

The Cyberinfrastructure Landscape: Systems, Providers, Technologies

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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–), CaRCC Emerging Centers Steering Committee (2024–)
- ▶ 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

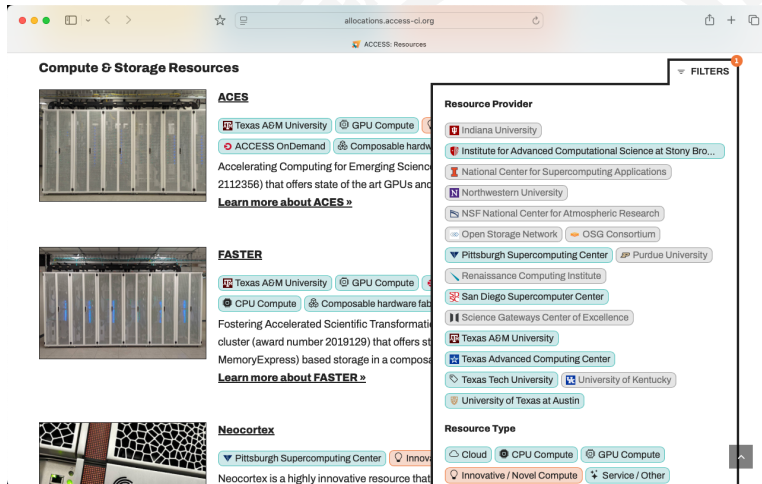
Discover 1.5M credits, 1-page proposal required

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

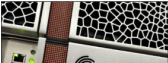



The screenshot shows a web browser window at `allocations.access-ci.org` displaying the "ACCESS: Resources" page. The page is titled "Compute & Storage Resources" and features a list of resources with a sidebar for filtering.

Compute & Storage Resources

ACES



 Texas A&M University  GPU Compute



 ACCESS OnDemand  Composable hardware

Accelerating Computing for Emerging Science (award number 2112356) that offers state of the art GPUs and

[Learn more about ACES »](#)

FASTER



 Texas A&M University  GPU Compute

 CPU Compute  Composable hardware

Fostering Accelerated Scientific Transformation (award number 2019129) that offers state of the art GPUs and


















[Learn more about FASTER »](#)

Neocortex






 Pittsburgh Supercomputing Center  Innovative / Novel Compute

Neocortex is a highly innovative resource that

Resource Provider

-  Indiana University
-  Institute for Advanced Computational Science at Stony Brook
-  National Center for Supercomputing Applications
-  Northwestern University
-  NSF National Center for Atmospheric Research
-  Open Storage Network  OSG Consortium
-  Pittsburgh Supercomputing Center  Purdue University
-  Renaissance Computing Institute
-  San Diego Supercomputer Center
-  Science Gateways Center of Excellence
-  Texas A&M University
-  Texas Advanced Computing Center
-  Texas Tech University  University of Kentucky
-  University of Texas at Austin

Resource Type

-  Cloud
-  CPU Compute
-  GPU Compute
-  Innovative / Novel Compute
-  Service / Other



New: DeltaAI at National Center for Supercomputing Applications (NCSA)

- ▶ 152 NVIDIA Grace-Hopper nodes, with 288 cores and 4 NVIDIA H100 GPUs (96 GB) each
- ▶ Superchip architecture
- ▶ 6 PB Lustre for \$HOME and \$SCRATCH
- ▶ 200 Gb HPE/Cray Slingshot networking



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
- ▶ Same storage and networking as DeltaAI



Stampede3 at Texas Advanced Computing Center (TACC)

- ▶ **New:** 24 Sapphire Rapids nodes with 1024 GB RAM, and 4 NVIDIA H100 (96 GB) GPUs
- ▶ 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



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
- ▶ **New:** 10 nodes with 104 Intel Sapphire Rapids cores, 2048 GB RAM, and 8 NVIDIA H100 GPUs (80 GB)
- ▶ 31 nodes with 40 Intel Cascade Lake cores, 102–512 GB RAM, and 8 NVIDIA V100 GPUs (16–32 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



Derecho at National Center for Atmospheric Research (NCAR)

- ▶ All using AMD 7763 CPUs
- ▶ 2488 nodes with 128 cores and 256 GB RAM
- ▶ 82 nodes with 64 cores, 512 GB RAM, and 4 NVIDIA A100 GPUs (40 GB)
- ▶ 200 Gb HPE/Cray Slingshot networking



Anvil at Purdue University

- ▶ Supporting CPU, GPU simulation and large memory simulation
- ▶ “Composable Subsystem” offers Kubernetes support for science gateways and other workloads
- ▶ All using dual AMD 7763 CPUs (128 cores)
- ▶ 1000 CPU nodes with 256 GB RAM, 32 with 1024 GB RAM
- ▶ 16 GPU nodes with 512 GB RAM and 4 NVIDIA A100 GPUs



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

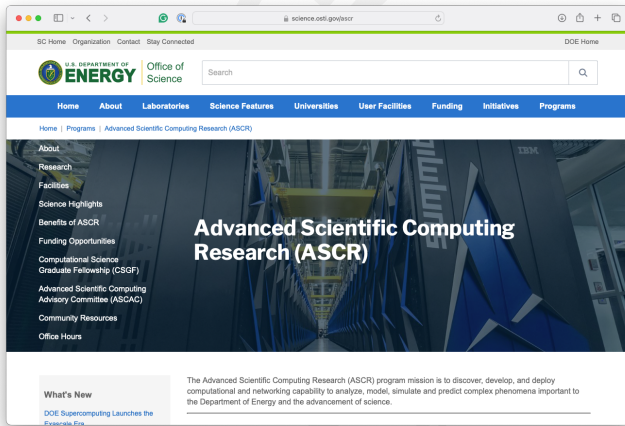


ACES at Texas A&M University

- ▶ 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 IPU: GC200, Bow-2000
 - ▶ NEC Vector Engine: Type 20B-P
- ▶ 2.3 PB Lustre
- ▶ 200 Gb Infiniband networking



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

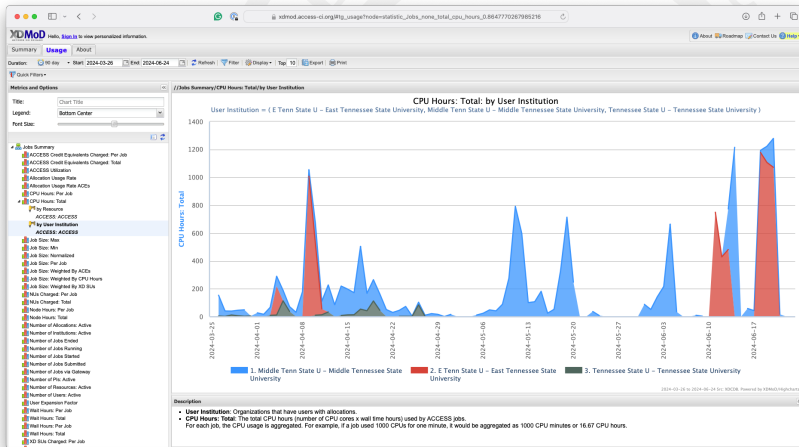
OpenHPC is a Linux Foundation Collaborative Project whose mission is to provide a reference collection of open-source HPC software components and best practices, lowering barriers to deployment, advancement, and use of modern HPC methods and tools.

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



Open OnDemand

The screenshot shows the Open OnDemand web interface. The top navigation bar includes links for Files, Jobs, Clusters, Interactive Apps, Develop, Help, and Log Out. The main content area features the Open OnDemand logo and a welcome message. Below this, the 'Active Jobs' section displays a table of running jobs. The 'Interactive Apps' sidebar on the right lists available applications like Jupyter Server, RStudio Server, MATLAB, Spark Jupyter Server, and VMD. A preview of a Jupyter Notebook is shown on the far right, displaying code for plotting a sine wave.

Active Jobs

ID	Name	User	Account	Time Used	Queue	Status
> 2904261	FW_job	petretto	lr_rnp	07:38:18	cd1	Completed
> 29054814	dlp	yanlanli	ac_aome	00:22:57	id3	Completed
> 29053319	AIEn.7984.115	rporter	alice	44:37:07	alice	Completed
> 29053253	AIEn.7984.115	rporter	alice	45:56:49	alice	Completed
> 29077609	AIEn.7984.115	rporter	alice	43:08:40	alice	Completed
> 29041210	13_opt_SA0032_protostated.in.sh	jialiang	mhg	03:50:10	mhg	Completed
> 28977391	start_all	khranki	nano	01:39:00	vulcan	Completed
> 29054279	swarm_56	sachlam	nano	00:07:16	extra-shared	Completed
> 29054280	swarm_57	sachlam	nano	00:07:15	extra-shared	Completed
> 29054281	swarm_58	sachlam	nano	00:07:12	extra-shared	Completed

Interactive Apps [Sandbox]

- Servers
- Jupyter Server
- RStudio Server
- MATLAB
- Spark Jupyter Server
- VMD

Plot:

Let's import the `numpy` module.

```
In [24]: import matplotlib
import matplotlib.pyplot as plt
import numpy as np

In [25]: # Data for plotting
x = np.arange(0.0, 2.0, 0.01)
y = 1 + np.sin(2 * np.pi * x)
fig, ax = plt.subplots()
ax.plot(x, y)

Out[25]: [<matplotlib.lines.Line2D at 0x2881cb9e490>]
```



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/>

