ACES Overview

ACES Workshop 2025

Lisa Perez

July 19, 2025

High Performance
Research Computing
DIVISION OF RESEARCH

Workshop Agenda

Friday, July 18	Check-in, Opening Remarks, Reception and Dinner
	Sonesta Columbus Downtown (2nd Floor) Map
3:00PM - 4:00PM	**Check-in** (Scioto Ballroom)
4:00PM - 4:10PM	**Opening Remarks** Bob Chadduck, National Science Foundation (Scioto Ballroom)
4:10PM - 5:00PM	**ACES Overview** Lisa Perez, Texas A&M High Performance Research Computing (Scioto Ballroom)
5:00PM - 6:00PM	Reception with Light Hors d'Deuvres (Pinnacle)
6:00PM - 9:00PM	Buffet Dinner (Pinnacle)

Workshop Agenda

Saturday, July 19	Tutorials and Lightning Talks
8:00AM - 9:00AM	Continental Breakfast (Pinnacle)
9:00AM - 9:30AM	**Introduction to the ACES Portal (Scioto Ballroom)** Lisa Perez, Texas A&M HPRC
9:30AM - 10:30AM	**Drona Workflow Engine (Scioto Ballroom)** Marinus Pennings, Texas A&M HPRC
10:30AM - 11:00AM	Break
11:00AM - 12:00PM	**Intro to Jupyter AI Assistant (Scioto Ballroom)** Keegan Smith, Texas A&M HPRC
12:00PM - 1:00PM	Lunch (Pinnacle)
1:00PM - 2:00PM	**Lightning Talks (Scioto Ballroom)**
2:00PM - 3:15PM	**AI/ML Workflows on ACES (Scioto Ballroom)** Zhenhua He, Texas A&M HPRC
3:15PM - 3:45PM	Break
3:45PM - 5:00PM	**AI/ML Workflows on ACES (Cont.)** Zhenhua He, Texas A&M HPRC
6:00PM - 9:00PM	Buffet Dinner (Pinnacle)

Workshop Agenda

Sunday, July 20	Tutorials and Special Session	
8:00AM - 9:00AM	Continental Breakfast (Pinnacle)	
9:00AM - 10:15AM	**AlphaFold3 Protein Stucture Prediction (Scioto Ballroom)** Michael Dickens, Texas A&M HPRC	***Ab initio* molecular dynamics on NEC VE (Scioto Ballroom)** Lisa Perez, Texas A&M HPRC
10:15AM - 10:45AM	Break	
10:45AM - 12:00PM	**Julia (Scioto Ballroom)** Wesley Brashear, Texas A&M HPRC	**LAMMPS on Intel PVC (Scioto Ballroom)** Richard Lawrence, Texas A&M HPRC
12:00PM - 1:00PM	Lunch (Pinnacle)	
1:00PM - 3:00PM	**ACES Office Hours (Pinnacle)**	**Advisory Board Meeting (Scioto Ballroom)**
3:00PM - 5:00PM	**ACES Office Hours (cont.) (Pinnacle)**	**CXL Meetup (Scioto Ballroom)**

NSF ACES

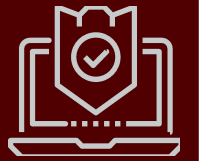
Accelerating Computing for Emerging Sciences

Our Goals:

- NSF ACSS CI testbed
- Offer an accelerator testbed for numerical simulations and **AI/ML workloads**
- Provide consulting, technical guidance, and training to researchers
- Collaborate on computational and data-enabled research.

ACES Partnerships

Equipment
- TAMU



Allocations
- TACC
- TAMU

User Services / Research
- TAMU
- UIUC

Training/Outreach
- TAMU
- TACC
- UIUC

Advisory Committee
- Independent

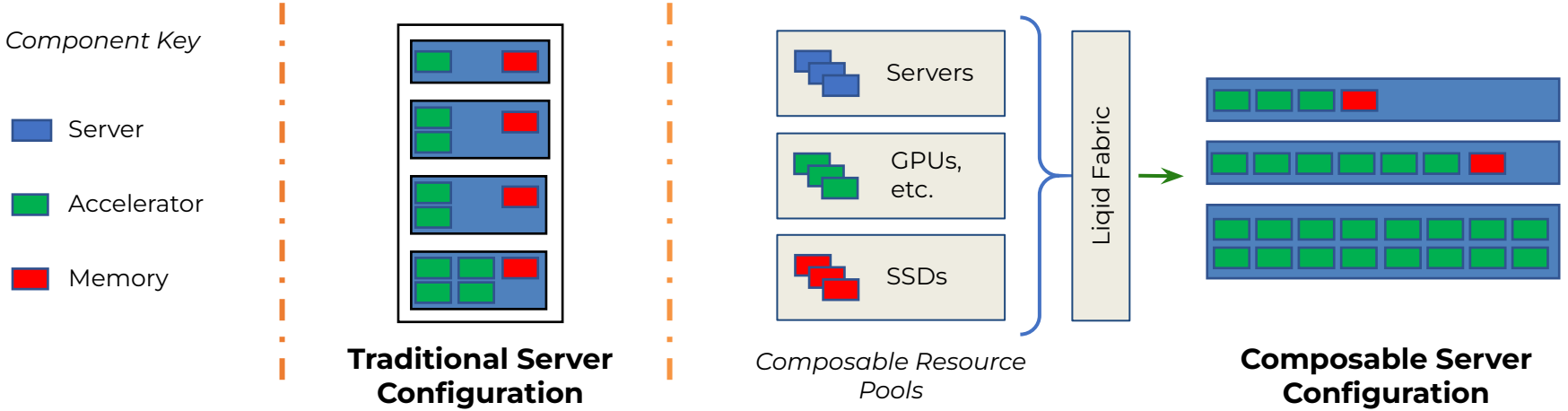
ACCESS

NSF

NAIRR Pilot

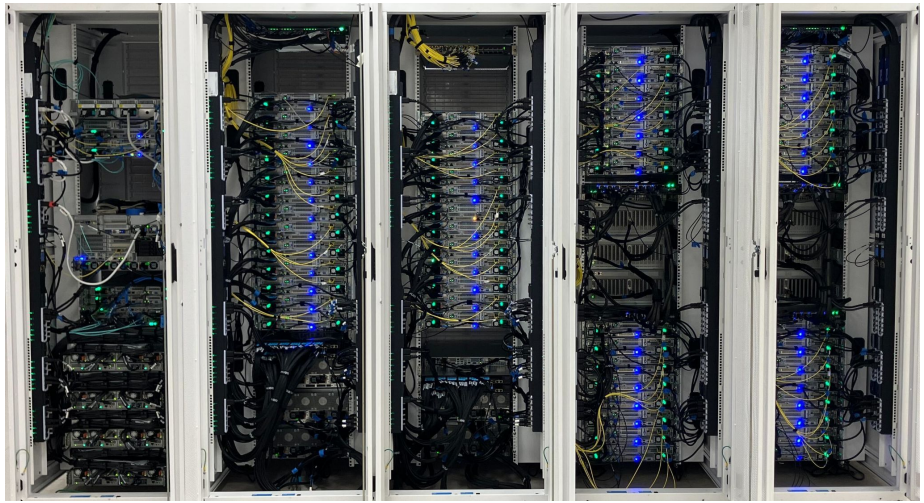
Composable HPC Architectures for AI/ML

- Built on Disaggregated Hardware
- Composable Hardware Platform
- Composable GPU/Accelerator
- Composable SSDs - Intel Optane
- Open Platform for various Accelerators



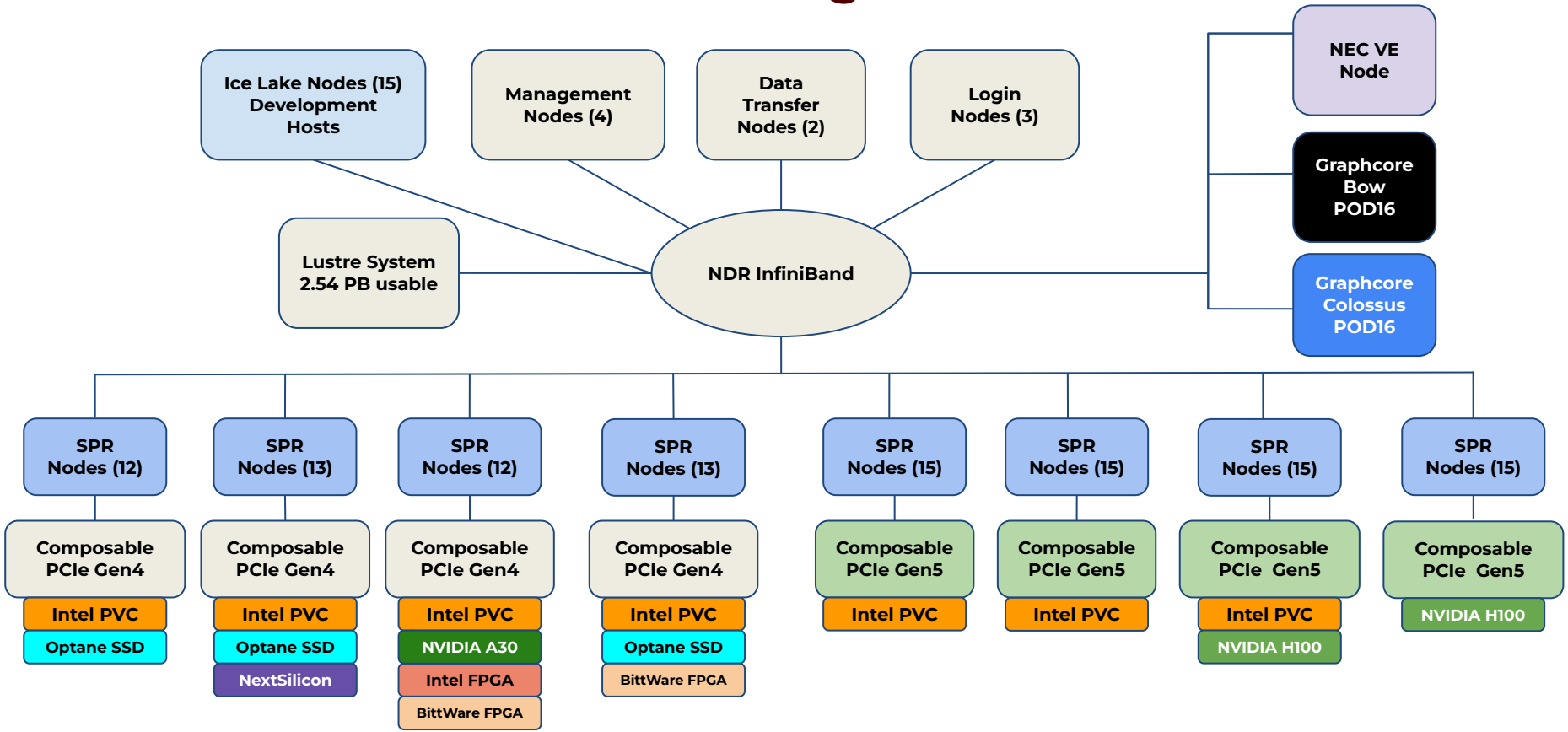
Industry Partners

LIQID intel DELL Technologies Red Hat ddn NVIDIA



NEC BittWare a molex company MemVerge slurm SchedMD GRAPHCORE NEXTSILICON

ACES Configuration

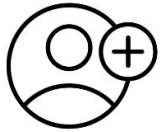


ACES Allocations

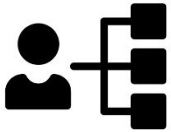
ACCESS

NAIRR Pilot

You can get allocations on ACES through both *ACCESS* and *NAIRR*



CREATE ACCOUNT



SELECT OPPORTUNITY

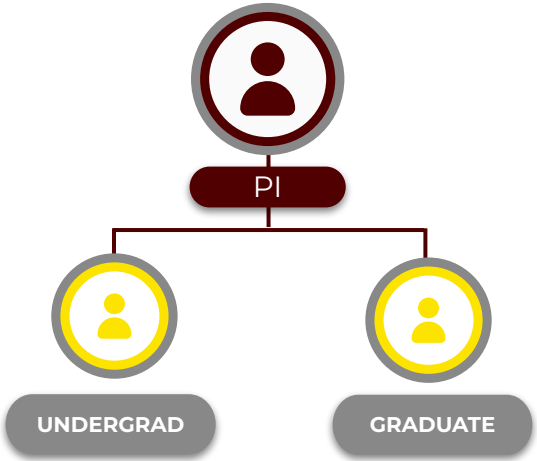
REQUEST ALLOCATION

RECEIVE CREDITS

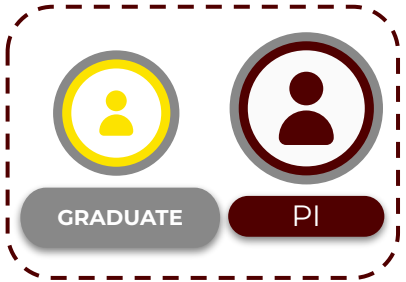
EXCHANGE CREDITS

Getting on ACES

- Using an ACCESS account
- Application for ACES is available through ACCESS: https://allocations.access-ci.org
- Email us at help@hprc.tamu.edu for questions, comments, and concerns.



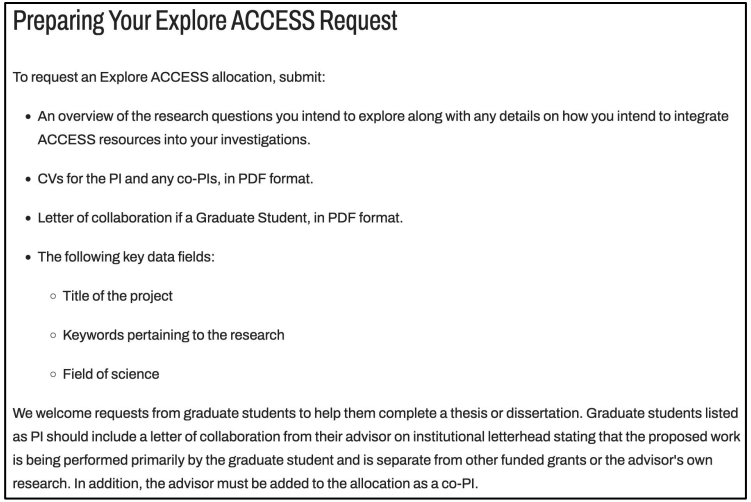
PIs can apply for an account and sponsor accounts for their researchers.



(Grad students may also apply directly with a letter of collaboration from their PI)

ACCESS Allocations Opportunities

See also:
https://hprc.tamu.edu/policies/allocations.html



Preparing Your Explore ACCESS Request

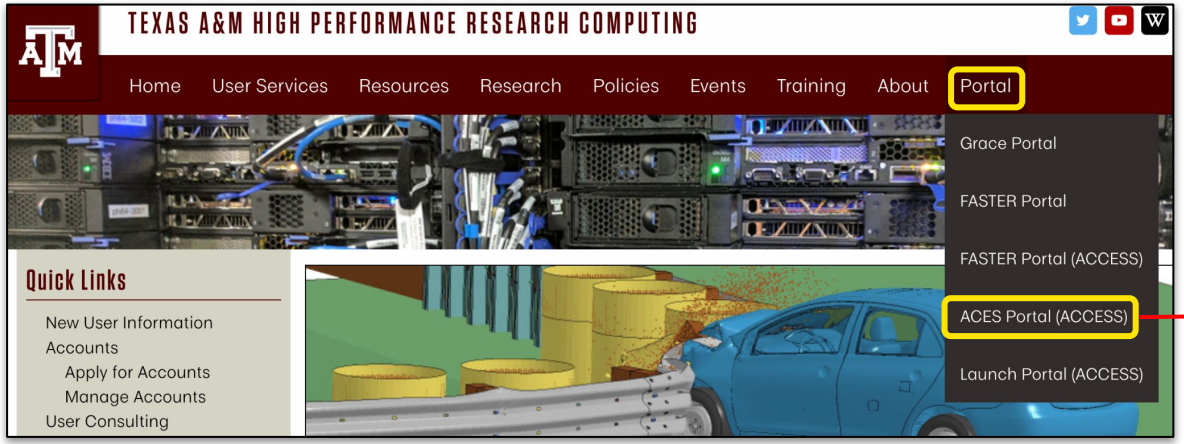
To request an Explore ACCESS allocation, submit:

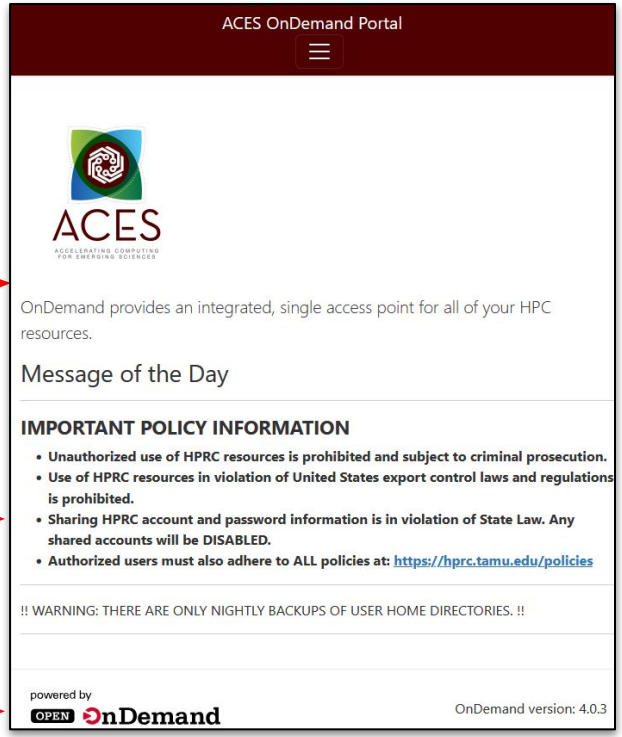
- An overview of the research questions you intend to explore along with any details on how you intend to integrate ACCESS resources into your investigations.
- CVs for the PI and any co-PIs, in PDF format.
- Letter of collaboration if a Graduate Student, in PDF format.
- The following key data fields:
  - Title of the project
  - Keywords pertaining to the research
  - Field of science

We welcome requests from graduate students to help them complete a thesis or dissertation. Graduate students listed as PI should include a letter of collaboration from their advisor on institutional letterhead stating that the proposed work is being performed primarily by the graduate student and is separate from other funded grants or the advisor's own research. In addition, the advisor must be added to the allocation as a co-PI.

	Explore	Discover	Accelerate
Purpose	Resource Evaluations, grad student projects, small classes, etc.	Large classes, benchmarking at-scale, Campus Champions	Multi-grant programs, Collaborations, Growing gateways
Requests Accepted	Continuously; multiple requests allowed		
Review requirements	Overview	1-page proposal	3-page (max) proposal

ACES Portal

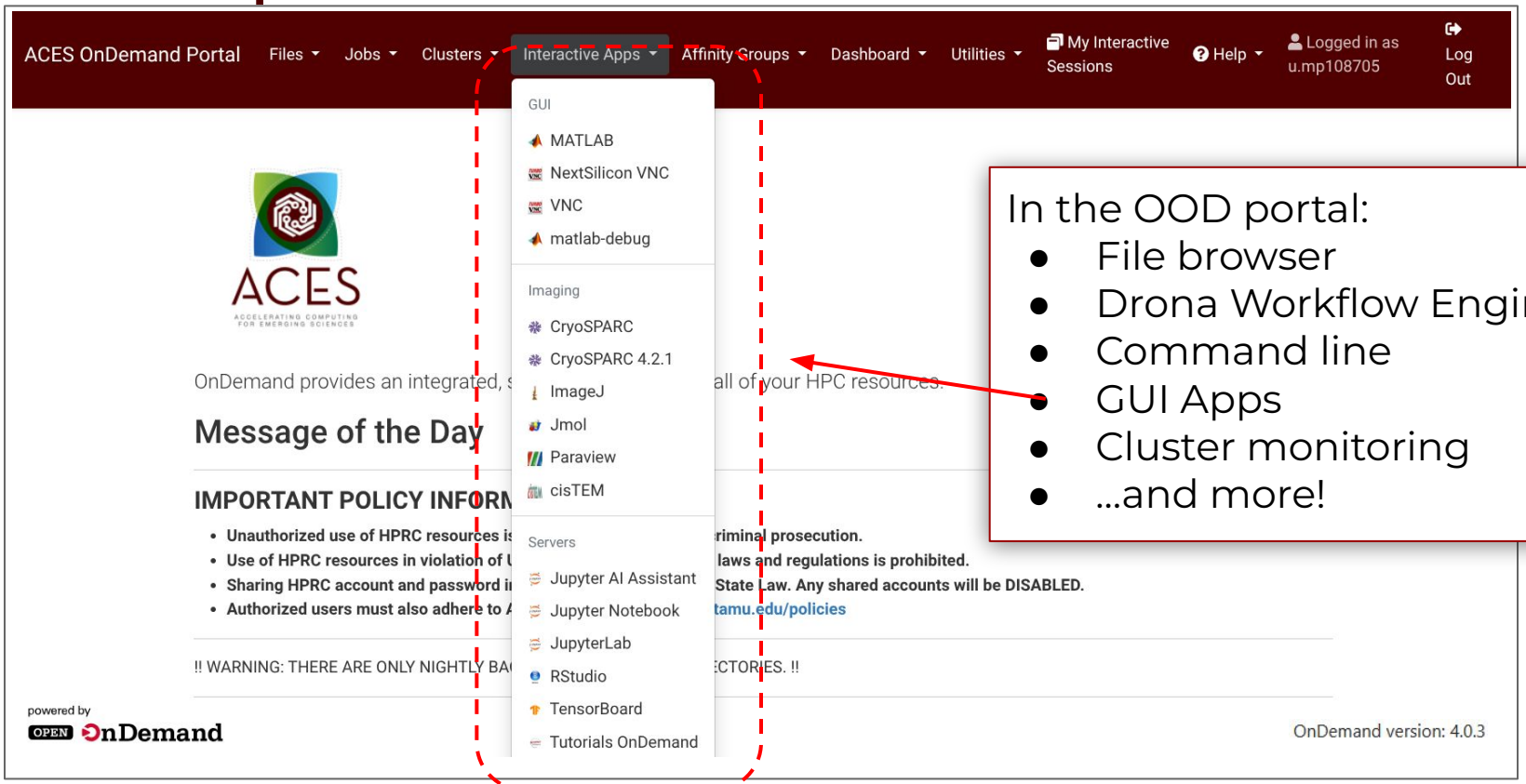




ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based graphical interface framework for HPC users

Open on Demand ACES Portal

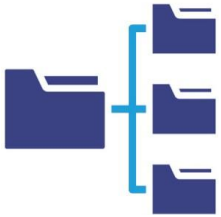


In the OOD portal:

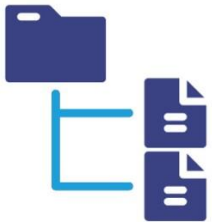
- File browser
- Drona Workflow Engine
- Command line
- GUI Apps
- Cluster monitoring
- …and more!

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit	Intended Use
/home/$USER	$HOME	10 GB	10,000	Small to modest amounts of processing.
/scratch/user/$USER	$SCRATCH	1 TB	250,000	Temporary storage of large files for on-going computations. Not intended for long-term storage. 6 month storage allocations granted.
/scratch/group/PROJECTID	$PROJECT	5 TB	500,000	High performance storage for specific storage allocation requests. Not purged while allocation is active. Available upon request.



Home and Scratch directories are not shared
Groups can share files in the Project directory



3,070+ Software Modules!

SOFTWARE MODULES ON THE ACES CLUSTER

ACES Software Modules | FASTER Software Modules | Grace Software Modules

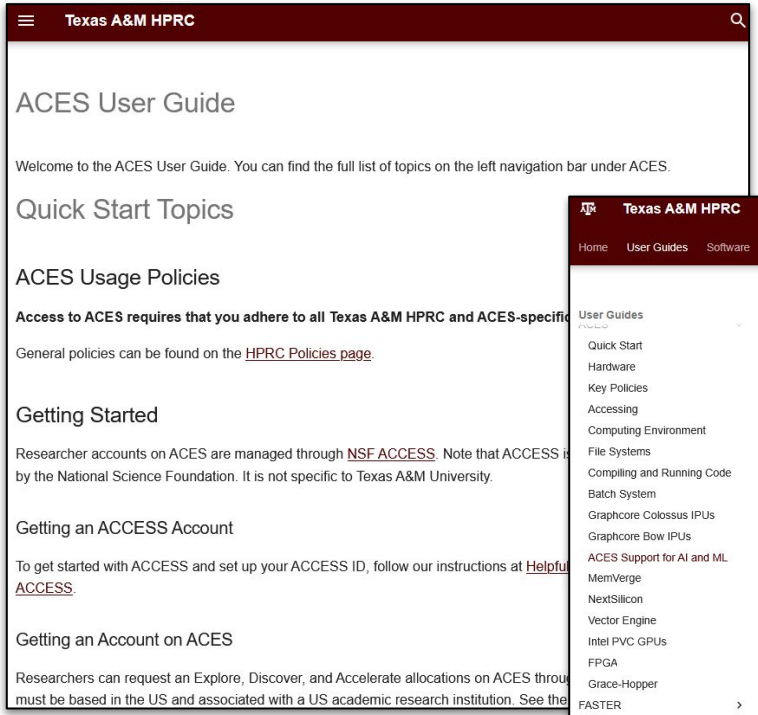
(Last Updated: Jul 2, 2025)

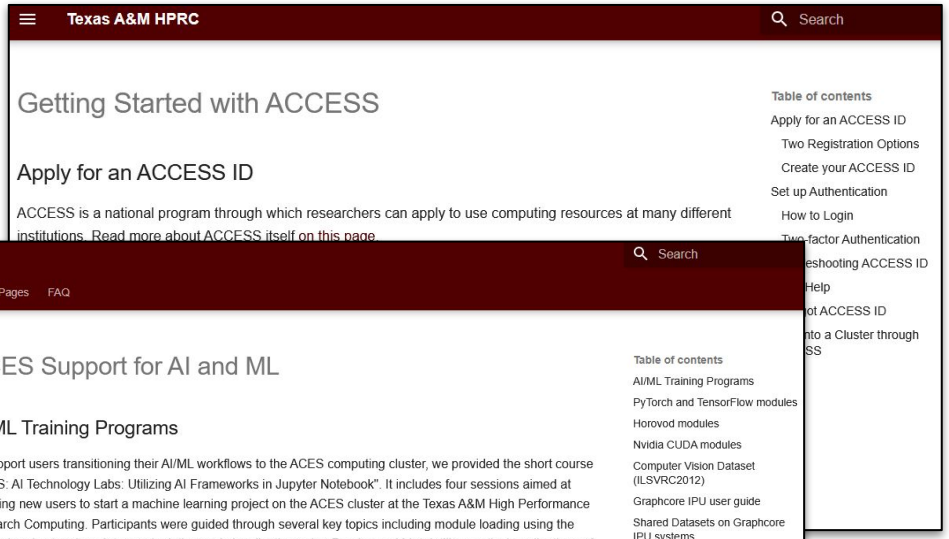
Name	Versions available	Description
ABYSS	ABySS/2.3.7	Assembly By Short Sequences - a de novo, parallel, paired-end sequence assembler
ACTC	ACTC/1.1	ACTC converts independent triangles into triangle strips or fans.
ADIOS2	ADIOS2/2.10.2	The Adaptable Input/Output (I/O) System transports data as groups of self-describing variables and attributes across different media types (such as files, wide-area-networks, and remote direct memory access) using a common application programming interface for all transport modes.
AI-TOOLS-GPU	AI-Tools-GPU/20240816	AI Tools from Intel (formerly referred to as the Intel AI Analytics Toolkit) give data scientists, AI developers, and researchers familiar Python tools and frameworks to accelerate end-to-end data science and analytics pipelines on Intel architecture. The components are built using oneAPI libraries for low-level compute optimizations. The AI Tools maximize performance from preprocessing through machine learning, and provides interoperability for efficient model development.
ANICALCULATOR	ANIcalculator/1.0	This tool will calculate the bidirectional average nucleotide identity (gANI) and Alignment Fraction (AF) between two genomes. Required input is the full path to the fna file (nucleotide sequence of genes in fasta format) of each query genome. Either the rRNA and tRNA genes can be excluded, or provided in a list with the -ignoreList option. This is necessary as the presence of tRNA and/or rRNA genes in the fna will artificially inflate the ANI.
ANTLR	ANTLR/2.7.7-Java-11	ANTLR, ANother Tool for Language Recognition, (formerly PCCTS) is a language tool that provides a framework for constructing recognizers, compilers, and translators from grammatical descriptions containing Java, C#, C++, or Python actions.
AOCC	AOCC/4.0.0	AMD Optimized C/C++ & Fortran compilers (AOCC) based on LLVM 13.0
APBS	APBS/3.4.1	APBS (Adaptive Poisson-Boltzmann Solver) solves the equations of continuum electrostatics for large biomolecular assemblages.

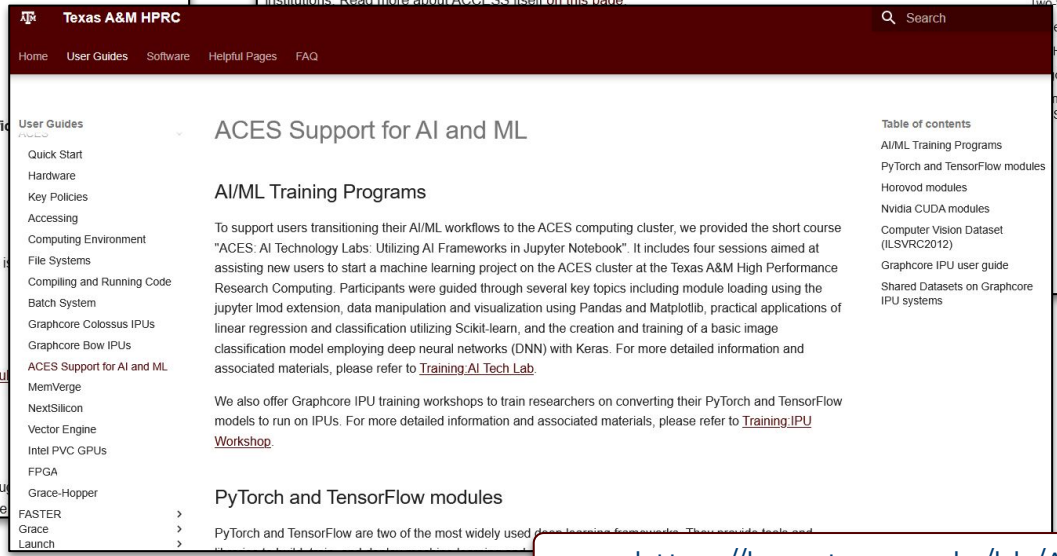
940 unique software packages – most with multiple version modules

hprc.tamu.edu/software/aces

Knowledge Base

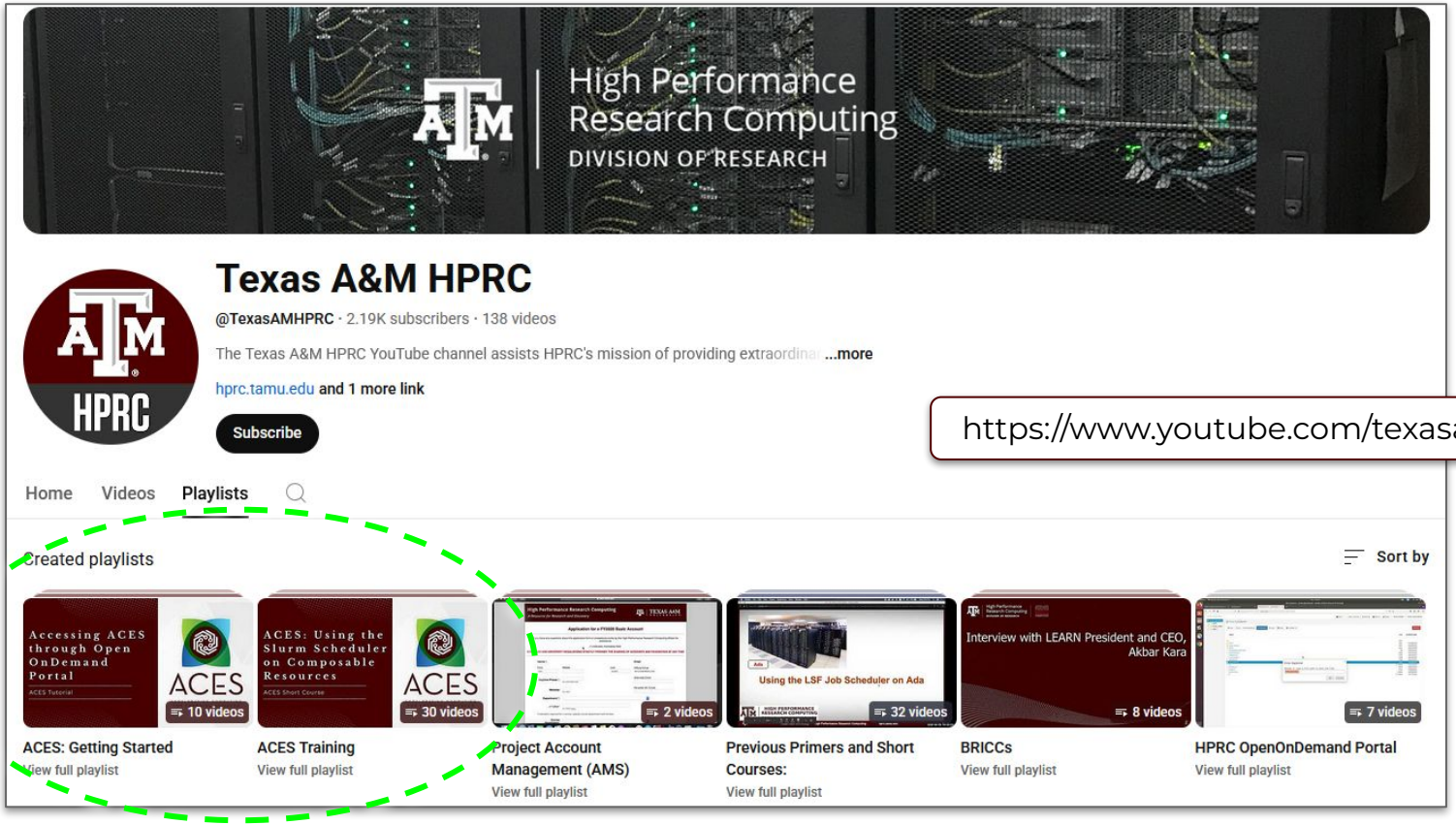






https://hprc.tamu.edu/kb/ACES

Training on YouTube



https://www.youtube.com/texasamhprc

Texas A&M at PEARC25

Tutorials and Workshop	Date/Time	Room
Tutorial: ACES Tutorial for using Graphcore Intelligence Processing Units (IPUs) for AI/ML Workflows	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room A213
Tutorial: Open OnDemand Overview, Customization, and App Development	Mon, July 21, 2025 1:30 AM-5:00 PM ET	Room A226
Workshop: Collaborating with K12 Schools: Supporting Secondary Students and Teachers in Computing	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room B132

Texas A&M at PEARC25

Presentations and BoF	Date/Time	Room
WFT&E-2-3: ByteBoost: An advanced cybertraining program designed to enhance research on testbed systems	Tue, July 22, 2025 11:50 AM-12:05 PM ET	Room A216
A&SW-2-5: Generating Scientific Workflows With Drona Environments	Tue, July 22, 2025 12:00 PM-12:15 PM ET	Room A220-A221
WFT&E-3-2: Empowering NAIRR "Pilots" of all skill levels to become "ACES" with HPC	Tue, July 22, 2025 2:15 PM-2:30 PM ET	Room A114-A115
WFT&E-5-4: Exploring the Role of Academics, Research and Workforce Development in Establishing Research Computing Collaborations	Wed, July 23, 2025 11:55 AM-12:10 PM ET	Room A114-A115
A&SW-6-2: Comparison of GPU Performance Scaling for Molecular Dynamics	Wed, July 23, 2025 2:15 PM-2:30 PM ET	Room A212-A213
BOF-18: Node to Joy: Finding the Right Compute Resources	Wed, July 23, 2025 4:15 PM-5:15 PM ET	Room A213-A215

High Performance
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DIVISION OF RESEARCH

Thank you

- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES), #2019129 (FASTER) and #19257614 (SWEETER)

- Please visit our talks and BoF at PEARC25
- Helpdesk: help@hprc.tamu.edu