

HIGH PERFORMANCE RESEARCH COMPUTING

HPRC Primer

Introduction to ACES: A Composable Cluster

September 23, 2025
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High Performance
Research Computing
DIVISION OF RESEARCH

ACES System Description

[ACES](#) (Accelerating Computing for Emerging Sciences) is a Dell cluster with a rich accelerator testbed:

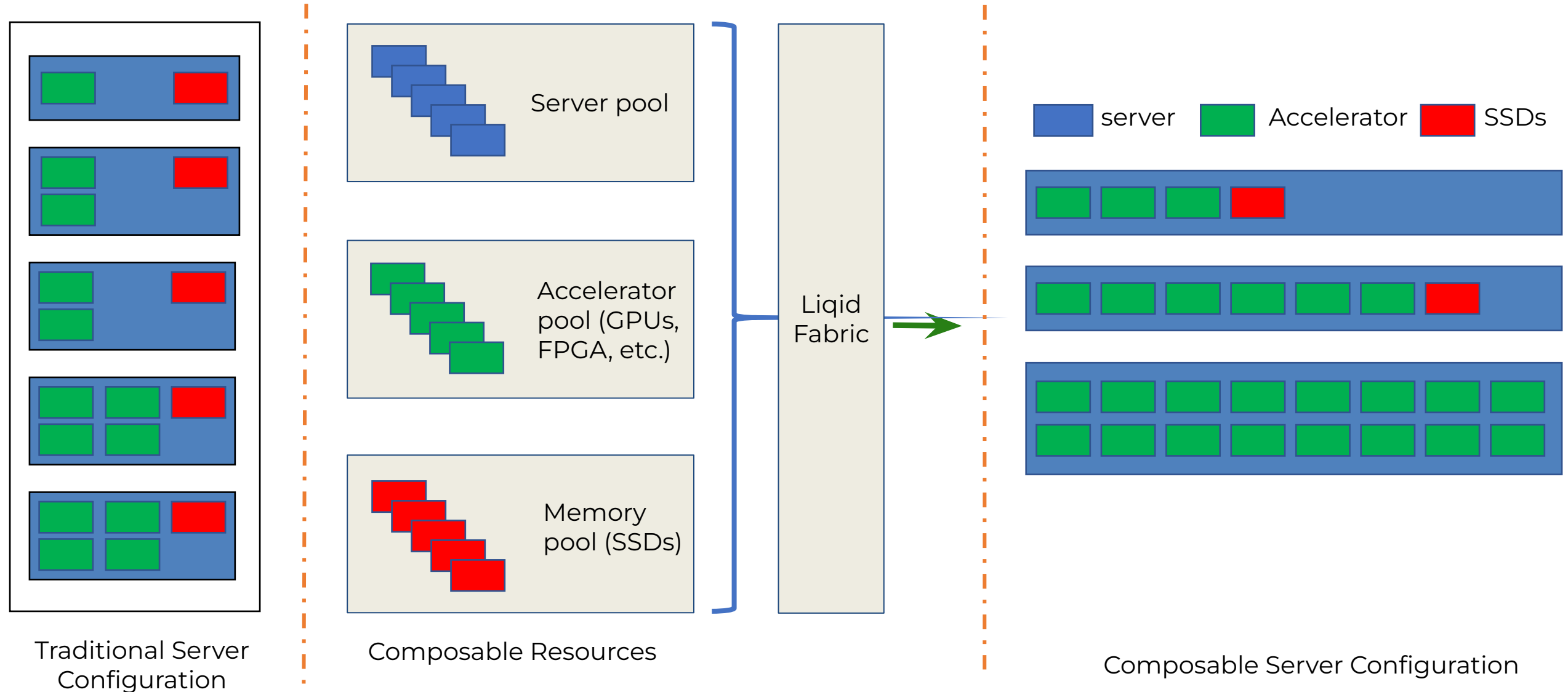
Compute nodes	• 110 Intel Sapphire Rapids Nodes • 17 Intel Ice Lake Nodes • 1 AMD Rome Graphcore Node with 16 Mk2 Colossus GC200 IPU's • 1 Intel Ice Lake Graphcore Node with 16 Bow-2000 IPU's • 1 Intel Cascade Lake Node with 8 NEC Vector Engine Type 20B-P cards	
Accelerators	• 30 NVIDIA H100 GPU's • 4 NVIDIA A30 GPU's • 3 Bittware Agilex FPGAs • 2 Intel D5005 FPGAs	• 2 NextSilicon coprocessors • 48 Intel Optane Memory • 120 Intel GPU Max 1100 (Formerly Ponte Vecchio)
Interconnect	NVIDIA Mellanox NDR200 InfiniBand (MPI and storage) Liquid PCIe Gen4 Fabrics (composability), Gen 5 Fabrics (Coming Soon)	



The Intel Optane SSDs and all accelerators (except the Graphcore IPU's and NEC Vector Engines) are accessed using Liquid's composable framework via PCIe (Peripheral Component Interconnect express) Gen4 and Gen5 fabrics.

Visit <https://hprc.tamu.edu/kb/User-Guides/ACES/> for more details.

Design: Composability at the Hardware Level



Accessing ACES via the HPRC Portal

- HPRC webpage - hprc.tamu.edu

TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING

Home User Services Resources Research Policies Events Training About Portal

Quick Links

- New User Information
- Accounts
 - Apply for Accounts
 - Manage Accounts
- User Consulting
- Training
- Knowledge Base
- Software
- FAQ

Grace Portal

FASTER Portal

FASTER Portal (ACCESS)

ACES Portal (ACCESS)

Launch Portal (ACCESS)

Use ACCESS ID

Using the ACES Portal - Shell Access

ACES OnDemand Portal Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ Affinity Groups ▾ Dashboard ▾ Utilities ▾ My Interactive Sessions

>_ acs Shell Access



Convenient shell access anywhere with a web browser.

Starts an in-browser Linux terminal on ACES.

OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

IMPORTANT POLICY INFORMATION

- Unauthorized use of HPRC resources is prohibited and subject to criminal prosecution.
- Use of HPRC resources in violation of United States export control laws and regulations is prohibited.
- Sharing HPRC account and password information is in violation of State Law. Any shared accounts will be DISABLED.
- Authorized users must also adhere to ALL policies at: <https://hprc.tamu.edu/policies>

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!

Hands-On Activity - 2 Minutes

1. Please try to access ACES through the portal.
2. What message do you see when you log on to the shell?

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	This is high performance storage intended to temporarily hold larger files and is for on-going processing that uses them. It is NOT backed up nor is it intended as long-term storage. Please delete or move out of these area any files that are not frequently used.
/scratch/group/PROJECTID	\$PROJECT	5 TB	500,000	This high performance storage is shared among to members of this particular group. It is not purged while the allocation is active. Data will be removed 90 days after allocation expiration.

View file usage and quota limits using the command:

showquota

Do NOT share your personal home or scratch directories.

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

Using the ACES Dashboard

ACES OnDemand Portal

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾

Affinity Groups ▾

Dashboard ▾

Utilities ▾

My Interactive Sessions

ACES Dashboard



ACES
ACCELERATING COMPUTING
FOR EMERGING SCIENCES

View your account
quota and projects

OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

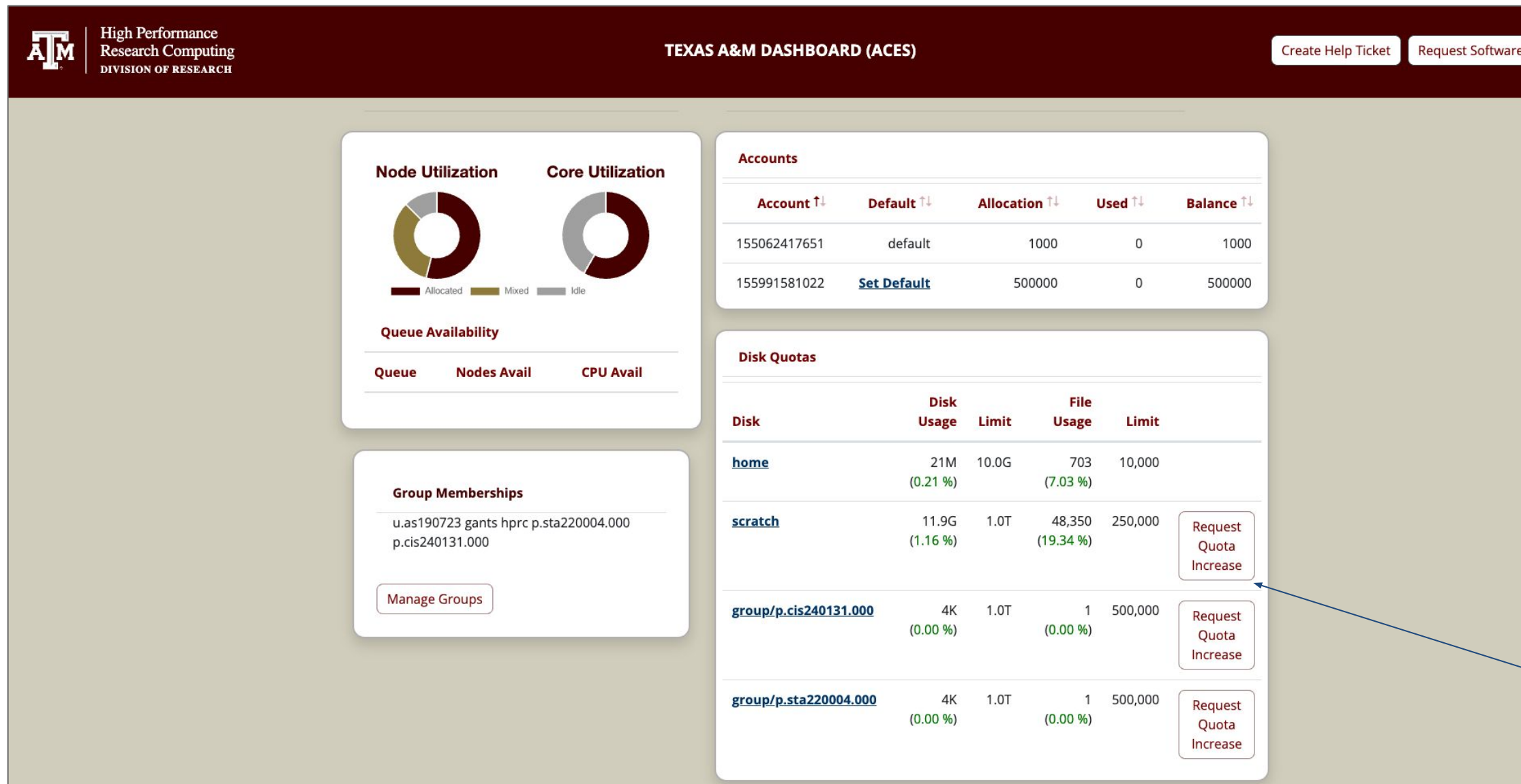
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Texas A&M Dashboard: ACES

View cluster utilization, storage quotas, & allocation balances



Quota and file limit increases considered for scratch directories.

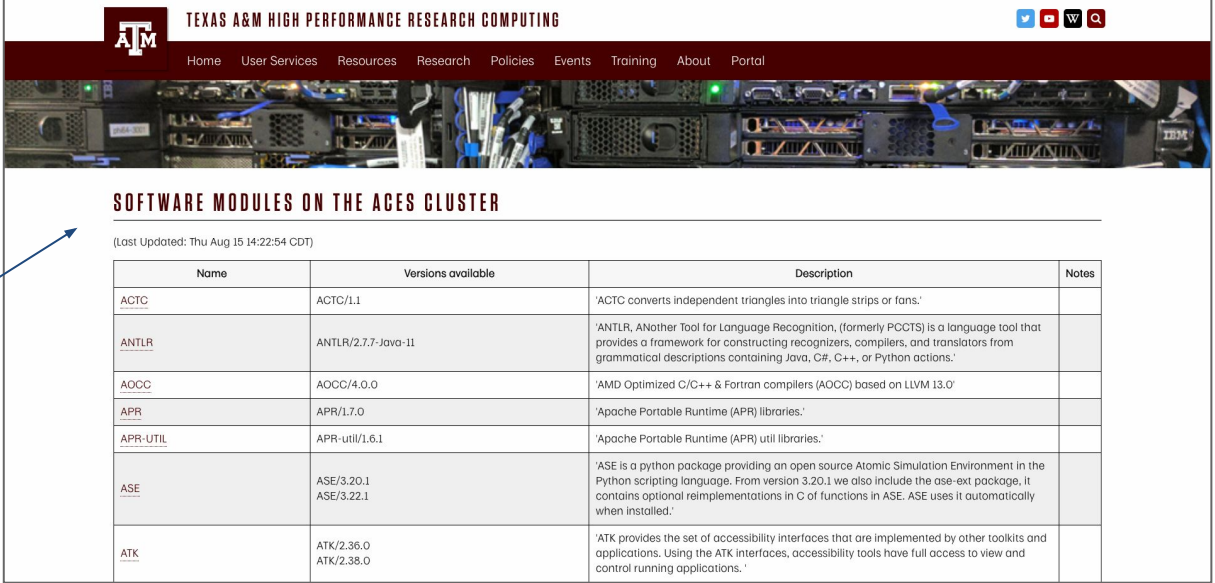
Preferred way to request *Quota Increases*

Hands-On Activity - 2 Minutes

1. Please try to access the dashboard now through the portal.
2. Where is the button to request a quota increase?

Software

- See the Software Knowledge Base page at <https://hprc.tamu.edu/kb/Software/> for instructions and examples.
- Search for software modules on <https://hprc.tamu.edu/software/aces/>.
- License-restricted software
 - Contact help@hprc.tamu.edu
- Contact HPRC for software installation help/requests.
 - User can install software in their home/scratch directory.
 - Do NOT run the `sudo` command when installing software.



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SOFTWARE MODULES ON THE ACES CLUSTER

(Last Updated: Thu Aug 15 14:22:54 CDT)

Name	Versions available	Description	Notes
ACTC	ACTC/1.1	'ACTC converts independent triangles into triangle strips or fans.'	
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.'	
APR	APR/1.7.0	'Apache Portable Runtime (APR) libraries.'	
APR-UTIL	APR-util/1.6.1	'Apache Portable Runtime (APR) util libraries.'	
ASE	ASE/3.20.1 ASE/3.22.1	'ASE is a python package providing an open source Atomic Simulation Environment in the Python scripting language. From version 3.20.1 we also include the ase-ext package. It contains optional reimplementations in C of functions in ASE. ASE uses it automatically when installed.'	
ATK	ATK/2.36.0 ATK/2.38.0	'ATK provides the set of accessibility interfaces that are implemented by other toolkits and applications. Using the ATK interfaces, accessibility tools have full access to view and control running applications.'	

Software: Application Modules

- Installed applications are made available with the module system.
- ACES uses a software hierarchy inside the module system.
- In this hierarchy, the user loads a compiler “toolchain” which then makes available software built with that compiler toolchain.

```
module list                # shows which software is ready
module load GCC/13.3.0     # load GCC compiler version 13.3.0
module list                # shows which software is now ready
module load OpenMPI/5.0.3  # load OpenMPI version 5.0.3
module list                # shows which software is now ready
```

Software: Modules and Toolchains

- Toolchains are what we call groups of compilers & libraries.
- There is a variety of toolchains on the clusters:

```
intel/2023a  
foss/2024.05  
GCCcore/13.3.0
```

*(more than just these versions)
(varies by cluster, as well)*

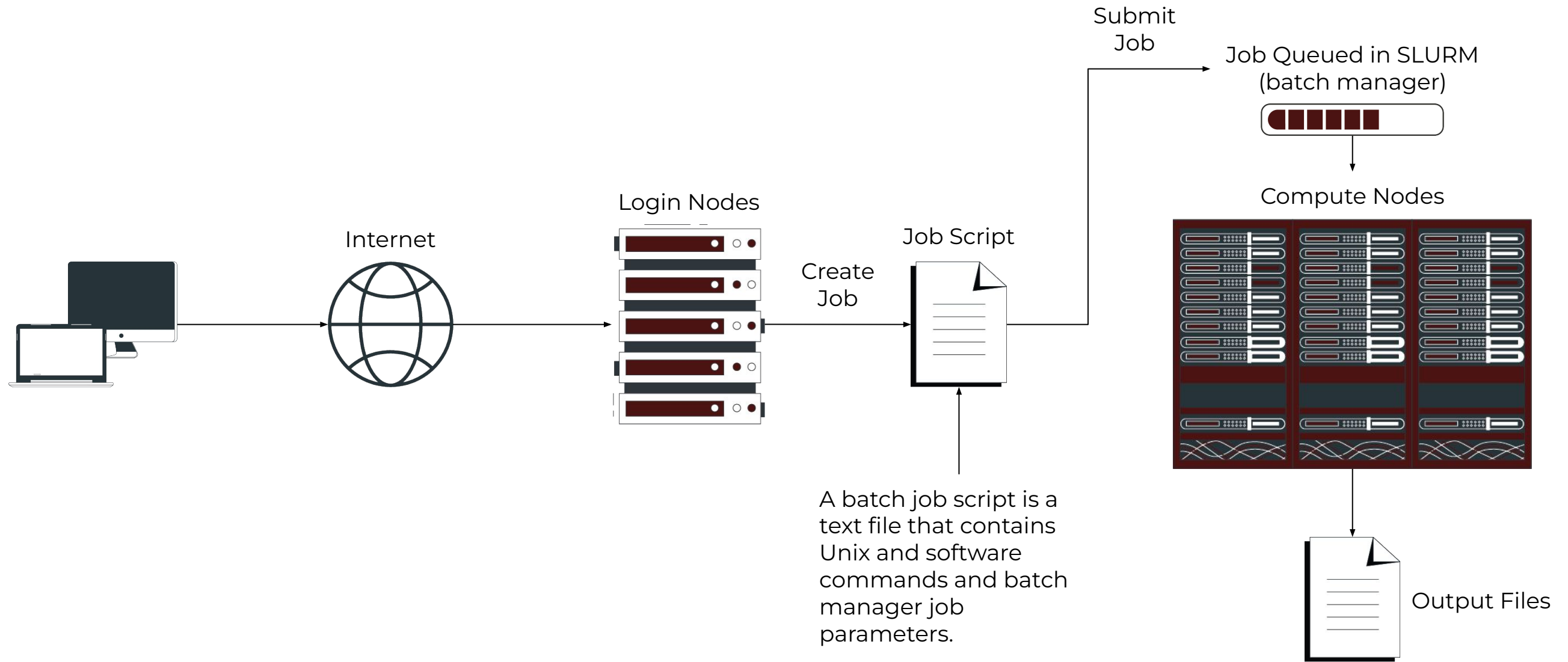
- Module management:

```
module spider      # Search for modules and their dependencies  
module purge       # removes all loaded modules from environment
```

Hands-on Exercise: Module Loading

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

Batch Computing on HPRC Clusters



Batch Queues

- Job submissions are auto-assigned to batch queues based on the resources requested (e.g. cpu vs. gpu).
- Use 'sinfo' to check on their status.

```
[u.as190723@aces-login2 ~]$ sinfo
PARTITION    AVAIL  TIMELIMIT  JOB_SIZE   NODES(A/I/O/T)  CPUS(A/I/O/T)
cpu*         up      3-00:00:00  1-64       54/0/0/54       3232/1952/0/5184
gpu          up      2-00:00:00  1-8        5/2/0/7         304/368/0/672
gpu_debug    up      2:00:00     1          0/3/0/3         0/288/0/288
pvc          up      2-00:00:00  1-30       0/27/5/32       0/2592/480/3072
bittware     up      2-00:00:00  1          0/0/2/2         0/0/192/192
memverge     up      2-00:00:00  1          0/4/6/10        0/384/576/960
nextsilicon  up      2-00:00:00  1          0/2/0/2         0/192/0/192
staff        up      2-00:00:00  1-110      59/36/13/108    3536/5584/1248/10368
```

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

Additional information:

<https://hprc.tamu.edu/kb/User-Guides/ACES/Batch/#batch-queues>

Sample Job Script Structure

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample1
#SBATCH --time=01:30:00
#SBATCH --ntasks-per-node=48
#SBATCH --nodes=2
#SBATCH --mem=488G
#SBATCH --output=Example1Out.%j
#SBATCH --partition=gpu
#SBATCH --gres=gpu:h100:1

##OPTIONAL JOB SPECIFICATIONS
##SBATCH --account=123456
##SBATCH --mail-type=ALL
##SBATCH --mail-user=email_address

# load required module(s)
module purge
module load GCCcore/13.3.0
module load Python/3.12.3
module load CUDA/12.6.0

# Run your program
python my_gpu_script.py
```

These parameters describe your job to the job scheduler.
The lines starting with #SBATCH are not just comments!

Account number to be charged
(if you are not using a default account).
(Note: having two '#' makes these lines comments;
reduce to one '#' to make Slurm read them)

Commands or scripts you want to run
Here, we set up the modules we need for our
environment and run a python program.

Hands-On Activity

- Navigate to the \$SCRATCH directory by running the following command:
cd \$SCRATCH
- Copy “hello_world.job” to your \$SCRATCH directory by running the following command:
cp -r /scratch/training/slurm_example \$SCRATCH
- Navigate inside the slurm_example directory by running the following command:
cd slurm_example/
- Now, you can submit the job by running the command:
sbatch hello_world.job

Submit Your Job and Check Job Status

Submit job

```
sbatch hello_world.job
```

```
sbatch: Job submitted using account 155062417651  
sbatch: Current account balance = 971468.947778  
Submitted batch job 981586
```

Check status

```
queue -u username
```

(or

```
queue --me
```

 as a shortcut for your own jobs)

JOBID	NAME	USER	PARTITION	NODES	CPUS	STATE	TIME	TIME_LEFT	START_TIME	REASON	NODELIST
981590	hello_world	u.as190723	cpu	4	384	PENDING	0:00	4:00:00	2025-03-05T11:00	Resources	
981589	hello_world	u.as190723	cpu	1	1	RUNNING	2:49	17:11	2025-03-05T10:12	None	ac091

Hands-On Activity - 5 Minutes

1. Create a submission file for a serial job; you can use the template shown previously or create your own.
2. Submit this job file using sbatch.
3. Check which queue the job is in using the command **squeue -u <username>**
4. When your job completes, check the contents of the output file. The name of the output file depends on the configuration in the job script.

Check your Service Unit (SU) Balance

- List the SU Balance of your Account(s).

```
myproject -m
```

=====							
List of u.lp46691's Project Accounts							

Account	FY	Default	Allocation	Used & Pending SUs	Balance	PI	

154669186753	2025	Y	951450.00	-2443.94	949006.06	Perez, Lisa	

155466915524	2025	N	602891.00	-3.51	602887.49	Perez, Lisa	

=====							
Account	Project						

154669186753	TRA220029						
155466915524	TRA240008						

- Run "myproject -d Account#" to change default project account.
- Run "myproject -h" to see more options.

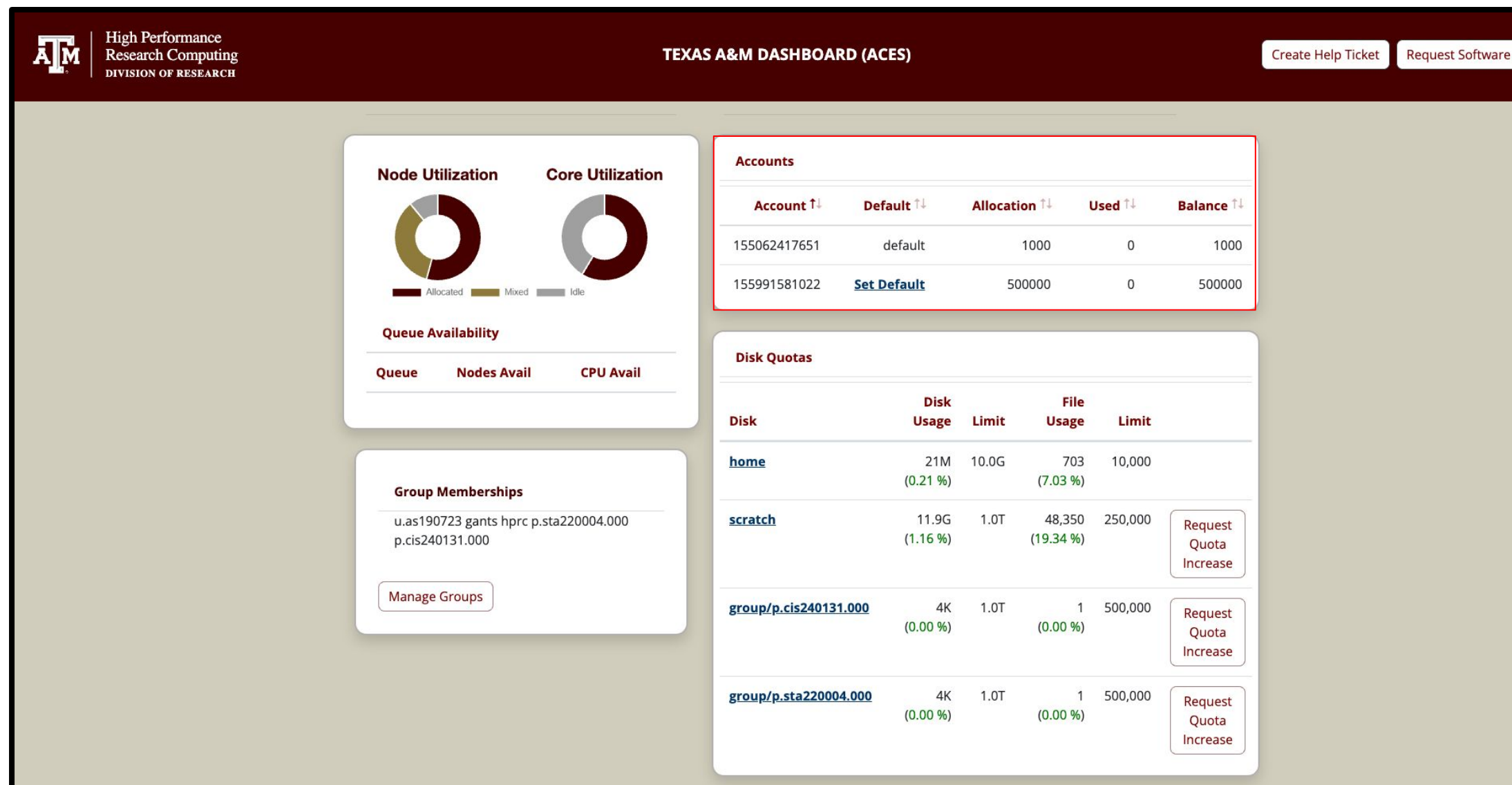
<https://hprc.tamu.edu/kb/User-Guides/AMS/#service-unit>

<https://hprc.tamu.edu/kb/User-Guides/AMS/#ams-user-interfaces>

(reminder)

Texas A&M Dashboard: ACES

Easily view Cluster utilization, Storage Quotas & Allocation Balances



Hands-On Activity - 2 Minutes

1. Use myproject to check the SU balance of your accounts.
2. Use the dashboard to check the same information.

Need Help?

First check the FAQ and our knowledge base -

- Accounts - <https://hprc.tamu.edu/kb/FAQ/Accounts/>
- ACES User Guide: <https://hprc.tamu.edu/kb/User-Guides/ACES/>
- Email your questions to help@hprc.tamu.edu

Contact our helpdesk

Email your questions to help@hprc.tamu.edu

Help us help you -- when you contact us, tell us:

- Which Cluster you are using
- Your 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
- Screenshots if possible



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<https://hprc.tamu.edu>

HPRC Helpdesk:
help@hprc.tamu.edu
Phone: 979-845-0219

Take our short course survey!

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