# High-Performance Cluster Computing:
# Learning the Applications of Computing Methodologies in STEM Disciplines

Spring 2023: Thomas Joseph, Ainara Garcia, Steven Lam, William Fey
Fall 2022: David Krasowska, Ethan Gindlesperger, Benjamin Schlueter, Charles Durham, Cooper Sanders, Moises Martinez Herrera
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## Abstract & Introduction


CI member's setup

- Students use Raspberry Pi clusters to learn supercomputing, like Clemson's Palmetto Cluster
- Students can showcase HPC skills in the Student Cluster Competition and research publications
- Students at SCC '22 work to build and optimize their cluster designs to get the best performance

**What is high performance computing (HPC)?**

- Computational Science uses advanced computing to understand and solve complex problems in all scientific fields through simulations and models
- **ALL** science is moving towards using computational methods
- HPC uses powerful computing resources to quickly process large amounts of data for complex situations, data analysis, and modeling in various fields such as science, engineering and finance

## Raspberry Pi Cluster

- Each student assembled 4 node Raspberry Pi Cluster.
- Pi Clusters contain resources similar to that in supercomputers at a fraction of the cost
- Building these clusters students we investigate HPC concepts such as strong and weak scaling
- By constructing their own clusters, students have the freedom to experiment with software configurations and applications
- Learning how to install software on these systems also helps students prepare for the Student Cluster Competition

| Hardware Used | |
|---|---|
| 4x Raspberry Pi 4 | 4x 32 GB micro SD card |
| 64 GB USB 3.1 Flash Drive | 4x Type C charge cables |
| 4x Cat 6 Patch cables | 4 node Pi rack |
| 5 port network switch | 4 port USB power supply |



Software Used:
- Ubuntu 20.04.2 LTS (Operating System)
- MPICH 3.3.2 (Communication Library)
- NFS 4.2 (Shared File System)

CI member's setup

## Student Cluster Competition

- International supercomputing contest: cultivating next-gen computational scientists[1]
- Collaborate with vendor partners to build optimal 3000W clusters
- Earn points through HPC benchmarks & real-world workflow performance
- Enhance knowledge of HPC architecture, programming techniques & performance measurement
- Gain comprehensive understanding: HPC usage patterns, methodologies & parallel performance
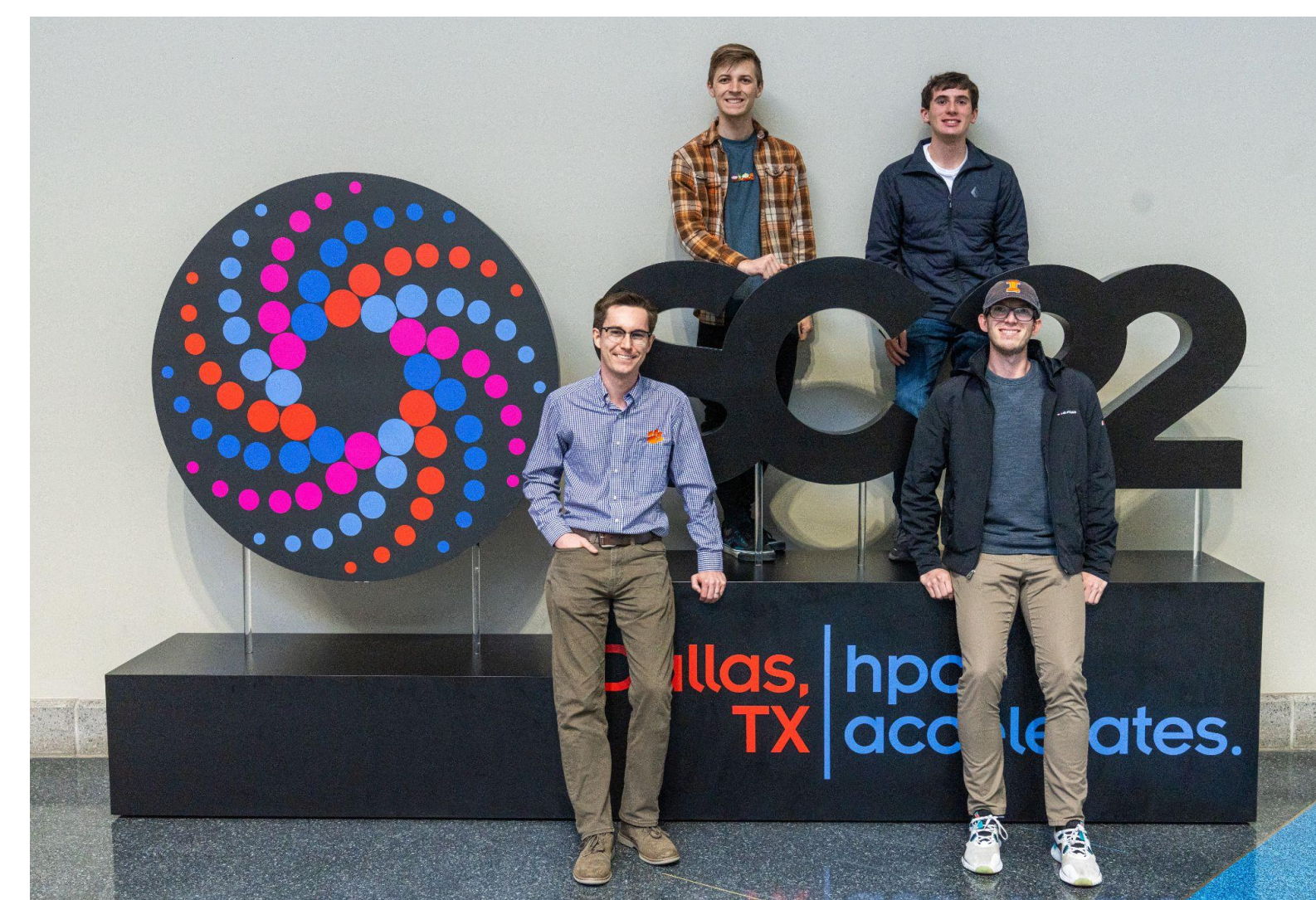- Valuable hands-on experience: manage large-scale HPC resources & common workloads



Presentation of undergraduate awards at SC22, including David Krasowska
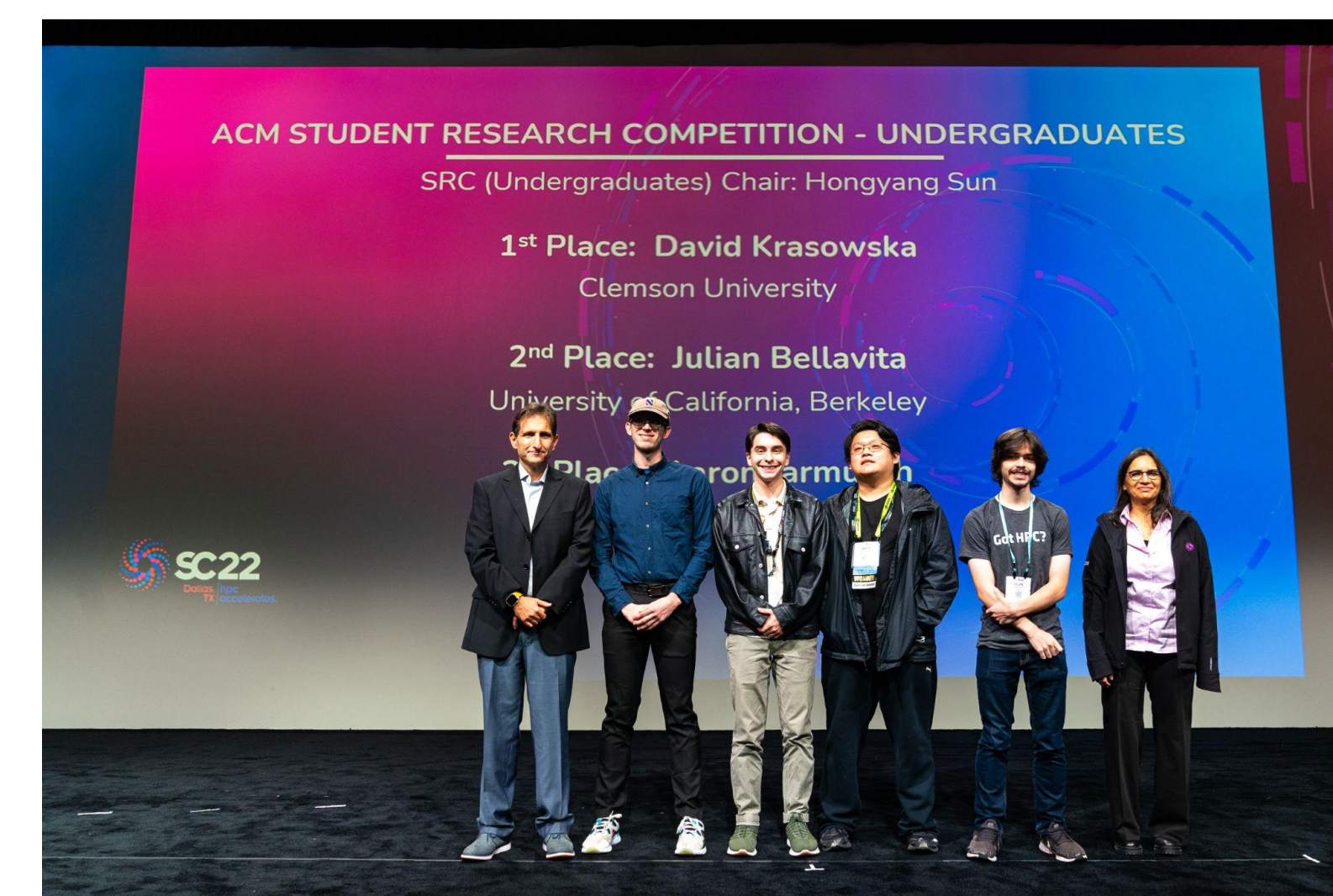
## IndySCC @ Supercomputing 2022

Team Members:
- Cooper Sanders
- David Krasowska
- Ethan Gindlesperger
- Logan Durham
- Moises Martinez Herrera
- Benjamin Schlueter


SC 22 members

Through partnerships between industry and academia, the Indy Student Cluster Competition (IndySCC) gives student teams the platform to compete in a 48-hour non-stop challenge involving the completion of scientific workloads and the demonstration of their proficiency in HPC to the judges as well as other attendees at the conference.

During Fall 2022, Clemson competed with teams from around the world in the IndySCC. Throughout the competition, we applied skills and knowledge from the CI to run benchmarks, run real-world applications such as NAMD, and to obtain the best performance scores.

## Applications of HPC
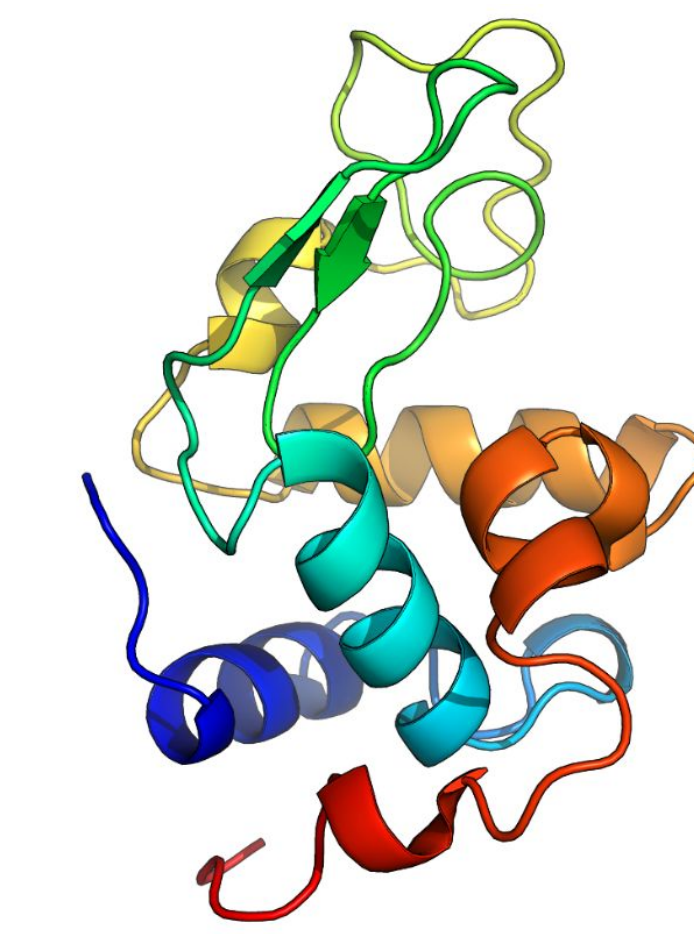

Lysozyme in Water modeled by Gromacs, a molecular dynamics simulator[3]

- Scientific Research
  - Simulate physical phenomena like weather patterns, galaxies, ocean currents
  - Simulate behavior of chemical compounds, drugs, and enable the prediction of efficacy and side effects of drugs
  - Study DNA sequence in genomic research[2]
- Commercial Applications
  - Clusters are used to analyze financial data and optimize oil and gas exploration to find cheaper and cleaner energy

## Accomplishments

**Awards / Accomplishments**

- Best Poster IndySCC
- 1st Place ACM SRC @ SC'22 - David Krasowska
- Journal submissions - Cooper Sanders and David Krasowska

**Internships / Graduate School**

- Intern (Su22) at Argonne National Laboratory - David Krasowska
- Ph.D. @ Northwestern - David Krasowska
- NSF REU Lehigh University - Ainara Garcia
- NSF REU Clemson University - Kristen Guernsey
- Intern (Su23) at Los Alamos National Laboratory - Benjamin Schlueter

## Future Work

- Preparing our SC'23 SCC application
- Discussing summer and fall research plans
- Preparing for graduate school



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**References**
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2. https://compbio.berkeley.edu/
3. http://www.mdtutorials.com/gmx/lysozyme/index.html