CENTER FOR ADVANCED RESEARCH COMPUTING

Internal Advisory Board Meeting
October 29, 2020

MINUTES

Present: **Susan Atlas** - Research Professor, Physics and Astronomy; **Karl Benedict**, Associate Professor & Director of Research Data Services, College of University Libraries and Learning Sciences; **Patrick Bridges** - Director of CARC; **Mary Jo Daniel** – Interim Associate Vice President of Research; **Jeremy Edwards** - Professor, Chemistry; **Hua Guo**- Distinguished Professor, Department of Chemistry and Chemical Biology, and Department of Physics and Astronomy; **Keith Lidke**- Associate Professor, Physics & Astronomy; **Monika Nitsche** - Professor, Mathematics and Statistics; **Marek Osinski** - Professor, Electrical & Computer Engineering; Center for High Technology Materials; **Brian Pietrewicz** - Interim Deputy CIO, Information Technologies; **Edl Schamiloglu** - Distinguished Professor, Electrical and Computer Engineering; Associate Dean for Research and Innovation, School of Engineering; **Tom Turner** - Professor, Biology; Associate Dean for Research, Arts & Sciences; **Tracy Wenzl** - CARC Business Manager

1. CARC 2019 Annual Report
    - Slides were presented (see attached)
2. Discussion:
    - Future System Acquisitions

Discussion of ways to acquire new machines, including via grant funding, PI condo purchase, and VPR support/match support. Noted that facilities need to be sufficient for expansion if pursuing large equipment grants and current building does not provide this. NSF MRI grants require substantial cost share.

Discussed potential plan to relocate machine room to Mesa Del Sol facility, in partnership with IT and UNMH – that facility is under contract with another prospective buyer so off the table for now. It was suggested that CARC get on the capital planning list, and pursue GO money to fund new facility if MDS is not an option.

Discussed plan to create space for CARC personnel in new research facility to be built on south campus in coming year. Facility would be shared with Sandia NL, AFRL, and other UNM research units.

- CARC/UNM Research Computing Support

Currently potential improvements to systems are delayed due to lack of available staff to complete them. CARC partners with Libraries to cross-train and share staff resources, this could be expanded to include Computer Science, Central IT. It was suggested that research computing be centralized.

Minutes submitted by Tracy Wenzl, 10/30/2020

Fall 2020 Internal Advisor Board Meeting

Patrick Bridges
Director

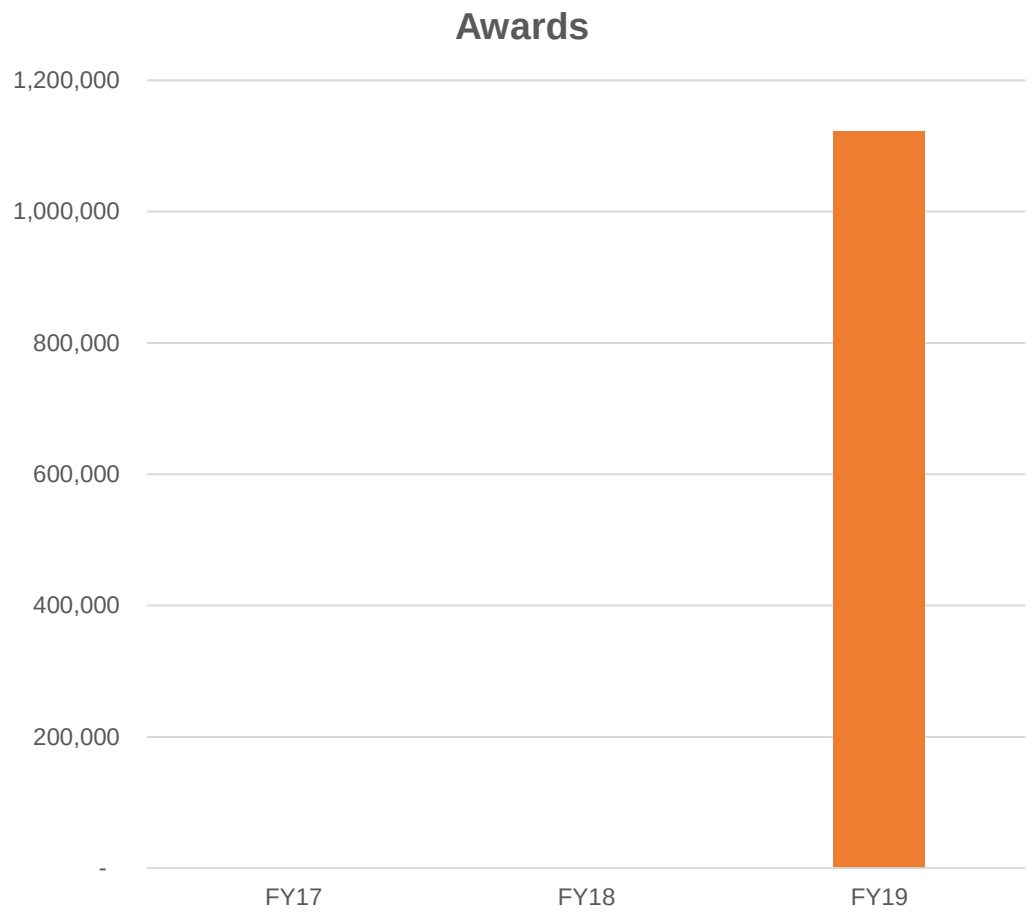
Agenda for today

- Review 2019 Accomplishments/Annual Report
- Discuss current challenges/needs
  - Facilities improvements
  - System renewal/acquisition
  - Capabilities/Staffing - Research IT Strategic Planning

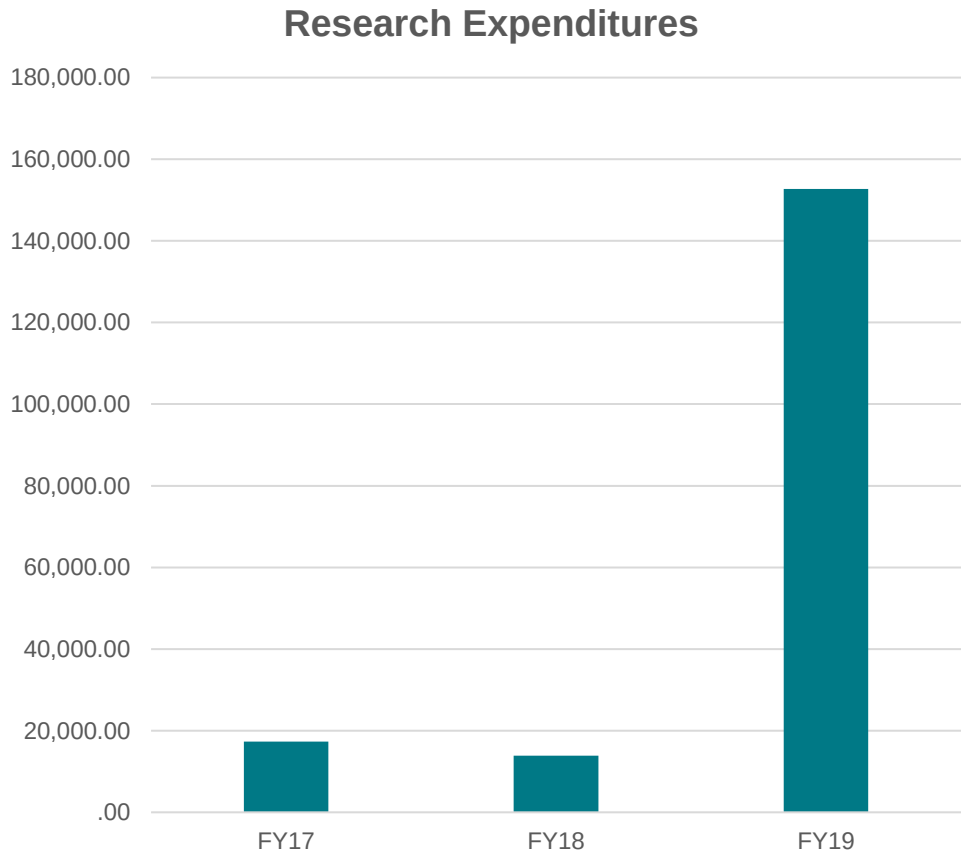
CY 2019 Goals and Status

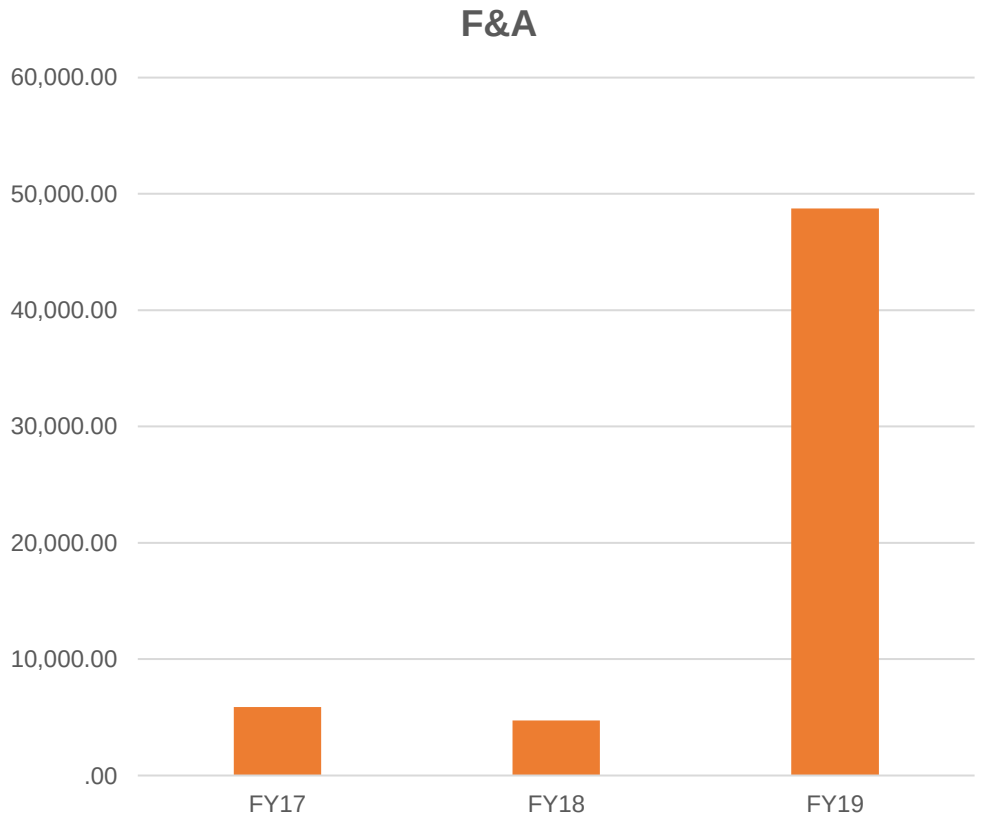
- Promote revised Computational Science and Engineering (CSE) graduate certificate program – outreach to affiliated faculty and departments, develop more specializations
  - Catalog updates completed May 2019. An admissions committee has been identified and we are working on creating an advisory board. Work has progressed on developing a data science specialization.
- Develop collaborative research community through outreach, workshops and symposia
  - 2019 saw 91 Introduction to Computing at CARC workshop attendees, a large increase over the 14 who attended in 2018
  - CARC Graduate Assistants held reNew Parallel MATLAB workshop was launched with 16 attendees
  - Research presentations in the Workshop room at the end of each semester
- Systems updates
  - Deployed a new NetApp enterprise storage system
  - Upgraded CARC core network infrastructure, making 10Gb Ethernet the default connection to all CARC HPC and storage systems
  - Launched Vivantio help ticket system
  - Deployed Jupyter notebooks, distributed MATLAB, and debugging queues to increase system accessibility
- Significant grant/contract opportunities
  - Submitted NSF cybertraining, NNSA MSIPP, HDR DSC, NSF IGE, NSF OAC, and PSAAP grant proposals in 2019
  - Received official notice in early 2020 that PSAAP was funded ($4 million)
  - Submitted revised application to NSF cybertraining in early 2020
  - Multiple additional opportunities going forward: NSF IUSE:CUE, Potential Mid-scale Infrastructure Collaboration with RMACC, Network infrastructure opportunities with regional partners

Proposals & Awards

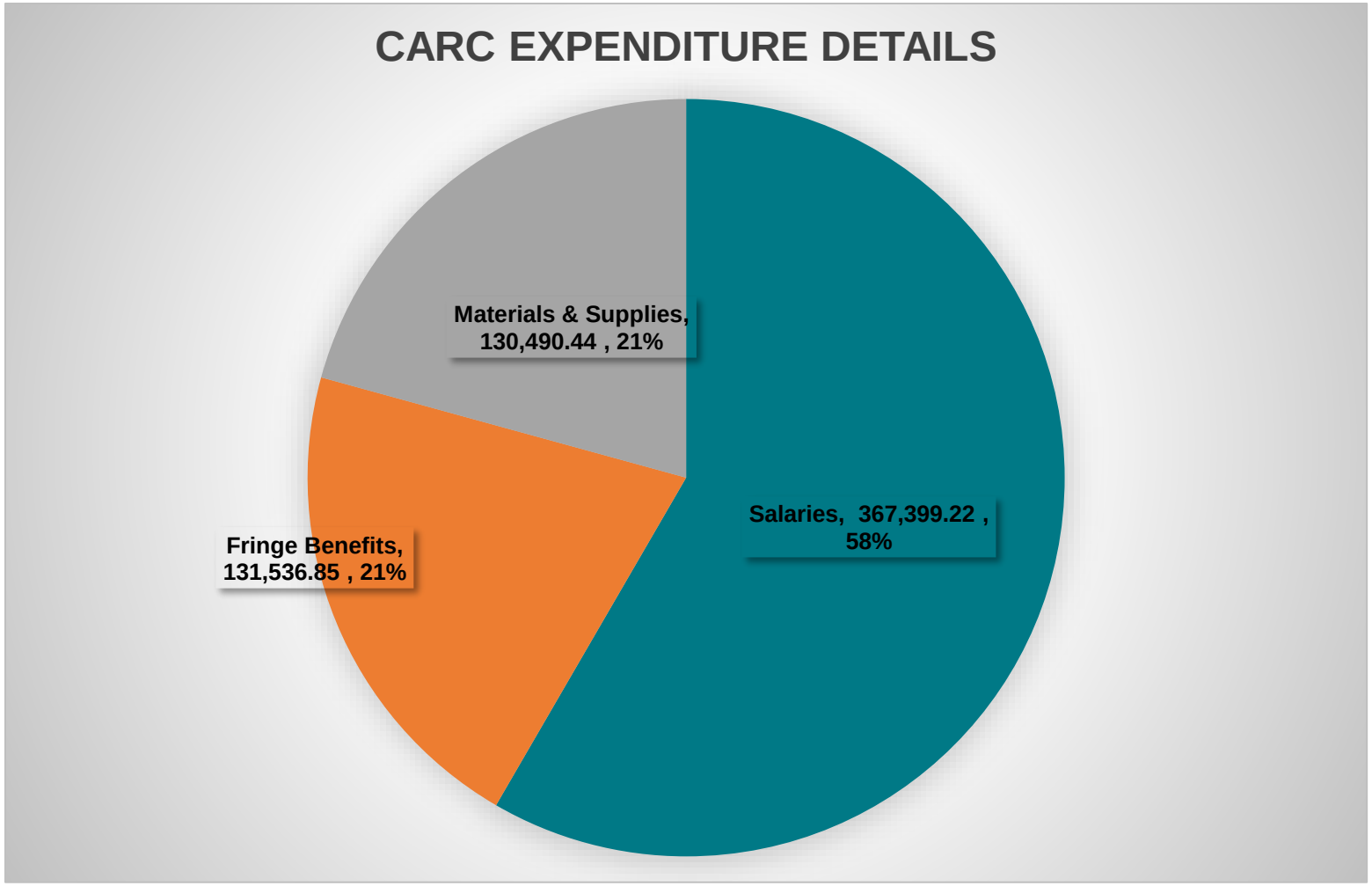


Research Expenditures and F&A





FY19 Sources of Revenue	
F&A Return	17,104.90
VPR Allocation	680,000.00
Other	4,000.00
FY18 to FY19 Reserves	26,424.18
Total	727,529.08



Research Center Impacts

- Trained 107 students, faculty and staff to use CARC resources in workshops held throughout the year
- Host and helped deploy the New Mexico Decedent Information Database, the first national searchable database of whole-body decedent CT scans
- The number of users, projects, jobs finished, and CPU hours provided to UNM continues to grow
  - 2017: 99,679 Jobs Finished; 7.2M CPU Hours provided
  - 2018: 217,427 Jobs Finished; 15.4M CPU Hours provided
  - 2019: 411,125 Jobs Finished; 17M CPU Hours provided
- CARC and multiple UNM PIs collaborated to begin acquiring new hardware to expand the Taos compute cluster
- Collaborating with NMSU via EPSCoR award to improve UNM and state computational research capabilities related to smart energy grids, including new storage at CARC

Research Center Impacts

- CARC supported 308 users and 92 PIs, with 411,125 jobs finished
- 56 publications in journals such as *Scientific Reports, Nanophotonics, Communications Physics, The Journal of Mathematical Physics, The Journal of Chemical Physics, The Astrophysical Journal, Materials Research Express, Radio Science, Viruses, Zoologica Scripta,* and *Water Resources Research*.
- Awards resulting in publications using CARC resources included funding from the National Science Foundation, National Institutes of Health, Department of Energy, Institute for Space and Nuclear Power Studies, Office of Naval Research, and the Air Force Research Lab among others.

Predictive Science Academic Alliance Program

PSAAP is managed by the NNSA Office of Advanced Simulation and Computing (ASC), in collaboration with Lawrence Livermore National Laboratory, Los Alamos National Laboratory and Sandia National Laboratories

- $4M 5 year NNSA award to CARC and subawardees (UTC, UAB)
- Focus is on research for next generation HPC communication system software
- Close collaboration with DOE national laboratories
- 8 other awardees: Colorado, Texas, MIT, Stanford, Illinois, Maryland, Buffalo, Oregon State

STRENGTHS

- 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

WEAKNESSES

- 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

OPPORTUNITIES

- 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

THREATS

- Staff loss to retirement, external competition
- Major system or facilities failure
- Decreasing price of cloud computing systems

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Facilities Needs

- Galles building and machine room are significantly aging
  - Poor office and research spaces
  - Spending tens of thousands of dollars on AC and UPS maintenance
  - Machine room size, reliability restrict ability to submit to and compete for large federal awards for running systems
- Possibilities
  - South campus collaboration space plan includes office space for CARC
  - Exploring shared data center possibilities
    - Large Mesa del Sol opportunity had potential, seller currently working with another potential buyer
    - Hospitals, IT still interested in pursuing joint data center opportunities

System renewal/acquisition

- Current system limitations
  - Current capacity system Wheeler is aging (10 years old)
  - Limited support for more diverse workloads
    - Data-intensive (e.g. Spark, Hadoop, etc.)
    - Large-scale data storage
    - Cloud and container-based workloads
    - Controlled unclassified information (e.g. PHI, PPI, export control)
  - Growing need for integrating instrumentation with data and analysis systems
- Current approach
  - Deploying BeeGFS scale-out data storage systems
  - Leverage PIs with need for specialized hardware and funding
  - Discussing OVPR matching PI system investments to grow campus capacity
- NSF MRI funding also a possibility to pursue – cost share the issue

Staffing Challenges, Campus Research IT needs

- Increasing need for research computing staff across campus
- Many potential CARC improvements delayed due to lack of staff
  - Authentication integration with main campus
  - Email migration to UNM IT (would need AIRS replacement)
  - NSF XSEDE L3 service provider integration
- Shared staffing/system efforts with Libraries have helped, could look to expand to include other partners (e.g. CS, IT, etc.)
- Ongoing Research IT strategic planning work a potential avenue for enabling broader collaboration