Introduction to Composable Computing on NSF ACES

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High Performance
Research Computing
DIVISION OF RESEARCH

Outline

- (Brief Disambiguation)
- ACES and Composability Overview
- Documentation and Training
- Getting Started on the ACES Cluster
- OOD Portal and Cluster Basics
- Software Infrastructure
- Batch Computing
- Composability, Accelerators, and AI/ML
- Bonus: ACES Configuration

Disambiguation

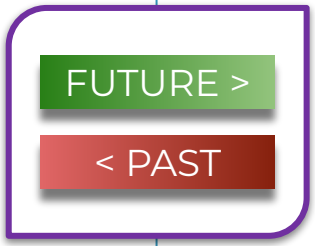
- **HPC** = “high performance computing”
  (a general field)
- **HPRC** = “High Performance Research Computing”
  (us – Texas A&M University’s HPC center)
- **TACC** = “Texas Advanced Computing Center”
  (unrelated to us – UT Austin’s HPC center)
- **ACES** = “Advancing Computing for Emerging Sciences”
  (one of HPRC’s clusters)
- **ACCESS** = “Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support”
  (nation-wide NSF program for HPC clusters)

ACES and Composability Overview

Composable HPC Architectures for AI

Common HPC

- Built on Converged Hardware
- Static Hardware Design
- Fixed GPU/Accelerator
- Fixed Memory
- Storage: SATA and SAS
- Vendor Lock

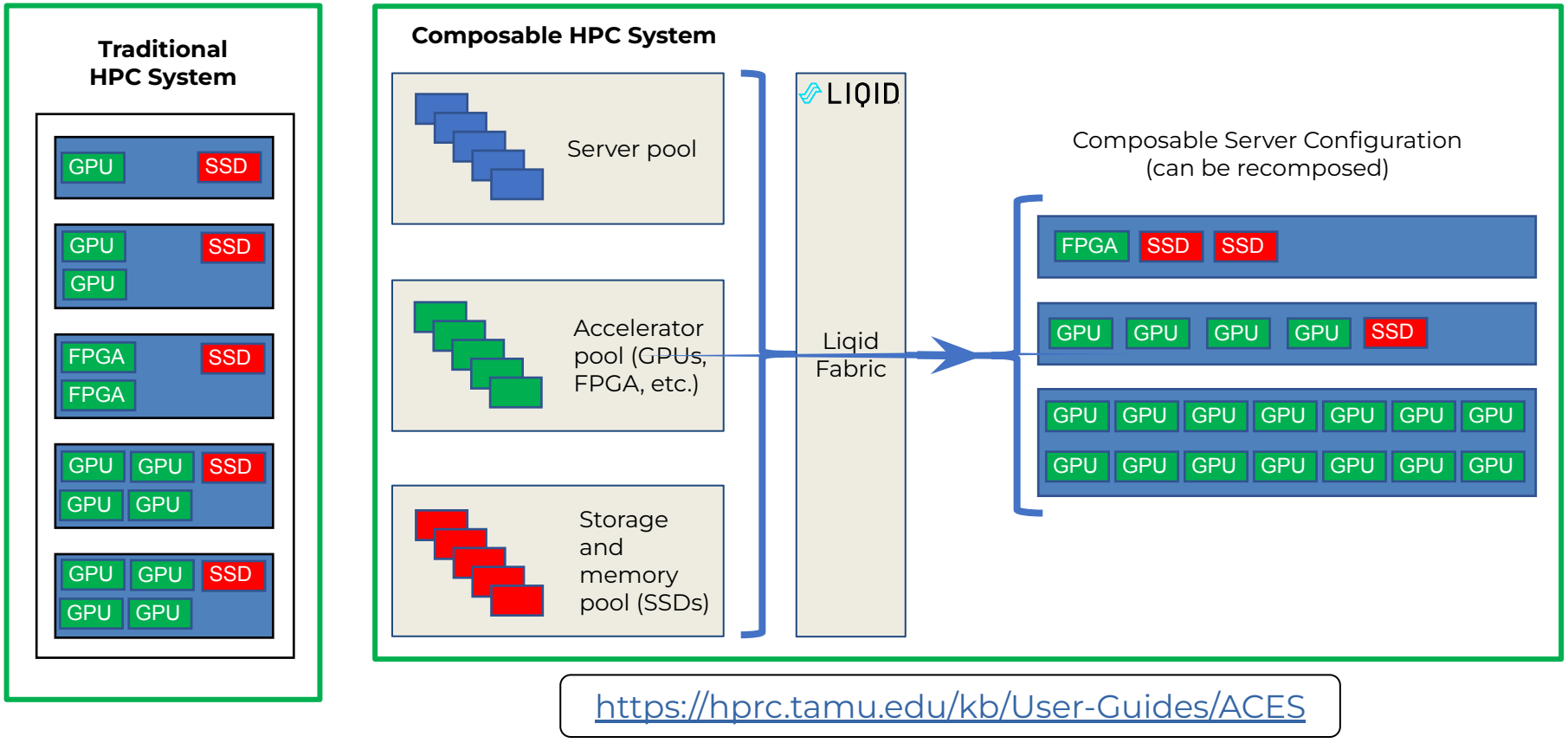


HPC for AI

- Built on Disaggregated Hardware
- Composable Hardware Platform
- Composable GPU/Accelerator
- Composable Memory - Optane
- Modern Storage: NVMe-oF
- Open Platform

Next Generation HPC/AI Platform Supports Composable Accelerators and Memory

Composability

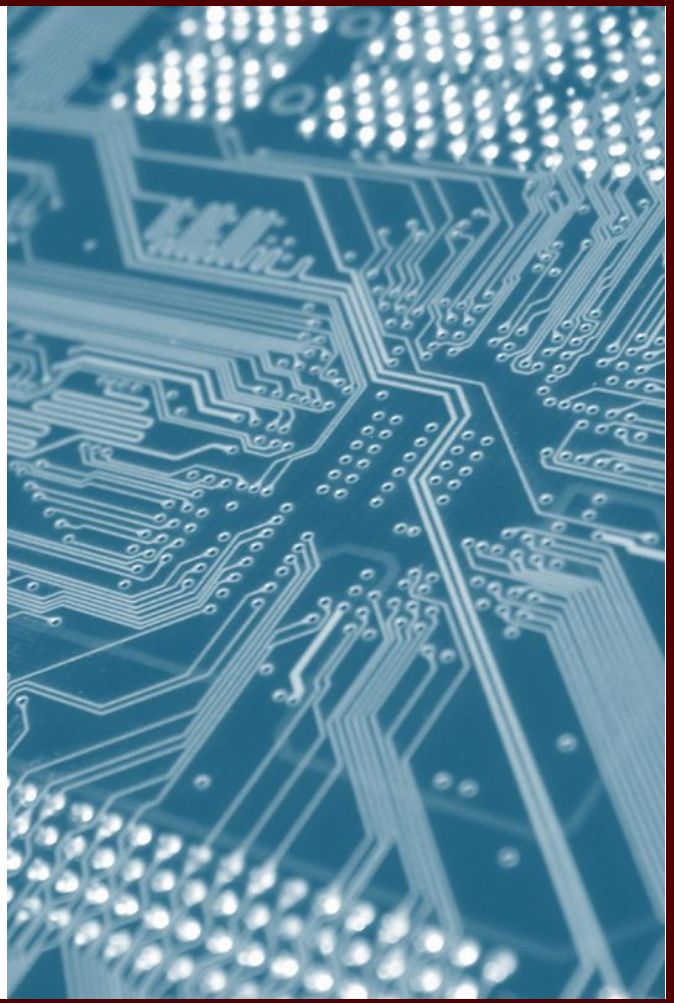


https://hprc.tamu.edu/kb/User-Guides/ACES

HPRC's Composable Clusters

- **FASTER** – First large-scale composable CPU/GPU system
- **ACES** – Composability for mixed-resource workflows

FASTER is not available through ACCESS, so we'll focus on ACES today



NSF ACES

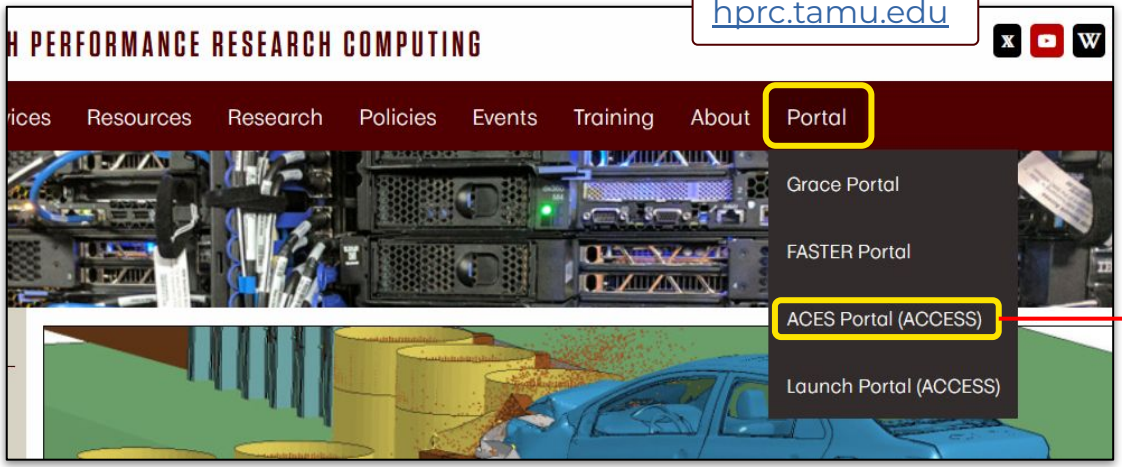
Accelerating Computing for Emerging Sciences

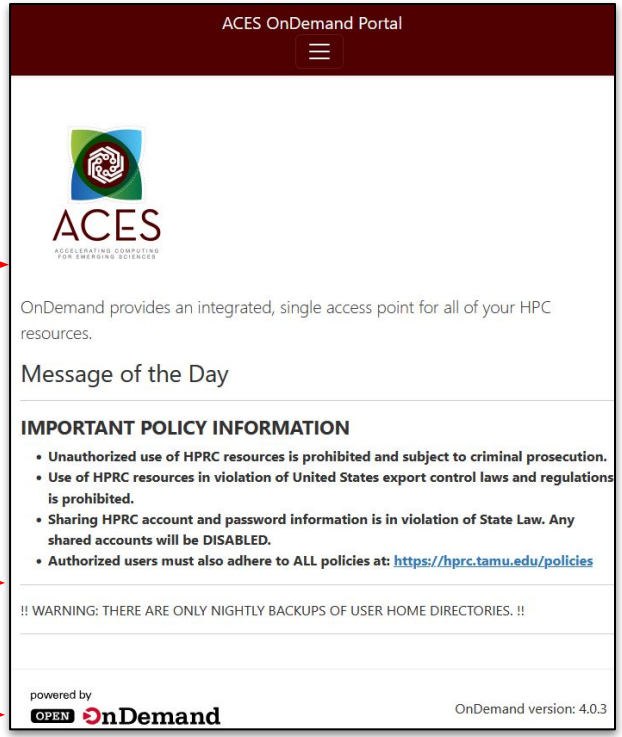
Our Mission:

- 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.

Login to ACES Portal

hprc.tamu.edu



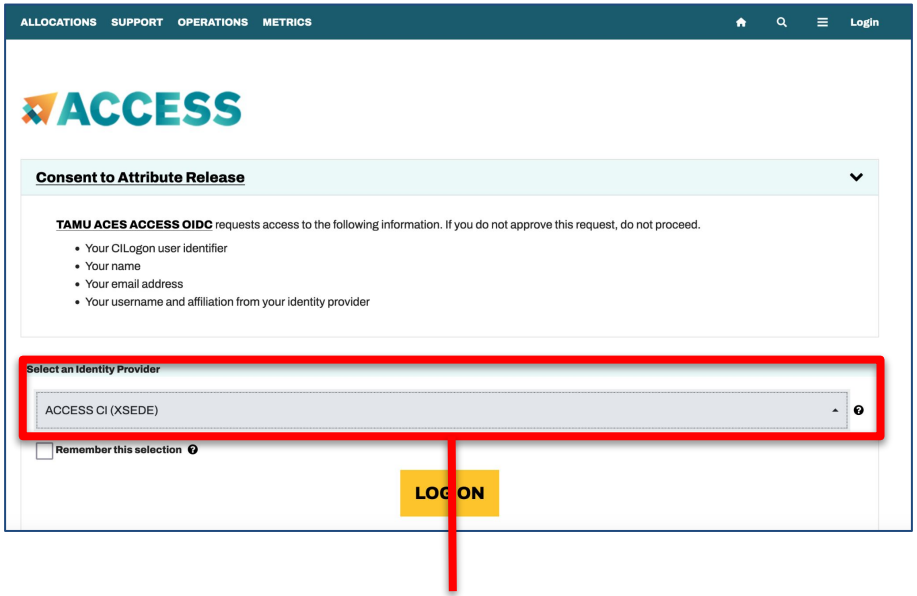


(You will have to log in with ACCESS if you haven't already)

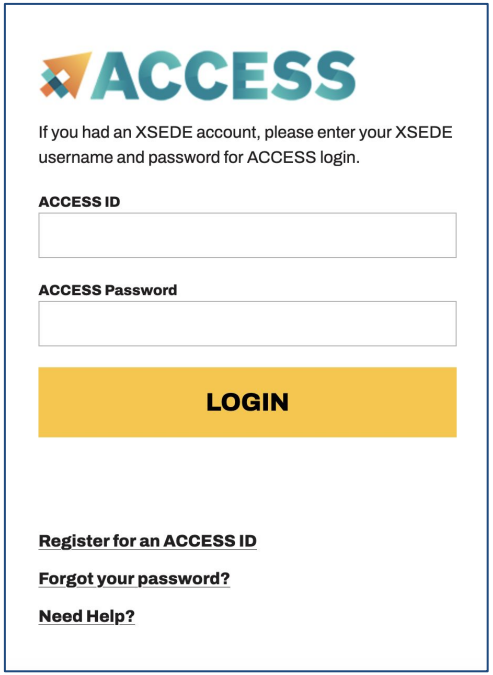
ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

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

Login to ACES Portal - ACCESS

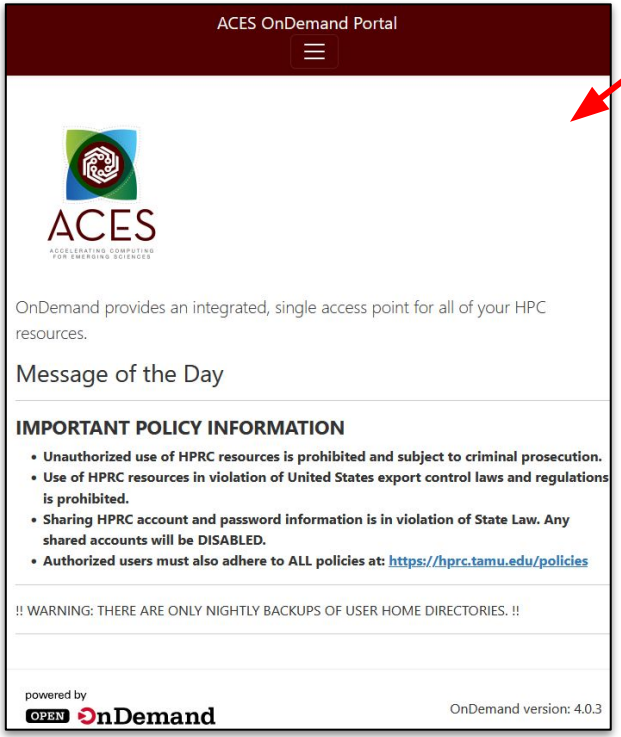


Select the Identity Provider appropriate for your account.



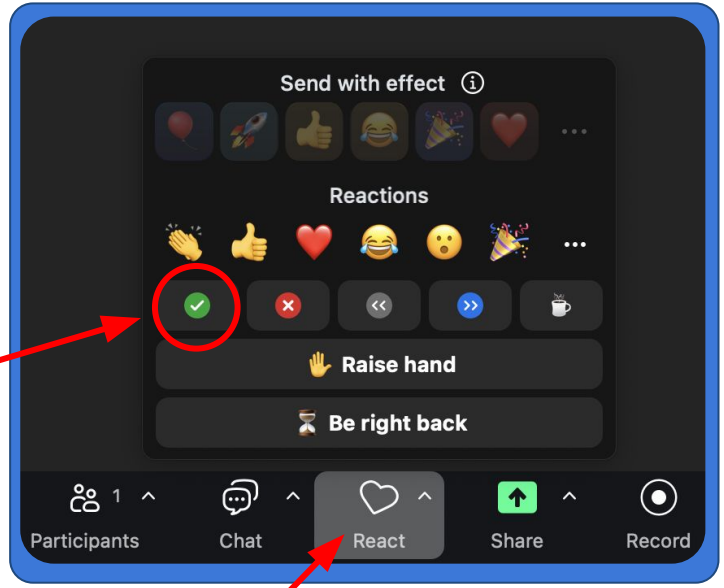
Log-in using your ACCESS or institutional credentials.

Login to ACES Portal



Once you're on this screen...

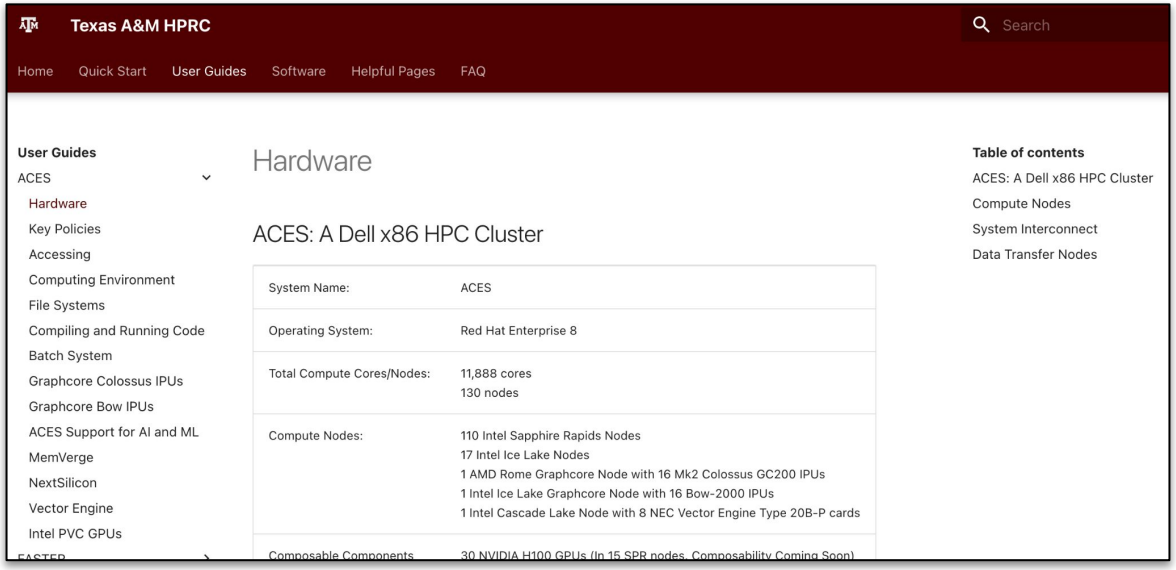
...Click the green checkmark reaction in Zoom



(find it here)

Documentation and Training

HPRC Knowledge Base



Knowledge Base for announcements, more hardware details, and more about the subjects we cover today

hprc.tamu.edu/kb
hprc.tamu.edu/kb/User-Guides/ACES

Training on YouTube

Texas A&M HPRC

@TexasAMHPRC · 1.35K subscribers · 107 videos

The Texas A&M HPRC YouTube channel assists HPR

hprc.tamu.edu and 1 more link

Subscribe

https://www.youtube.com/texasamhprc

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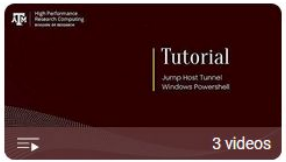
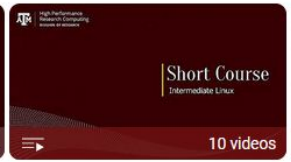
Created playlists



ACES: Getting Started

View full playlist



ACES

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

Accelerator Training

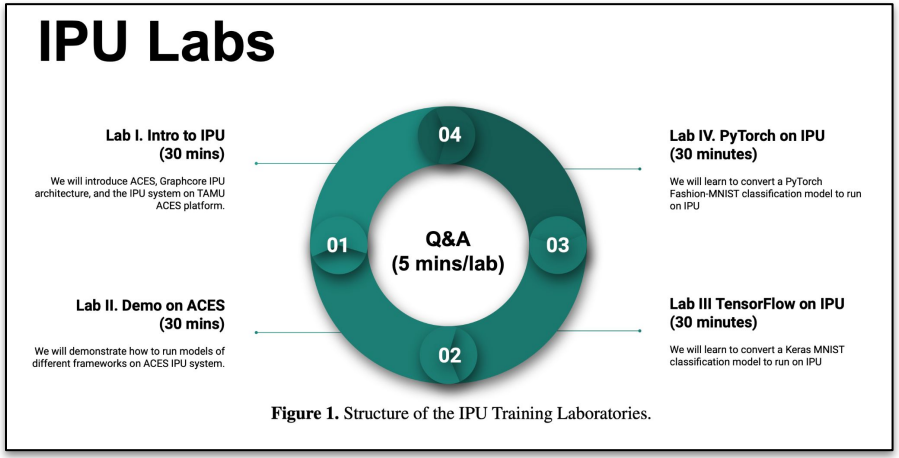
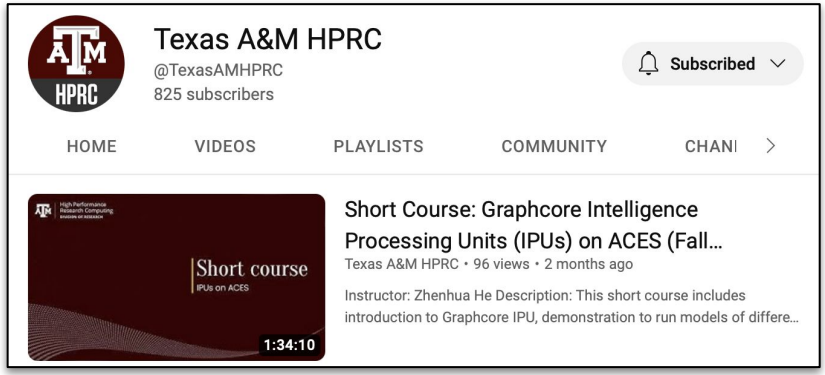


Figure 1. Structure of the IPU Training Laboratories.



This semester we will have training sessions for several accelerators:

- PVCs - https://hprc.tamu.edu/training/aces_intel_pvc.html
- IPUs - https://hprc.tamu.edu/training/aces_ipus.html
- Vector Engines - TBA

See also our “ACES Training” YouTube Playlist for previous courses:

- https://www.youtube.com/@TexasAMHPRC/playlists

Getting Started on the ACES Cluster

Usage Policies
(Be a good compute citizen)

- It is illegal to share computer passwords and accounts
- Clusters must not be used in any manner that violates the United States export control laws and regulations, EAR & ITAR
- Abide by the license restrictions when using commercial software

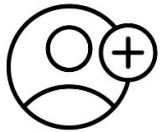
hprc.tamu.edu/policies

Allocations Management

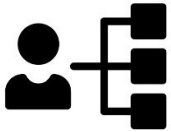
ACCESS

NAIRR Pilot

You can get allocations on ACES through both ACCESS and the NAIRR Pilot.



CREATE ACCOUNT



SELECT OPPORTUNITY

REQUEST ALLOCATION

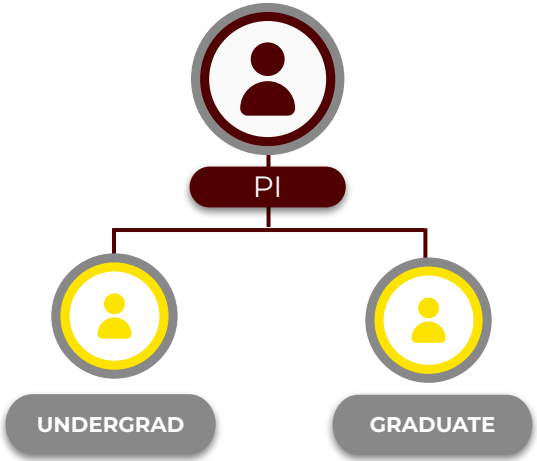
RECEIVE CREDITS

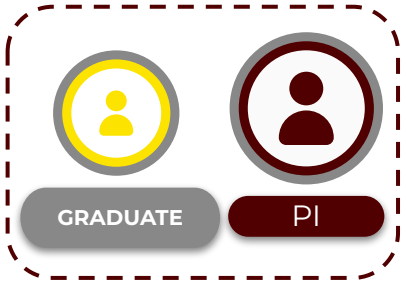
EXCHANGE CREDITS

This is all free!

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.



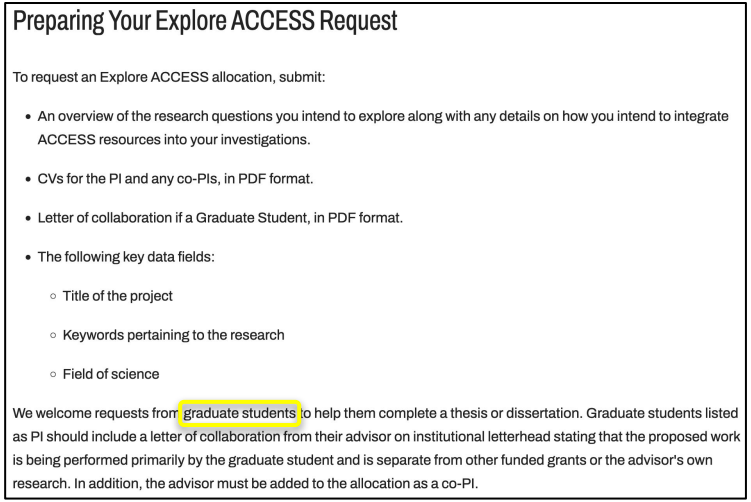


PIs can apply for an account and sponsor accounts for their researchers.

(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.

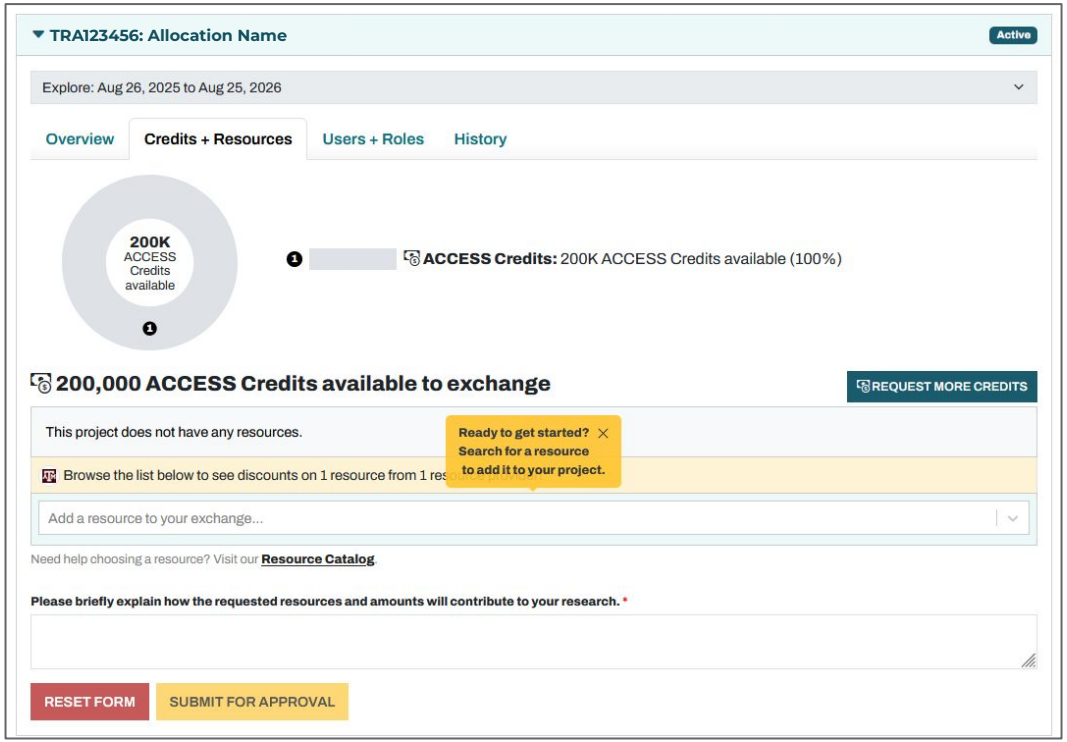
	Explore	Discover	Accelerate	Maximize
Purpose	Resource Evaluations, grad student projects, small classes, etc.	Large classes, benchmarking at-scale, Campus Champions	Multi-grant programs, Collaborations, Growing gateways	Large-scale research requiring more resources
Requests Accepted	Continuously; multiple requests allowed			Every 6 months; usually only 1 allowed
Review requirements	Overview	1-page proposal	3-page (max) proposal	10-page (max) proposal

ACCESS to ACES

Once your ACCESS allocation is approved, you request credits on ACES.

Once the resource provider (us) approves, we will set up your accounts on the cluster.

From then on, you can log into the cluster using your ACCESS credentials.

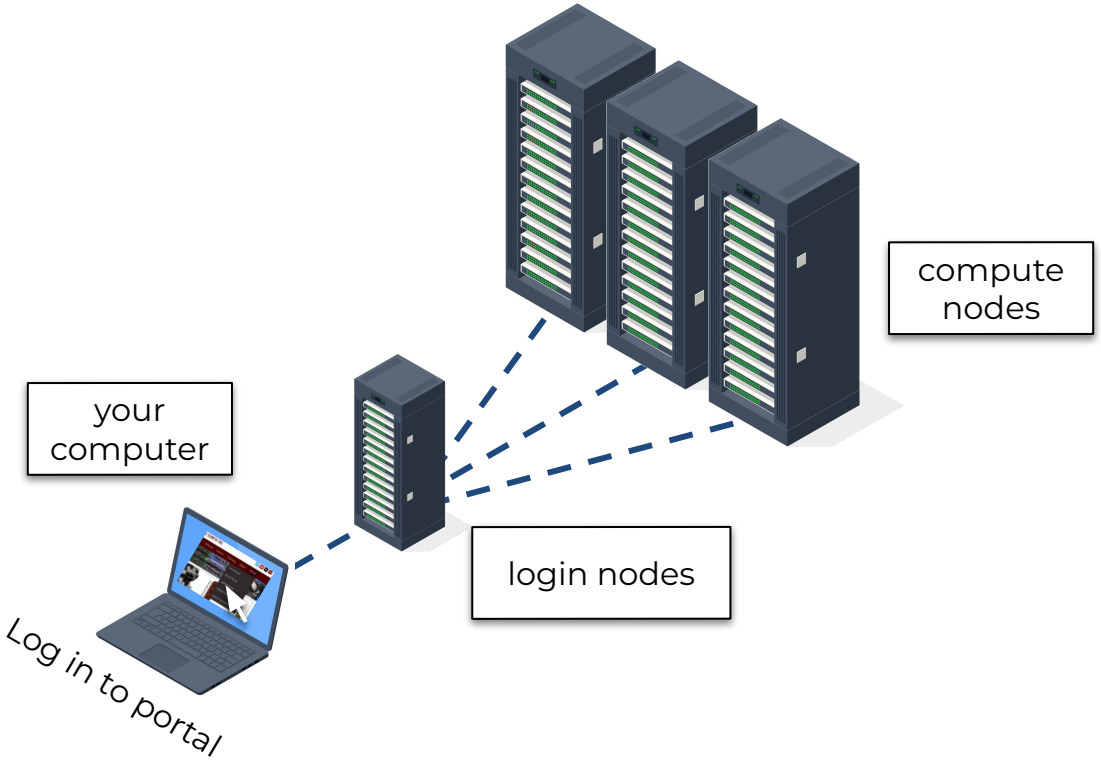


Portal and Cluster Basics

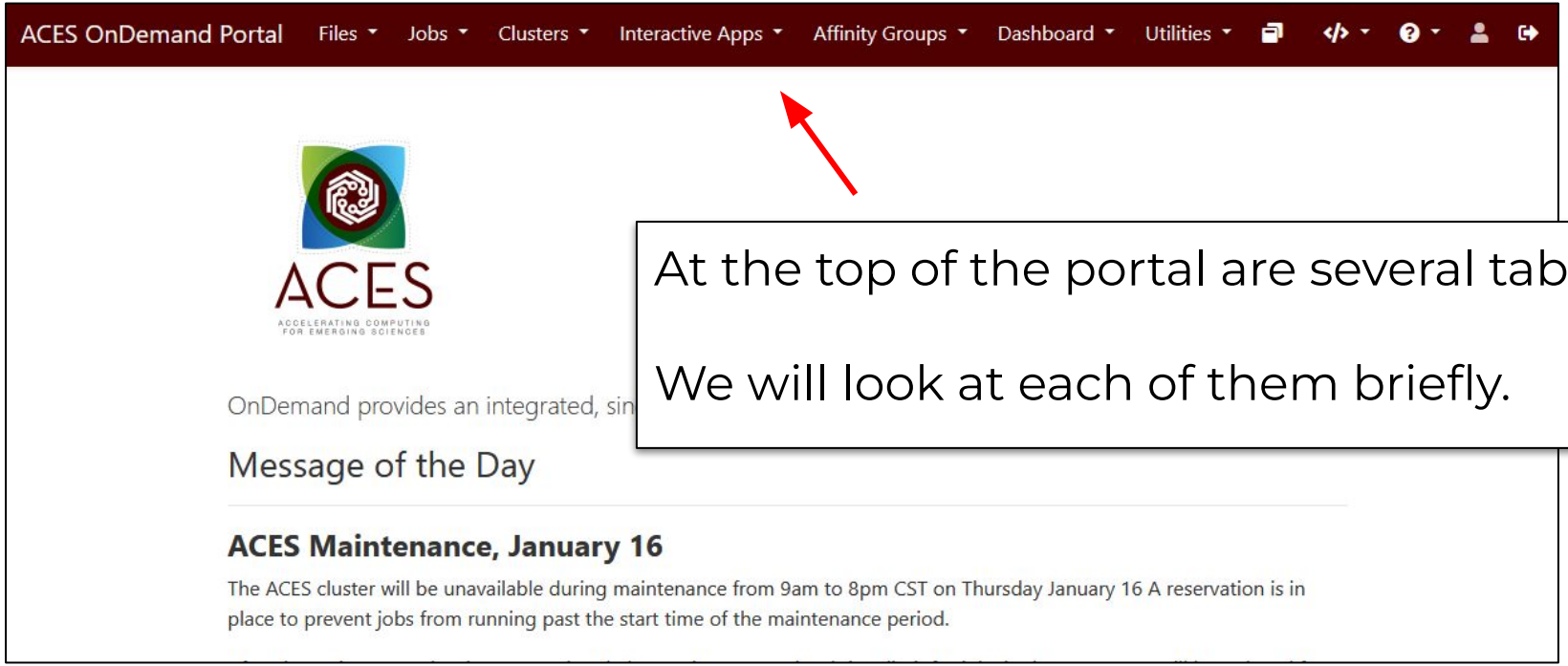
- Portal Walkthrough
- Quotas and SUs

Batch Computing on Clusters

- Interact via **your own machine**.
- Log in to the cluster's **OOD portal** (on the **login nodes**) and write instructions.
- Send instructions to **compute nodes** to do the heavy-lifting (spending credits/SUs).



HPRC Portal Overview

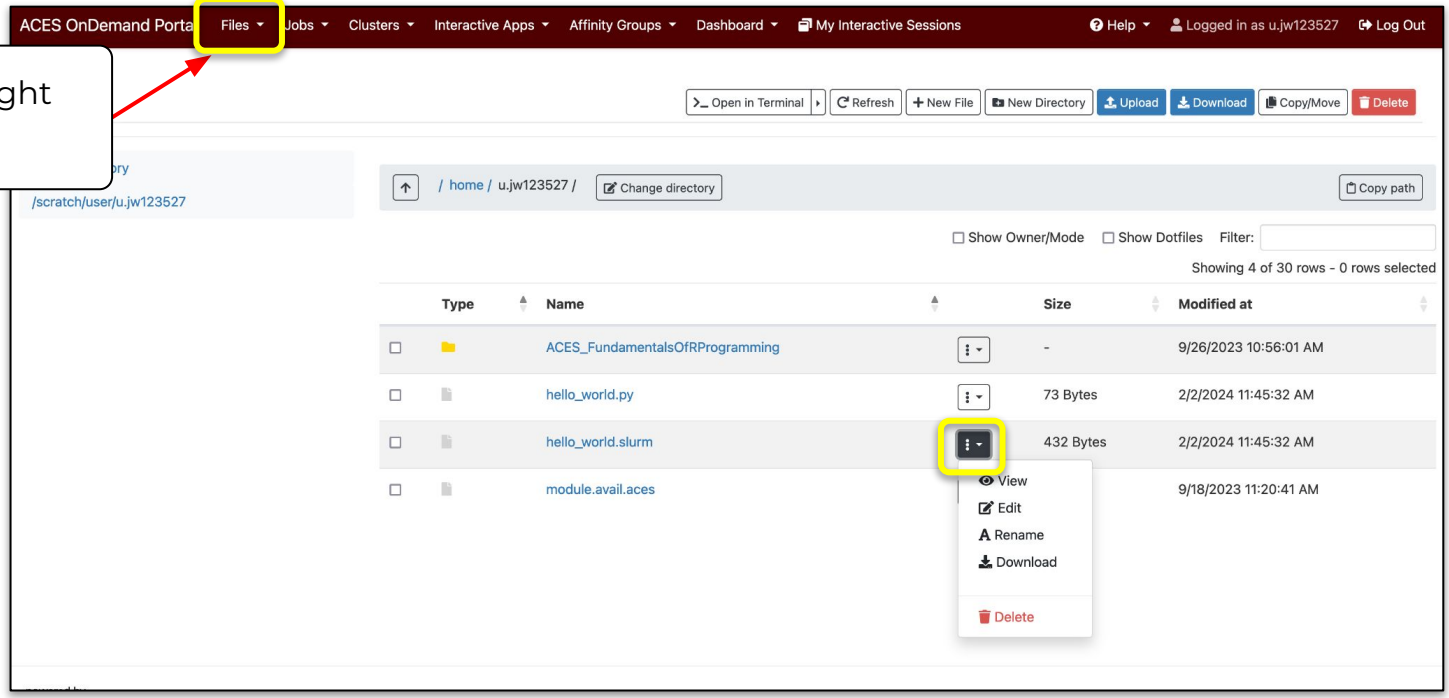


At the top of the portal are several tabs.

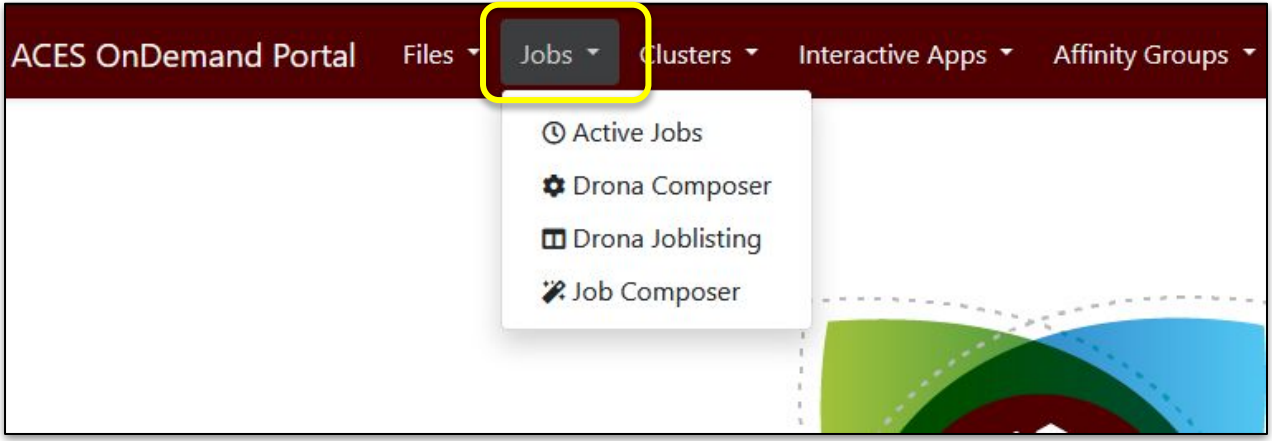
We will look at each of them briefly.

File Browsing, Viewing, and Editing

Manage your files right in your browser



Portal Job Composers



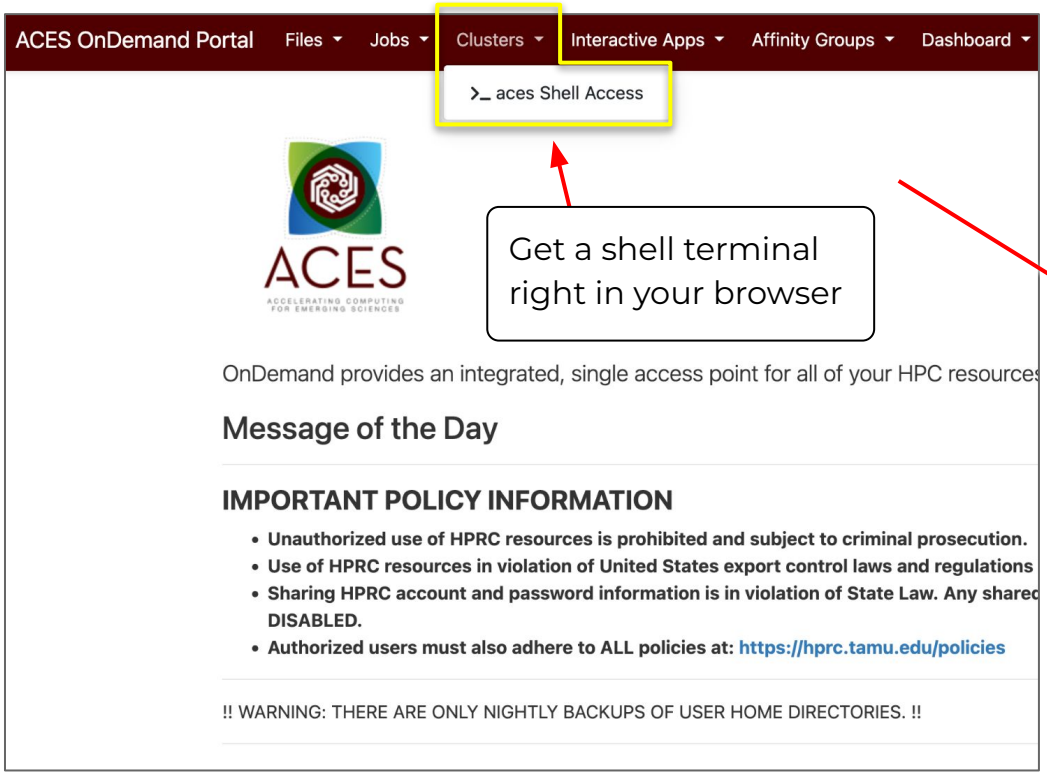
Manage jobs without using the command line (will talk more about these later)

- "Active Jobs" is like `squeue`.
- "Job Composer" lets you:
  - Create job scripts
  - Save job templates
  - Monitor your own jobs

We will focus on the new "Drona" options:

- "Drona Joblisting" shows current and past jobs.
- "Drona Composer" helps you build workflows and manage job scripts.

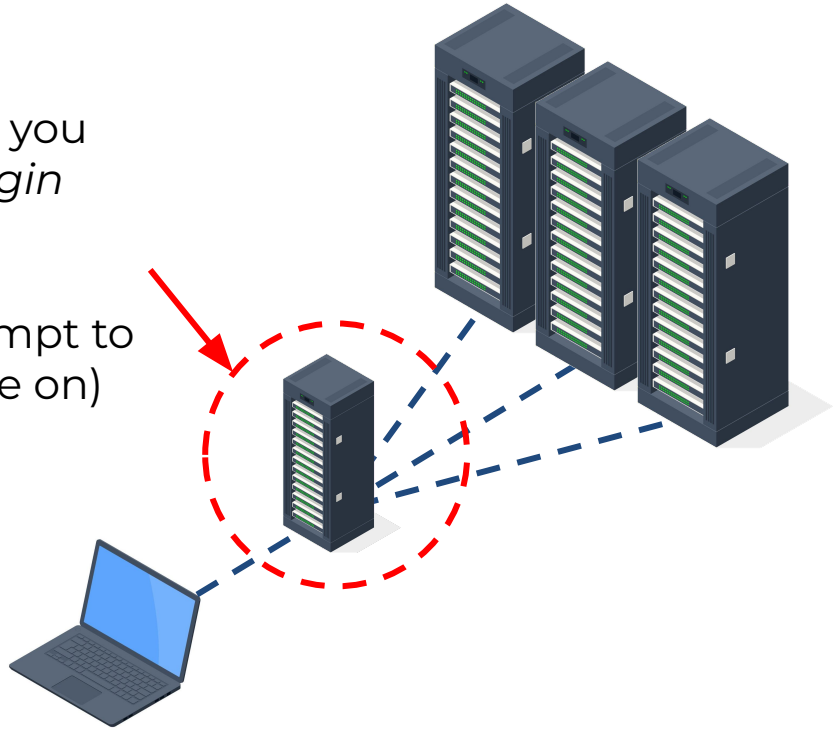
Shell Access via the Portal



Shell Access via the Portal: Logging In

When you first log in, you are on a dedicated *login node*.

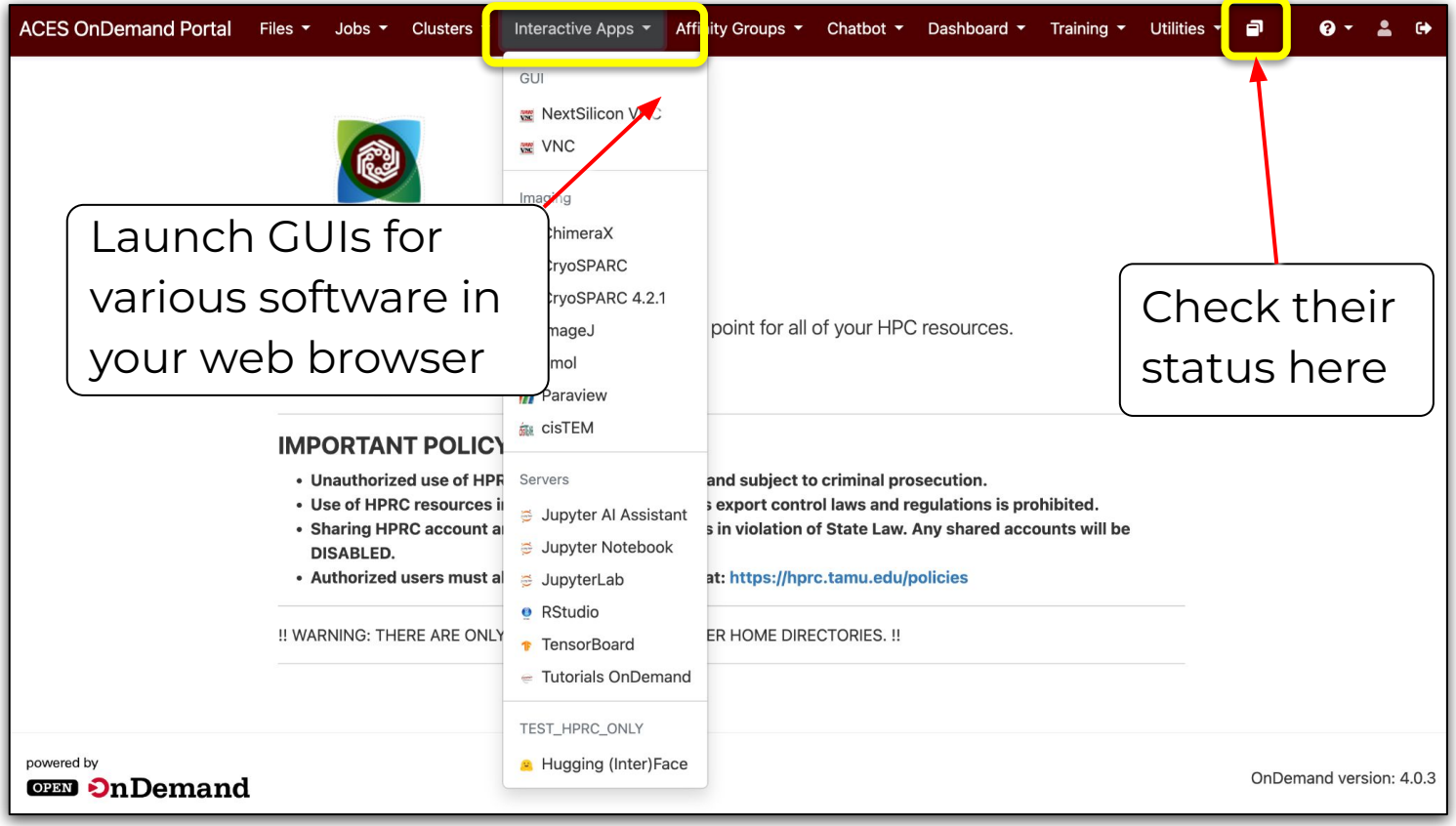
(check your shell prompt to see which one you are on)



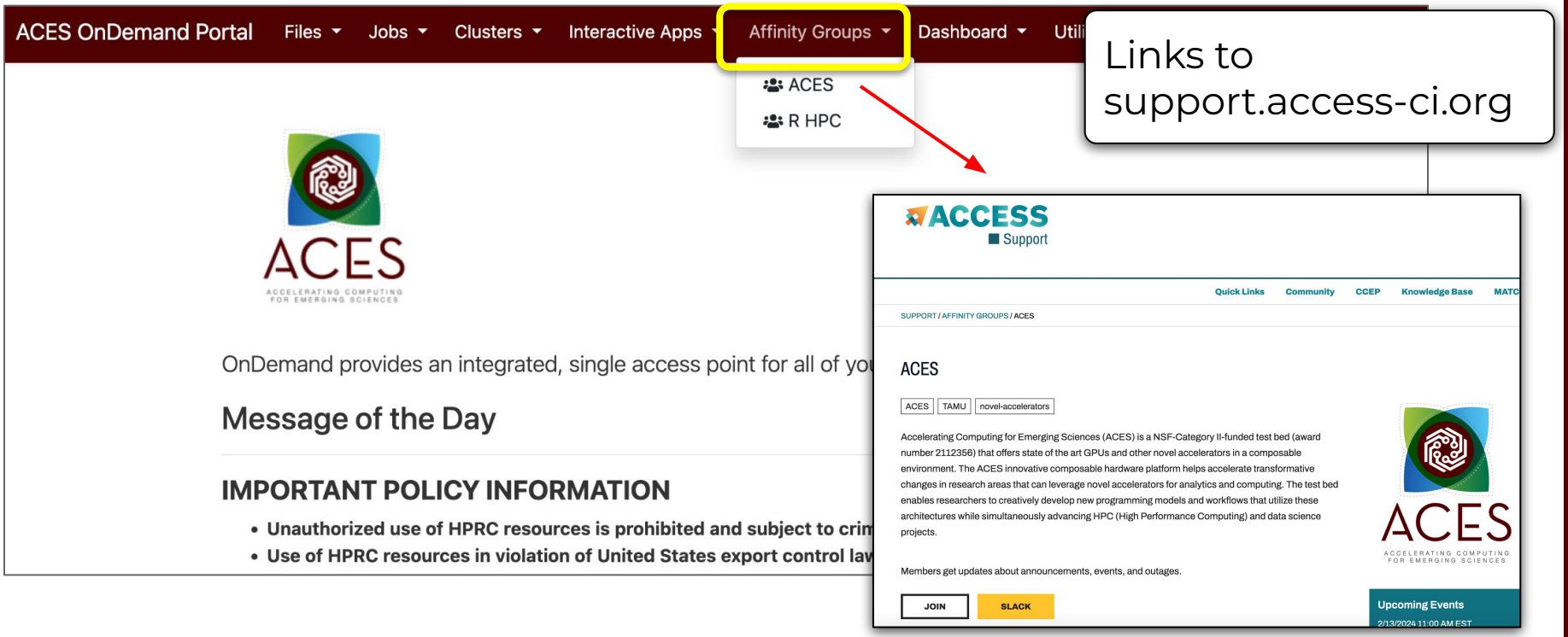
Login nodes are not for running big processes!
There are rules:

- No processes longer than 1 hr
- Sessions idle for 1 hr will be killed
- Do not use more than 8 cores.
- Do not use "`sudo`"

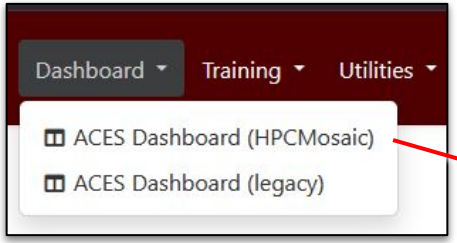
Interactive Apps



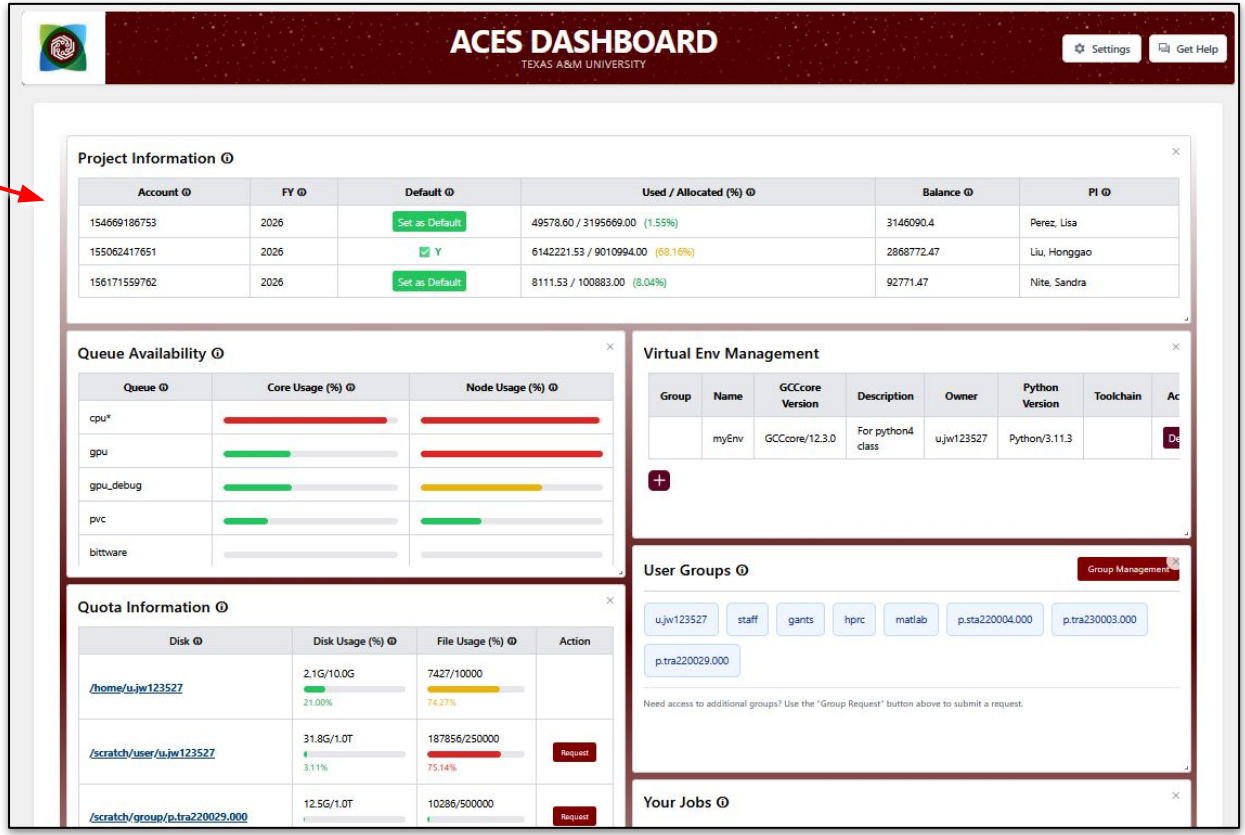
Join Affinity Groups



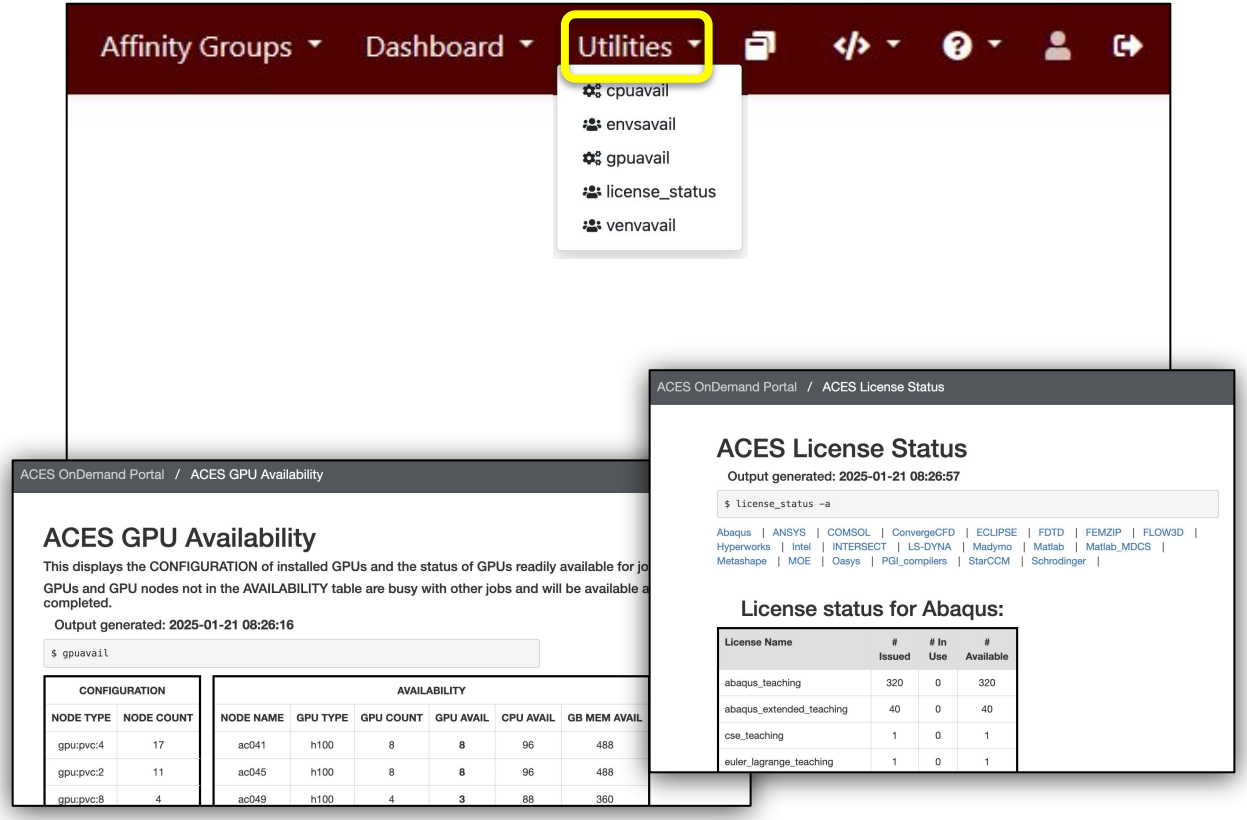
ACES Dashboard



- Request help or new software
- Request quota increases
- Manage user groups
- Check job and cluster status



Utilities



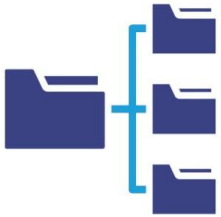
- Convenient collection of command-line tools
- Check availability of gpus, licenses, and other resources

Portal and Cluster Basics

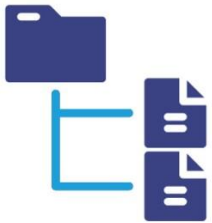
- Portal Walkthrough
- Quotas and SUs

File Systems and User Directories

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



Do not share your Home or Scratch areas!
Use Project to collaborate and share files!



Command-line Tools: Quota Usage

Check your file and storage use with the “showquota” command:

```
[username@aces ~]$ showquota

Your current disk quotas are:
Disk                    Disk Usage      Limit   File Usage   Limit
/home/username               1.4G      10.0G         3661   10000
/scratch/user/username     117.6G       1.0T        24226  250000
/scratch/group/projectid   510.5G       5.0T       128523  500000
```

Service Units

- Service Units (SUs) are part of our account management system (AMS).
  - **You spend SUs to run jobs on compute nodes**
- 1 SU ~ 1 core-hour on a CPU … more if using accelerators or extra memory
- Number of SUs you start with depends on which ACCESS allocation you got
- SUs are charged as your jobs spend time on the compute nodes.
  (we will see how later).
  (Work on login nodes is not charged, but you cannot do big computing there!)
- You can check your SU balance on both:
  - The command line
  - The HPRC Portal

https://hprc.tamu.edu/kb/User-Guides/AMS/#service-unit
https://hprc.tamu.edu/kb/User-Guides/AMS/#ams-user-interfaces
https://hprc.tamu.edu/policies/allocations.html

Command-line Tools : Allocation Usage

Check your allocation balances with the “myproject” command:

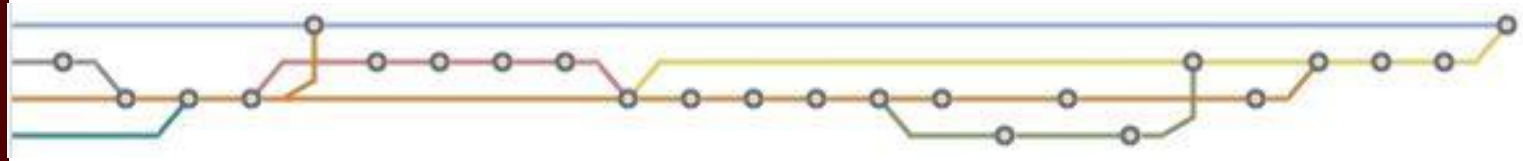
```
[username@aces ~]$ myproject
 ==========================================================================================
 List of user's Project Accounts
 ------------------------------------------------------------------------------------------
 |  Account    | Default | Allocation |Used & Pending SUs|   Balance  |          PI       |
 ------------------------------------------------------------------------------------------
 |1228000223136|       N|   150000.00|              0.00|    10000.00| Last, First       |
 ------------------------------------------------------------------------------------------
 |1428000243716|       Y|    20000.00|              0.00|    20000.00| Last, First       |
 ------------------------------------------------------------------------------------------
 |1258000247058|       N|     5000.00|              0.00|     5000.00| Last, First       |
 ------------------------------------------------------------------------------------------
```

(Run with the `-h` flag for more information.)

ACES Charging Scheme

Resource(s)	SUs (per hour)	ACCESS Credits (per hour)
Intel SPR / Icelake	1	0.1
Intel PVC GPUs	30	3.75
Bittware Agilex FPGA	30	3.75
Intel Optane Memory	30	3.75
Graphcore IPU Classic	45	5.625
NextSilicon Co-processor	50	6.25
Graphcore IPU Bow	60	7.5
NVIDIA A30	64	8
NEC Vector Engine	75	9.375
NVIDIA H100	128	16

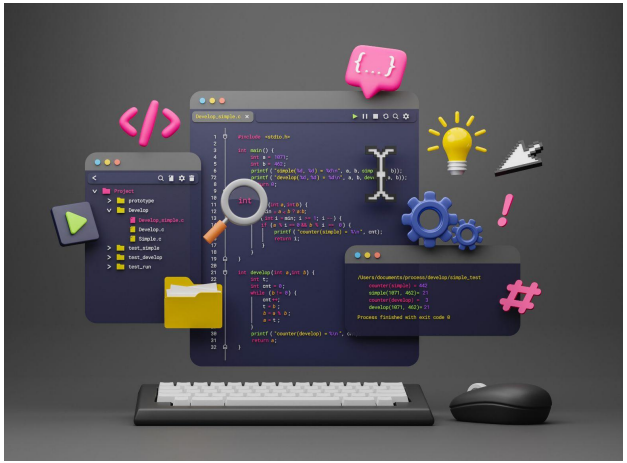
Software Infrastructure



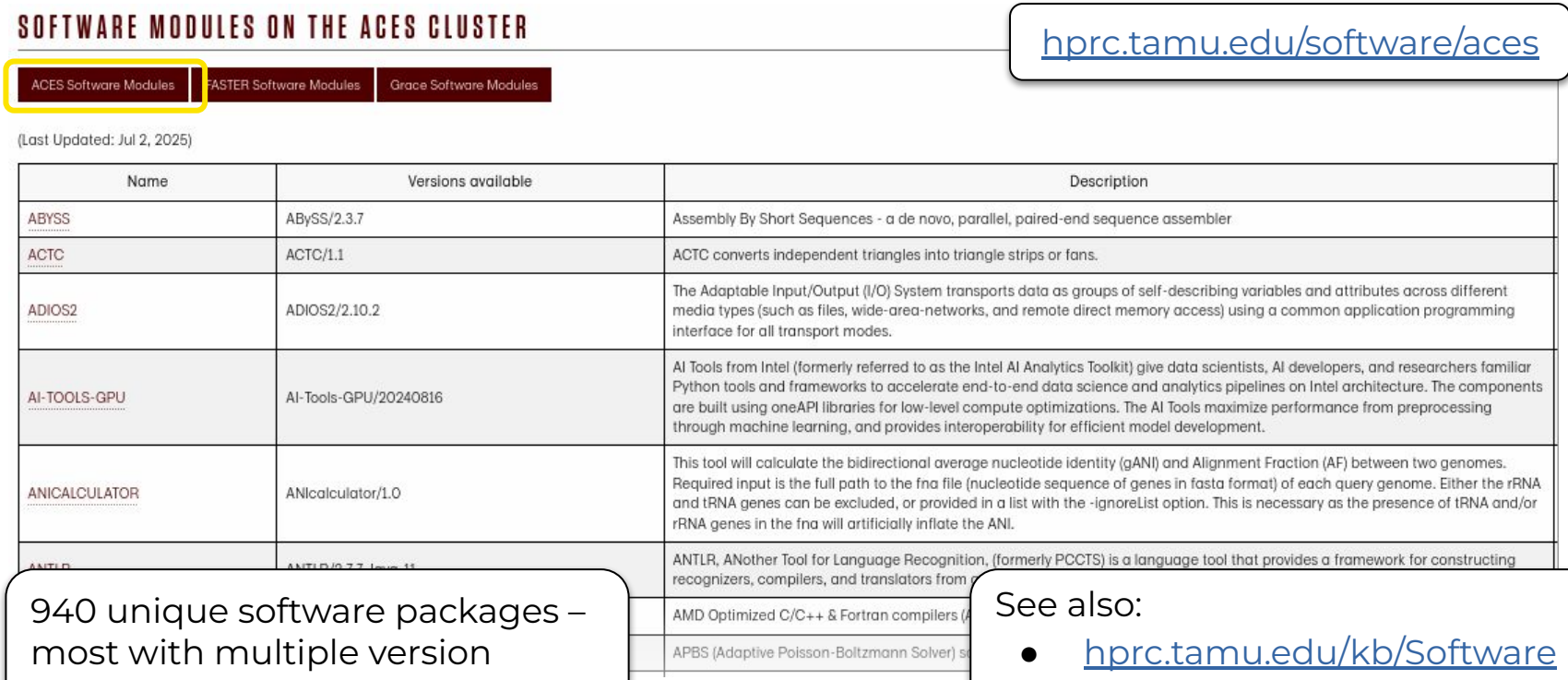
Getting Software

You need software! How to get it?

1. Check to see if we have it installed as a ‘module’ already.
2. If not, see about getting it installed:
   a. Install for yourself in your $SCRATCH.
   b. Ask us to install system-wide as a module.



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
AOCC	AOCC/4.2.0	AMD Optimized C/C++ & Fortran compilers (
APBS	APBS/3.4.1-gompi-2023a	APBS (Adaptive Poisson-Boltzmann Solver) s

hprc.tamu.edu/software/aces

940 unique software packages – most with multiple version modules (over 3,040 total)

See also:

- hprc.tamu.edu/kb/Software
- hprc.tamu.edu/software

Computing Environment

Managing software versions using Lmod and Easybuild

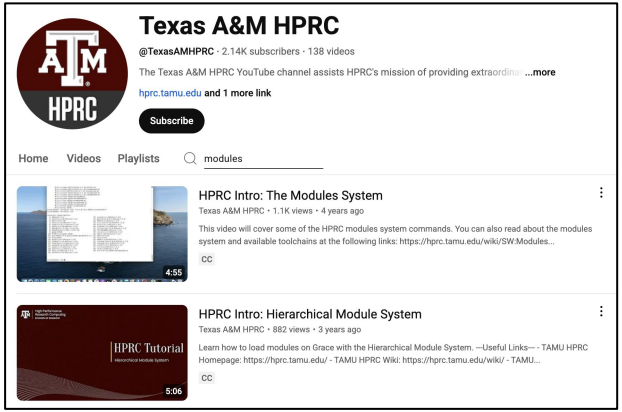
- Uses the command: **module**
- Each version of a software, application, library, etc. is available as a module.
  - Module names have the format:

toolchain-name / version toolchain-name / version

GCC/14.2.0 OpenMPI/5.0.7

software-name / version-spec

PyTorch/2.7.0-CUDA-12.6.0



- module sets the correct environment variables for you

hprc.tamu.edu/kb/Software/useful-tools/Modules/

Module Usage Basics

`module avail`

- Lists all available modules (may be slow).
- Navigation:
  -spacebar, arrows, or `j` and `k`
  -quit with `q`
- Case-sensitive search: `/`
- Use **`mla`** instead to save results to a file as well (will be named `module.avail.aces` or similar)

`module spider <word>`

- Case-sensitive search for modules with “word” in name.
- Provide an exact name to see dependencies.

```
[u.jw123527@aces-login2 ~]$ module spider Python

----------------------------------------------------------------------------------------------------------------
  Python:
----------------------------------------------------------------------------------------------------------------
    Description:
      Python is a programming language that lets you work more quickly and integrate your systems more effectively.

     Versions:
        Python/2.7.18-bare
        Python/2.7.18
        Python/3.8.6
        Python/3.9.5-bare
        Python/3.9.5
        Python/3.9.6-bare
        Python/3.9.6
        Python/3.10.4-bare
        Python/3.10.4
        Python/3.10.8-bare
        Python/3.10.8
        Python/3.11.3
        Python/3.11.5
     Other possible modules matches:
        Biopython  Boost.Python  Brotli-python  IPython  LASSO-Python  Python-bundle-PyPI  flatbuffers-python  graphvi

----------------------------------------------------------------------------------------------------------------
  To find other possible module matches execute:

      $ module -r spider '.*Python.*'
```

Module Usage Basics

`module list`

- See what modules are loaded in your current session

`module load <module>`

- add <module> paths to the current environment variables

`module purge`

- Unload all modules

```
[u.jw123527@aces-login2 ~]$ module load GCCcore/13.2.0
[u.jw123527@aces-login2 ~]$ module list

Currently Loaded Modules:
  1) GCCcore/13.2.0



[u.jw123527@aces-login2 ~]$ module purge
[u.jw123527@aces-login2 ~]$ module list
No modules loaded
[u.jw123527@aces-login2 ~]$
```

There is also a shorthand:

`ml`
`ml <module>`
`ml purge`

Hands-on Exercise: Module Loading

1. `mla blast+` -See which versions of BLAST+ are available.
2. `ml BLAST+/2.14.1` -error! You cannot do that yet.
3. `module spider BLAST+/2.14.1` -Learn how to load this module.
4. `ml _____ BLAST+/2.14.1` -Fill in the blank (with the correct toolchains) to load this module.
5. `ml list` -List all loaded modules.
6. `ml GCC/10.2.0` -Change version of a loaded Toolchain module (GCC); notice the message about reloaded modules.
7. `ml list` -List all loaded modules.
8. `ml purge` -Remove all loaded modules.

Installing Software

- Researchers can install software in their own directories.
  - Exact steps depend on the software.
  - You CANNOT run the "sudo" command when installing software.
  - Watch your file quotas! Install in $SCRATCH!

- Contact us if you need help
  - We can install software *cluster-wide*.
  - Requests can be sent from the Dashboard.

- License-restricted software
  - Check on command line with `license_status`
  - Contact help@hprc.tamu.edu

Python and Virtual Environments

Python is a language which supports many external libraries in the form of extensions. (called Python Packages).

Some commonly used packages:

- SciPy & NumPy
- Jupyter notebook
- Scikit-learn

Once you have loaded the appropriate Python module, you can install these additional packages yourself using the *Virtual Environment* feature. Instructions are on our KB:

- https://hprc.tamu.edu/kb/Software/Python/#hprc-venv-management-tools
- https://hprc.tamu.edu/kb/Software/ModuLair/ (special HPRC tool!)

Hands-on Exercise: Python Software Install

1.
```
ml purge
create_venv myEnv -d "Example Env" -t “GCCcore/14.3.0 Python/3.13.5”
```

Start from a clean environment and use ‘create_venv’
The **-d** arg is optional Use the **-t** arg if you haven’t loaded modules already

2.
```
source activate_venv myEnv
```
-Activate virtual environment.

3.
```
python -c "import pytime"
```
-Check if python-time is installed (it is not).

4.
```
pip install python-time
```
-Install python-time.

5.
```
python -c "import pytime; print(pytime)"
```
-Where is python-time installed?

6.
```
deactivate
```
-Close virtual environment.

Batch Computing

- Command Line
- Job Management Tools

Batch Computing on HPRC Clusters: Overview

Since the cluster is a shared resource, jobs have to be moderated somehow so everyone has a turn. In short:

1. Write instructions on the login node
2. Give the instructions to Slurm
3. Slurm sends everybody's instructions to compute nodes (in an orderly fashion!)

Sample Job Script Structure

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=hello_world
#SBATCH --time=00:15:00
#SBATCH --ntasks=2
#SBATCH --ntasks-per-node=2
#SBATCH --nodes=1
#SBATCH --mem=3G
#SBATCH --output=hello_world_log.%j

# load required module(s)
module purge
module load GCCcore/13.3.0
module load Python/3.12.3
python hello_world.py

# Job Environment variables
echo $SLURM_JOBID
echo $SLURM_SUBMIT_DIR
echo $TMPDIR
echo $SCRATCH
```

- This is a single-line comment and not run as part of the script.
- These parameters describe your job to the job scheduler.
- The lines starting with #SBATCH are comments to the shell, but NOT to Slurm!
- See the Knowledge Base for more info.
- Whatever commands or scripts you want to run. Here, we set up the modules we need for our environment, run a python program, and print out some environment variables.

Submit a Job and Check Job Status

Submit job

```
sbatch example01.job
```

```
Submitted batch job 6853258
(from job_submit) your job is charged as below
              Project Account: 122792016265
              Account Balance: 1687.066160
              Requested SUs:   3
```

Check status

```
squeue -u $USER
```

or

```
squeue --me
```

```
JOBID    NAME      USER       PARTITION  NODES  CPUS  STATE    TIME         TIME_LEFT  START_TIME          REASON     NODELIST
6853258  jobname   someuser   cpu        2      96    RUNNING  3-07:36:50   16:23:10   2025-01-23T17:27:3  None       ac[180,202]
6853257  jobname   someuser   cpu        2      96    RUNNING  3-07:36:56   16:23:04   2025-01-23T17:27:2  None       ac[523-524]
```

Hands-on Exercise: Job Submission

1. `cp -r /scratch/training/slurm_example/ $SCRATCH` -Copy example files to $SCRATCH
2. `cd $SCRATCH/slurm_example` -Go to the example files
3. `vi hello_world.job` -View/edit job file (optional)
4. `sbatch hello_world.job` -Submit job
5. `squeue --me` -Check job
6. `cat <output file name>` -Check output when done

Checking Resources for Jobs

`sinfo` `pestat` `maxconfig`

There are several command-line tools available to check what you can use in your jobs...

Checking Resources for Jobs: Queues

sinfo pestat maxconfig

```
PARTITION       AVAIL  TIMELIMIT    JOB_SIZE    NODES(A/I/O/T)     CPUS(A/I/O/T)
cpu*            up     3-00:00:00   1-64        69/1/3/73          5960/760/288/7008
gpu             up     2-00:00:00   1-8         6/0/1/7            211/365/96/672
gpu_debug       up     2:00:00      1           1/1/1/3            16/176/96/288
pvc             up     2-00:00:00   1-30        15/13/2/30         892/1796/192/2880
bittware        up     2-00:00:00   1           0/2/0/2            0/192/0/192
nextsilicon     up     2-00:00:00   1           1/1/0/2            51/141/0/192
nec             up     2-00:00:00   1           0/1/0/1            0/48/0/48
staff           up     2-00:00:00   1-110       86/18/6/110        6696/3288/576/10560
```

Shows job queue status

For the NODES and CPUS columns:
- A = Active (in use by running jobs)
- I = Idle (available for jobs)
- O = Offline (unavailable for jobs)
- T = Total

Checking Resources for Jobs: Nodes

sinfo | **pestat** | maxconfig

```
[u.jw123527@aces-login2 ~]$ pestat -p gpu -G
Print only nodes in partition gpu
GPU GRES (Generic Resource) is printed after each JobID
Hostname       Partition     Node Num_CPU  CPUload  Memsize  Freemem  GRES/node       Joblist
                            State Use/Tot  (15min)     (MB)     (MB)                  JobID User GRES/job ...
ac041              gpu      mix   64  96   29.40*   500000   193421  gpu:h100:8(S:0) 220099 u.xw127610 gpu:h100=8 220026 u.xw127610 gpu:h100=8 *
ac045              gpu      mix   64  96   14.21*   500000   256566  gpu:h100:8(S:0) 220099 u.xw127610 gpu:h100=8 239377 u.ch204012 gpu:h100=2 239432 u.ch204012 gpu:h100=2 *
ac049              gpu      mix   32  96   14.81*   500000   260781  gpu:h100:4(S:0) 220001 u.xw127610 gpu:h100=8 *
ac055              gpu      mix   32  96   14.78*   500000   260220  gpu:h100:4(S:0) 220001 u.xw127610 gpu:h100=8 *
ac064              gpu    down*    0  96    0.00    500000   511159  gpu:a30:2(S:0)
ac065              gpu    down*    0  96    0.00    500000   511187  gpu:a30:2(S:0)
ac096              gpu      mix   32  96   14.58*   500000   256768  gpu:h100:4(S:0) 220026 u.xw127610 gpu:h100=8 *
[u.jw123527@aces-login2 ~]$
```

Shows status of nodes

Notable options:

- -p <partition name> show only a specific partition
- -u $USER show only specified user's jobs
- -G show "generic resources" (e.g., the gpus used)

Checking Resources for Jobs: SUs

sinfo pestat **maxconfig**

If you ask for too many resources, your job will not run. You can check beforehand:

```
[u.ab12345@aces-login2 ~]$ maxconfig

  ACES partitions:   cpu  gpu  gpu_debug  pvc  bittware  memverge  nextsilicon
  ACES GPUs in gpu partition:  a30:2  h100:2  h100:4  h100:8  pvc:2  pvc:4  pvc:6  pvc:8

  Showing max parameters (cores, mem, time) for partition cpu

#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --time=7-00:00:00
#SBATCH --nodes=1       # max 64 nodes for partition c
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=96
#SBATCH --mem=488G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
```

Check specific partitions with:

maxconfig -p <partitionName>

Estimate the SUs a job will require with:

maxconfig -f <jobScriptName>

Job Summary: myjob

Command-line tool to show you details of a specific job:

```
myjob
```

Shows, e.g.:

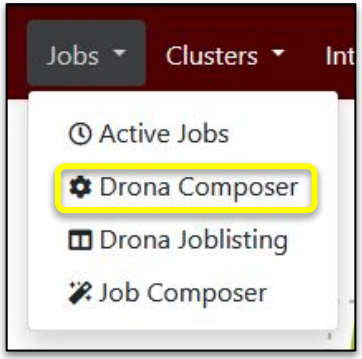
- Submission details
- Resource usage of finished jobs
- Status of pending job

```
>$ myjob 1234701

Job ID: 1234701
               Cluster: aces
          User/Group: u.ab123456/u.ab123456
             Account: 123455963789
               State: COMPLETED (exit code 0)
           Partition: gpu
          Node Count: 1
            NodeList: ac098
      Cores per node: 48
        CPU Utilized: 11:25:16
      CPU Efficiency: 2.68% of 17-18:31:12 core-walltime
         Submit time: 2025-07-20 21:37:13
          Start time: 2025-07-21 02:42:10
            End time: 2025-07-21 11:35:19
 Job Wall-clock time: 08:53:09
     Memory Utilized: 6.41 GB
   Memory Efficiency: 2.63% of 244.00 GB (244.00 GB/node)
            Job Name: GPU_Analysis
Job Submit Directory: /scratch/user/u.ab123456/job_scripts
         Submit Line: sbatch
ratpose_video_analysis_job.slurm
```

Batch Computing

- Command Line
- Job Management Tools

Portal: Drona Composer GUI

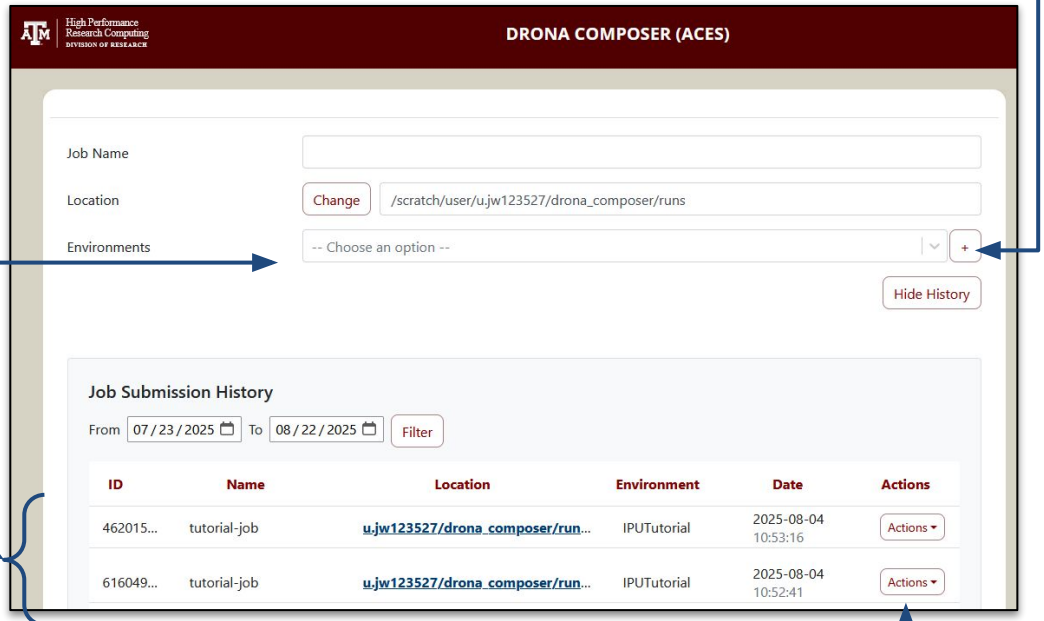


Import additional environments

Select customizable environments or workflows

History of previously submitted jobs

Rerun jobs



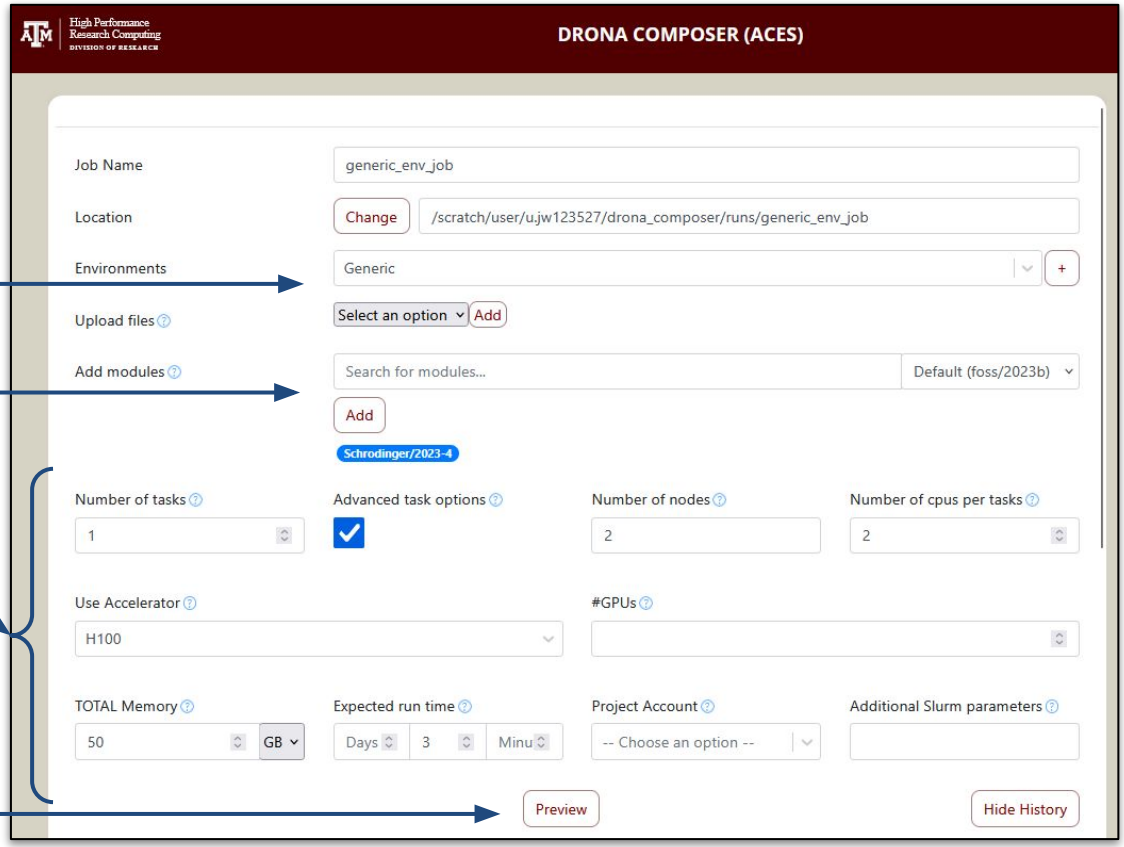
Portal: Drona Composer GUI

Generic environment to create custom Slurm batch job

Add modules for job

Fill out info that Slurm would need

Hit ‘Preview’



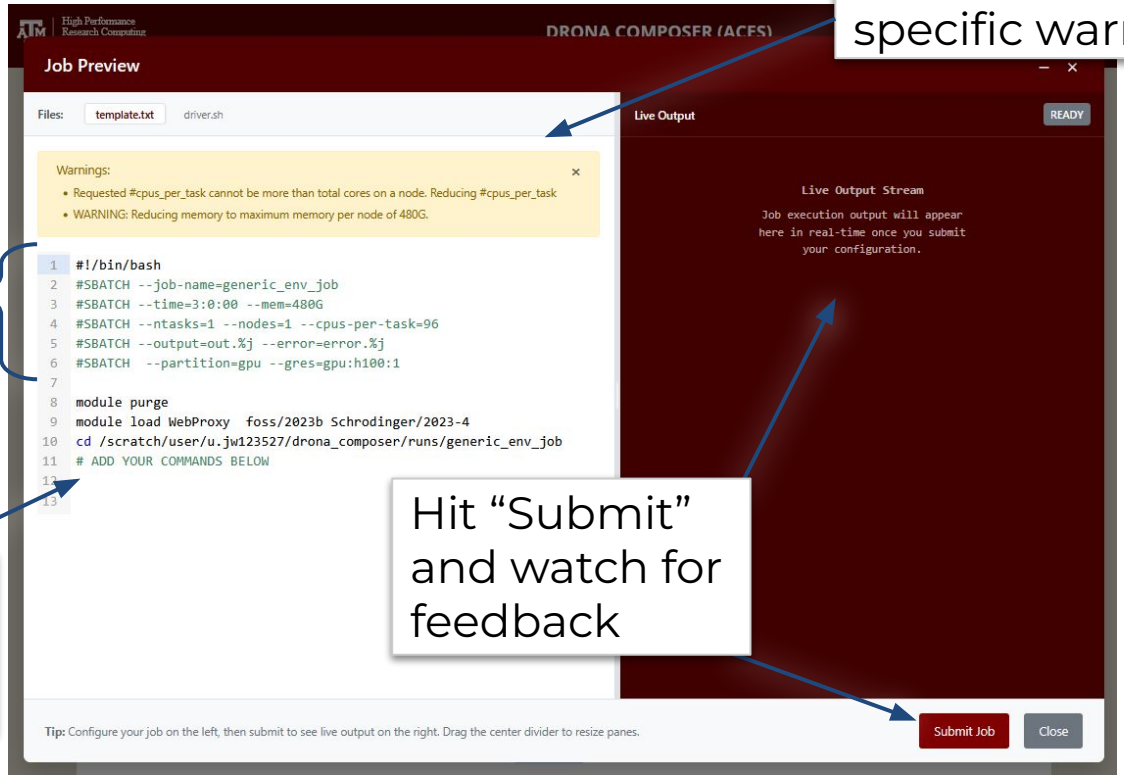
Portal: Drona Composer GUI

Generated Slurm directives and module loads

Add commands directly into editable window

Pane with input-specific warnings

Hit “Submit” and watch for feedback



TAMULauncher

- A more robust and cluster-efficient way to submit “array” jobs

```
tamulauncher commands_file.txt
```

- Use when you have hundreds or thousands of commands to run, each utilizing a single-core or a few cores.
  - tamulauncher keeps track of which commands completed successfully and can pick up where it left off
  - Can be run in a batch script or interactively (for <8 login node cores)
  - You can check the --status on the command line from the working directory.
- More information: https://hprc.tamu.edu/kb/Software/tamulauncher
(See also our Slurm course this afternoon!)

TAMULauncher Multi-Node Single-Core Commands

commands.txt (500 lines for example)

```
spades.py -1 s1_R1.fastq.gz -2 s1_R2.fastq.gz -o s1_out --threads 1
spades.py -1 s2_R1.fastq.gz -2 s2_R2.fastq.gz -o s2_out --threads 1
spades.py -1 s3_R1.fastq.gz -2 s3_R2.fastq.gz -o s3_out --threads 1
spades.py -1 s4_R1.fastq.gz -2 s4_R2.fastq.gz -o s4_out --threads 1
spades.py -1 s5_R1.fastq.gz -2 s5_R2.fastq.gz -o s5_out --threads 1
spades.py -1 s6_R1.fastq.gz -2 s6_R2.fastq.gz -o s6_out --threads 1
spades.py -1 s7_R1.fastq.gz -2 s7_R2.fastq.gz -o s7_out --threads 1
spades.py -1 s8_R1.fastq.gz -2 s8_R2.fastq.gz -o s8_out --threads 1
spades.py -1 s9_R1.fastq.gz -2 s9_R2.fastq.gz -o s9_out --threads 1
spades.py -1 s10_R1.fastq.gz -2 s10_R2.fastq.gz -o s10_out --threads 1
spades.py -1 s11_R1.fastq.gz -2 s11_R2.fastq.gz -o s11_out --threads 1
spades.py -1 s12_R1.fastq.gz -2 s12_R2.fastq.gz -o s12_out --threads 1
spades.py -1 s13_R1.fastq.gz -2 s13_R2.fastq.gz -o s13_out --threads 1
spades.py -1 s14_R1.fastq.gz -2 s14_R2.fastq.gz -o s14_out --threads 1
spades.py -1 s15_R1.fastq.gz -2 s15_R2.fastq.gz -o s15_out --threads 1
spades.py -1 s16_R1.fastq.gz -2 s16_R2.fastq.gz -o s16_out --threads 1
spades.py -1 s17_R1.fastq.gz -2 s17_R2.fastq.gz -o s17_out --threads 1
spades.py -1 s18_R1.fastq.gz -2 s18_R2.fastq.gz -o s18_out --threads 1
spades.py -1 s19_R1.fastq.gz -2 s19_R2.fastq.gz -o s19_out --threads 1
spades.py -1 s20_R1.fastq.gz -2 s20_R2.fastq.gz -o s20_out --threads 1
spades.py -1 s21_R1.fastq.gz -2 s21_R2.fastq.gz -o s21_out --threads 1
spades.py -1 s22_R1.fastq.gz -2 s22_R2.fastq.gz -o s22_out --threads 1
```

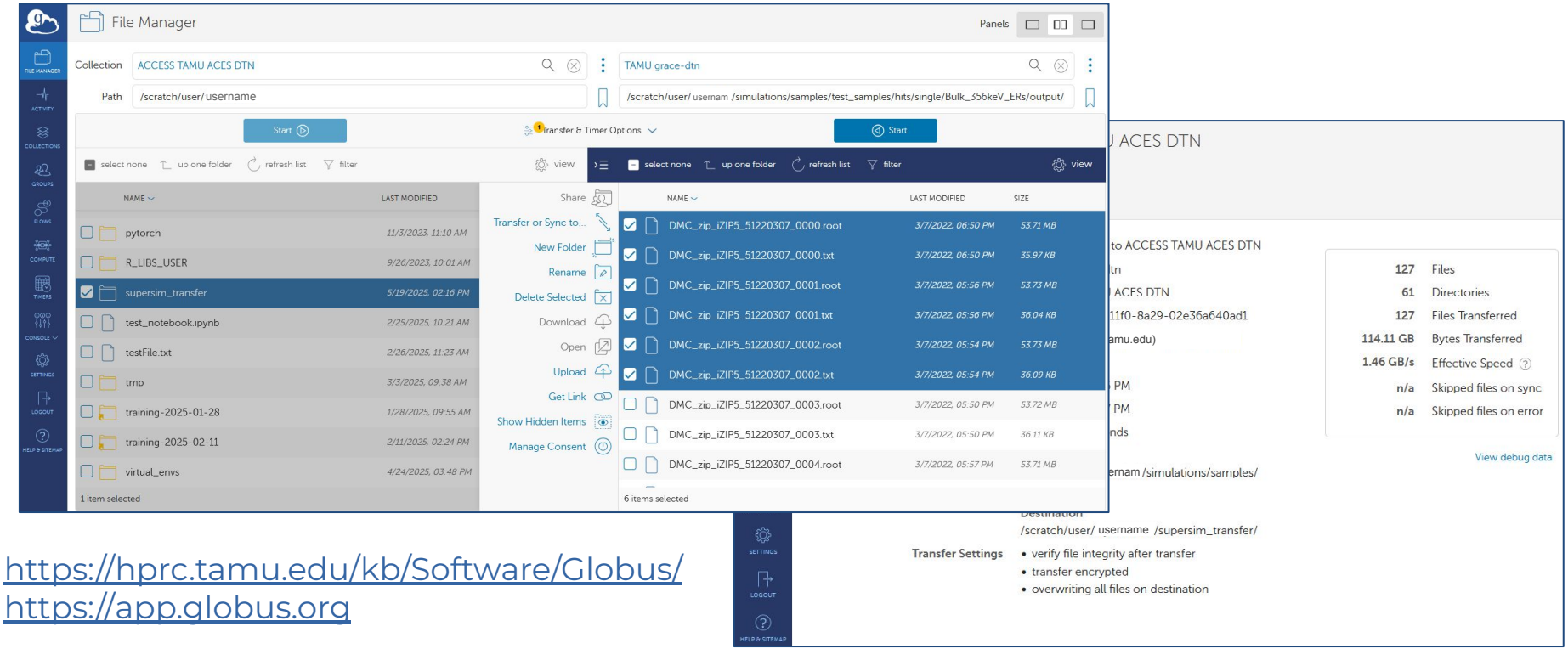
run_spades_tamulauncher.sh

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=96
#SBATCH --cpus-per-task=1
#SBATCH --mem=488G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.3.0  SPAdes/3.15.5

tamulauncher commands.txt
```

Run 96 spades.py commands per node with each command using 1 core.
Requesting all 96 cores on ACES reserves entire node for your job.

- Run 96 single-core commands per node; useful when each command requires <= 5GB memory.
- Create a commands file (named whatever you want) to go with the the job script.
- The commands.txt file will contain one command per line.
- Load the software module in the job script not the commands file.

Data Transfers Using Globus



https://hprc.tamu.edu/kb/Software/Globus/
https://app.globus.org

Composability, Accelerators, and AI/ML

Status of Composability

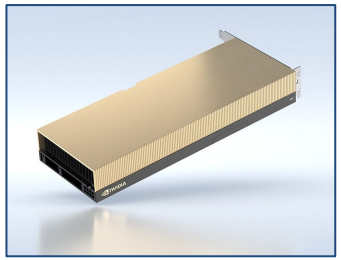
Composability is currently handled by sysadmins.

- Contact help@hprc.tamu.edu to request a given composable configuration for a cluster.
- After the composed node has been created, simply specify the relevant resources in your Slurm job file.
- In-progress: making Slurm and Liqid handle it automatically
- *Note*: The IPUs and NEC Vector Engines cannot be composed.

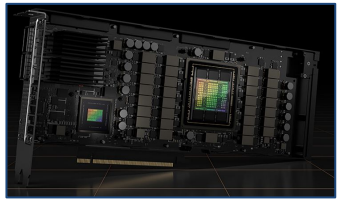
Accelerator Access

Component	Access	node or partition
NVIDIA A30 GPUs and H100 GPUs	Slurm	--partition=gpu --partition=gpu_debug
Intel GPU Max 1100 (PVC)	Slurm	--partition=pvc
BittWare IA-840F FPGA	Slurm	--partition=bittware
Intel Optane SSD	Slurm	--partition=memverge
NextSilicon Coprocessor	Slurm	--partition=nextsilicon
NEC Vector Engine	Slurm	--partition=nec
Graphcore Bow IPUs	Interactive	ssh poplar2
Graphcore Colossus IPUs	Interactive	ssh poplar1
Kubernetes & Development Cluster	Interactive	upon request (pilot)

NVIDIA GPUS on ACES



A30s: Support less intense workloads relying on numerical simulations and AI/ML methods.

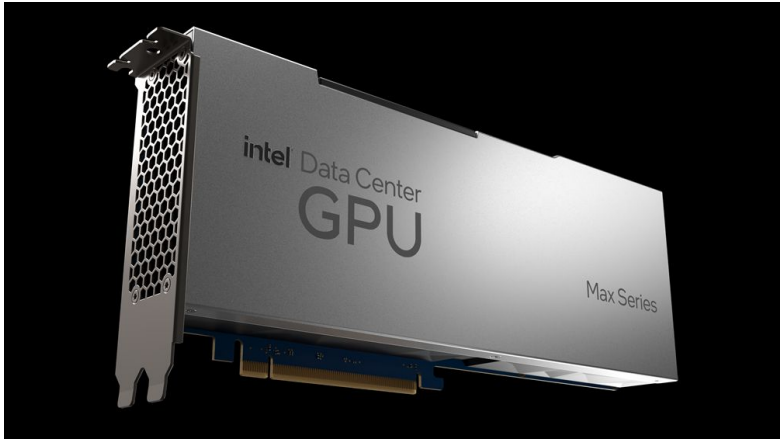


H100s: Supports computationally intensive workloads employing numerical simulations and AI/ML methods.

Specify in Slurm file:

```
#SBATCH --partition=gpu
#SBATCH --gres=gpu:<gpu type>:<number>
```

Intel Data Center Max GPU 1100 GPUs (PVC GPUs)



We are planning to have a PVC training event in March!

See also our YouTube channel for previous PVC training sessions!

Intel GPUs for HPC, DL Training, AI Inference

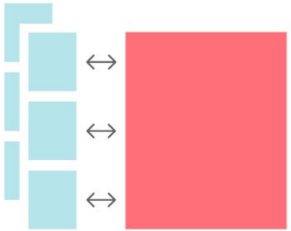
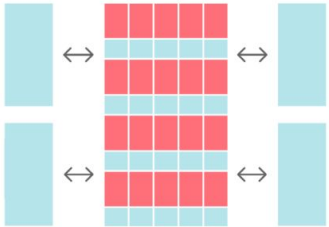
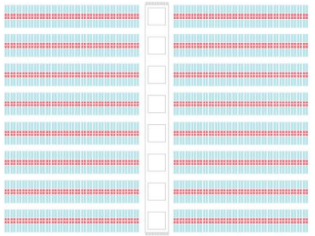
Specify in Slurm file:

```
#SBATCH --partition=pvc
#SBATCH --gres=gpu:pvc:<number>
```

See also our command-line tool to check configuration:

```
$ show_pvc_features
HOSTNAME AVAIL_FEATURES           GRES          STATE
ac010    gen4_fabric              gpu:pvc:4     mixed
...
ac024    gen4_fabric              gpu:pvc:8     idle
ac025    gen4_fabric              gpu:pvc:4     mixed
ac026    gen5_fabric              gpu:pvc:6     reserved
ac030    gen5_fabric              gpu:pvc:8     reserved
ac081    gen5_fabric,xelink4      gpu:pvc:4     reserved
ac082    gen5_fabric,xelink2      gpu:pvc:2     reserved
...
```

Graphcore IPUs

	CPU	GPU	IPU
Parallelism	Designed for scalar processes	SIMD/SIMT architecture. Designed for large blocks of dense contiguous data	Massively parallel MIMD. Designed for fine-grained, high-performance computing
			
Memory Access	Off-chip memory	Model and data spread across off-chip and small on-chip cache, and shared memory	Model and data tightly coupled, and large locally distributed SRAM

www.graphcore.ai/bow-processors

further documentation: docs.graphcore.ai/en/latest

Accessing Graphcore IPUs

- SSH into poplar1 or poplar2 from ACES
  - **`[username@login ~]$ ssh poplar2`**

Contact us first to be given access to poplar.

- Enable the SDK environment. See our KB for details:
  - hprc.tamu.edu/kb/User-Guides/ACES/Graphcore_Colossus_IPUs/
  - hprc.tamu.edu/kb/User-Guides/ACES/Graphcore_Bow_IPUs/

- Type **`gc-monitor`** to view the status of the IPUs:

```
mouse@poplar1:~$ gc-monitor
+-------------+-----------------------------------------------------------------------------------+
| gc-monitor  |                Partition: p16 [active] has 16 reconfigurable IPUs                 |
+-------------+-----------------+---------+--------------+----------+---------+----+------+-------+
|    IPU-M    |      Serial     |IPU-M SW|Server version|  ICU FW  |  Type   | ID | IPU# |Routing|
+-------------+-----------------+---------+--------------+----------+---------+----+------+-------+
| 10.1.5.1    | 0010.0002.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 0  |  3   |  DNC  |
| 10.1.5.1    | 0010.0002.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 1  |  2   |  DNC  |
| 10.1.5.1    | 0010.0001.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 2  |  1   |  DNC  |
| 10.1.5.1    | 0010.0001.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 3  |  0   |  DNC  |
+-------------+-----------------+---------+--------------+----------+---------+----+------+-------+
| 10.1.5.2    | 0030.0002.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 4  |  3   |  DNC  |
| 10.1.5.2    | 0030.0002.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 5  |  2   |  DNC  |
| 10.1.5.2    | 0030.0001.8213921 |        |    1.9.0     |  2.4.4   | M2000   | 6  |  1   |  DNC  |
```

We are planning to have an IPU training event in March!

See also our Youtube channel for previous IPU training sessions!

NEC Vector Engine

- 300W PCIe Gen3 x16 card
- 8 cores, 48 GB HBM2 with 1.5 TB/s memory bandwidth
- 2.45 TFLOPS FP64 peak performance
- Eight (8) NEC Vector Engine Type 20B-P cards hosted in a Dell DSS8440 server
- Links to further documentation at hprc.tamu.edu/kb/User-Guides/ACES/vectorengine/
- Slurm access: `--partition=nec`

VE training event is currently planned for April!

See also our Youtube channel for previous training sessions!

NextSilicon Coprocessors

- 300W PCIe Gen5 x8 card (i.e. 300W per card)
- 64 GB HBM2e memory,
  1.6 TB/s memory bandwidth
- Maverick-1 coprocessor
- Hardware integer compute units
- 2 TFLOPS FP64 peak performance
- Slurm Access: `--partition=nextsilicon`

BittWare FPGAs

BittWare IA-840F FPGA

Supported Tools:

- Intel FPGA OneAPI
- Intel Quartus Prime

Slurm access: `--partition=bittware`

Composing Memory

MemVerge Memory Machine installed on 8 nodes:

- Base nodes:
  - 96 Intel Xeon 8468 processors
  - ~488 Gb DRAM
- Intel Optane SSDs provide additional memory for large jobs –up to 18 TB
- Best for jobs that infrequently access data in memory

Slurm access:

```
#SBATCH --partition=memverge
```

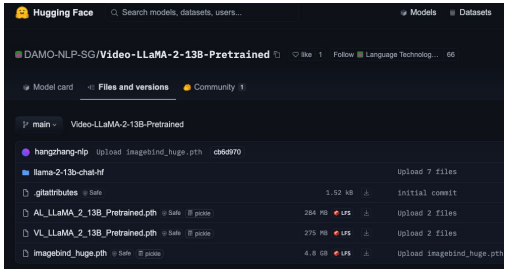
hprc.tamu.edu/kb/User-Guides/ACES/memverge

AI Workflows: Hugging Face Hub on ACES

Hugging Face Hub

- huggingface_hub (models, datasets, etc)
- git-lfs (Git Large File Storage)

Using Git LFS (Large File Storage) with the Hugging Face Hub is crucial for handling large files like machine learning models and datasets.




```
[u.zh108696@aces-login3 ~]$ ml spider git-lfs

----------------------------------------------------------
  git-lfs:
----------------------------------------------------------
     Description:
       Git Large File Storage (LFS) replaces large files
       while storing the file contents on a remote server

     Versions:
        git-lfs/3.2.0
        git-lfs/3.3.0
        git-lfs/3.5.1
```

huggingface_hub

```
[u.zh108696@aces-login3 ~]$ module load GCC/13.2.0 huggingface_hub/0.27.1
[u.zh108696@aces-login3 ~]$ huggingface-cli login

    _|    _|  _|    _|    _|_|_|    _|_|_|  _|_|_|  _|      _|    _|_|_|      _|_|_|_|    _|_|      _|_|_|  _|_|_|_|
    _|    _|  _|    _|  _|        _|            _|    _|_|    _|  _|            _|        _|    _|  _|        _|
    _|_|_|_|  _|    _|  _|  _|_|  _|  _|_|      _|    _|  _|  _|  _|  _|_|      _|_|_|    _|_|_|_|  _|        _|_|_|
    _|    _|  _|    _|  _|    _|  _|    _|      _|    _|    _|_|  _|    _|      _|        _|    _|  _|        _|
    _|    _|    _|_|      _|_|_|    _|_|_|  _|_|_|  _|      _|    _|_|_|      _|        _|    _|    _|_|_|  _|_|_|_|

    A token is already saved on your machine. Run `huggingface-cli whoami` to get more information or `huggingface-cli logout` if you want to log ou
t.
    Setting a new token will erase the existing one.
    To log in, `huggingface_hub` requires a token generated from https://huggingface.co/settings/tokens .
Enter your token (input will not be visible):
```

AI Workflows: Hugging Face Hub on ACES

Hugging Face Libraries

- Transformers
- Datasets
- Tokenizers
- Accelerate
- Diffusers
- …

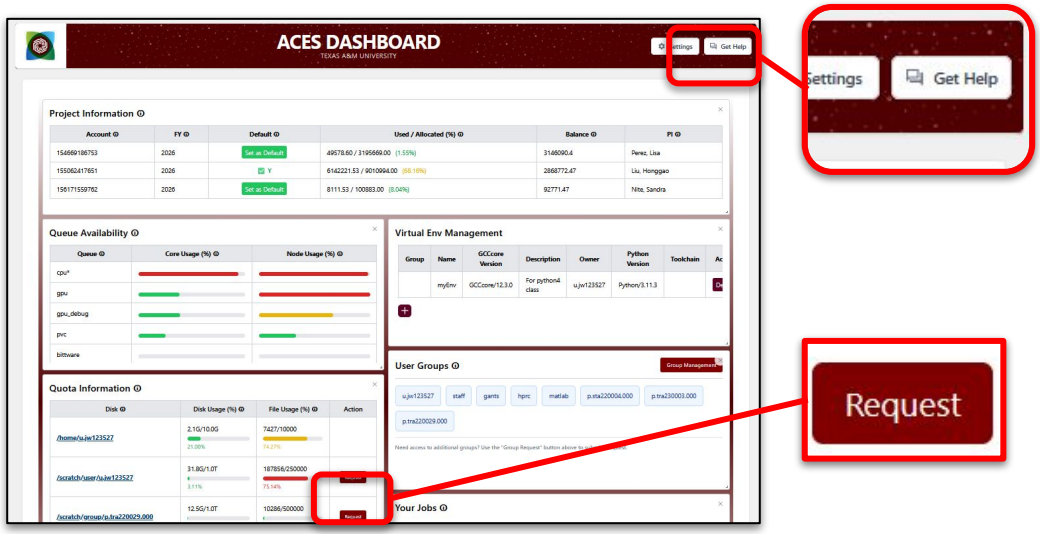

```
(hgf-env) [u.zh108696@aces-login3 huggingface]$ pip install transformers datasets tokenizers
Looking in indexes: https://pypi.org/simple, https://pypi.ngc.nvidia.com
Collecting transformers
  Downloading transformers-4.48.0-py3-none-any.whl.metadata (44 kB)
     ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 44.4/44.4 kB 5.7 MB/s eta 0:00:00
Collecting datasets
  Downloading datasets-3.2.0-py3-none-any.whl.metadata (20 kB)
Collecting tokenizers
```

```python
from transformers import AutoTokenizer, AutoModelForSequenceClassification

# Choose a model, e.g., BERT for sentiment analysis
model_name = "distilbert-base-uncased-finetuned-sst-2-english"

# Load tokenizer and model
tokenizer = AutoTokenizer.from_pretrained(model_name)
model = AutoModelForSequenceClassification.from_pretrained(model_name)

# Tokenize input
inputs = tokenizer("I love ACES!", return_tensors="pt")

# Perform inference
outputs = model(**inputs)
predictions = outputs.logits.argmax(dim=-1)
print(predictions)  # 1 for positive sentiment
```

Need Help?

First check the FAQ: https://hprc.tamu.edu/kb/FAQ/Accounts

- ACES user Guide: https://hprc.tamu.edu/kb/User-Guides/ACES
- FASTER user Guide: https://hprc.tamu.edu/kb/User-Guides/FASTER



Remember the Dashboard!

These buttons have automations that help us address your issue faster!

Need Help? - Email

You can also contact our helpdesk at help@hprc.tamu.edu

Help us help you -- tell us:

- Which cluster
- Username
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- Steps you have taken, so we can reproduce the problem

High Performance
Research Computing
DIVISION OF RESEARCH

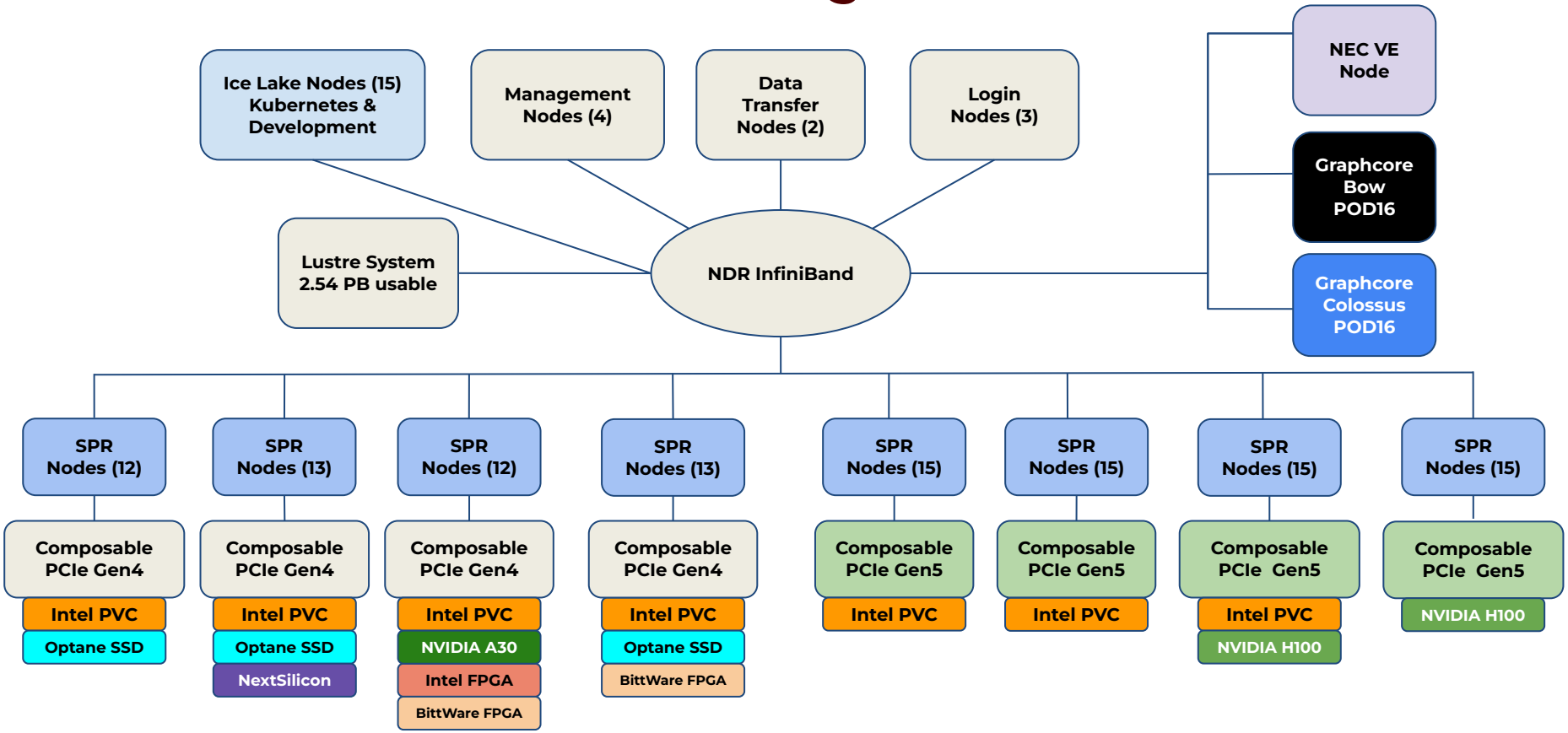
Give us feedback on the class with this survey:
https://u.tamu.edu/hprc_shortcourse_survey

Thank you!

Questions?

ACES Configuration

ACES Configuration



ACES System Description

Component	Quantity	Description
Sapphire Rapids Nodes: Compute Nodes Data Transfer Nodes Login & Management Nodes	 110 nodes 2 nodes 5 nodes	96 cores per node, dual Intel Xeon 8468 processors 512 GB DDR5 memory 1.6 TB NVMe local storage Compute: NVIDIA Mellanox NDR 200 Gbps InfiniBand adapter DTNs & Login & Management nodes: 100 Gbps Ethernet adapter
Ice Lake Login & Management Nodes	2 nodes	64 cores per node, dual Intel Xeon 8352Y processors 512 GB DDR4 memory 1.6 TB NVMe local storage NVIDIA Mellanox NDR 200 Gbps InfiniBand adapter
PCIe Gen4 Composable Infrastructure	50 SPR nodes	Dynamically reconfigurable infrastructure that allows up to 20 PCIe cards (GPU, FPGA, etc.) per compute node
PCIe Gen5 Composable Infrastructure	60 SPR nodes	Dynamically reconfigurable infrastructure that allows up to 16 H100s or 14 PVCs per compute node
NVIDIA InfiniBand (IB) Interconnect	110 nodes	Two leaf and two spine switches in a 2:1 fat tree topology
DDN Lustre Storage	2.5 PB usable	HDR IB connected flash and disk storage for Lustre file systems

ACES Accelerators

Component	Quantity	Description
Graphcore IPU: Colossus GC200 Bow	 16 16	Each IPU group hosted with a CPU server as a POD16 on a 100 GbE RoCE fabric
NVIDIA GPUs: H100 A30	 30 4	 For HPC, DL Training, AI Inference For AI Inference and Mainstream Compute
BittWare IA-840F FPGA	3	Accelerator with Agilex AGF027 FPGA and 64 GB of DDR4
NextSilicon Coprocessor	2	Reconfigurable accelerator with an optimizer continuously evaluating application behavior.
NEC Vector Engine	8	Vector computing card (8 cores and HBM2 memory)
Intel Optane SSD	48	18 TB of SSDs addressable as memory w/ MemVerge Memory Machine.
Intel PVC GPUs	120	Intel GPUs for HPC, DL Training, AI Inference