

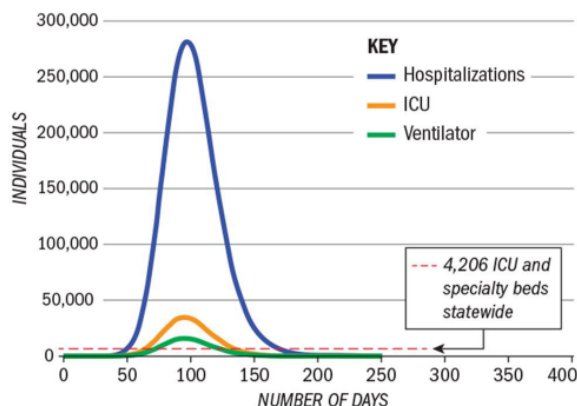
# Center for Research Computing Research of Impact 2019-2020



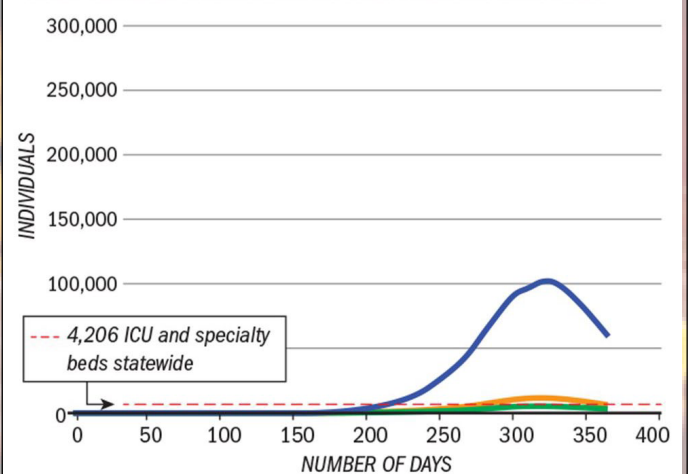
## Statewide projections for COVID-19 hospitalizations

The Framework for Reconstructing Epidemiological Dynamics (FRED), a disease modeling platform developed at the University of Pittsburgh Graduate School of Public Health, has forecasted surprisingly high hospitalization rates statewide, based on different scenarios for COVID-19 transmission.

### WITHOUT SOCIAL DISTANCING



### WITH SOCIAL DISTANCING OF DECREASING INTENSITY



Source: University of Pittsburgh  
Graduate School of Public Health

James Hilston/Post-Gazette

CRC resources helped Pitt's Public Health Dynamics Laboratory create models used to guide Pennsylvania's responses to the COVID-19 pandemic. Above are models as of March 26, reflecting outcomes with and without social distancing. Read more at "Epidemiology" on page 3.

## Center for Research Computing 2019-2020

In 2019-2020, CRC expanded our reach, impact, and capabilities.

### Reach

- CRC now hosts **889 active individual users**, a **10 percent increase** over 2018-2019.
- CRC enabled **184 grants** in FY 2020, supported by **\$143 million in outside funding** – in FY 2019 CRC documented **\$81 million in outside funding** (Note: the 2020 figure is based upon responses from 72 percent of CRC collaborators who are PIs on funded grants).
- **Overall usage** on CRC's four computing clusters **increased by 18 percent** based on service units (corresponding with compute hours).
  - Usage of **SMP** (Shared Memory Processing) **increased by 82 percent**.
  - Usage of **GPU** (Graphic Processing Units) **increased by 78 percent**.

### Impact

- CRC supports **302 group accounts in 54 departments, centers, and institutes**.
- CRC collaborators published more than **150 papers** that we are aware of in CY 2019 using CRC resources, including **more than 65 in high-impact journals** in the top 7 percent of rankings of scientific research journals (based upon an impact factor criterion of 5 and above).
- CRC hosts **46** departments, laboratories, and research offices that **pay for data storage space** on CRC's storage systems.

### Capabilities

- CRC will host computing for the **Center for Craniofacial and Dental Genetics** in the School of Dental Medicine, which is **investing in hardware** that will become part of CRC resources
- CRC **added 56 nodes in 2020** to the SMP cluster to address high utilization pressure.
- CRC **expanded data storage in 2019** with a new parallel file system and retired an aging storage system, migrating existing files to allow all users to access the updated data storage system.

CRC provides priority consultation, access, and computing allocations for several Pitt groups working on COVID-19 projects.

Public Health Dynamics Laboratory  
Biomedical Informatics  
Mechanical Engineering and Materials Science  
School of Pharmacy  
Center for Vaccine Research

## Research of Impact

### Epidemiology

PA policymakers facing the onset of the COVID-19 pandemic called on Pitt's Public Health Dynamics Laboratory to create models used in the state's first mitigation responses. The Laboratory, directed by Graduate School of Public Health professor Mark Roberts, relied heavily on the computing resources of CRC to model millions of scenarios, using a priority computing allocation, part of CRC's policy to facilitate COVID-19 research.



*PA Secretary of Health Rachel Levine and Governor Tom Wolf.*

### Biomedical Informatics

CRC put together a high-priority, complex set of resources for a COVID-19-related project led by Professor Greg Cooper from the Department of Biomedical Informatics, supported by the a team under Professor Jonathan Silverstein, to apply machine learning to analyze emergency department reports during the COVID-19 outbreak in order to the estimate magnitude and timing of outcomes, such as the daily number of cases.. The team needed powerful computing, and because they work with Protected Health Information, they needed a customized route to submit data. Within only a few hours, CRC and Pitt IT carved out resources and storage, configured and tested the software, and put in place security protocols. With CRC support, the team completed in four days an analysis which would otherwise take more than a month. The analysis is being used to develop models for identifying patients who may develop COVID-19, and to identify patients who may have had undetected COVID-19 in the past.

### Humanities

Ruth Mostern, associate professor of history and director of Pitt's World History Center collaborated with CRC to develop the World Historical Gazetteer, a platform for historians to search and share files. It creates multiple layers of data on human habitations and natural features, with ever-expanding references of events, figures, and artwork.

### Chemical and Petroleum Engineering

CRC resources help create novel nanomaterials in the Computer-Aided Nano and Energy Lab headed by Yanni Mpourmpakis, associate professor of chemical and petroleum engineering. They develop computational methods to design nanomaterials exploring safe storage and disposal of radioactive waste, formation of kidney stones, and creation of plastics. The lab designs catalysts that address real problems via simulations and collaborate with experimentalists who use these simulations as a basis for the physical design of nanomaterials, minimizing the slow, costly trial-and-error inherent in experimentation.

### Bioengineering

Pitt's Radiofrequency Research Facility relies on CRC to support development, human imaging studies, and clinical trials of one of the most powerful MRI devices in existence, able to reveal unprecedented levels of detail. The collaboration between Bioengineering and Psychiatry and directed by directed by Tamer Ibrahim, professor of bioengineering, radiology, and psychiatry, works with brain markers in which the MRI's electromagnetic waves must enter the skull in a uniform pattern, or heat can concentrate dangerously. CRC supported simulating hundreds of thousands of configurations to find the most even and safe magnetic field.

## From our collaborators – Why work with CRC?

### Support

*“CRC is one of the few places where you can ask a question and the consultants will investigate, instead of the researcher being forced to take time away from the project to work out a computational problem.”*

*-Lucas Mentch, assistant professor of statistics*

### Responsiveness

*“With the outstanding support from CRC, we get a response within a few hours for tickets that might otherwise take days at other supercomputing resources we have used. CRC is a fantastic resource.”*

*-Xiaosong Wang, associate professor of pathology and biomedical informatics, head of the Wang Cancer Genomics & Molecular Targeting Lab*

### Speed and capacity

*“To create an epidemiological model, we carry out many runs of the entire state person by person, adding different characteristics and events into each calculation, which makes modeling very computationally expensive. At CRC, we were able to use a flexible set of software that could handle a wide range of data. CRC created a reservation that allowed us to jump the queue and save a lot of time. Without CRC resources we could not run the entire state in the short timeframe necessary.”*

*-Mary Krauland, research assistant professor, Public Health Dynamics Laboratory*

### Wide-ranging

*“CRC is invaluable to humanities and social science researchers. It is hard to find a place for social scientists and humanists to meet the need for computing. I’m incredibly grateful for CRC.”*

*-Ruth Mostern, Director of Pitt’s World History Center*

### Multipurpose

*“CRC is necessary for us not just for simulation and optimization, but also for processing human imaging data produced in the clinical trials.”*

*-Tamer Ibrahim, professor of bioengineering, radiology, and psychiatry*

### Freedom to explore

*“Our lab works with thousands of combinations of regulatory t-cells in cancers. Using CRC gives me time to explore, to take risks, and make mistakes that don’t cost tens of thousands of dollars. That freedom to explore is part of the research culture of the university.”*

*-Anthony Cillo, post-doctoral associate in Immunology’s Dario Vignali Laboratory*

### Flexibility

*“For our studies of supernovae, dedicated facilities exist but they have a very narrow tailored scope and are expensive. We need the in-between scale of CRC.”*

*-Carles Badenes, associate professor of astrophysics and astronomy*

## **CRC's five faculty research consultants**

- Authored and co-authored 20 academic papers and conference proceedings.
- Are PIs, co-PIs, and senior personnel on eight research grants:
  - Associate professor Kim Wong: Leveraging Existing Humanware for Research in the Cloud Through Judicious Bursting, Indiana University initiative Humans Advancing Research in the Cloud
  - Associate professor Kim Wong: MIDAS Network Coordination Center, NIH
  - Associate professor Kim Wong: Advancing Drug-lead and Chemical probe Discovery Using Weighted-ensemble Simulations and Biophysical Validation, NIH
  - Assistant professor Shervin Sammak: Development of Real Gas Kinetic Chemistry at High Pressure, Pitt Momentum Funds Seedling Grant, SVCR-Momentum Fund
  - Assistant professor Fangping Mu: Correcting Pathogenic TGF Beta Activity in the Airway, NIH/NHLBI
  - Assistant professor Leonardo Bernasconi: Modeling of Adsorption and Diffusion of Warfare Agents and Related Molecules in Pristine and Defective Metal Organic Framework Materials, Army Research Office
  - Assistant professor Leonardo Bernasconi: Design, Synthesis and Characterization of Hybrid Stratified MOF-Plasmonic Nanoparticle Materials for Detection and Destruction of Chemical Agents, Defense Threat Reduction Agency
  - Assistant professor Barry Moore II: AudioXD: Seeding a new multi-disciplinary, multi-university network of data scientists working with audio recordings locating and counting terrestrial wildlife with an open source, automated acoustic survey platform, National Science Foundation
- Provided 175 one-on-one consultations with collaborators in person and online.
- Presented 22 workshops in person and online to more than 190 attendees.
- Workshops were expanded to include the University Library System, Health Science Library System and Pitt-Johnstown.
- Hosted well-attended workshops by industry representatives from Intel and Nvidia and by researchers from Biomedical Informatics and UPMC Children's Hospital.