Carnegie Mellon University

Computing support and Infrastructure for Academic Scientific Research at the Mellon College of Science

OCTOBER 22, 2025

Nuno Chagas

Agenda

- Computing support
- Infrastructure
- Academic Scientific Research
- Mellon College of Science

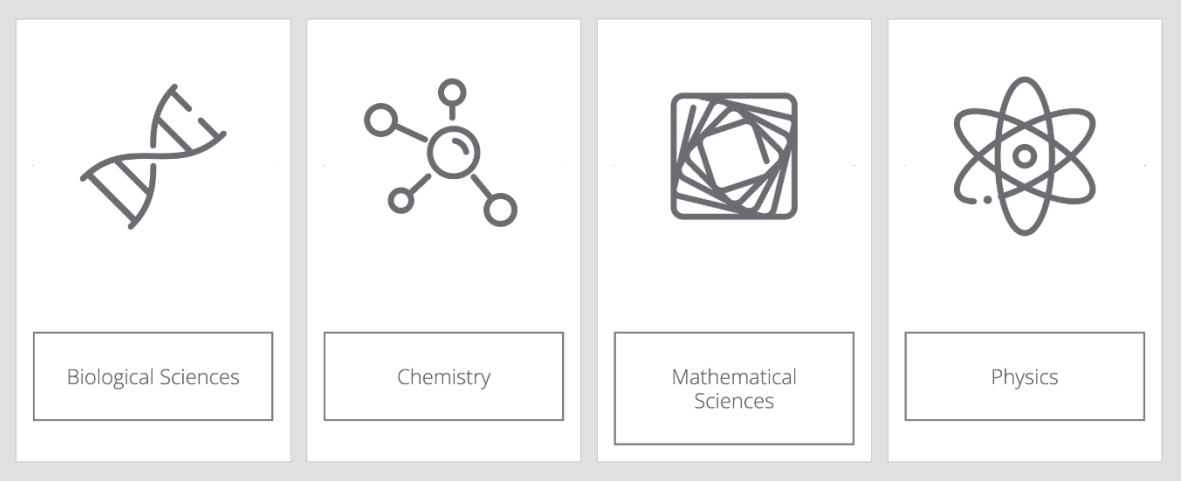
Agenda

1. Mellon College of Science
2. Academic Scientific Research
3. Computing support
4. Infrastructure

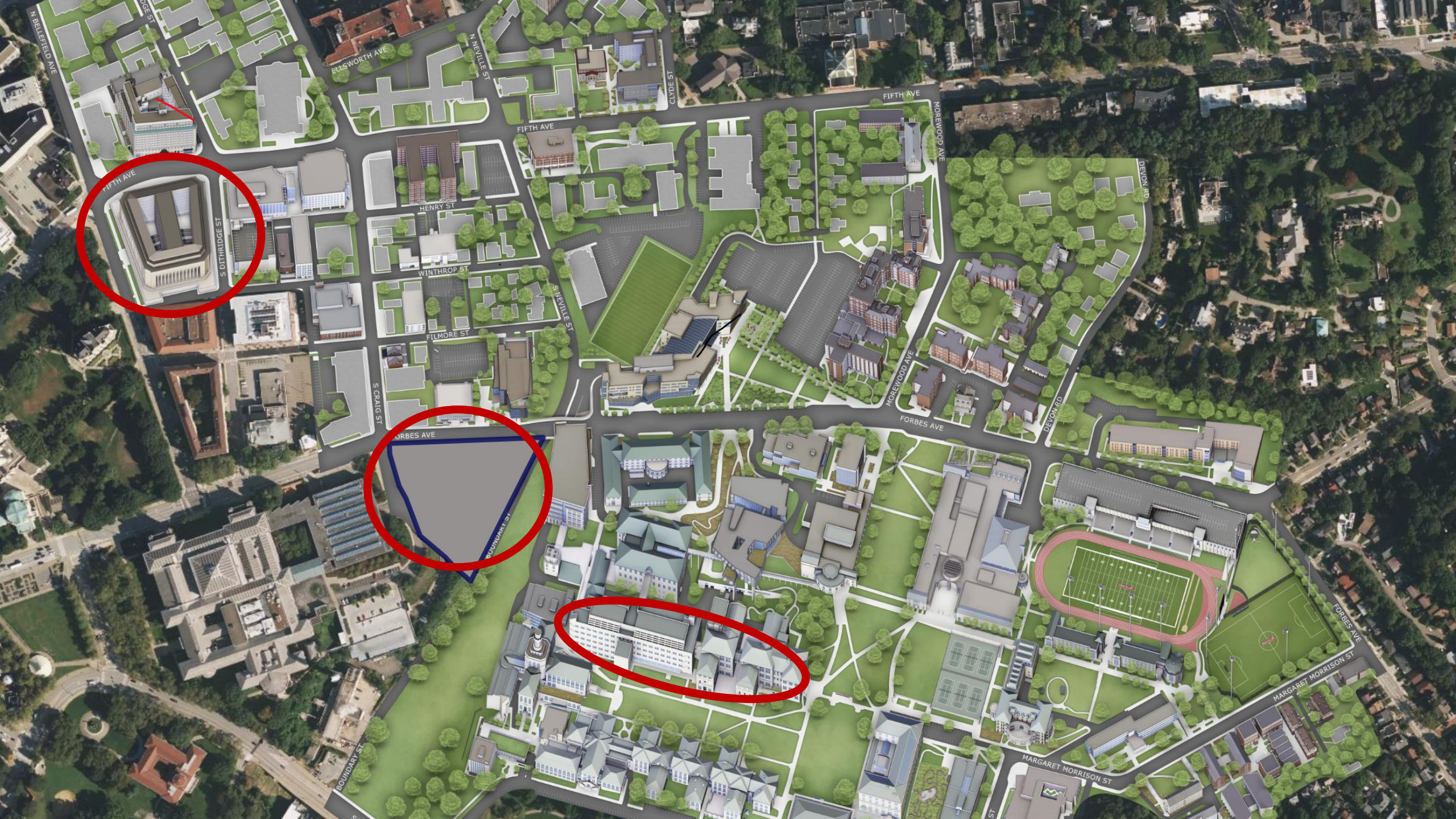
Mellon College of Science

Carnegie Mellon University

4	departments
1000+	undergrads
450+	grad students
135	faculty
34	staff
7	IT staff



N BELLEFIELD AVE
ELLSWORTH AVE
N NEVILLE ST
CLYDE ST
FIFTH AVE
MOREWOOD AVE
DEVON RD
S DITHRIDGE ST
HENRY ST
WINTHROP ST
S NEVILLE ST
FILMORE ST
S CRAIG ST
FORBES AVE
BOUNDARY ST
MARGARET MORRISON ST


N BELLEFIELD AVE
ELLSWORTH AVE
N NEVILLE ST
CLYDE ST
FIFTH AVE
MOREWOOD AVE
DEVON RD
FIFTH AVE
S DITHRIDGE ST
HENRY ST
WINTHROP ST
S NEVILLE ST
FILMORE ST
S CRAIG ST
MOREWOOD AVE
FORBES AVE
DEVON RD
FORBES AVE
BOUNDARY ST
FORBES AVE
MARGARET MORRISON ST
MARGARET MORRISON ST

HAMERSCHLAG DR.

BOUNDARY ST

FORBES AVE
MARGARET MORRISON ST

N BELLEFIELD AVE
ELLSWORTH AVE
N NEVILLE ST
CLYDE ST
FIFTH AVE
HENRY ST
WINTHROP ST
S NEVILLE
FIFTH AVE
MOREWOOD AVE
DEVON RD
MOREWOOD AVE
FORBES AVE
DEVON RD

HAMERSCHLAG DR.

Mellon College of Science – computing support scope

- college-specific support for research labs, admin, faculty, students
- Mediator, partner and 2nd level support for general computing queries, software-licensing, netOps, facilities management, infosec, physicalsec, mediatech

7 people?

- Backed by self-serve websites, many CMU central services and resources
- This allows us to concentrate on quality subject-matter-focused hardware and application support
- Flexible-work and 24h coverage (ticketing systems)– WFH pervasive post-covid

Academic Scientific Research

Academic Scientific Research

- Stakehoders: Undergrad, grad, postgrad, faculty, collaborator
- One size does not fit all
  - Agility
  - Diverse requirements and budgets
  - Value-for-money: Repurposing -- hand-downs thru e-waste
- Their job is “throwing spaghetti at the wall”, support’s job is to help them to do it efficiently & effectively
  - Trial and error
  - Blameless culture
  - Post-mortem

Academic **Scientific** Research

- Science *lingua franca*
  - Build trust
- Emphasis on documentation and reproducibility and research integrity&quality
  - Computer architectures
  - ECC or scale
  - git
  - Conda environments

Academic Scientific **Research**

- Lab/group epoch management
  - Must survive transient members
- Success defined by
  - Publications
  - Citations
  - Patents
  - Number of students
  - Funding
  - Established/sustained lifecycle

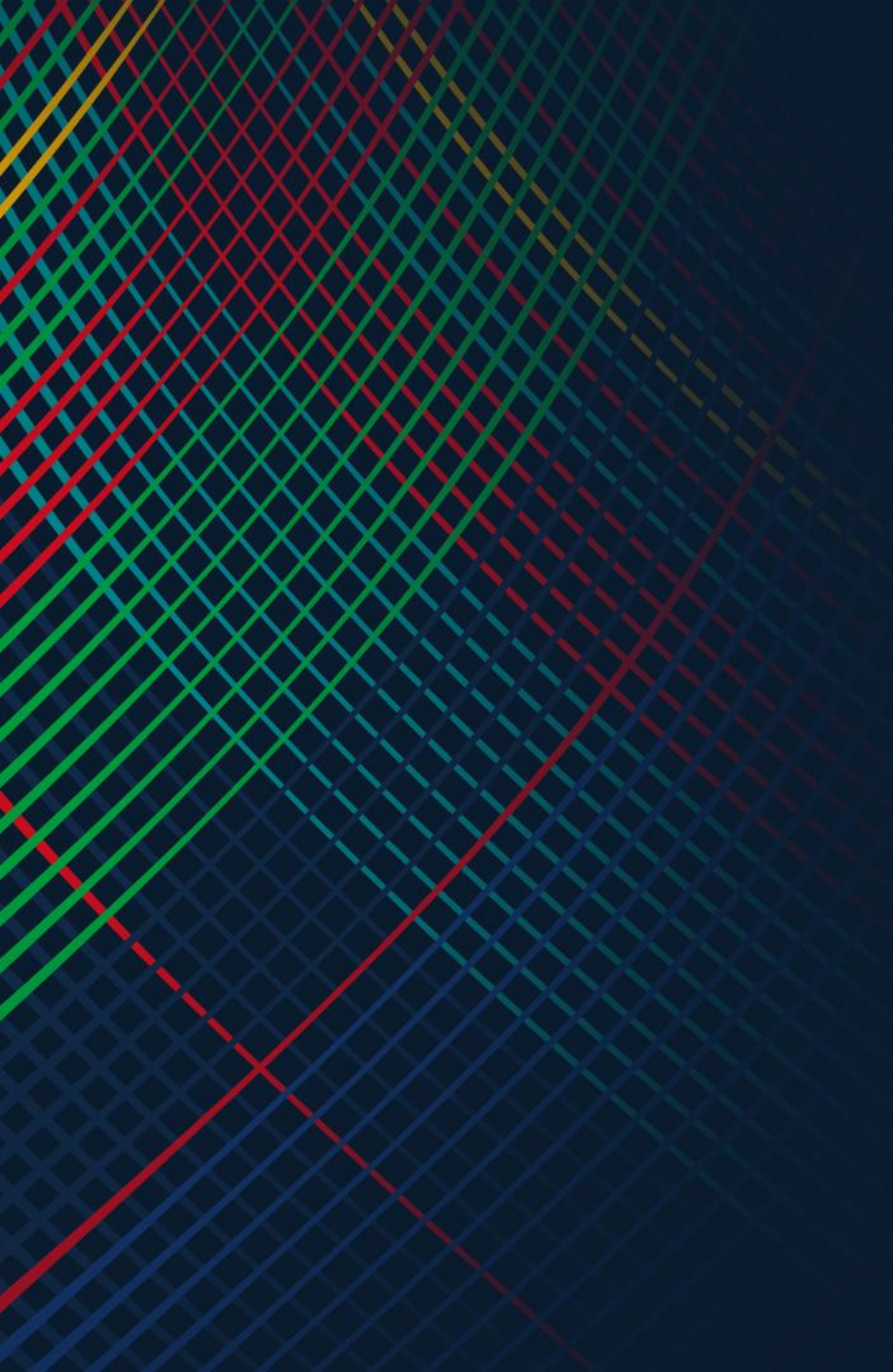
Computing Support

College Computing Support

- We are on your side
  - responsiveness
  - in-person in every building
  - Dedicated helpdesk email queues backed by ticketing systems
- Consumables – stock, charging(payments), specifying, sourcing
- Workstation provision inc. loaners (mac, windows, linux, ipads, pens, adapters, peripherals)
- Scientific software support and optimization
  - You’re not a computer scientist and that’s OK, we’re not chemists, biologists, astrophysicists, mathematicians…

College Computing Support

- Interfacing with lab instruments
- Lab inductions and check-outs (lifecycle)
- external collaborators
    - Logins
    - Data interfacing
- Lab establishment (requirements, specification, phasing, ordering)
    - Liase with pre-award grant proposals, CMU-FMS Power/HVAC, CMU-NetOps
- Lifecycle: Install/maintain/operate/repurpose/e-waste



Infrastructure

Infrastructure

- Ticketing queues (helpdesks for departments and for admin, e.g expense reimbursements)
- Monitoring systems
- MCS-Linux distro – Ubuntu LTS-based preinstalled with commercial scientific software licensed by CMU (Workstation, Server, Laptop variants)
    - Common platform for ease of maintenance
    - Quickly deployable (thousands of machines)
    - Allow sudo access to users if requested
    - Dual –boot, VM and container support

Infrastructure MCS managed and operated

- 7 server rooms, 5 sites --- furthest 20miles
- 16 clusters --- largest with 988 users
- 270 computing nodes
- 43 file servers across 5 physical locations (inc backup)
- 250+ linux workstations
- 2000 HDDs
- 3 dead hard drives per week

Infrastructure MCS operated – mathematics

- Student cluster + research cluster boostable to cloud
- Firedrake
- Matlab
- Mathematica
- General purpose nodes
- Single-processor optimized nodes
- Large memory nodes (4TB)
- GPU nodes

Infrastructure MCS operated – cosmology and physics

- slurm private clusters
- CERN xrootd (cosmology/physics) P2P ipv6
- REANA (Reusable and Reproducible Data Analysis) is a platform designed to facilitate the execution of computational workflows in scientific research using containerization and cloud computing
    - help to structure research data analysis in reusable manner
    - instantiate computational workflows on remote clouds
    - rerun analyses with modified input data, parameters or code
    - support for several compute clouds (Kubernetes/OpenStack)
    - support for several workflow specifications (CWL, Yadage)
    - support for several shared storage systems (Ceph, EOS)
    - support for several container technologies (Docker, singularity)

Infrastructure MCS operated – chemistry

- Lab clusters (dedicated funding)
- cp2k
- gromacs
- matlab
- mathematica
- Pmemd.cuda (ambermd)
- Python / conda
- 140 nodes over 3 research groups with 2PB storage
- ECC and non ECC nodes (VRAM)

Infrastructure MCS operated – biology

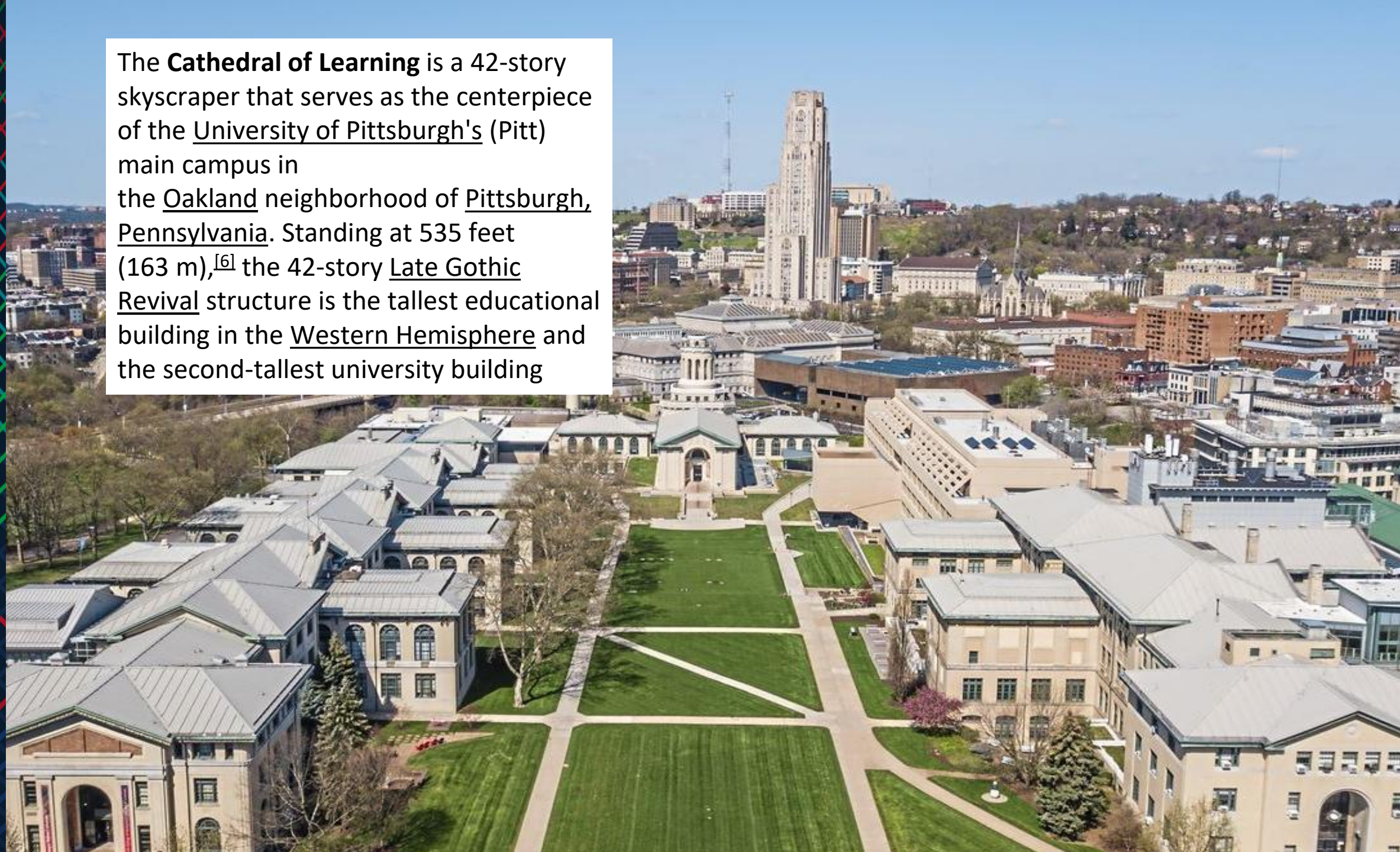
- Lab clusters (dedicated funding)
- matlab
- mathematica
- Kilosort (spike sorting electrophysiological data)
- Video processing
- non ECC nodes (VRAM)
- Storage bandwidth and data reduction

Infrastructure MCS operated – humanities and social sciences

- LLM
- slurm
- 3x 8x Nvidia L40 – Infiniband RDMA 200gpbs
- 1PB fileserver

Infrastructure MCS supercomputing

- PSC.EDU – lower the error bars
  - 70 staff
  - Joint centre between MCS & University of Pittsburgh
  - Co-location
  - Offsite backups
  - 4th supercomputing center in the US



The **Cathedral of Learning** is a 42-story skyscraper that serves as the centerpiece of the University of Pittsburgh's (Pitt) main campus in the Oakland neighborhood of Pittsburgh, Pennsylvania. Standing at 535 feet (163 m),[6] the 42-story Late Gothic Revival structure is the tallest educational building in the Western Hemisphere and the second-tallest university building

Challenges / Opportunities

- Attitude / culture
- Self-insuring
- Self-build vs integrator
- Supplier relations
- Purchasing agility / Bureaucracy
- Pre-deploy stress-testing
- Pocicies / Cluster-policing
- Donations
- Decision Discretion
- Scale

Carnegie Mellon University

Computing support and Infrastructure for Academic Scientific Research at the Mellon College of Science

OCTOBER 22, 2025

Nuno Chagas