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High Performance Research Computing Core
https://research.vcu.edu/cores/

What is the HPRC Core?

- The Office of the Vice President for Research and Innovation (OVPRI) operates core laboratories & facilities.
  - OVPRI provides these core laboratories to maximize resource sharing across VCU schools/colleges.
  - The High Performance Research Computing (HPRC) Core is one of these core facilities.
  - HPRC can positively impact almost every college & school's research due to applicability of high performance computing.

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What is the HPRC Core?

- The High Performance Research Computing (HPRC) Core
  - Mission: "In support of VCU's Quest 2025 Strategic plan, the primary mission of the HPRC core facility is to advance scientific research at VCU in areas that benefit from *large-scale computation*. These areas span *mathematics and computational sciences, the physical and chemical sciences, engineering, the life sciences, medicine, and the arts and humanities*. The HPRC core facility will provide the **supercomputing clusters**, **large-scale storage systems**, specialized software, technical expertise in the use of such software and expertise in developing new software for this compute intensive environment."

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Some Table Setting: What is HPC?

- The HPRC core is a High Performance Computing (HPC) organization based on its mission.

- HPC is "High Performance Computing most generally refers to the practice of aggregating computing power in a way that **delivers much higher performance than one could get out of a typical desktop computer or workstation** in order to solve **large problems** in science, engineering, or business."

  – https://www.usgs.gov/core-science-systems/sas/arc/about/what-high-performance-computing

- HPRC is not a cloud computing or enterprise computing resource.

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What is the HPC?

- Historically, these systems are referred to as clusters, HPC clusters, or supercomputers.

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438

» https://www.top500.org/lists/top500/list/2020/11/

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What is the HPC?

- Used to solve complex systems of Partial Differential Equations, Machine Learning (ANNs), and more recently used for Image and Natural Language Processing.
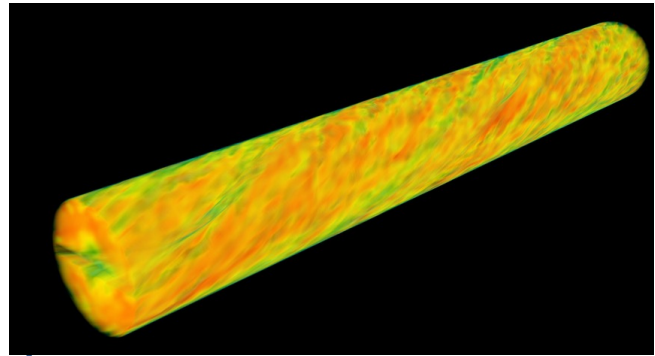
Partial Difference Equation

$$\nabla^* \cdot u^* = 0$$

$$\frac{\partial u^*}{\partial t^*} + u^* \cdot \nabla^* u^* = -\nabla^* p^* + \frac{1}{Re} \nabla^{*2} u^*$$

$$\frac{\partial T^*}{\partial t^*} + u^* \cdot \nabla^* T^* = \frac{1}{RePr} \nabla^{*2} T^*$$

Numerical Solution calculated on HPC Resources

Visualization of Flow in a Clean Energy Component
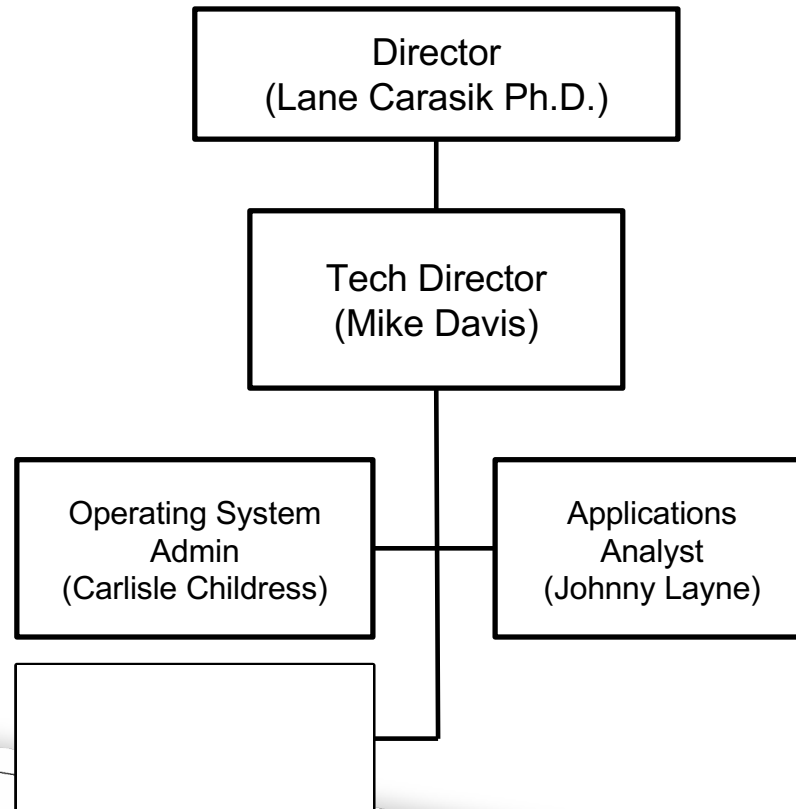
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What do we have at HPRC?

We currently have four clusters.

- Teal (teal.vcu.edu)
  - General use computing cluster (~3700 CPUs & 2 GPU nodes)
- Godel (godel.vcu.edu)
  - Data Science/Bioinformatics focused cluster (~1768 CPUs)
- Fenn (fenn.vcu.edu)
  - HIPAA deidentified compliant cluster (~912 CPUs)
- Bach (bach.vcu.edu)
  - Historic version of Fenn to be retired later this year. (~848 CPUs)

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What is the current organization?

Director
(Lane Carasik Ph.D.)

Tech Director
(Mike Davis)

Operating System Admin
(Carlisle Childress)

Applications Analyst
(Johnny Layne)

What is the vision of HPRC's Future?

It is my vision that HPRC will obtain a national profile within five years (2025-2026) as an innovative core of research, educational, and outreach areas leveraging existing and future resources & personnel at VCU.

- Objectives:
  - Near Term (1-2 years)
  - Medium Term (3-4 years)
  - Long Term (5-7 years)

Near Term Objectives

- Modernization of software & hardware on HPRC clusters including a modern queue system
  - Current hardware and software needs a full audit
  - Updating the OS on each cluster is going to take time but doable.
- Increase usership within all VCU colleges/schools
  - Requires outreach to colleges/schools of capabilities at HPRC
  - Requires developing potential user buy-in
- Update strategic plan for HPRC Core and develop stakeholdership
  - Integrate vision of President, VPRI, Deans/Provosts of academic units
  - Buy-in from research active faculty

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Medium Term Objectives

- Instituting an allocation system for each cluster
    - Start-up allocations, small/medium/large allocations, and director allocations
    - Ensures equitable usage of clusters
- HPRC core join the XSEDE community
    - Enable VCU focused researchers to use XSEDE community computing for research not enabled by existing and future HPRC capabilities
- Involve HPRC core in educational and outreach programs
    - Integrate HPC/programming on clusters into courses across the university to support future research
    - Examples: Bioinformatics, Epidemical Modeling, Financial Modeling, Computational Fluid Dynamics, and others

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Long Term Objectives

- Build the next major HPC cluster (HERO Class) in Virginia at VCU
  - Enables us to be part of the larger national discussions around HPC
  - Enables us to attract and retain HPC focused researchers
  - Enables us to attract funding opportunities made possible through HPC
- Establishing VCU as a nationally recognized HPC focused institution
  - Enabling better faculty recruitment and retention
  - Enabling further growth of VCU Research Activities involving the support of at least 10-15 million in extramural research funding

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What's the current activities?

- Reconstitute the HPRC Core Oversight Committee.

- Taking initial steps to establish a system for the systematic allocation and prioritization of processor and storage resources for HPRC users similar to those deployed at HPC centers at peer institutions
  - Implement a new submission system (Slurm).
  - Implement an allocation system (Coldfront).

- Working with OVPRI communications/PR staff to develop a VCU-wide communications strategy to raise the visibility of the HPRC
  - New Website at https://research.vcu.edu/cores/.
  - Outreach and Educational Videos for VCU Researchers.
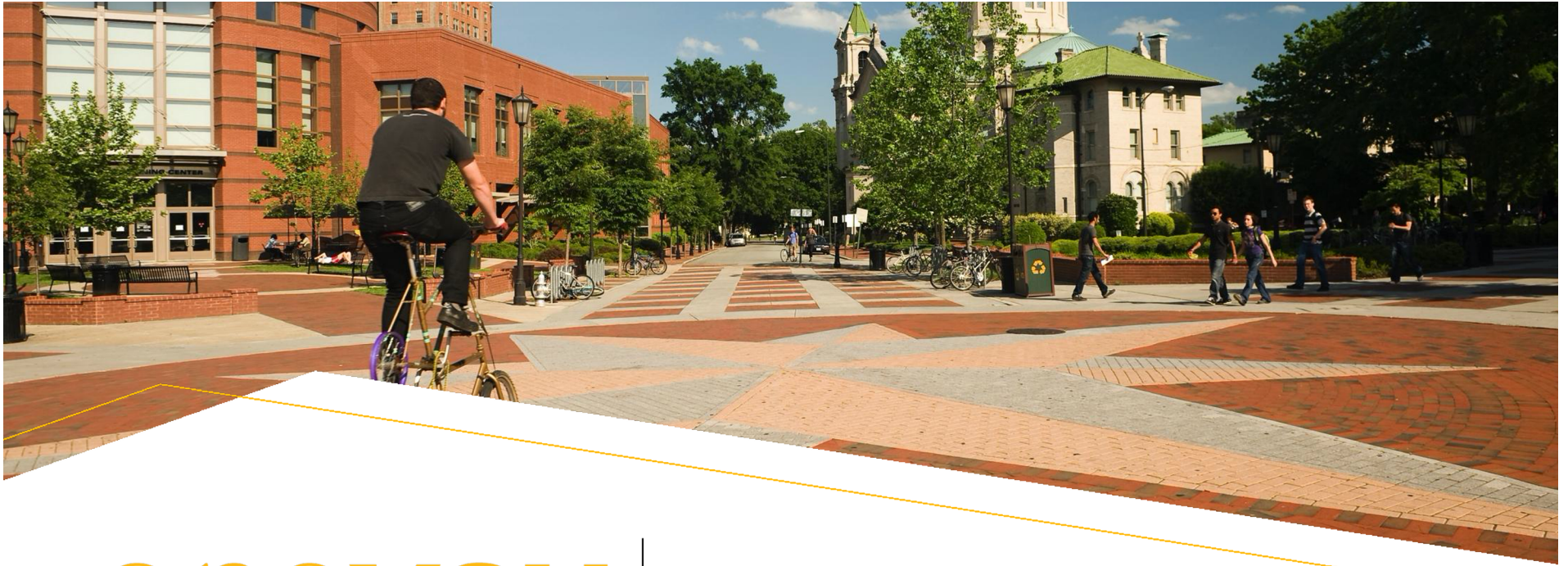
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What's the current activities?

- Hiring additional staff to support HPRC mission

- Specializing existing staff responsibilities

- Bring online the newest cluster (Huff) and reduce total number of HPRC clusters
  - Intended to replace existing aging equipment (pre-2015).
  - Reduce four (five) clusters to two/three clusters.

- Reduce barriers to larger usership of VCU research community
  - Create new and improve existing guides, how-tos, tutorials for HPRC resources (hardware and software).
  - Set up workshops to encourage usage and get past obstacles to usage.

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What is the current future of HPRC Resources?

- We will reduce four (five) clusters to two/three clusters.
  - Remove older hardware (pre-2013)
    - Bach, Godel, and Teal clusters
  - The need for multiple specialized clusters has been reduced due to current state-of-art programming and software practices.
    - Software generally will run on most common (AMD and Intel) processors and GPUs (Nvidia) found in HPC applications.
  - Reduce overhead associated with maintaining multiple clusters

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Demo (If Time)

- Share screen

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Director
(Lane Carasik Ph.D.)

Administrative Assistant
(Core Shared)
(Vacant)

Tech Director
(Mike Davis)

Senior User
Support Lead
(Vacant)

Senior System
Admin
(Carlise Childress)

Senior Dev Ops
(Johnny Layne)

System Admin
(Brad Freeman)

Dev Ops
Engineer
(Vacant)

System Admin
(Vacant)

Dev Ops
Engineer
(Vacant)

User Support
Specialist
(Bioinformatics)
(Vacant)

User Education
Specialist
(Brad Freeman*)

User Support
Specialist
(Physics)
(Vacant)

User Support
Specialist
(Bioinformatics)
(Vacant)

User Support
Specialist
(Chemistry)
(Vacant)

User Support
Specialist
(Engineering)
(Vacant)

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What is HPC?

- Types of software that is commonly run on HPC
  - CPU bound

  - GPU bound

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What software is available?

- Full List being compiled

How can I access HPRC clusters?

- See website