

# Research of Impact

## Center for Research Computing Annual Report 2021-2022

This year stands out for CRC for expanded collaborations, resource growth, and a new level of transparency and service in the Center's operations and planning, both for users and the CRC team as well. The appointment of Kim Wong and Adam Hobaugh as co-directors helps deepen connections between Pitt's research computing community and Pitt IT. That collaboration soon bore fruit in IT's development of CRC's user dashboard providing a striking graphical representation of CRC's operations in near real time, with a wealth of data representing granular operations and trends over time.

CRC's resources grew thanks in large part to grants from both the NSF and NIH – an NSF Major Research Instrumentation Grant that put the center in a new class of AI applications with state-of-the-art GPUs and an NIH S10 instrumentation grant that significantly grew the center's high throughput computing resources.

And as in every year, CRC enabled researchers to do work impacting the world around us – analyzing legal decisions, developing advanced medical imaging, exploring genomic approaches to cancer immunotherapy, revealing the effects of gender on economic dislocation, and designing computing systems to withstand the extreme conditions of space exploration.

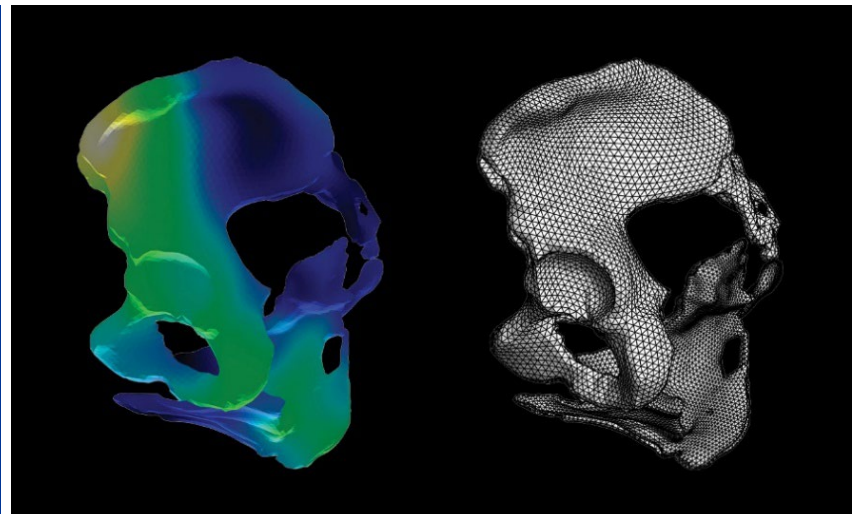


CRC co-directors Adam Hobaugh and Kim Wong

### Our Users

CRC collaborators published more than 170 papers and book chapters.

*This image created using CRC resources was a winner in the Coalition for Academic Scientific Computation brochure 2022 competition. The lab of Steven D. Abramowitch, associate professor of bioengineering, developed a statistical computer model of the female pelvis and pelvic floor muscles using thousands of points from MRI scans to model pelvic shape variation in pregnant women.*



# New Resources

## NSF MRI grant opens the ceiling for creativity

CRC collaborated with a multi-disciplinary team of Pitt researchers led by associate chemistry professor Geoffrey Hutchison to land a \$1.2 million NSF MRI grant for computing resources (internal Pitt funding pushed the entire award to \$1.5 million). The center is acquiring an unprecedented volume of high-end graphics processing units (GPU) that are twice as fast as the previous generation, giving researchers across the university access to new capabilities in speed, power, and scope.

More than 30 existing research groups across the university will benefit from the new resources, with over \$18 million in NSF grants in fields including chemistry, computational biology, materials science, psychology, astrophysics, weather forecasting, energy, and sustainability.

## High throughput computing receives boost thanks to NIH grant

CRC collaborator Adrian Lee, professor in Pharmacology and Chemical Biology and Pittsburgh Foundation Chair in Precision Medicine was awarded a \$573,647 NIH grant to the Institute for Precision Medicine, via an NIH S10 instrumentation award that will allow replacement of CRC's High Throughput Computing (HTC) Cluster with a new cluster made up of Central Processing Units (CPU) and Graphic Processing Units (GPU), along with associated data storage. Use of the HTC cluster is provided without charge to all Pitt biomedical researchers.



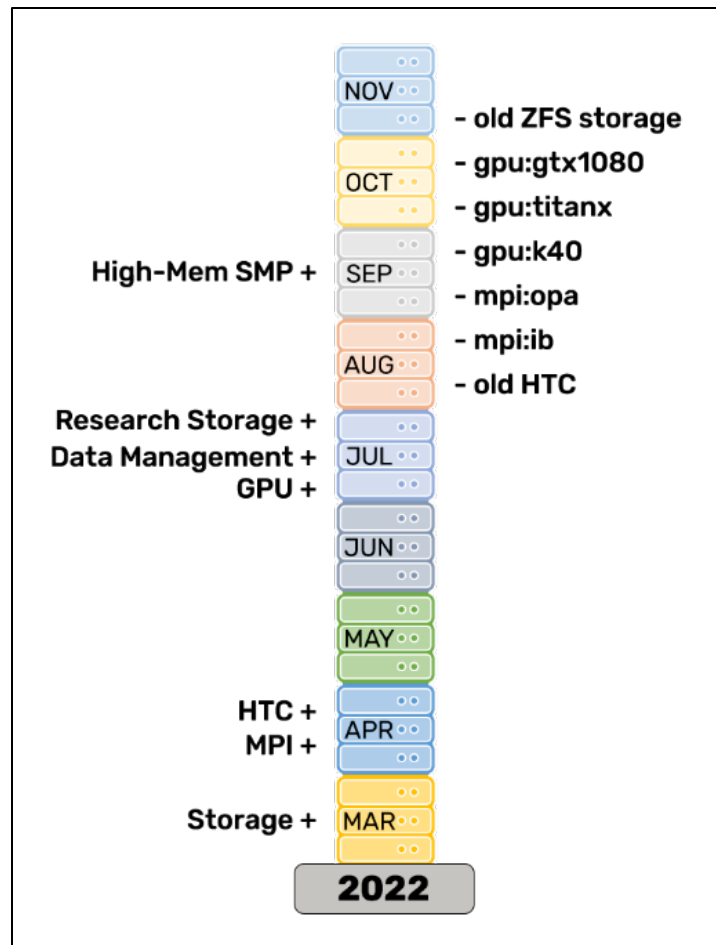
Geoffrey Hutchison



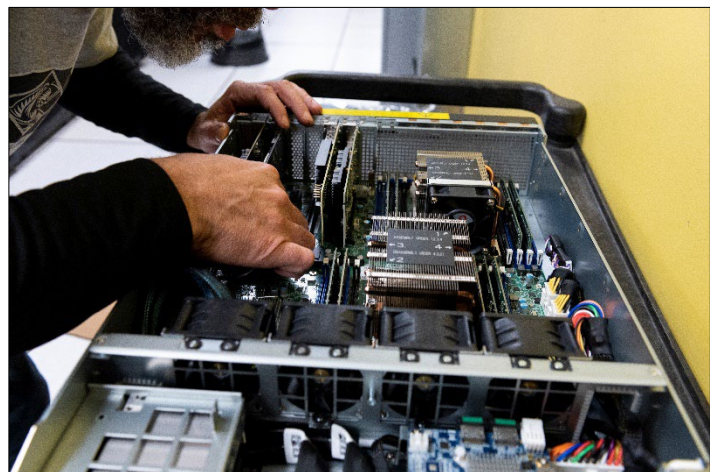
*This simulation done with CRC resources of sustainable catalysts based on tungsten oxide was featured on the cover of the Journal of the American Chemical Society (JACS) created by a team from the Department of Chemical and Petroleum Engineering.*

# Operations Planning & Improvements

CRC's plan for acquiring and retiring equipment in 2022 are outlined in the graphic at right: items denoted by + on the left side show equipment being added and items denoted by - on the right side indicate equipment being retired. The upgrades touch all segments of the CRC ecosystem, including compute, storage, and data management. Funding for these improvements comes from a complement of NIH S10 and NSF MRI big instrumentation awards, and the budgets of CRC and Pitt IT. The center's overall data storage capacity will increase by 2 petabytes. An additional 1 PB will replace existing aging lower-performance storage. Importantly, these new storage systems can scale up across all parts of Pitt's research enterprise, providing CRC a flexible path for future expansion and upgrades.



To establish an internal culture of continuous and sustainable improvements, CRC leveraged the University's GitHub Enterprise platform to host our operations codebase, Standard Operation Procedures documentation, and Continuous Integration and Continuous Delivery processes. The downstream effects include the creation of more effective onboarding material for new team members, a codebase that adheres to best practices standards for development, and integrated workflow for testing and deploying new code to production and rolling back when users report errors.

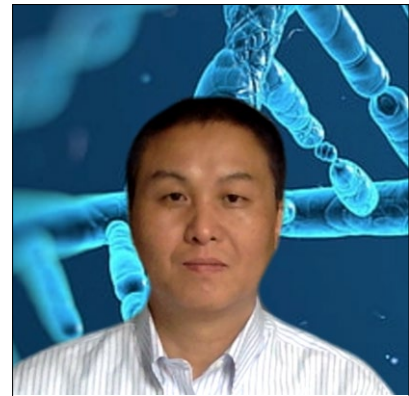


# Our Team

- CRC research faculty **presented and hosted 32 workshops** in Fall 21 to Spring 22 With an estimated attendance of 366 faculty, students, and staff, including an estimated 15 non-Pitt attendees, primarily from Howard University.
- From June 2021 to May 2022, Pitt faculty researchers **provided an estimated 322 individual consultations** lasting at least one hour.
- Between June 2021 and May 2022, Pitt faculty researchers were **co-authors on six published papers**.

## Fangping Mu created computational genomics program

Assistant research professor and CRC consultant **Fangping Mu** was awarded Pitt Seed funding to create a university-wide **Computational Genomics Training Program** to address the lack of bioinformatics expertise to take advantage of technologies such as next generation sequencing. The project involves designing and teaching 40 three-hour hands-on computational genomics workshops during 2021-2022. Mu's project also deployed a web forum platform to allow Pitt researchers to exchange questions and experience in bioinformatics-related research.



**CRC found new team members** with the backgrounds in computing and domain science that are vital to CRC's unique service. **Nickolas Comeau** is a research computing specialist with a background in neurobiology and computer science who manages user accounts and helps plan operating system updates and improvements in software and processes. **Cheng-nian Xiao** joined CRC as an engineering HPC consultant from a postdoc position in the Department of Mechanical Engineering and Materials Science in the Swanson school of Engineering, bringing experience in theoretical engineering, fluid dynamics, and scientific computing.

## CRC hosted a technical workshop for astronomical surveys

In November 2021, CRC faculty researchers led by assistant research professor and CRC consultant Daniel Perrefort hosted a 3-day technical workshop on the community-developed broker **systems supporting ground-based astronomical surveys** like the Zwicky Transient Facility (ZTF) and the Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST). The workshop focused on the technological challenges involving the ingestion, storage, processing, and distribution of live alert data that are presented in building a broker system. The workshop facilitated discussion among Broker teams of the technological challenges and sharing of expertise that will promote the development of broker-related services that benefit the broader scientific community. Participants and presenters came from leading research universities from Chile, Northern Ireland, Berlin, as well as the Goddard Space Center and other industry and non-university organizations.

# Transparency

In July CRC unveiled a system status display on our homepage that presents at one glance **far more data, at more granular levels, than before possible**. Both users and CRC team members can retrieve in-depth data on the status of utilization for individual clusters and user groups, including searching within defined time periods. Displayed here are status updates for the period Jan. 1, 2021 to May 31, 2022.

