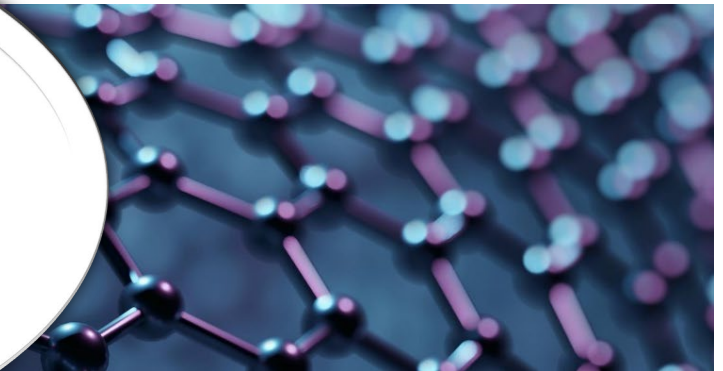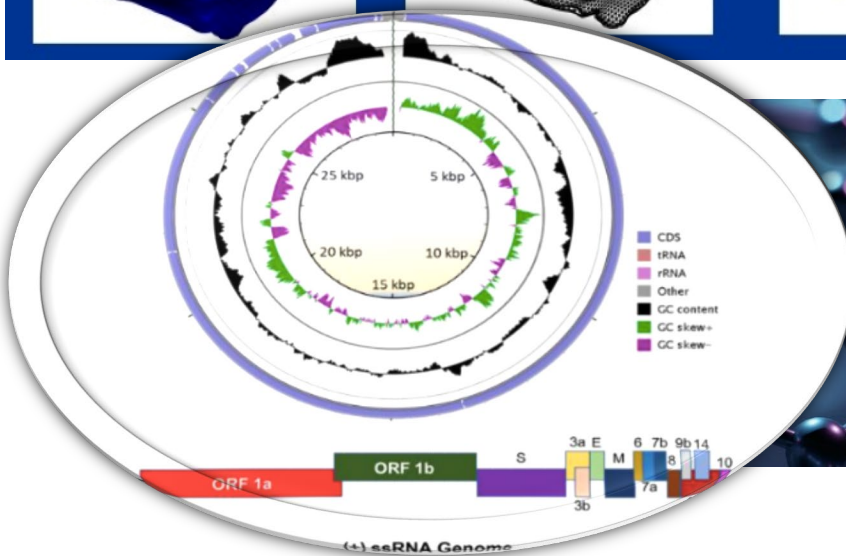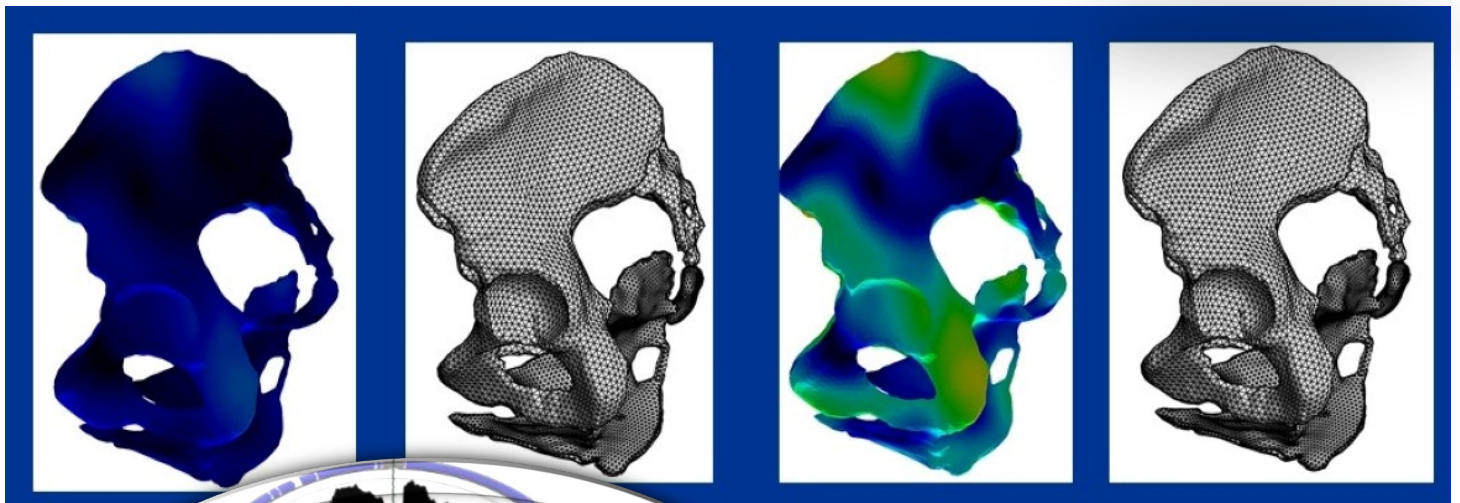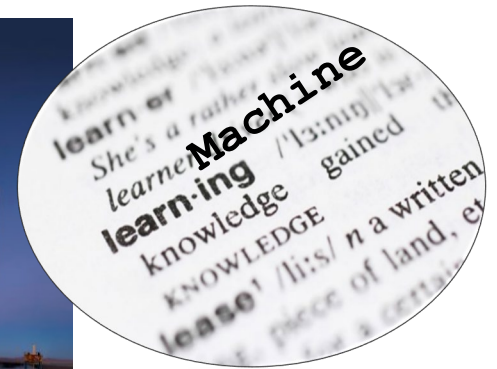# Research of Impact 2020-2021

Center for Research Computing 2020-2021

Pitt researchers faced a great many challenges in 2020-21 owing to the COVID-19 pandemic – closed and partly-staffed laboratories, restricted access to equipment, and team communication that had to adjust to an almost wholly online model. In the midst of much adjustment and improvising, there were not many resources researchers could count on consistently.

In spite of these challenges, the Center for Research Computing (CRC) continued high productivity and success. We quickly adjusted to virtual operations, enabled, and configured resources tailored for researchers working on projects related to the COVID-19, and continued to provide reliable and seamless access and support for all researchers across the Pitt community. Researchers who for months could not efficiently access specialized computing resources in their labs could always rely on CRC to bring advanced computing power to a laptop in their living rooms.

Research supported by CRC in 2020-2021 included:

- **Transcribing the genomes** of progressive mutations of COVID-19 variants within the body of a cancer patient with long-term COVID.
- **Modeling the effects of women's pelvic shapes** on long-term injuries from pregnancy and delivery.
- **Studying the origins of galaxies** based on spectra of eight-billion-year old light.
- **Predicting the patterns of decaying toxic substances** in soil.

CRC's education and training mission continued with a full schedule of online workshops and the addition of summer workshops in 2020 and 2021. The CRC's online workshops achieved great reach due to expanding our outreach to other institutions, including HBCUs Howard University and Spelman College. Faculty and students at Howard particularly were well represented at our Fall workshops and virtual Advancing Research through Computing Symposium in April. The online symposium roughly doubled in attendance from the 2019 symposium, with 279 individual logins by attendees from academic and industry institutions nationwide.

New Equipment Funding

CRC successfully secured major funding for equipment upgrades.

- $574K from the NIH S10 Instrumentation Programs for upgrading the HTC cluster to support health sciences research.
- $1.5M from the NSF Major Research Instrumentation Program to upgrade the GPU and MPI clusters

Usage

Our four [primary] computing clusters performed at consistently high volume while also accommodating regular surges in utilization owing to patterns of the academic calendar and research cycle.

- MPI: 76% annual average, 98% surge
- SMP: 66% annual average, 98% surge
- HTC: 50% annual average, 98% surge
- GPU: 78% annual average, 100% surge

Impact

CRC hosts 1624 active individual users on our resources.

CRC supports 338 accounts in 112 departments, centers, and institutes.

CRC supports computing accounts for 15 individual courses.

CRC hosts 17 departments, laboratories, and research offices that pay for data storage space on CRC's storage systems.

CRC documents that our collaborators published more than 310 papers, book chapters and conference presentations in 2020-2021 using CRC resources, including more than 60 papers in high-impact journals in the top 7 percent of rankings of research journals. [1]

CRC enabled over 154 grants in FY 2021, supported by 124.4 million dollars in external funding.[2]

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1. Owing to a greatly increased volume of published research on COVID-19, including pre-prints, the number of papers is considerably higher than in 2019-2020.

2. This dollar figure is based upon grants documented by CRC collaborators in proposals for computing allocations. This figure does not include grants that were not documented in proposals, grants for which it was not possible to document a dollar amount, and omnibus proposals that may include grants that are documented elsewhere.

New Outreach

CRC expanded both the scope and reach of our workshops on topics ranging from basic cluster usage to data science and machine learning **to online tutorial**s in response to the COVID-related shutdown and increasing interest in computational research, **first to Howard University** faculty, staff, students, and postdocs. The CRC team is collaborating with our Pitt faculty as well as faculty at Howard, other HBCUs, and beyond for our **workshops, tutorials, biennial meeting, access to CRC computing resources, and access to CRC support consultants** .

CRC's expanded outreach programs to HBCUs and regional undergraduate research groups made a significant contribution toward securing $1.5M in NSF funding for equipment upgrades.
CRC's outreach is an opportunity for Pitt to recruit previously untapped students and faculty, and to develop rich collaborations.
CRC is now exploring leveraging relationships with Pitt's Center for Latin American Studies to work with partners in Latin America.

CRC's collaborations include faculty at:

- Spelman College and other HBCUs in the Atlanta University Center Consortium
- University of Richmond and others in the undergraduate research MERCURY consortium
- Regional undergraduate colleges and universities, including Pitt Johnstown, Chatham University, Penn State Fayette, and Frostburg State University in Maryland
- High schools with diverse student bodies in the urban Pittsburgh Public School district, including nearby Pittsburgh Science and Technology Academy and Taylor Allderdice.

In 2020-2021, CRC research faculty consultants

Presented and hosted **42 online workshops** with **497 registrants.**

Provided **213 individual consultations.**

Delivered **invited lectures** for graduate courses.

Save the Date
April 6, 2021

Advancing Research through Computing 2021

CRC hosted our biennial symposium online in April with nationally prominent speakers from UC Berkeley and Argonne National Laboratory, as well as speakers from Pitt and Carnegie Mellon University, exploring Advanced Computing in the fields of Materials Design and Precision Medicine.

We attracted 279 participants – nearly twice as many as the last in-person symposium. Registrants came from industry, including Nvidia and PPG, and universities across the nation, including UC San Diego, UCLA, Montana State, University of Illinois, Case Western, the Ohio Supercomputing Center, Howard University, Columbia, Florida A&M, and of course our neighbors Carnegie Mellon, Duquesne, and the Pittsburgh Supercomputing Center.
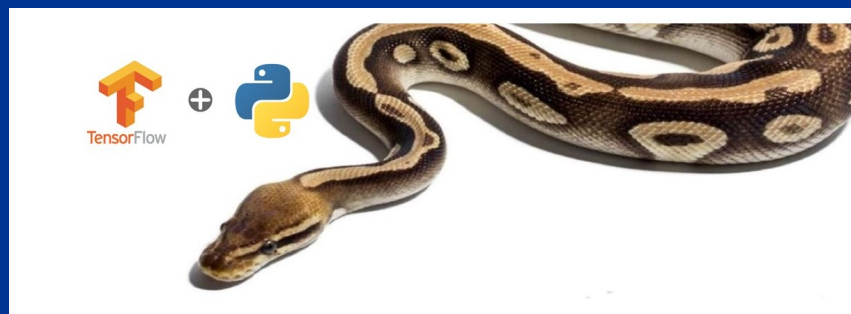
In June, CRC hosted a 5-day workshop on using the Python and Tensor Flow packages for advanced scientific computing and artificial intelligence. We attracted over 130 participants from the engineering, computing and scientific community at Pitt, CMU, and the Pittsburgh Supercomputing Center.

What our collaborators say about CRC

"The collaboration CRC creates is important. Researchers share expertise, we share problems. Sharing **the center creates community. Working together makes life much easier."**

– Peter Brusilovsky PhD, professor in the School of Computing and Information.

"This kind of research would not be feasible without CRC resources. **We can use CRC without already being funded, especially if you need a preliminary study** *before applying for the grant. A lot of the shape modeling is not possible at all on any of our machines. We didn't have funding and I needed to first try every free resource – a colleague told me about CRC. I didn't know CRC is free."*

– Megan Routzong, PhD candidate in Bioengineering on the team of Steven Abramowitch, PhD

The project on modeling galactic formation would have taken a very different approach – and a lot more time – without access to CRC. I was able to take **time to learn, try new ideas, and demonstrate that the model worked. The CRC staff has been great.** *I was new and I had a lot to learn, and Barry was a big help with writing the code and Kim Wong helped us get set up."*

– Yasha Kaushal, graduate student in the group of Rachel Bezanson, assistant professor of Physics and Astronomy (Kim Wong is associate research professor and CRC's co-director; Barry Moore II was formerly a research faculty consultant at CRC).

"The Public Health Dynamics Laboratory **needed large memory nodes to simulate the possible pandemic responses in Pennsylvania,** *which the state government implemented. Kim Wong set us up so that we are able to use a flexible set of software, which means we can use a wide range of data to run the simulation. CRC created a reservation that allowed us to jump the queue, as part of their policy to facilitate COVD-19 research. That saved a lot of time.* **Without CRC resources we could not model the entire state of Pennsylvania."**

– David Galloway, research programmer at the Public Health Dynamics Laboratory under Mark Roberts, MD, MPP, Professor of Health Policy and Management. The Laboratory advised the Pennsylvania Department of Health in on the state's initial March 2020 shutdown in response to the COVID-19 pandemic.