The Cyberinfrastructure Landscape: Systems, Providers, Technologies

Mike Renfro[1,2]

[1]Tennessee Tech University

[2]Campus Champions Leadership Team

2024-06-25

Who am I? (Who are any of us, really?)

Back in the day

- ME student at a medium-sized public STEM-ish university who should have studied more instead of helping people do things in computer labs.
- Sysadmin/CAD/FEA co-op student at Oak Ridge National Lab before SGI Irix got its cameo in "Jurassic Park" ("It's a Unix system: I know this!").

Figure 1: Some skinny nerd, 1990

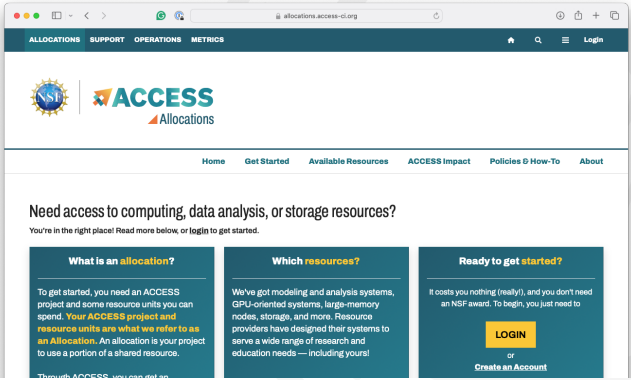
Who am I? (Who are any of us, really?)

Now

- Three ME degrees from the now-R2 university (1995, 1998, 2018)
- Mostly-solo practitioner of all things RCD at the same university (2000–2017, 2017–)
- Perpetually online member of multiple RCD organizations (2018–)
- Member of Campus Champions Leadership Team (2022–)
- Compulsive advice-giver

Figure 2: Same nerd, not remotely skinny, 2023

ACCESS Allocations Portal



https://allocations.access-ci.org/

ACCESS Project Types

Explore for resource evaluation, grad student projects, small classes/training events, benchmarking, development/porting, other small-scale cases

Discover for grants with modest needs, Campus Champions, large classes/training events, NSF graduate fellowships, gateway development

Accelerate for experienced users with mid-scale needs, multi-grant programs, collaborative projects, growing gateways

Maximize largest-scale research activities

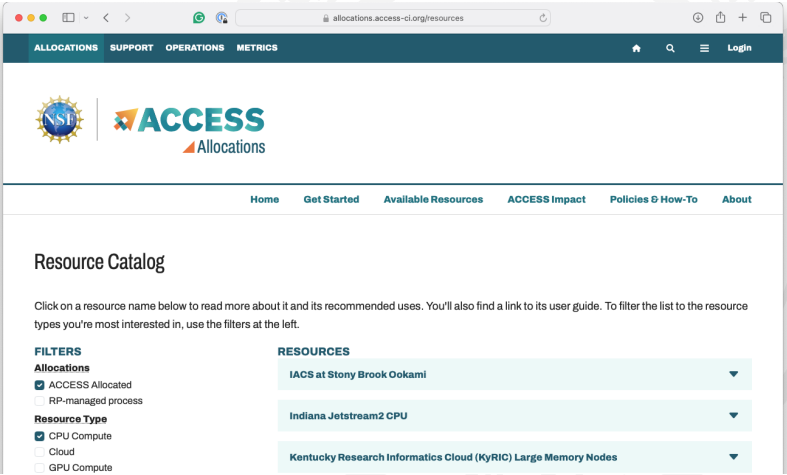
ACCESS Project Types

Explore, Discover, Accelerate:

- run for grant duration or 12 months
- can be requested any time
- allow multiple projects

Explore	400k credits, only an overview required
Discover	1.5M credits, 1-page proposal required
Accelerate	3M credits, 3-page max proposal required, subject to merit review
Maximize	usually only 1 project allowed, 10-page max proposal required, subject to merit review, requests accepted every 6 months

ACCESS Resource Catalog



Stampede3 at Texas Advanced Computing Center (TACC)

- 20 Intel Sapphire Rapids nodes each with 4 Intel GPUs, 128 GB HBM
- 560 Intel Sapphire Rapids nodes (no GPUs), 128 GB HBM
- 1060 Intel Skylake nodes, 192 GB RAM
- 224 Intel Ice Lake nodes, 256 GB RAM
- 10 PB VAST (`$SCRATCH`) + 1 TB Lustre (`$WORK`)
- 100 Gb Omni-Path networking
- Intended for:
  - parallel applications scalable to 10,000+ cores
  - general purpose computing
  - throughput computing

Delta at National Center for Supercomputing Applications (NCSA)

- All using AMD 7763 CPUs
- 132 nodes with 128 cores and 256 GB RAM
- 100 nodes with 64 cores, 256 GB RAM, and 4 NVIDIA A40 CPUs
- 100 nodes with 64 cores, 256 GB RAM, and 4 NVIDIA A100 GPUs
- 6 nodes with 128 cores, 2048 GB RAM, and 8 NVIDIA A100 GPUs
- 1 node with 128 cores, 2048 GB RAM, and 8 AMD MI100 GPUs
- 6 PB Lustre for `$HOME` and `$SCRATCH`
- 200 Gb HPE/Cray Slingshot networking

Bridges-2 at Pittsburgh Supercomputing Center (PSC)

- 488 nodes with 128 AMD 7742 cores and 256 GB RAM
- 16 nodes with 128 AMD 7742 cores and 512 GB RAM
- 4 nodes with 96 Intel Cascade Lake cores and 4096 GB RAM
- 24 nodes with 40 Intel Cascade Lake cores, 512 GB RAM, and 8 NVIDIA V100 GPUs (32 GB)
- 9 nodes with 40 Intel Cascade Lake cores, 192 GB RAM, and 8 NVIDIA V100 GPUs (16 GB)
- 1 node with 48 Intel Skylake cores, 1536 GB RAM, and 16 NVIDIA V100 GPUs (32 GB)
- 15 PB Lustre for `$PROJECT`
- 200 Gb Infiniband networking

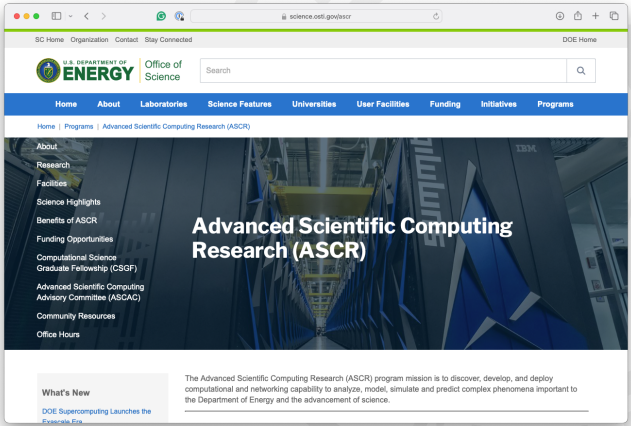
ACES at Texas A&M University

- 130 nodes, 11888 cores
- Mostly Intel Sapphire Rapids, some Intel Ice Lake, Intel Cascade Lake, and AMD Rome
- Tons of mostly-composable accelerators:
  - GPUs: NVIDIA H100 and A30, Intel (coming soon)
  - FPGAs: Bittware Agilex, Intel D5005
  - Coprocessors: NextSilicon
  - Optane memory modules
- Non-composable accelerators:
  - Graphcore IPUs: GC200, Bow-2000
  - NEC Vector Engine: Type 20B-P
- 2.3 PB Lustre
- 200 Gb Infiniband networking

Jetstream2 at Indiana University

- Hybrid-cloud platform for flexible, on-demand, programmable cyberinfrastructure tools
- Interactive virtual machine services
- Infrastructure and orchestration services for research and education
- AMD Milan CPUs (128 per node)
- 360 NVIDIA A100 GPUs
- 512–1024 GB RAM
- 100 Gb Ethernet

Advanced Scientific Computing Research (ASCR)



Accessing ASCR Facilities

- Innovative and Novel Computational Impact on Theory and Experiment (INCITE): multi-year awards for open science using majority of machine at Oak Ridge or Argonne
- ASCR Leadership Computing Challenge (ALCC): 1-year awards for advancing DOE mission or broadening the community capable of using large computing resources at Oak Ridge, Argonne, or NERSC
- Energy Research Computing Allocations Process (ERCAP): 1-year awards for advancing DOE Office of Science and SBIR/STTR mission at NERSC
- Center Reserves: 1-year awards for advancing science and engineering fields at Oak Ridge, Argonne, or NERSC

Multi-tier Assistance, Training & Computational Help (MATCH) Plus

MATCH Plus:

- takes requests from researchers with a support need,
- identifies a student and mentor that can provide that support,
- connects the researcher to the student and mentor with regular meetings and updates,
- for 5–10 student hours and 2–3 mentor hours per week for 3–6 months,
- at **no charge**.

Multi-tier Assistance, Training & Computational Help (MATCH) Premier

MATCH Premier:

- takes requests from already-funded projects,
- identifies an expert consultant and arranges payment,
- for a 6–12 month period.

Engagement and Performance Operations Center (EPOC)

EPOC provides researchers with a holistic set of tools and services needed to debug performance issues and enable reliable and robust data transfers. By considering the full end-to-end data movement pipeline, EPOC is uniquely able to support collaborative science, allowing researchers to make the most effective use of shared data, computing, and storage resources to accelerate the discovery process.

– https://epoc.global/

Science Gateways

[Science g]ateways are online interfaces that give researchers, educators, and students easy access to shared resources that are otherwise inaccessible or unaffordable for a large segment of the scientific community.

. . .

The SGCI was founded to provide services and resources that advance the state of the art in science gateways, that help gateway creators use accepted practices in developing and operating gateways, and that catalyze the formation of a community that may be diverse in discipline but has a common need to advance science through gateways.

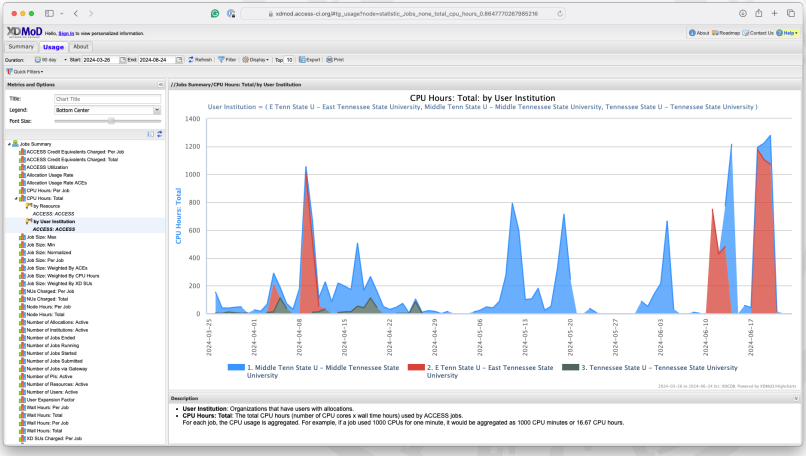
OpenHPC

OpenHPC is a Linux Foundation Collaborative Project whose mission is to provide a reference collection of open-source HPC software components and best practices, lowering barriers to deployment, advancement, and use of modern HPC methods and tools.

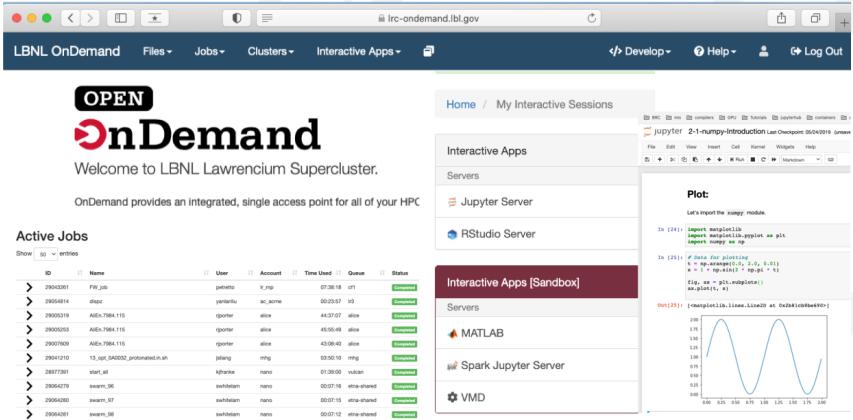
OpenHPC components and best practices will enable and accelerate innovation and discoveries by broadening access to state-of-the-art, open-source HPC methods and tools in a consistent environment, supported by a collaborative, worldwide community of HPC users, developers, researchers, administrators, and vendors.

– https://openhpc.community/about-us/

Open XDMoD


CPU Hours: Total: by User Institution
User Institution = (E Tenn State U – East Tennessee State University, Middle Tenn State U – Middle Tennessee State University, Tennessee State U – Tennessee State University)
CPU Hours: Total
1400
1200
1000
800
600
400
200
0
2024-03-15
2024-04-01
2024-04-08
2024-04-15
2024-04-22
2024-04-29
2024-05-06
2024-05-13
2024-05-20
2024-05-27
2024-06-03
2024-06-10
2024-06-17
1. Middle Tenn State U – Middle Tennessee State University
2. E Tenn State U – East Tennessee State University
3. Tennessee State U – Tennessee State University
Description
User Institution: Organizations that have users with allocations.
CPU Hours: Total: The total CPU hours (number of CPU cores x wall time hours) used by ACCESS jobs.
For each job, the CPU usage is aggregated. For example, if a job used 1000 CPUs for one minute, it would be aggregated as 1000 CPU minutes or 16.67 CPU hours.

Open OnDemand



Spack

- Spack is a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments.
- It was designed for large supercomputing centers, where many users and application teams share common installations of software on clusters with exotic architectures, using libraries that do not have a standard ABI.
- Spack is non-destructive: installing a new version does not break existing installations, so many configurations can coexist on the same system.

– https://spack.readthedocs.io/