CRCF Annual Public Report

VILLANOVA UNIVERSITY
CENTRALIZED RESEARCH
COMPUTING FACILITY

Academic Year 2026
Last updated 5/11/26

Contents

Overview

The Centralized Research Computing Facility (CRCF) is Villanova's first core facility (established November 2021) and provides support for computational research. Most research support is in the form of high performance computing (HPC), but other forms of support are available as well. We encourage all Villanova researchers to contact us if they are interested in research computing but do not yet have a strategy towards achieving their goals.

CRCF supports two HPC clusters and their users:

- Augie: this is CRCF's largest and newest cluster. It was procured through an NSF Campus Cyberinfrastructure (CC*) grant in Summer 2020. The cluster was installed in March 2021. Augie is open to all Villanova researchers and Villanova students.
- Clusty: this is the Astrophysics cluster that has been opened up to all users. The cluster is managed by Andrej Prsa in the Astrophysics and Planetary Science department.

A third cluster, Alipi, was restricted to COE users and was retired in Summer 2025.

CRCF emphasizes that *centralized computing is more than just HPC equipment*. CRCF currently provides the following to the Villanova community:

- State-of-the-art HPC resources
- A central knowledge base/pool of expertise for research computing resources
- A partner to help faculty integrate HPC into their coursework and proposals
- A resource for developing computer programming and software applications skills for students, staff, and faculty. This resource follows Augustinian values of helping others (akin to service learning)

In summary, *CRCF is a partnership of faculty, technical staff and students that empowers Villanova to maximize its computational research potential.*

CRCF has three thrusts as part of this mission/vision:

Thrust #1: HPC Support through a Collaboration of Faculty and IT Staff. This thrust involves the management of Augie, Alipi, and Clusty.

Thrust #2: Research Computing Center of Expertise. CRCF provides training opportunities including on-demand new user training, webinars for research computing topics of interest, and a point of contact for interaction with experts at other institutions. All researchers interested in research computing or HPC should approach CRCF to help develop a strategy to meet their goals.

Thrust #3: HPC Peer User Support. A wealth of research computing expertise exists on campus, and CRCF strives to facilitate communication between users seeking help and the experts that can help them. These volunteer experts personify Villanova's Augustinian tradition, providing support for commonly used programming languages and applications.

CRCF HPC Cluster Specifications

Augie

Item	Values
Compute Nodes/Cores	37 compute nodes/2,368 AMD EPYC Series
RAM	17.4 TB Main Memory
Disk Space	292 TB
GPU	2x Tesla A100: 13.8k CUDA cores for throughput of 19.5 TFLOPS
Interconnect	Mellanox 200 Gbps
Software	ANSYS-Fluent, ANSYS-Mechanical, COMSOL, C, Fortran, OpenMPI/MVAPICH/Intel MPI, Gnuplot, MATLAB, Python, PyTorch, Tensorflow, VASP, CUDA, R, IQTREE

The status of Augie's applications is as follows:

1. The following software applications have been installed and performance tested, with sample scripts available to users: ANSYS-Fluent, ANSYS-Mechanical, COMSOL, CUDA, Intel MPI, IQTREE, MATLAB, Python, VASP, Fortran/MVAPICH, GCC/MVAPICH, GnuPlot, R, PyTorch, and Tensorflow.
2. The following software applications are slated for installation: Abaqus, AOCC, CP2K, Gaussian, GCC/MPICH, GCC/OpenMPI, LAMMPS, OpenFOAM, PAML, PyHEA, QE, RAXML, SageMath, and Singularity.
3. The following software applications need further exploration or discussion prior to initiating an installation effort: Mathematica, Open OnDemand, and Anjuta.

Only those software packages listed in Items 1 and 2 above are currently supported by CRCF. Users are encouraged to install their own software packages in their home directories for their own use.

Users are encouraged to visit the Coding Resources and Scripts folder on the AugieUsers SharePoint site, which contains lessons learned and names of power users for many of the software applications listed above.

Clusty

Cores: 212
RAM: 208 GB
Disk space: 15 TB
GPU: none
Interconnect: 10 Gbps
Software: Python, Perl, R, sqlite3, octave

Key Personnel (AY 2026)

CC* Committee: Matt Morrissey (UTS - Asst VP Tech. Infra. & Research Computing), Josh Poinsett (UTS – Exec. Director of Cloud & Research Computing), Chris Washburn (Research Computing Administrator), Aaron Wemhoff (COE, Administrative Director)

Key UTS Support (Augie): Leo Nelson, Peter Palladino, Gavin Printz

Key Provost Support: Amanda Grannas, Haiyan Li, Amanda Bilinsky, Matt Kirsch

HPC Advisory Board: David Cereceda (COE), Justin DiBenedetto (CLAS), Andrej Prsa (CLAS), Michael Robson (Smith College), Jason Simms (Swarthmore College), Raisa Velthuis (VSB)

Strategic Plan (5-year, 2023-2028)

Mission: Support and promote computational research for Villanova researchers and their collaborators

Vision: CRCF, as a center of expertise in computational research, is one of the top contributors to Villanova's research enterprise.

Goals & Metrics (5-year goal in parentheses, AY2026 value after colon):

1. CRCF is a significant enabler of research productivity
    a. Number of grant proposals submitted that use CRCF resources (10/yr.): 8 external + 4 internal
    b. Number of peer-reviewed publications produced using CRCF resources (10/yr.): 8 + 8 in progress
2. CRCF is the center of expertise for computational research
    a. Number of workshops or tutorials offered (4/yr.): 2 (Google Colab, Using AI for Developing Web-based Apps)
    b. Number of researchers using external services (OSG, PATh, XSEDE/ACCESS) (5/yr.): 1 user achieved research using ACCESS with Texas Advanced Computing Center (TACC).
    c. Number of CI grant proposals stemming from the center (1/yr.): 1 in progress
3. CRCF has a robust multidisciplinary community of computational researchers
    a. Number of total users (170): 266
    b. Number of active users (40/mo.): average of 17 per month, max 27
    c. Number of departments represented by active CRCF researchers (12): 12
    d. Number of power users per software application (3): 0 or 1
    e. Number of software applications with power users (12): 3
    f. Number of classes that use Augie for instruction (8/yr.): 2 in the past year.
4. CRCF's resources grow to match demand
    a. Low idle time (< 15%): 39%
    b. Small average job wait time (< 12 hours): we are still looking on ways to track this

    c. Number of new condoers per year (2): None (program on hold)
    d. Acting as a host site for REDCap: pushed to data storage investigation
    e. Dedicated HPC IT Admin: done
5. CRCF operates for the good of all humankind beyond research
    a. Request that hosting data center must meet energy efficiency requirements (PUE < 1.5): Netrix does not track PUE; request made for them to do so
    b. Request that data center have PPA in place for renewable energy: Netrix does not do this; request has been made for them to do so

Accomplishments

CRCF's accomplishments for the AY have been split into administrative and technical categories.

Administrative

The team spent the AY continuing to grow CRCF to ensure long-term use and management of the facility. Highlights of the facility's administrative accomplishments include:

1. Ran webinars on Google Colab, Using AI for Developing Web-based Apps
2. Achieved another NSF ACCESS allocation to help researchers with OS transition
3. Hosted intern to explore Globus file management service: Arielle Korn
4. Renewed COMSOL and ANSYS-Fluent licenses
5. Procured Gaussian & distributed to faculty group
6. Updated short names for websites: villanova.edu/crcf, villanova.edu/augie

Technical

1. Transitioned all nodes from CentOS to Ubuntu
2. Updated SLURM by several versions
3. InfiniBand update done
4. BeeGFS updated on compute nodes
5. Updated new user provisioning script for Ubuntu
6. Progress in app installation in Ubuntu
7. Established ability to launch jobs using MATLAB

Metrics

Total number of users (as of 3/9/26)

- Augie: 266
- Clusty: 127 (note: all students in astrophysics & planetary science are on by default)

Active Departments

The following departments contain active users since March 2023:

- CLAS: Biology, Chemistry, Computing Sciences, Mathematics and Statistics, Physics, Psychological and Brain Sciences, Sociology
- COE: Civil and Environmental Engineering, Chemical and Biological Engineering, Electrical and Computer Engineering, Mechanical Engineering
- VSB: Finance

Publications using CRCF resources in the past year

Bazurto, Eric; Kumar, Revati; Jorn, Ryan, "Toward a Transferable Coarse-Grained Model for Glyme Electrolytes" The Journal of Physical Chemistry B, (2026) 130, 2226-2235.

S Benouadah, M Vaezi, R Shen, H Jafarkhani "End-to-End NOMA with Perfect and Quantized CSI Over Rayleigh Fading Channels" accepted for publication in ICC 2026. arXiv preprint arXiv:2602.13446

Justin DeBenedetto. Linearization Order Matters for AMR-to-Text Generation Input. In *Proc. UMR Parsing Workshop*. 2024.

Hiep Nguyen, Lynn Yip, Justin DeBenedetto. Automatic Quality Estimation for Data Selection and Curriculum Learning. In *Proc. BabyLM Challenge at CoNLL*. 2024.

Byte-ranked Curriculum Learning for BabyLM Strict-small Shared Task 2023. In *Proc. BabyLM Challenge at CoNLL*. 2023.

Additional publications/presentations:

- Presentation to Southern Finance Association annual meeting
- Two papers by Venkat Margapuri.
- Muhammad Qadri publication.
- 8 additional papers are in progress.

Proposals submitted in the past year that would utilize CRCF resources

- Venkat Margapuri: 2 (internal)
- Raisa Velthuis: 1 (internal)
- Peter Palenchar: 0
- Ryan Jorn: 0
- Mojtaba Vaezi: 0
- Anthony Rice: 0
- Kyle Juretus: 2 (1 funded, $258k)
- Qianhong Wu: 6 (2 funded, $898k)
- Justin Debenedetto: 1 (internal)

Courses where Augie, Alipi, or clusty have been integrated

- BL 2149 TOP:Cyber Law
- CHM 9947 Computational Chemistry
- CSC 2405 Computer Systems II
- CGS 5990 Fairness in AI
- CGS 5900/PSY 8900 Cognitive Science Seminar
- ECE 8487 - Advanced Machine Learning
- Mathematics Senior Seminar
- ME 3600 Fluid Mechanics
- ME 3950 Heat Transfer I
- ME 7030: Numerical Methods in Engineering Simulation

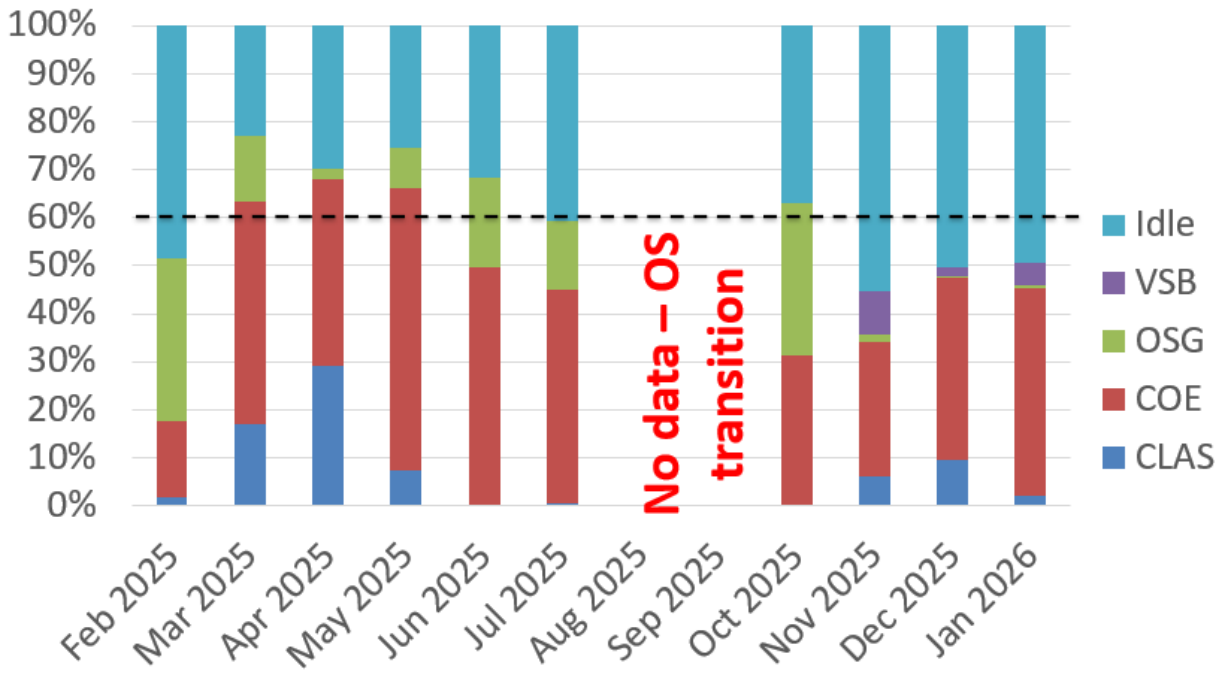
- SPA 3200 Introduction to Spanish Translation

CRCF workshops offered in the past year

- Google Colab (Justin Debenedetto)
- Using AI for Developing Web-based Apps (Aaron Wemhoff)

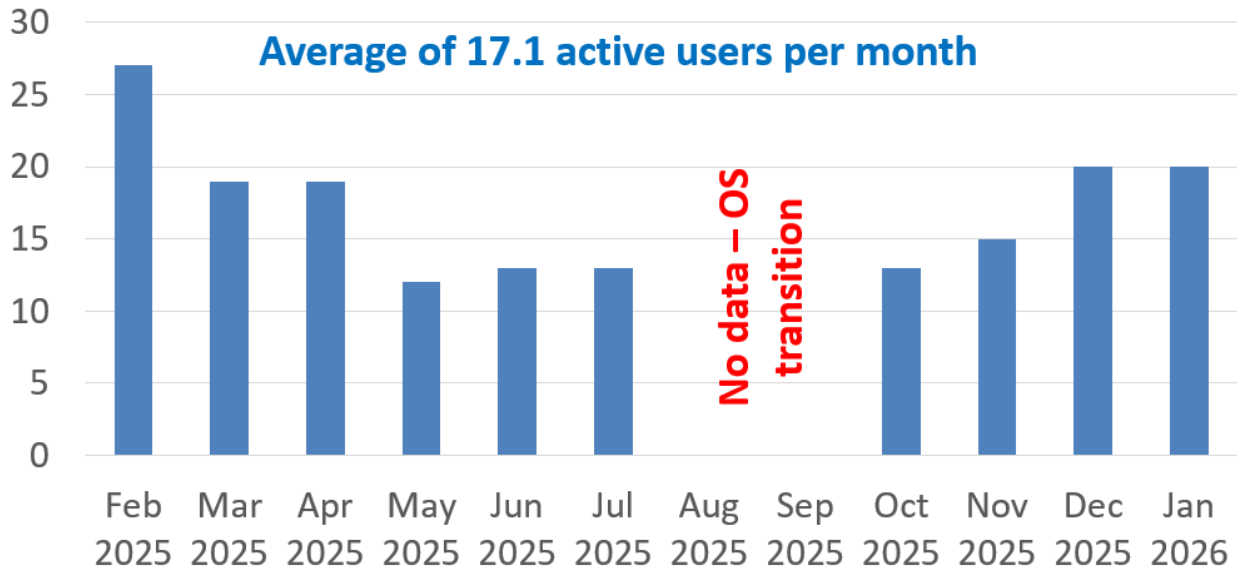
Augie Usage

The average usage goals for Augie are (1) less than 20% idle time, and (2) less than 20% usage by the Open Science Grid (OSG). Note that data for August and September 2025 are missing due to the OS transition. In the last 12 months, the idle time is high (39%), and the OSG usage is under the limit (12%). The idle time is high primarily due to the OS transition, where software packages had to be rebuilt. The usage was more consistent with goals prior to the OS transition data blackout period. While CLAS and COE demand vary widely, the average Augie usage per college is 7% for CLAS and 39% for COE, 2% for VSB, and zero usage by FCON.



Number of Active Users

Active users are defined as those that submitted jobs to Augie within a specified month. The annual average is 17.3 users, which is slightly down from 20.3 users in the previous 12 months.



Work in Progress

The following efforts are currently ongoing:

- File system update
- Data management
- Archival (large data sets, electronic lab notebook, formatted datasets for public distribution)
- Automated transfers (Globus)
- Use of Internet2 connection
- MRI proposal development (if selected to move forward), which would increase GPU availability
- Provide better means to track papers, proposals, and integration into courses
- Hold at least 1 workshop per semester
- Recruit power users
- Track average job wait time
- Check viability of connecting GPU node to internet resources

User Survey

A survey was provided to the Augie Users in March 2026. No feedback was garnered outside of indications of satisfaction with the current state of affairs. We will continue to provide an annual survey in March 2027.

Final Points

Good Citizenship

Some reminders:

- No running jobs on the head node – submit batch jobs instead
- Don't use the debug queue for production runs
- Don't submit lots of jobs to occupy a large percentage of cores on the cluster
- Be sure to acknowledge use of the HPC clusters – see user terms and conditions documents:
    - Augie: Augie Users SharePoint, file Administrative/Augie-HPC-TC_20210507.pdf
    - Clusty: contact Andrej Prsa
- Need help on Augie or Clusty?
    - Don't contact UNIT directly or put in a ticket
    - Augie:
        - Find appropriate document in the Coding Resources and Scripts documents. See if the document specific to your app has the information you need.
        - Some documents have listed power users; contact the power user for help.
        - If the above two items don't work, then email ccstarcommittee@villanova.edu.
    - Clusty: contact Andrej Prsa

Interested in Helping CRCF?

Contact ccstarcommittee@villanova.edu if you are interested in…

- Supporting other Villanova researchers as a power user
- Collaborating with a researcher at a small local college
- Providing additional feedback on CRCF operations
- Working as an undergrad support software technician during the summer
- Providing your thoughts about how to make AugieFest a popular, fun event
- Providing ideas for tutorials

Acknowledgements

Funding and support for CRCF from the Office of the Provost, the College of Liberal Arts and Sciences, the College of Engineering, and UNIT are gratefully acknowledged.