

Center for Advanced Research Computing

Patrick Bridges

Director

2017 Annual Review Of Category 3 Research Centers/Institutes | March 9, 2018

Mission

To lead and grow the computational research community at UNM.

To fulfill our mission, we will:

- Provide access to high-end computing resources and associated infrastructure;
- Offer specialized expertise and technical support;
- Coordinate and collaborate with other UNM programs that support the community; and
- Grow the collaborative user community through education, workshops, and outreach events.

2017 Goals And Status

- Develop a strategic plan for CARC
 - In keeping with the University's Research 2020 plan, we have developed a strategic plan to better meet the needs of our users. We are also working to develop a sustainable funding model to enable the expansion of our systems and services as demand for CARC services grows and evolves.
- Develop and advertise cost center models for above baseline CARC systems and services
 - A cost model was developed in 2017 and received approval from the Internal Advisory Board. It was approved by the Executive Advisory Board and Unrestricted Accounting in 2018 and is now posted on our website.
- Work with PIs and other units and departments on sharing resources to grow capacity
 - Acquired joint enterprise storage system and virtualization system in collaboration with University Libraries
 - Recruited students from UNM departments to increase campus expertise and user support capacity
- Pursue cyber-infrastructure grant and contract research opportunities to enhance system capabilities
 - Submitted an NSF OAC proposal (pending) for researching new HPC system software approaches
 - Submitted an NSF CNS preproposal (encouraged) to deploy a system for research with streaming data

Membership of Advisory Committee

Karl Benedict, Ph.D. - Associate Professor, Director of Research Data Services. College of University Libraries and Learning Sciences

Vince Calhoun, Ph.D. - Distinguished Professor, Electrical and Computer Engineering, Biology, Computer Science, Neurosciences, and Psychiatry; Executive Science Officer, The Mind Research Network

Jed Crandall, Ph.D. - Associate Professor, Computer Science

Laura Crossey, Ph.D. - Interim Associate Dean for Research, Arts & Sciences and Professor, Earth and Planetary Sciences

Jeremy Edwards, Ph.D. - Professor, Chemistry

Miguel Gandert, M.A. - Director, Interdisciplinary Film and Digital Media (2017)

Hua Guo, Ph.D. - Distinguished Professor, Department of Chemistry and Chemical Biology, and Department of Physics and Astronomy

Patricia Henning, Ph.D. - Associate Vice President for Research; Professor of Physics and Astronomy

Jane Lehr, Ph.D. - Professor, Electrical and Computer Engineering

Keith Lidke, Ph.D. - Associate Professor, Physics & Astronomy

Barbara McCrady, Ph.D. - Distinguished Professor, Psychology; Director, Center on Alcoholism, Substance Abuse, and Addictions (CASAA)

Monika Nitsche, Professor, Mathematics and Statistics

Brian Pietrewicz, M.B.A. - Deputy CIO, Information Technologies

Edl Schamiloglu, Ph.D. - Distinguished Professor, Electrical and Computer Engineering; Associate Dean for Research, School of Engineering

Gregory Taylor, Ph.D. - Director, Long Wavelength Array; Director, Center for Astrophysical Research and Technology; Professor, Department of Physics and Astronomy

Lee Taylor, Ph.D. - Associate Professor, Biology

2017 Highlights

- Major awards
 - Received gifted computer system from Los Alamos National Laboratories, which includes 228 nodes, each featuring two quad-core 2.66 GHz Intel Xeon 5550 CPUs and 48 GB of memory. The new system, named Wheeler, was launched in two phases in 2017.
- Publicity
 - Hosted a booth at UNM Day at the Roundhouse
 - Hosted NM Supercomputing challenge student evaluations
 - Developed and deployed center communications strategy, including re-launch of social media accounts
- Major conferences
 - UNM/Los Alamos National Labs Computational Symposium
 - ACM/IEEE International Conference on Supercomputing
 - I-IWG Working Group on New Mexico Computational Science Pathway

Proposals & Awards

In prior years, CARC did not run grants through the Center; named staff were paid from funds held in other UNM departments.

In 2017, two grant applications, to be run through the Center, were submitted:

- CRI Preliminary: II-EN: Research Infrastructure for Continuous Analysis of High-Intensity Data Streams, \$656,956 (encouraged, full proposal submitted in early 2018)
- CDS&E: Optimization of Advanced Cyberinfrastructure through Data-driven Computational Modeling, \$523,644 (pending)

FY 2017 Budget

Salary (72%)

- All CARC staff, temp costs, and director

Infrastructure (14%)

- Computers, software, equipment and storage maintenance contracts

SC Conference (6%)

- Exhibition booth & staff travel to supercomputing conference – expenses overlap FY, most expenses from SC16*

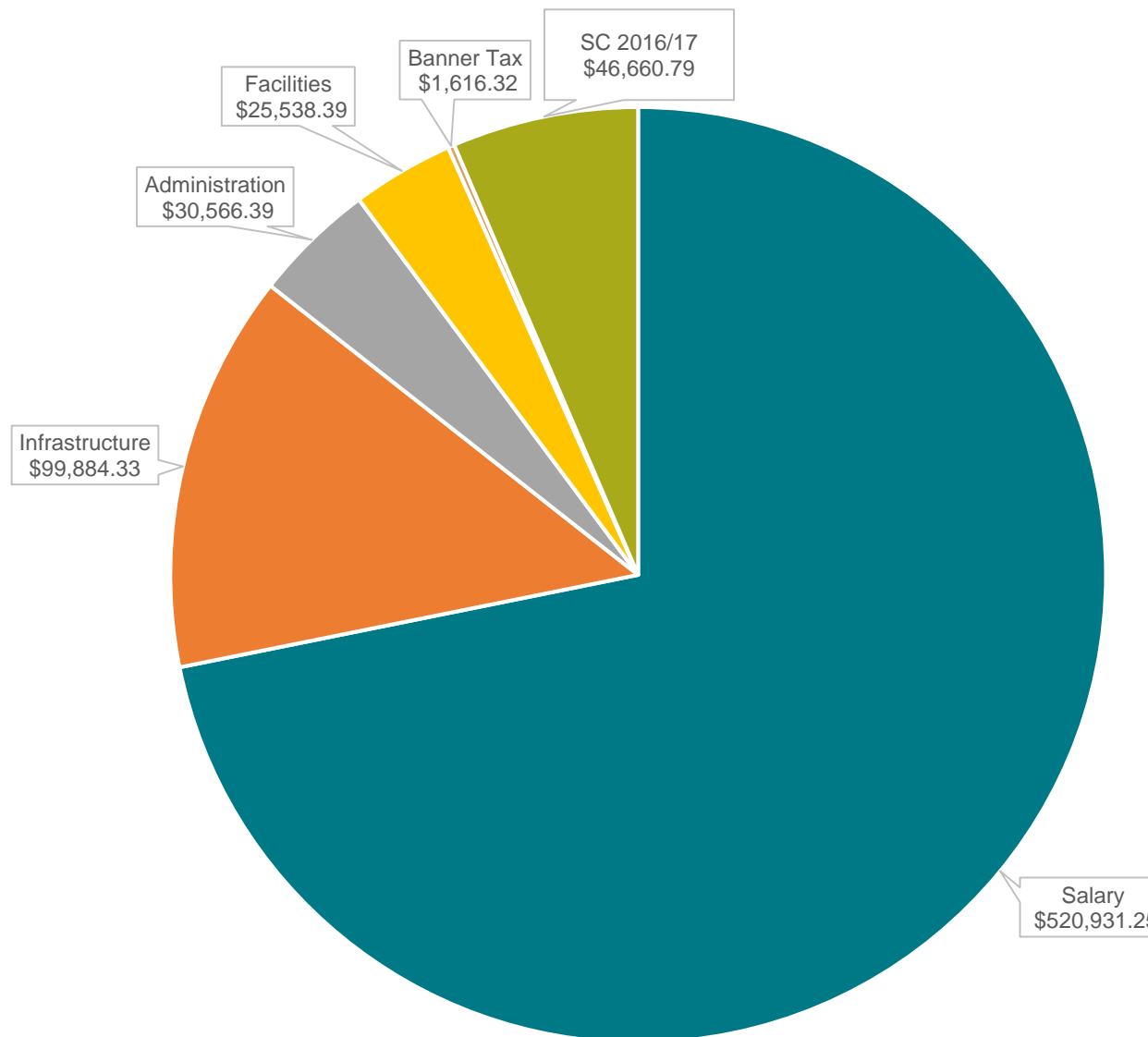
Administration (4%)

- Office supplies, phones, copier, travel, legal fees

Facilities (4%)

- Machine room (MMR) electrical work, cooling system repair

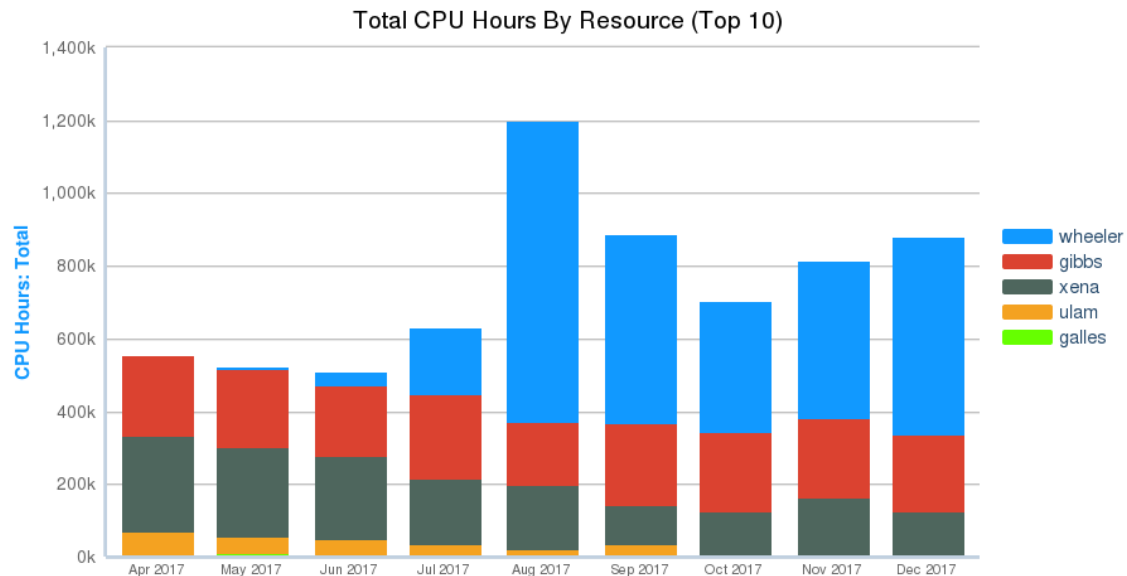
Banner Tax (0%)



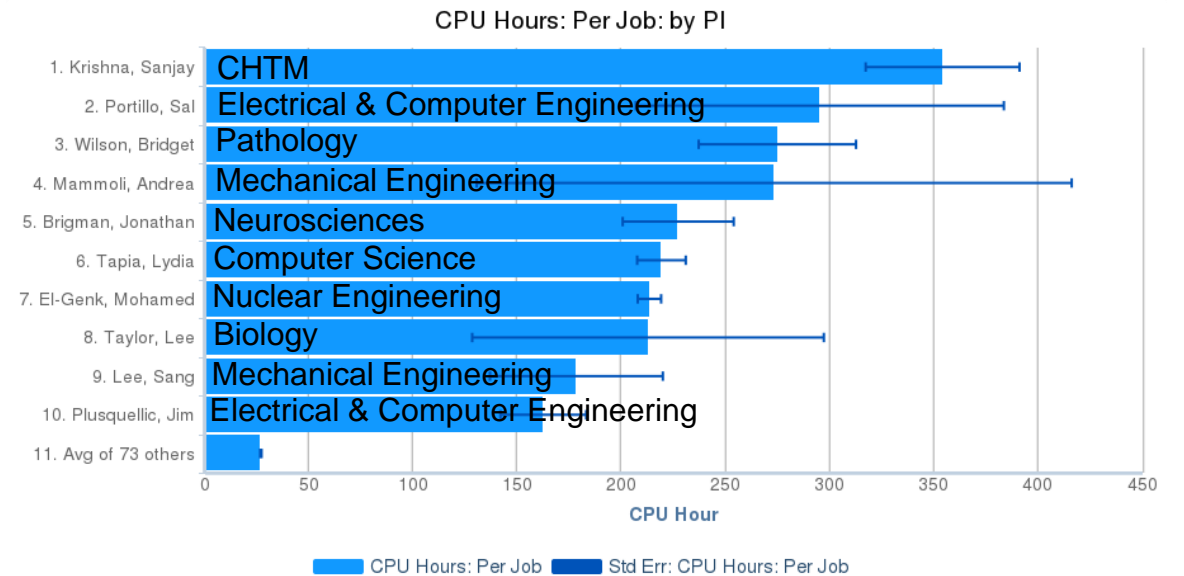
*Booth size and overall costs for SC18 reduced

Research Center Impacts

- Resources provided for the campus
 - Resources available include the 280-node/2240-core Wheeler capacity compute cluster, the 32-node Xena NVIDIA GPU cluster, and the 1.5PB Research Storage Consortium storage system.
 - Computational science application advice from expert staff
 - Computational research support for active grants
 - In-house workshops and presentations in UNM courses



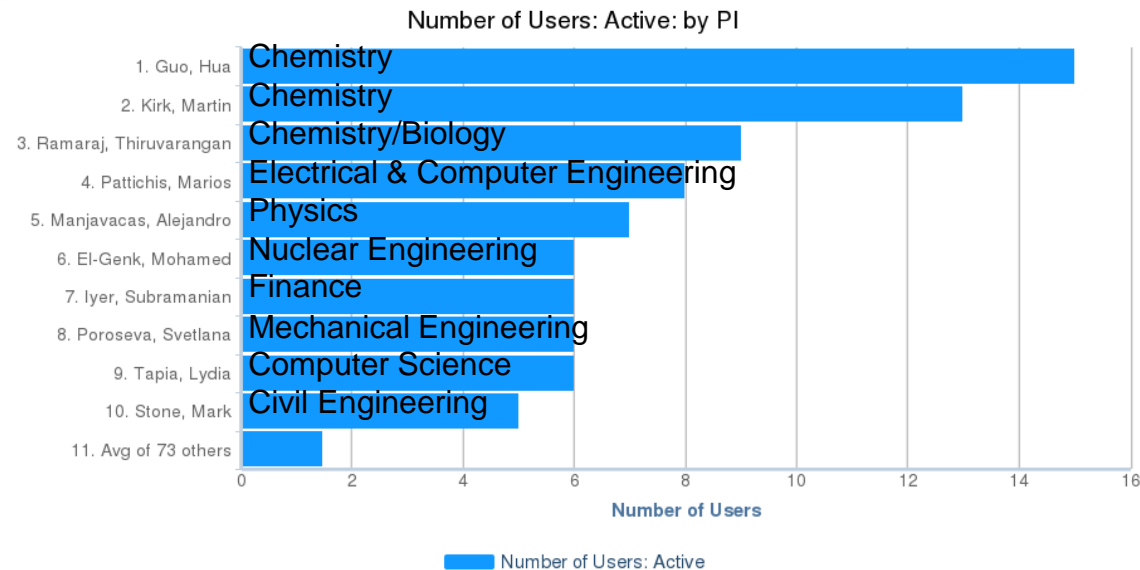
2017-04-01 to 2017-12-31 Src: HPCDB. Powered by XDMoD/Highcharts



2017-04-01 to 2017-12-31 Src: HPCDB. Powered by XDMoD/Highcharts

Return On Investment

- Average of 80 active facility users, mostly students, across 40 active PIs per month
- 34 publications in journals such as *PLOS One*, *The Journal of Chemical Physics*, *The Journal of Immunology*, *Journal of Materials Chemistry*, and *Journal of Biogeography*
- Awards resulting in publications using CARC resources included funding from the National Science Foundation, National Institutes of Health, Department of Energy, Army Research Office MURI grant, and Ministerio de Economía y Competitividad (Spain) among others.



Support a broad range of computational research activities by the UNM community

Provide substantial computational resources to researchers free of charge

Expert user support staff

STRENGTHS

Aging systems and facilities

Understaffed to meet campus demand

Building with significant security, maintenance, and utilization challenges

Underutilized CSE program

Lack of support for research with specialized needs or that handle sensitive data

WEAKNESSES

Computational science workforce demand

Increase collaboration with other computational units on campus (Libraries, IT)

External collaboration with Labs (SNL, LANL) and Industry

Leverage cloud computing resources to handle specialized research needs and sensitive data

OPPORTUNITIES

Staff loss to retirement, external competition

Major system or facilities failure

Decreasing price of cloud computing systems

THREATS



Looking Ahead To 2018

- Significant grant/contract opportunities
 - NSF CISE Research Infrastructure (submitted)
 - NSF OAC Cyberinfrastructure for Sustained Scientific Innovation (submission planned jointly with UNM Libraries)
- New partnerships/relationships
 - Deploy and publicize system cost model to UNM main campus units
 - Develop LANL research and workforce development relationship
 - Revitalize CSE certificate program in collaboration with UNM Math, Mechanical Engineering, and Computer Science departments
- Significant plans for space
 - Consolidate systems staff into a single working space
 - Explore renovating available space in Galles building into a LANL/SNL/AFRL research collaboration facility in concert with New Mexico Consortium

Summary

The gift of our new system, Wheeler, represents a significant increase in computing capacity for the Center. This will allow more users to complete bigger and more complex projects with relative ease.

The development of a strategic plan is setting the direction for the Center in 2018. One priority is developing sustainable funding models. We have developed a cost model to address specialized computing needs by users as a first step towards this, and are actively seeking grant funding that will support equipment and staff in the future.

The revision and re-focusing of our Computational Science and Engineering certificate will allow us to begin to create a pathway from university to employment. This includes future work on creating partnerships with employers such as the New Mexico National Labs and private industry.