

Center for Advanced Research Computing

Patrick Bridges

Director

2020 Annual Review of Category 3 Research Centers/Institutes | February 12, 2021

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.

CY 2020 Goals and Status

- \$4 million, 5-year DOE NNSA award to create the Center for Understandable, Performant Exascale Communication Systems (CUP-ECS) was awarded September 30, 2020.
- Computational Science and Engineering graduate certificate application moved into UNM's ApplyYourself system, admissions committee established, data science specialization roadmap published to CARC website
- Goal of becoming an NSF XSEDE basic service provider (SP) and assessing requirements/benefits of further integration with NSF XSEDE services deferred to 2021 or later
- Plan to develop and submit an NSF MRI proposal for a new HPC CARC-hosted capacity HPC system deferred pending identifying sufficient cost share funds

Membership of Advisory Committee

- **Susan Atlas, Ph.D.** - Research Professor, Physics and Astronomy
- **Patrick Bridges, Ph.D.** - Director, CARC; Professor, Computer Science
- **Karl Benedict, Ph.D.** - Associate Professor & Director of Research Data Services, College of University Libraries and Learning Sciences
- **Mary Jo Daniel, Ph.D.** - Associate Vice President for Research
- **Jeremy Edwards, Ph.D.** - Professor, Chemistry
- **Hua Guo, Ph.D.** - Distinguished Professor, Department of Chemistry and Chemical Biology, and Department 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, Ph.D.** - Professor, Mathematics and Statistics
- **Marek Osinski, Ph.D.** - Distinguished Professor, Electrical & Computer Engineering; Center for High Technology Materials
- **Brian Pietrewicz, MBA** - Deputy CIO, Information Technologies
- **Andrea Polli, Ph.D.** - Mesa Del Sol Endowed Chair of Digital Media Professor, Fine Arts and Engineering University of New Mexico Department of Art and Art History
- **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
- **Tom Turner, Ph.D.** - Associate Dean for Research, Arts & Sciences; Professor, Biology

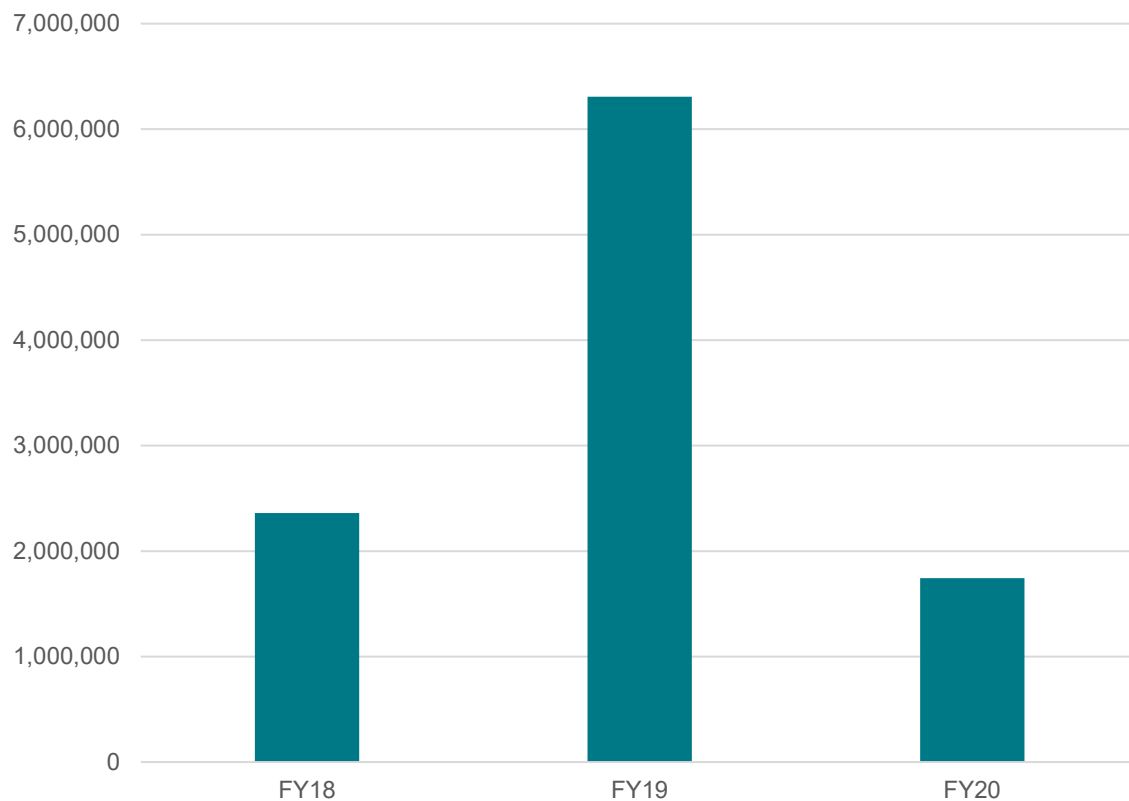
Date of CY2020 annual review: pending

CY 2020 Highlights

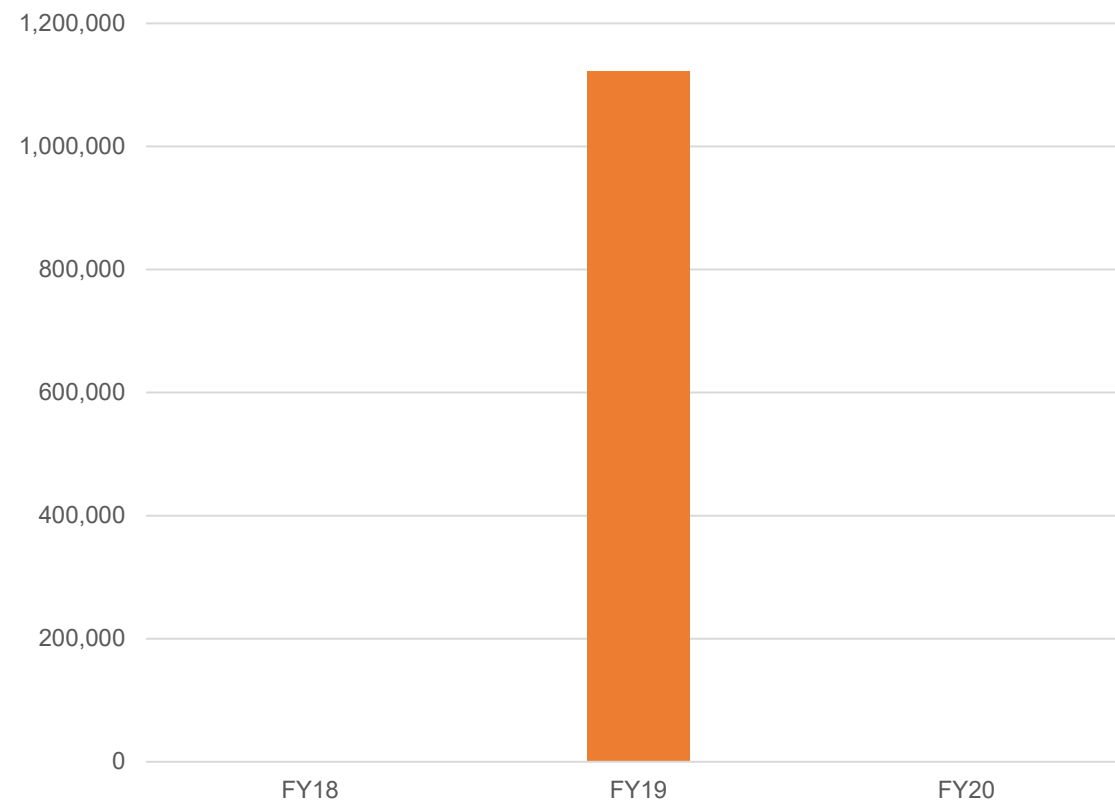
- Systems Expansion
 - Taos cluster expansion using funds from PIs and their sponsored research projects
 - Prototyping and deployment of center-wide parallel filesystem
- CARC support for UNM COVID-19 research efforts
 - Analysis of COVID gene sequences collected in New Mexico and Wyoming
 - Deidentifying CT scans of pneumonia and COVID victims for pathology research
 - Simulation of COVID-19 spread in human lung tissue
 - <https://carc.unm.edu/news--events/News/researchers-study-covid-19.html>
- Awarded \$4 million DOE NNSA PSAAP III research center
- Introduction to Computing at CARC goes online (Youtube, Learn)

Proposals & Awards

Proposals

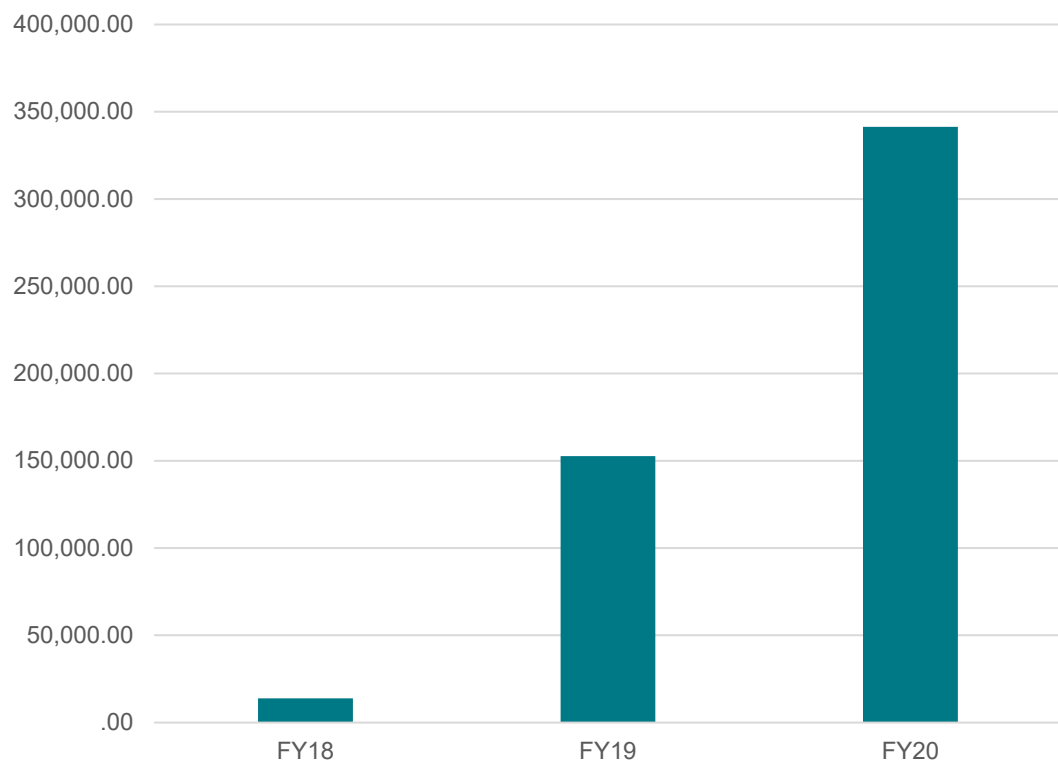


Awards

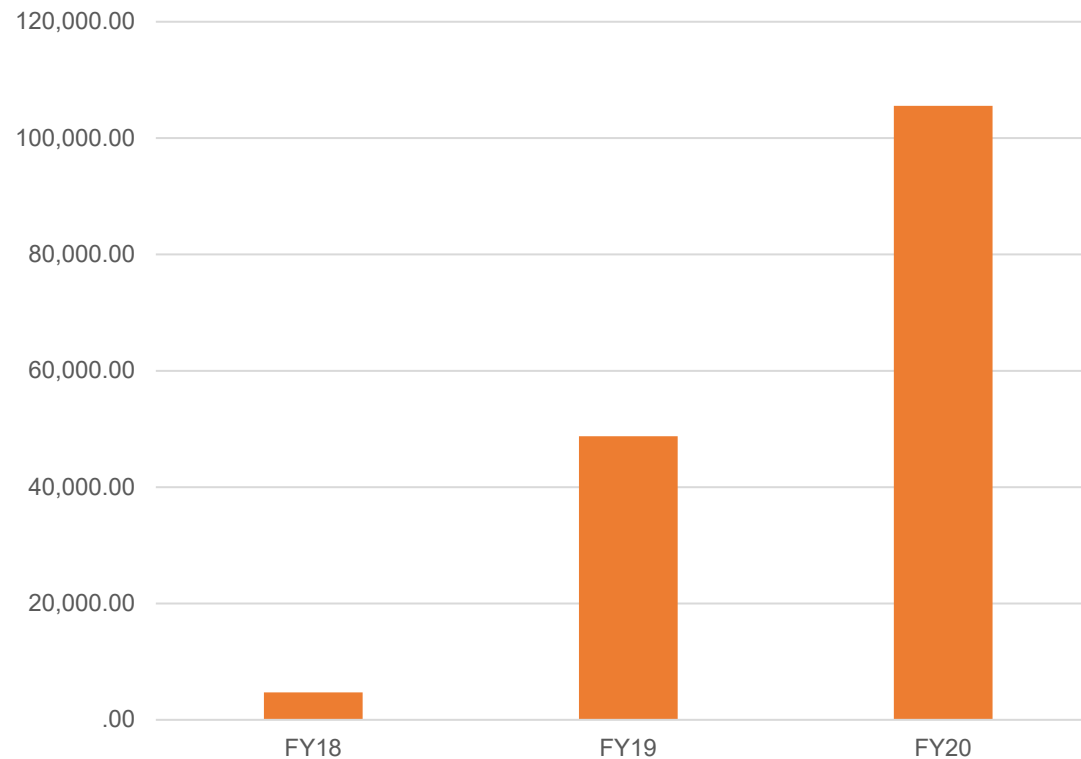


Research Expenditures and F&A

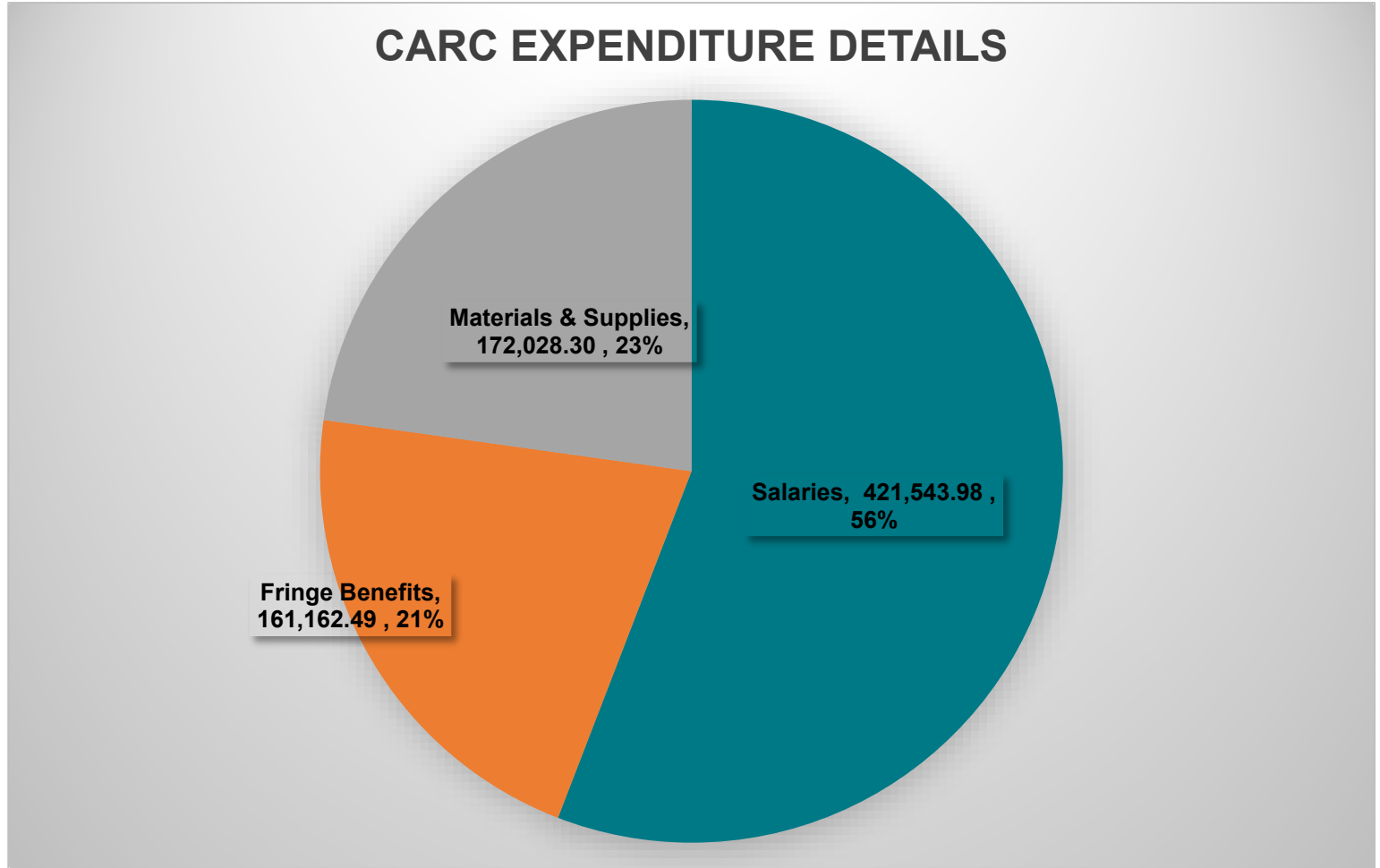
Research Expenditures



F&A



FY20 Sources of Revenue	
F&A Return	36,946
VPR Allocation	680,000
Service Center	36,292
Other	4,500
FY19 to FY20 Reserves	98,102
Total	855,840



Research Center Impacts

- Trained 32 students in-person in Spring 2020 on use of CARC systems
- 832 views of QuickBytes YouTube series that replaced in-person training this summer; Dr. Fricke estimates he's oriented 40-70 new users online since March
- NSF-funded research projects supported multiple graduate students, publication of papers, and design/prototyping of platform for handling controlled unclassified research information SAMPRA impact
- CARC-trained graduate student ambassadors completing research, actively training lab members, and being placed in jobs
- The number of users, projects, jobs finished, and CPU hours provided to UNM continues to grow
 - 2018: 217,427 jobs finished; 15.4M CPU hours provided
 - 2019: 411,125 jobs finished; 17M CPU hours provided
 - 2020: 545,309 jobs finished; 16.9M CPU hours provided
- Collaborating with NMSU via EPSCoR award to improve UNM and state computational research capabilities related to smart energy grids, including new storage at CARC

Return on Investment

- CARC supported 408 users and 104 PIs, with 545,309 jobs finished
- 53 publications in journals such as *Nature*; *Chemical Science*; *Journal of Volcanology and Geothermal Research*; *The Journal of Chemical Physics*; *Journal of Applied Physics*; *Journal of Chemical Theory and Computation*; *Applied Materials Today*; *Current Robotics Reports*; *Journal of the American Chemical Society*; *ACS Nano*; *Journal of Geophysical Research: Space Physics*; *G3: Genes, Genomes, Genetics*; *NeuroImage*; *Proceedings of the National Academy of Sciences of the United States of America*
- Awards resulting in publications using CARC resources included funding from the National Science Foundation, Department of Energy, Defense Advance Research Projects Agency, Air Force Office of Scientific Research, and Army Research Office 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

Graduate student ambassador training program

STRENGTHS

Aging systems and facilities

Understaffed to meet campus demand

Building with significant security, maintenance, and utilization challenges

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

WEAKNESSES

Utilize CSE program to expand research computing expertise on campus

Computational science workforce demand

Research and Education Funding opportunities within NSF Harnessing the Data Revolution Big Idea calls

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

External collaboration with Labs (SNL, LANL) and industry

OPPORTUNITIES

Staff loss to retirement, external competition

Major system or facilities failure

Unnecessary use of expensive cloud computing systems by UNM researchers

Pandemic could push already short staffing into a bigger problem

THREATS



Looking Ahead to 2021

- Continue to promote and improve revised CSE program – outreach to affiliated faculty and departments, develop more specializations
- Become an NSF XSEDE basic service provider (SP) and assess the requirements and potential benefits of further integration with NSF XSEDE services, as preparation for potential submission of NSF system acquisition and management awards.
- Develop and begin executing systems refresh plan using combination of state funds, institutional funds, and potential federal funds (e.g. NSF MRI awards)

Summary

- Made considerable progress on the immediate goals outlined in our strategic plan
- Engaged in major collaborative projects, strengthening cross-campus collaborations that increase center impact for the benefit of the UNM community
- Submitted multiple sponsored research proposals, resulting in the selection of UNM CARC to lead a prestigious DOE NNSA PSAAP center in collaboration with researchers at the University of Tennessee at Chattanooga and the University of Alabama at Birmingham