Machine Learning approaches.

Student Outcomes



Madeleine Oliver

Science outcome: MC Oliver, et al., “Exploring the Limits of Empirical Correlations for the Design of Energy Systems with Complex Fluids: Liquid Sulfur Thermal Energy Storage as a Case Study,” *J. of Energy Resources Technology*, 145,121704, 2023.

Current position: Modeling & Simulation Engineer, Amentum, supporting NASA projects.



Kevin Menear

Science outcome: K Menear, et al., “One System, Many Models: Designing a Surrogate Model for Sulfur Thermal Energy Storage,” *2022 AAI Fall Symposium, Washington, DC* .

Current position: Researcher/Data Scientist, NLR.

Summary

National laboratory internships in computational science and engineering provide meaningful learning opportunities beyond what is available in academia.

Interns make meaningful contributions to national laboratory research as they complete their internships.

Internship “alumni” contribute to the entire US science and technology enterprise, including the national laboratory system.