

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	<i>Ab initio</i> 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

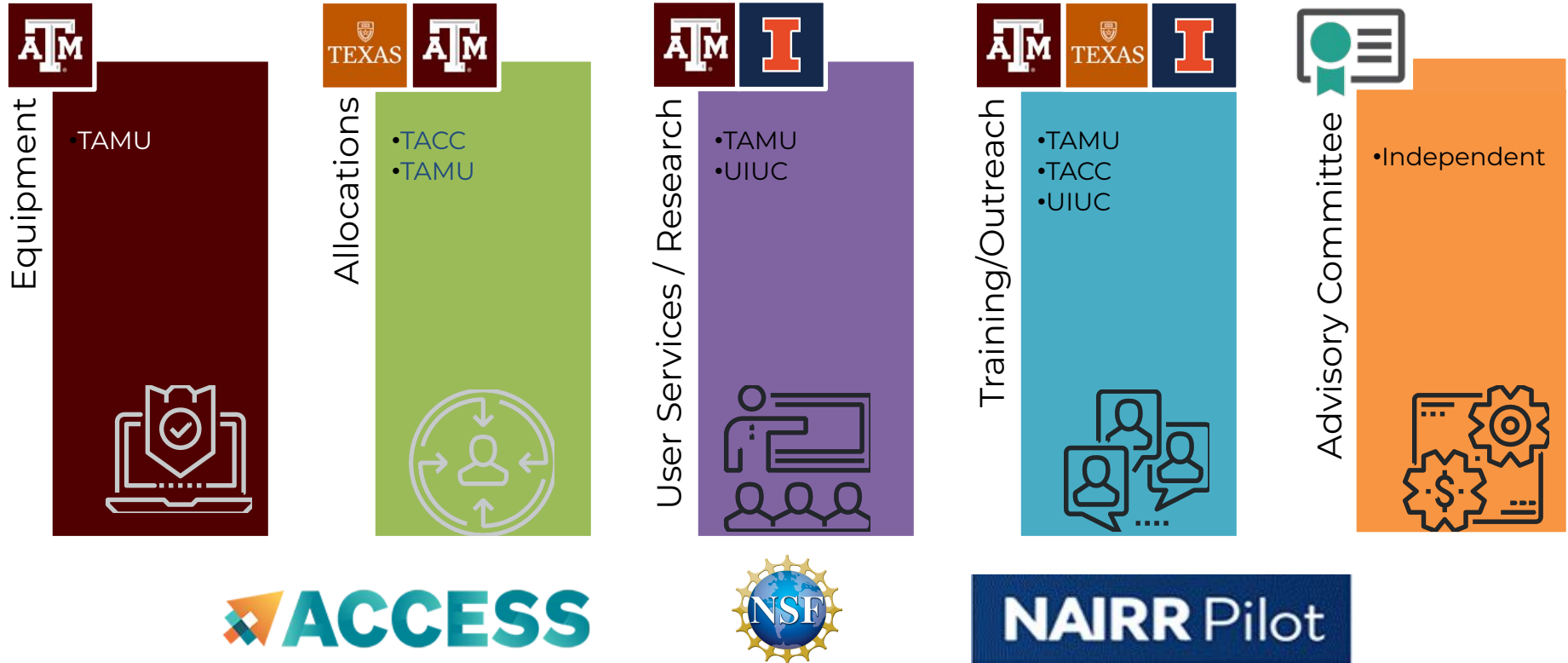
Accelerating Computing for Emerging Sciences

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.



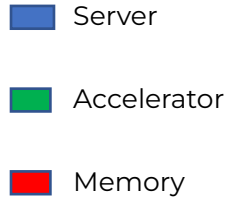
ACES Partnerships



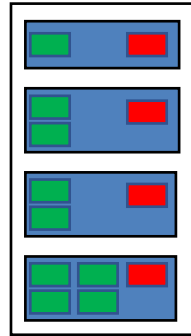
Composable HPC Architectures for AI/ML

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

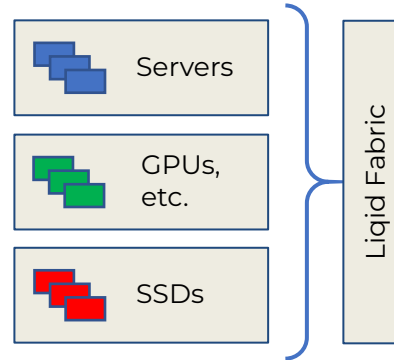
Component Key



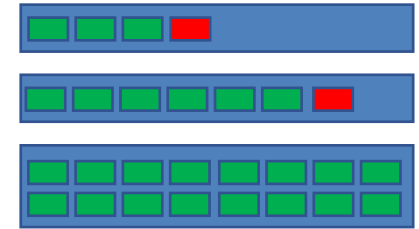
Traditional Server Configuration



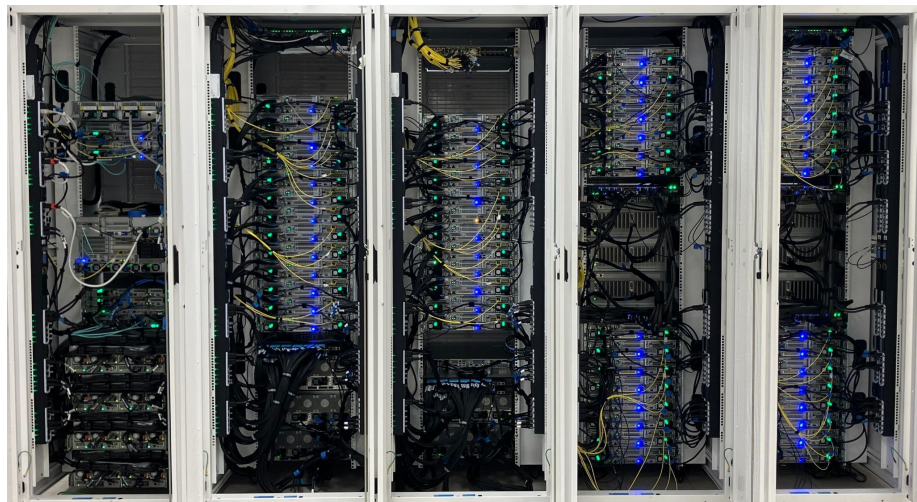
Composable Resource Pools



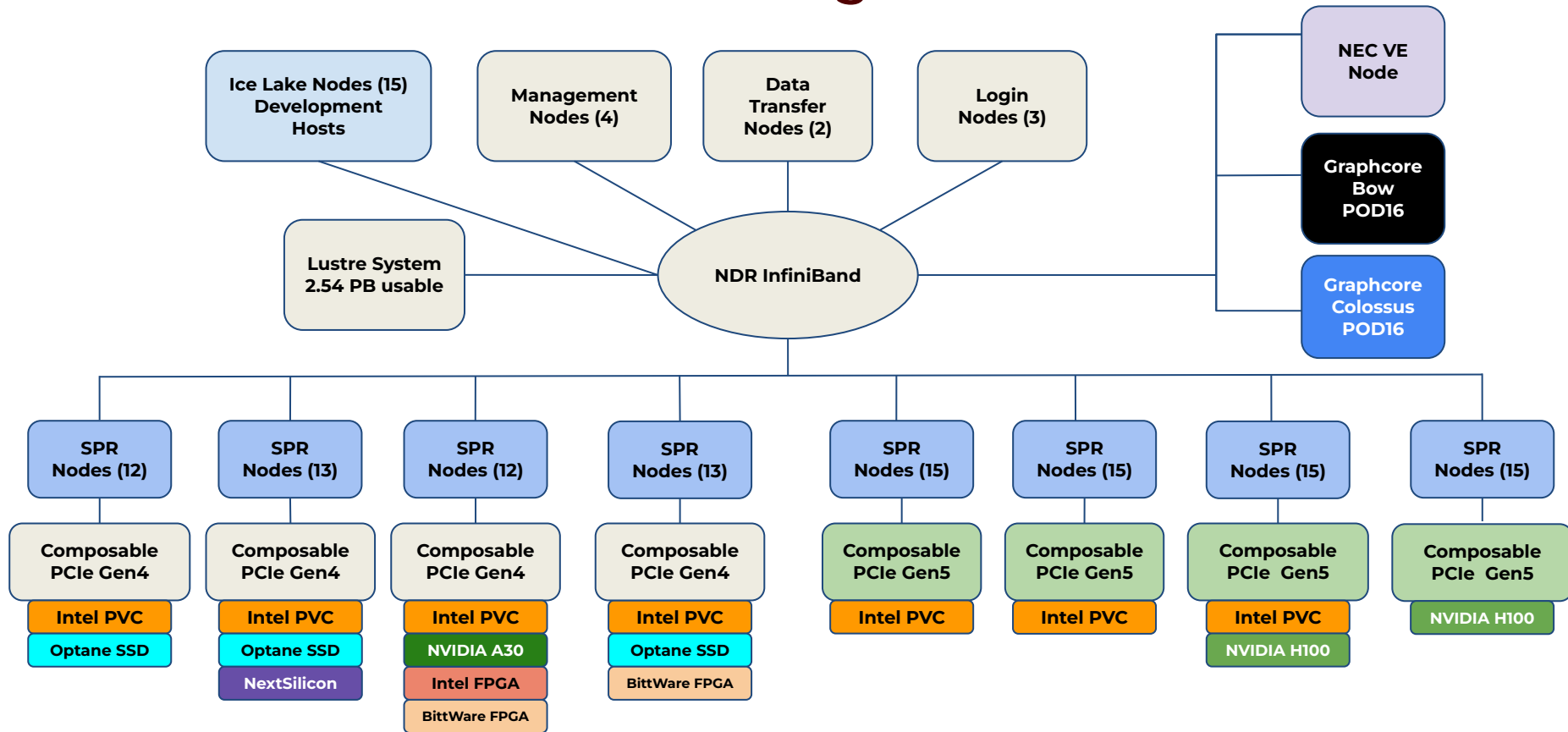
Composable Server Configuration



Industry Partners



ACES Configuration



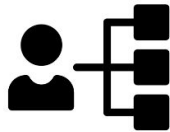
ACES Allocations



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



CREATE
ACCOUNT



SELECT
OPPORTUNITY



REQUEST
ALLOCATION



RECEIVE
CREDITS

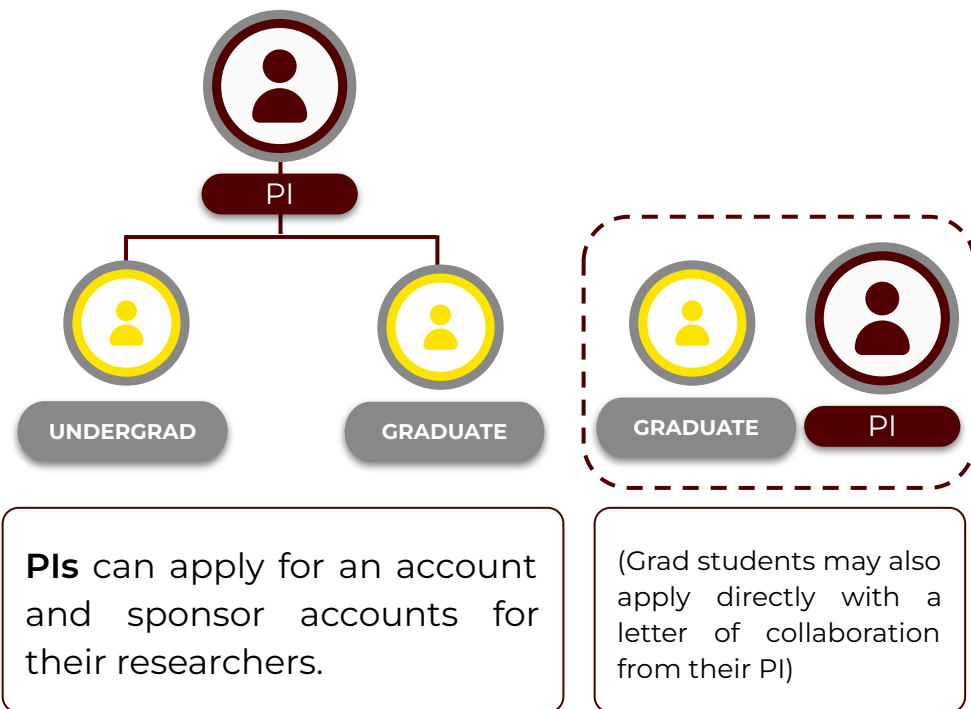


EXCHANGE
CREDITS



Getting on ACES

- Using an [ACCESS](https://access-ci.org) 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.





Allocations Opportunities

See also:

<https://hprc.tamu.edu/policies/allocations.html>

Preparing Your Explore ACCESS Request

To request an Explore ACCESS allocation, submit:

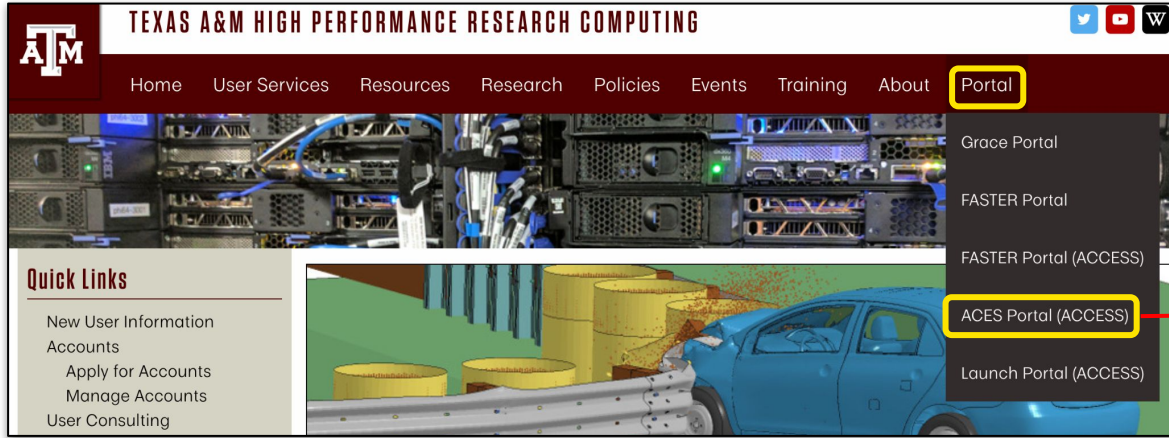
- An overview of the research questions you intend to explore along with any details on how you intend to integrate ACCESS resources into your investigations.
- CVs for the PI and any co-PIs, in PDF format.
- Letter of collaboration if a Graduate Student, in PDF format.
- The following key data fields: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

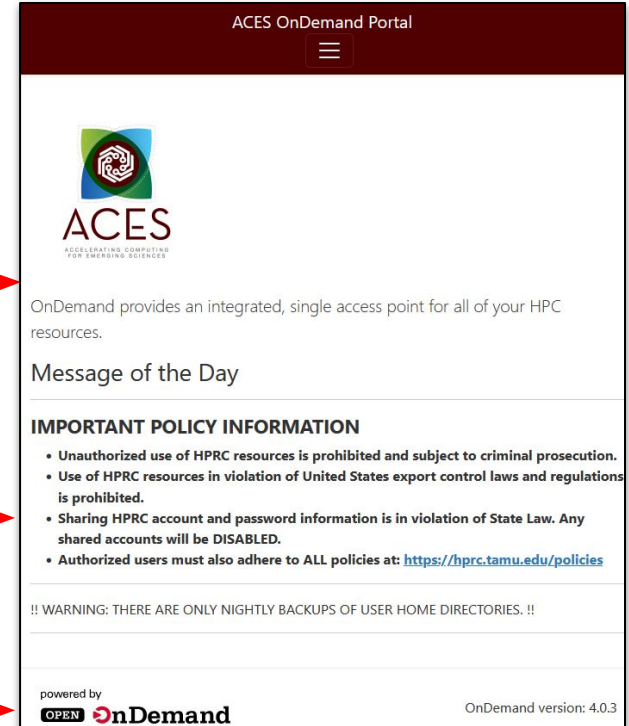


ACES Portal



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

ACES OnDemand Portal Files Jobs Clusters **Interactive Apps** Affinity Groups Dashboard Utilities My Interactive Sessions Help Logged in as u.mp108705 Log Out

GUI

- MATLAB
- NextSilicon VNC
- VNC
- matlab-debug

Imaging

- CryoSPARC
- CryoSPARC 4.2.1
- ImageJ
- Jmol
- Paraview
- cisTEM

Servers

- Jupyter AI Assistant
- Jupyter Notebook
- JupyterLab
- RStudio
- TensorBoard
- Tutorials OnDemand

ACES
ACCELERATING COMPUTING
FOR EMERGING SCIENCES

OnDemand provides an integrated, secure environment for all of your HPC resources.

Message of the Day

IMPORTANT POLICY INFORMATION

- Unauthorized use of HPRC resources is prohibited.
- Use of HPRC resources in violation of University of Texas at Austin State Law is prohibited.
- Sharing HPRC account and password information is prohibited.
- Authorized users must also adhere to all applicable laws and regulations.

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS !!

powered by **OPEN OnDemand**

OnDemand version: 4.0.3

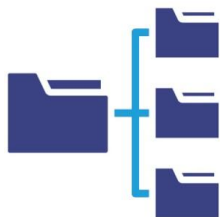
In the OOD portal:

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

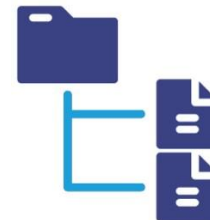


File Systems and User Directories

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

940 unique software packages – most with multiple version modules

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 <i>fna</i> 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 <i>-ignoreList</i> option. This is necessary as the presence of tRNA and/or rRNA genes in the <i>fna</i> 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.

hprc.tamu.edu/software/aces



Knowledge Base

Texas A&M HPRC

ACES User Guide

Welcome to the ACES User Guide. You can find the full list of topics on the left navigation bar under ACES.

Quick Start Topics

ACES Usage Policies

Access to ACES requires that you adhere to all Texas A&M HPRC and ACES-specific policies. General policies can be found on the [HPRC Policies page](#).

Getting Started

Researcher accounts on ACES are managed through [NSF ACCESS](#). Note that ACCESS is managed by the National Science Foundation. It is not specific to Texas A&M University.

Getting an ACCESS Account

To get started with ACCESS and set up your ACCESS ID, follow our instructions at [Helpful ACCESS](#).

Getting an Account on ACES

Researchers can request an Explore, Discover, and Accelerate allocations on ACES through the [ACES Request Portal](#). All requests must be based in the US and associated with a US academic research institution. See the [ACES User Guide](#) for more details.

Texas A&M HPRC

Getting Started with ACCESS

Apply for an ACCESS ID

ACCESS is a national program through which researchers can apply to use computing resources at many different institutions. [Read more about ACCESS itself on this page.](#)

ACES Support for AI and ML

AI/ML Training Programs

To support users transitioning their AI/ML workflows to the ACES computing cluster, we provided the short course "ACES: AI Technology Labs: Utilizing AI Frameworks in Jupyter Notebook". It includes four sessions aimed at assisting new users to start a machine learning project on the ACES cluster at the Texas A&M High Performance Research Computing. Participants were guided through several key topics including module loading using the jupyter lmod extension, data manipulation and visualization using Pandas and Matplotlib, practical applications of linear regression and classification utilizing Scikit-learn, and the creation and training of a basic image classification model employing deep neural networks (DNN) with Keras. For more detailed information and associated materials, please refer to [Training AI Tech Lab](#).

We also offer Graphcore IPU training workshops to train researchers on converting their PyTorch and TensorFlow models to run on IPU. For more detailed information and associated materials, please refer to [Training IPU Workshop](#).

PyTorch and TensorFlow modules

PyTorch and TensorFlow are two of the most widely used deep learning frameworks. They provide tools and

- Table of contents
- Apply for an ACCESS ID
 - Two Registration Options
 - Create your ACCESS ID
- Set up Authentication
 - How to Login
 - Two-factor Authentication
- Resetting ACCESS ID
- Help
- Get ACCESS ID
- Join a Cluster through ACCESS

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- AI/ML Training Programs
- PyTorch and TensorFlow modules
- Horovod modules
- Nvidia CUDA modules
- Computer Vision Dataset (ILSVRC2012)
- Graphcore IPU user guide
- Shared Datasets on Graphcore IPU systems

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



Training on YouTube

Texas A&M HPRC
@TexasAMHPRC · 2.19K subscribers · 138 videos
The Texas A&M HPRC YouTube channel assists HPRC's mission of providing extraordinary ...more
hprc.tamu.edu and 1 more link

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- ACES: Getting Started**
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- ACES Training**
View full playlist
- Project Account Management (AMS)**
View full playlist
- Previous Primers and Short Courses**
View full playlist
- BRICCs**
View full playlist
- HPRC OpenOnDemand Portal**
View full playlist

<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
Research Computing
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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

