

Working on



ACES

ACCELERATING COMPUTING
FOR EMERGING SCIENCES

Josh Winchell

Wednesday, 26 February 2025

PACES Research Training Workshop

Outline

- ACES System Overview
- Basic Usage
 - Open OnDemand Portal
 - File Systems and Quotas
 - Software Infrastructure
- Interactive Jobs
- Setting up workshop files

Outline

- **ACES System Overview**
- Basic Usage
 - Open OnDemand Portal
 - File Systems and Quotas
 - Software Infrastructure
- Interactive Jobs
- Setting up workshop files

NSF ACES

Accelerating Computing for Emerging Sciences

Our Mission:

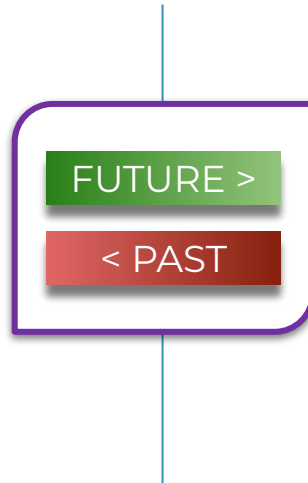
- NSF ACSS CI testbed
- Offer an accelerator testbed for numerical simulations and **AI/ML workloads**
- Provide consulting, technical guidance, and training to researchers
- Collaborate on computational and data-enabled research.



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

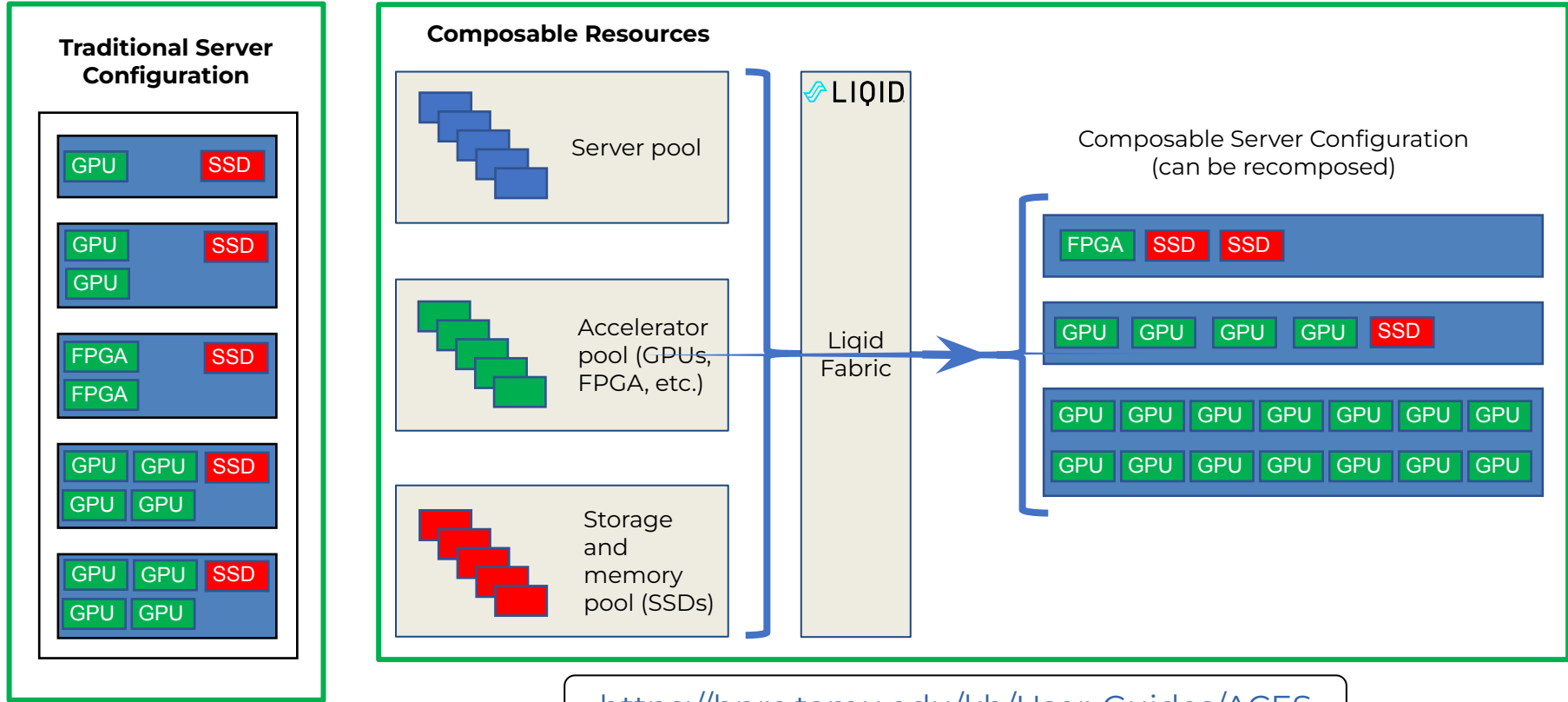


HPC for AI

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

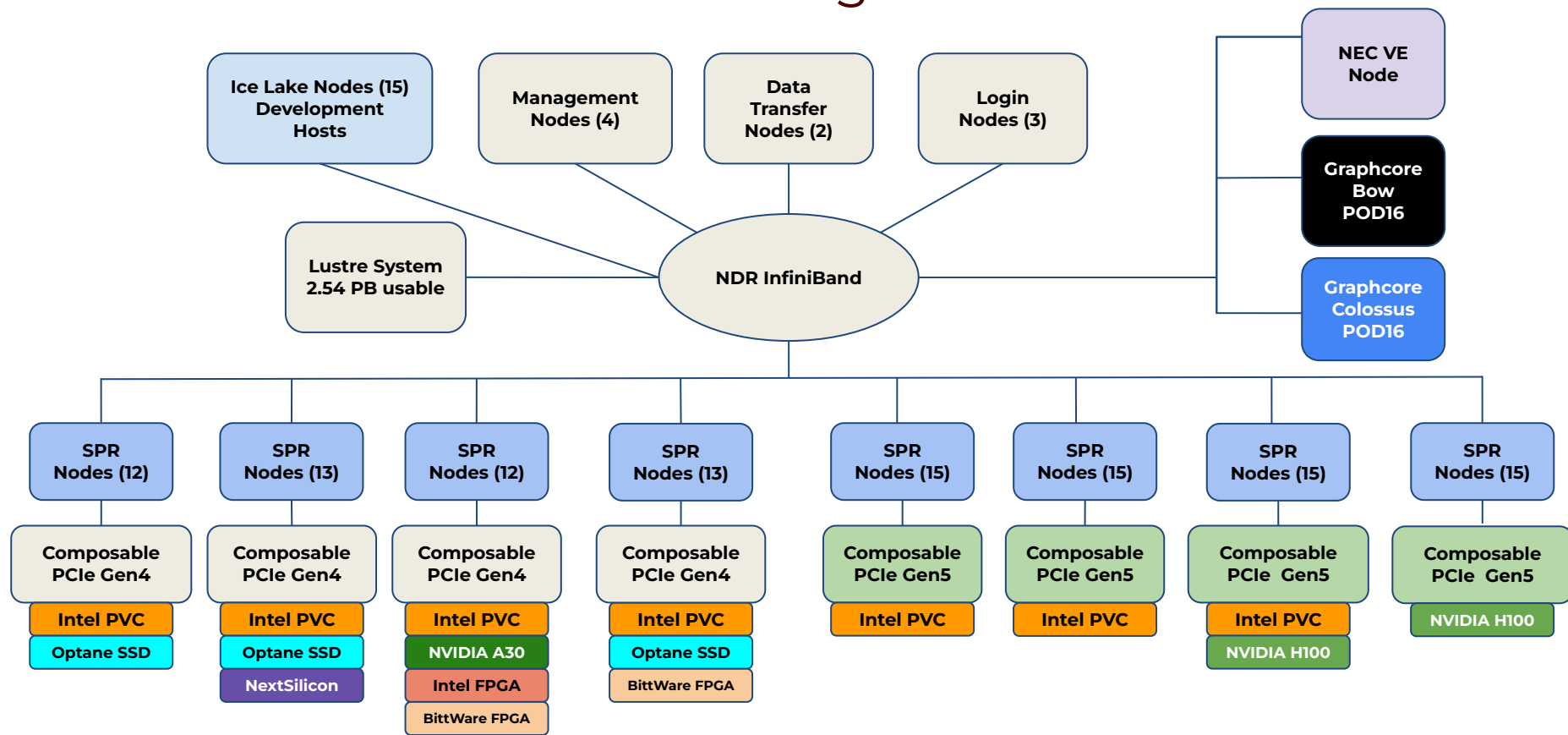
Next Generation HPC/AI Platform Supports Composable Accelerators and Memory

Composability



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

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 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 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/Components

Component	Quantity	Description
Graphcore IPU	32	16 Colossus GC200 IPUs, 16 Bow IPUs. Each IPU group hosted with a CPU server as a POD16 on a 100 GbE RoCE fabric
<i>FPGAs:</i>		
Intel PAC D5005	2	Accelerator with Intel Stratix 10 GX FPGA and 32 GB DDR4
BittWare IA-840F	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.
<i>NVIDIA GPUs:</i>		
H100	30	For HPC, DL Training, AI Inference
A30	4	For AI Inference and Mainstream Compute
Intel PVC GPUs	120	Intel GPUs for HPC, DL Training, AI Inference

Refer to our Knowledge Base for more:

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

System Software Stack

Function	Component	Version
Cluster Management	xCAT	2.16.4
Primary OS	Red Hat Enterprise Linux	8.9
HPC Scheduler	Slurm	22.05.11
InfiniBand Subnet Manager	UFM	6.12
OFED	Mellanox OFED	23.10-2.1.3
Storage Client	Lustre	2.12.9_ddn38
Software Management	Lmod	8.7
Software Build Framework	EasyBuild	4.9.2
Web Portal Software	Open OnDemand	3.0
Data Movement Software	Globus Connect Server	5.4
Job Reporting Software	Open XDMoD	10.5

Outline

- ACES System Overview
- **Basic Usage**
 - **Open OnDemand Portal**
 - File Systems and Quotas
 - Software Infrastructure
- Interactive Jobs
- Setting up workshop files

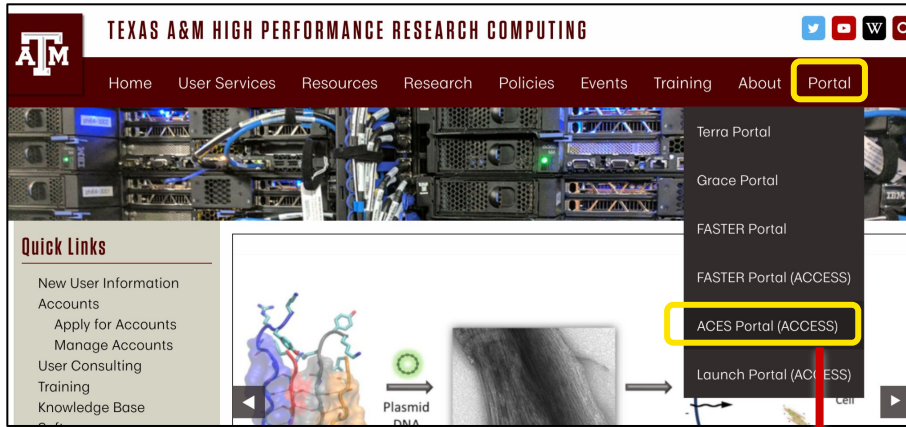
Usage Policies

(Be a good compute citizen)

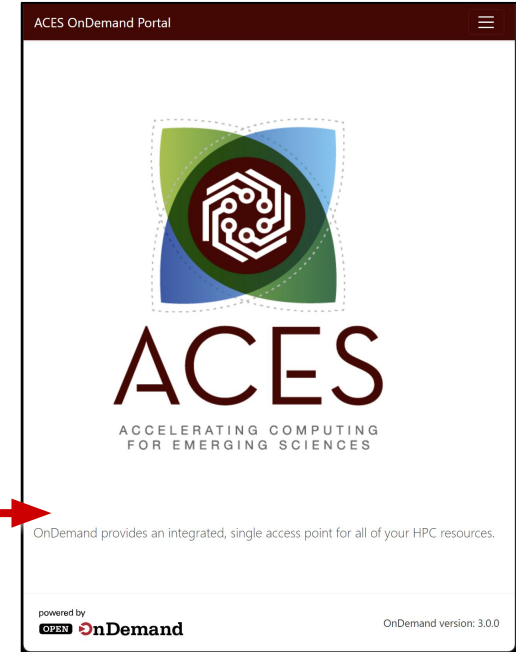
- It is illegal to share computer passwords and accounts
- Clusters must not be used in any manner that violates the United States export control laws and regulations, EAR & ITAR
- Abide by the license restrictions when using commercial software

hprc.tamu.edu/policies

ACES Access - Portal



- Navigate from HPRC homepage
- Login via ACCESS
- Open-OnDemand Portal



HPRC Portal Overview

File Browsing, Viewing, and Editing

ACES OnDemand Portal

Files Jobs Clusters Interactive Apps Affinity Groups Dashboard My Interactive Sessions

Help Logged in as u.jw123527 Log Out

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

/home / u.jw123527 / Change directory Copy path

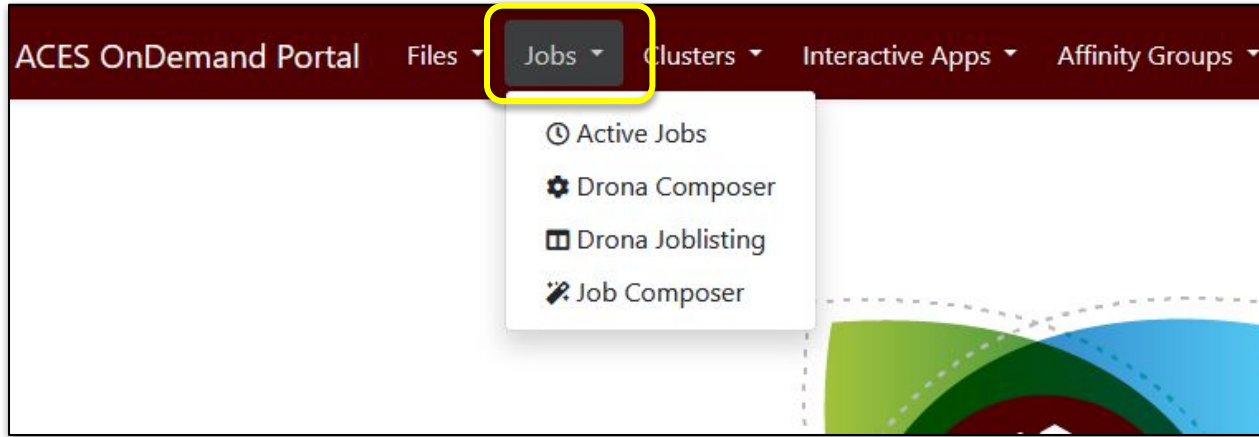
Show Owner/Mode Show Dotfiles Filter: Showing 4 of 30 rows - 0 rows selected

Type	Name	Size	Modified at
Folder	ACES_FundamentalsOfRProgramming	-	9/26/2023 10:56:01 AM
File	hello_world.py	73 Bytes	2/2/2024 11:45:32 AM
File	hello_world.slurm	432 Bytes	2/2/2024 11:45:32 AM
File	module.avail.aces		9/18/2023 11:20:41 AM

View Edit Rename Download Delete

Manage your files right in your browser

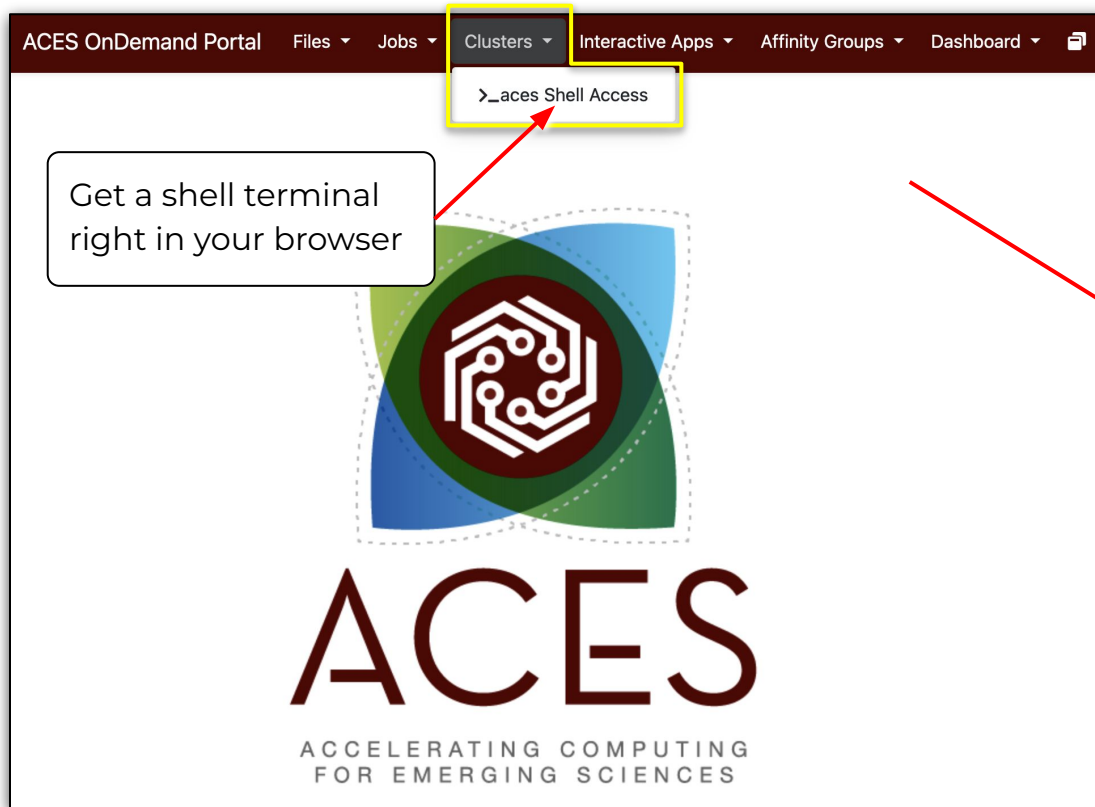
Portal Job Composers



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 Slurm files via a form.

Shell Access via the Portal



```
Host: login.aces
Warning: Permanently added 'login.aces,10.71.1.13' (ECDSA) to the list of known hosts.
*****
This computer system and the data herein are available only for authorized
purposes by authorized users. Use for any other purpose is prohibited and may
result in disciplinary actions or criminal prosecution against the user. Usage
may be subject to security testing and monitoring. There is no expectation of
privacy on this system except as otherwise provided by applicable privacy laws.
Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.
*****

Last login: Mon Feb 12 13:11:13 2024 from 10.71.1.6

=====
Texas A&M University High Performance Research Computing
=====
Website:      https://hprc.tamu.edu
Consulting:   help@hprc.tamu.edu (preferred) or (979) 845-0219
ACES Documentation: https://hprc.tamu.edu/kb/User-Guides/ACES
FASTER Documentation: https://hprc.tamu.edu/kb/User-Guides/FASTER
Grace Documentation: https://hprc.tamu.edu/kb/User-Guides/Grace
Terra Documentation: https://hprc.tamu.edu/kb/User-Guides/Terra
YouTube Channel: https://www.youtube.com/texasamhprc
=====

*****
===== 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. Current HPRC staff members are
*   US citizens and legal residents.
* - Sharing HPRC account and password information is in violation of
*   Texas State Law. Any shared accounts will be DISABLED.
* - Authorized users must also adhere to ALL policies at:
*   https://hprc.tamu.edu/policies/
*****

*** ACES Partial Availability, February 12 ***

We are still troubleshooting issues for various compute nodes that were
reconfigured for PCIe fabric connectivity to the H100 and PVCs.

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

Please restrict usage to 8 CORES across ALL login nodes.
Users found in violation of this policy will be SUSPENDED.

To see these messages again, run the moitd command.

Your current disk quotas are:
Disk          Disk Usage    Limit    File Usage    Limit
/home/u.jw123527 165M         10.0G    499          10000
/scratch/user/u.jw123527 28.1G       1.0T     102472       250000
Type 'showquota' to view these quotas again.
[u.jw123527@aces-login3 ~]$
```

Interactive Apps

The screenshot shows the ACES OnDemand Portal interface. The top navigation bar is dark red with white text. It includes links for 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Affinity Groups', 'Dashboard', and 'My Interactive Sessions'. The 'Interactive Apps' link is highlighted with a yellow box, and a red arrow points from a text box to it. The 'My Interactive Sessions' link is also highlighted with a yellow box, and a red arrow points from another text box to it. A dropdown menu is open under 'Interactive Apps', showing categories: 'GUI' (with sub-items 'VNC' and 'Nextsilicon VNC'), 'Imaging' (with sub-items 'CryoSPARC', 'ImageJ', and 'cisTEM'), and 'Servers' (with sub-items 'Jupyter Notebook', 'JupyterLab', 'RStudio', and 'TensorBoard').

Launch GUIs for various software in your web browser

Check their status here

Join Affinity Groups

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

Links to support.access-ci.org

ACES
R HPC



ACCESS
Support

Quick Links Community CCEP Knowledge Base MATC

SUPPORT / AFFINITY GROUPS / ACES

ACES

ACES TAMU novel-accelerators

Accelerating Computing for Emerging Sciences (ACES) is a NSF-Category II-funded test bed (award number 2112356) that offers state of the art GPUs and other novel accelerators in a composable environment. The ACES innovative composable hardware platform helps accelerate transformative changes in research areas that can leverage novel accelerators for analytics and computing. The test bed enables researchers to creatively develop new programming models and workflows that utilize these architectures while simultaneously advancing HPC (High Performance Computing) and data science projects.

Members get updates about announcements, events, and outages.

JOIN SLACK

ACES
ACCELERATING COMPUTING
FOR EMERGING SCIENCES

Upcoming Events
2/13/2024 11:00 AM EST

ACES Dashboard

ACES OnDemand Portal

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾

Affinity Groups ▾

Dashboard ▾

My Interactive Sessions

ACES Dashboard

High Performance Research Computing
DIVISION OF RESEARCH

TEXAS A&M DASHBOARD (ACES)

Create Help Ticket

Request Software

Node Utilization



Allocated Mixed Idle

Core Utilization



Allocated Mixed Idle

Queue Availability

Queue

Nodes Avail

CPU Avail

Group Memberships

u.ab123456 matlab p.sta220004.000

Manage Groups

Accounts

Account ▴▾	Default ▴▾	Allocation ▴▾	Used ▴▾	Balance ▴▾
155062417651	default	1000	0	1000

Request higher storage limits

Disk Quotas

Disk	Disk Usage	Limit	File Usage	Limit
home	179M (1.75 %)	10.0G	707 (7.07 %)	10,000
scratch	37.6G (3.67 %)	1.0T	140,232 (56.09 %)	250,000
group/ p.sta220004.000	4K (0.00 %)	1.0T	1 (0.00 %)	500,000

Request Quota Increase

Request or change user groups

Request help or new software

D. Pham et al. (2022) PEARC '22
<https://doi.org/10.1145/3491418.3535182>

Utilities

The screenshot shows the ACES OnDemand Portal interface. The top navigation bar includes 'Affinity Groups', 'Dashboard', and 'Utilities' (highlighted with a yellow box). The 'Utilities' dropdown menu lists: 'cpuavail', 'envsavail', 'gpuavail', 'license_status', and 'venvavail'. Below the menu, two utility pages are displayed:

ACES GPU Availability
This displays the CONFIGURATION of installed GPUs and the status of GPUs readily available for...
Output generated: 2025-01-21 08:26:16
\$ gpuavail

CONFIGURATION		AVAILABILITY					
NODE TYPE	NODE COUNT	NODE NAME	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVA
gpu.pvc:4	17	ac041	h100	8	8	96	488
gpu.pvc:2	11	ac045	h100	8	8	96	488
gpu.pvc:8	4	ac049	h100	4	3	88	360

ACES License Status
Output generated: 2025-01-21 08:26:57
\$ license_status -a

Abaqus | ANSYS | COMSOL | ConvergeCFD | ECLIPSE | FDTD | FEMZIP | FLOW3D |
Hyperworks | Intel | INTERSECT | LS-DYNA | Madymo | Matlab | Matlab_MDCS |
Metashape | MOE | Osays | PGL_compilers | StarCCM | Schrodinger |

License status for Abaqus:

License Name	# Issued	# In Use	# Available
abacus_teaching	320	0	320
abacus_extended_teaching	40	0	40
cse_teaching	1	0	1
euler_lagrange_teaching	1	0	1

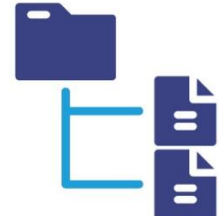
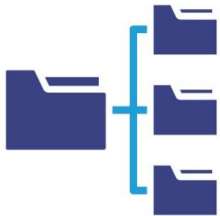
- Convenient collection of command-line tools
- check availability of gpus, licenses, and other resources

Outline

- ACES System Overview
- **Basic Usage**
 - Open OnDemand Portal
 - **File Systems and Quotas**
 - Software Infrastructure
- Interactive Jobs
- Setting up workshop files

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 to be a long-term storage area.
/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.



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

(Or check on the Dashboard in the OOD portal)

Service Units

- Service Units (SUs) are part of our account management system (AMS).
- 1 SU ~ 1 core-hour on a CPU
(using accelerators or extra memory will cost additional SUs)
- 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'll see how later).
(Work on login nodes is not charged, but you can't 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/UI/>

<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

```
-----
```

(Or check on the Dashboard in the OOD portal)

ACES Charging Scheme

Resource	Service Units (per hour)	ACCESS Credits (per hour)
Intel SPR / Icelake	1	0.1
NVIDIA H100	120	15
NVIDIA A30 and Intel PVC GPUs	60	7.5
Bittware Agilex FPGA	100	12.5
Intel D5005 FPGA	50	6.3
NEC Vector Engine	150	18.8
NextSilicon Co-processor	100	12.5
Graphcore IPU Classic	90	11.3
Graphcore IPU Bow	120	15
Intel Optane Memory	60	7.5

Outline

- ACES System Overview
- **Basic Usage**
 - Open OnDemand Portal
 - File Systems and Quotas
 - **Software Infrastructure**
- Interactive Jobs
- Setting up workshop files

2,400+ Software Modules!

SOFTWARE MODULES ON THE ACES CLUSTER

ACES Software Modules

FASTER Software Modules

Grace Software Modules

Over 740 unique software packages – most with multiple version modules

(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 applications.'	

hprc.tamu.edu/software/aces

Installing Software

- Software pages for instructions and examples:
 - <https://hprc.tamu.edu/kb/Software>
 - hprc.tamu.edu/software
- Researchers can install software in their home/scratch directories
 - Do **NOT** run the "sudo" command when installing software
 - Watch your file quotas! Install in \$SCRATCH!
- Contact us if you need help or want to request software
 - 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

Computing Environment

Managing software versions using Lmod

- 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

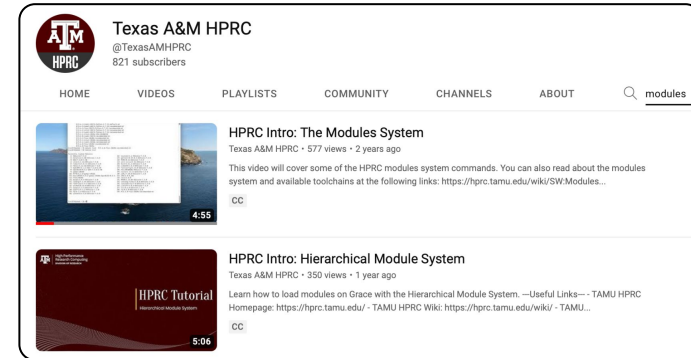
GCC/12.3.0 OpenMPI/4.1.5

software-name / version-spec

PyTorch/2.1.2-CUDA-12.1.1

- 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 module 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 load <module>

- add <module> paths to the current environment variables

module list

- See what modules are loaded in your current session

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 ~]$
```

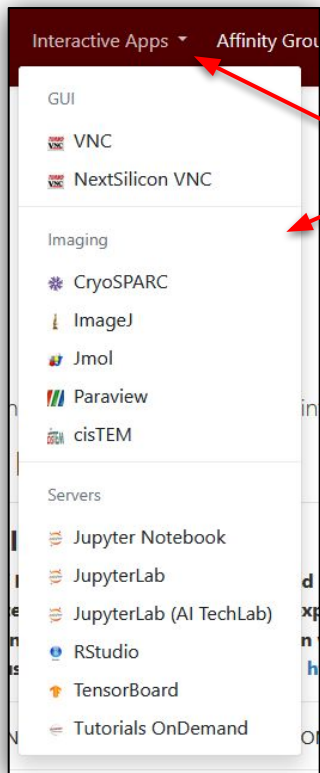
Hands-on Exercise: Module Loading

1. `m1a blast+` -See which versions of BLAST+ are available.
2. `m1 BLAST+/2.14.1` -error! You cannot do that yet.
3. `module spider BLAST+/2.14.1` -Learn how to load this module.
4. `m1            BLAST+/2.14.1` -Fill in the blank (with the correct toolchains) to load this module.
5. `m1 list` -List all loaded modules.
6. `m1 GCC/10.2.0` -Change version of a loaded Toolchain module (GCC); notice the message about reloaded modules.
7. `m1 list` -List all loaded modules.
8. `m1 purge` -Remove all loaded modules.

Outline

- ACES System Overview
- Basic Usage
 - Open OnDemand Portal
 - File Systems and Quotas
 - Software Infrastructure
- **Interactive Jobs**
- Setting up workshop files

Running an Interactive App



In the portal, select an app from the “Interactive Apps” dropdown.

You’ll get a form in which to specify what resources to use (this is specifying a Slurm job behind the scenes)

Jupyter Notebook

This app will launch a Jupyter Notebook server on the ACES cluster.

Type of Environment

Python module + virtualenv

Select the type of environment in which Jupyter is installed. [Help me choose](#)

Select Python Module Version

Python/3.10.8

Optional Python virtualenv to be activated

Enter the full path to a python virtual environment "activate" script to be activated. This field is optional. If used, it will override the default Jupyter.

E.g. /scratch/user/netid/...path-to-env/bin/activate

Your optional environment must have been previously built with the Python module selected in the Module option above. It is expected to have a Jupyter package installed. Please see [instructions](#).

Node type

CPU only

Select a GPU node for software that supports GPU processing.

Number of hours (max 168)

2

Number of cores (max 96)

1

Total GB memory (max 485)

5

Account

This field is optional.

Email

This field is optional.

Launch

* The Jupyter Notebook session data for this session can be accessed under the [data root directory](#).

Hit ‘Launch’

My Interactive Sessions

Launching an interactive app
(or clicking this in the toolbar) →
shows you the status of your apps:



The image displays four overlapping cards representing the lifecycle of a Jupyter Notebook session. Each card has a title bar, metadata, and a status indicator.

- Card 1 (Queued):** Title "Jupyter Notebook (690828)", status "Queued". Metadata: "Created at: 2025-02-20 16:18:07 CST", "Time Requested: 1 hour", "Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f". A red "Delete" button is present.
- Card 2 (Starting):** Title "Jupyter Notebook (690828)", status "1 node | 1 core | Starting". Metadata: "Created at: 2025-02-20 16:18:07 CST", "Time Remaining: 59 minutes", "Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f". A red "Delete" button is present.
- Card 3 (Running):** Title "Jupyter Notebook (690828)", status "1 node | 1 core | Running". Metadata: "Host: >... ac005", "Created at: 2025-02-20 16:18:07 CST", "Time Remaining: 59 minutes", "Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f". A red "Delete" button and a blue "Connect to Jupyter" button are present.
- Card 4 (Completed):** Title "Jupyter Notebook (690828)", status "Completed". Metadata: "Created at: 2025-02-20 16:18:07 CST", "Time Requested: 1 hour", "Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f". A red "Delete" button is present.

When this shows up,
connect to the GUI here

My Interactive Sessions

Until your job turns grey, you're being charged SUs!
Be sure to close your program when you're done.

The image displays four overlapping screenshots of the 'My Interactive Sessions' interface, illustrating the lifecycle of a Jupyter Notebook session. A red arrow points from the text 'Be sure to close your program when you're done.' to the 'Completed' state.

- Queued:** The session is in a light blue state. It shows 'Created at: 2025-02-20 16:18:07 CST', 'Time Requested: 1 hour', and 'Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f'. A 'Delete' button is visible.
- Starting:** The session is in a light blue state with '1 node | 1 core | Starting'. It shows 'Created at: 2025-02-20 16:18:07 CST', 'Time Remaining: 59 minutes', and 'Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f'. A 'Delete' button is visible.
- Running:** The session is in a green state with '1 node | 1 core | Running'. It shows 'Created at: 2025-02-20 16:18:07 CST', 'Time Remaining: 59 minutes', and 'Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f'. A 'Delete' button is visible.
- Completed:** The session is in a grey state with 'Completed | [icon]'. It shows 'Created at: 2025-02-20 16:18:07 CST', 'Time Requested: 1 hour', and 'Session ID: fcf55438-0b20-45c0-ac6a-78873c8ee85f'. A 'Delete' button is visible.

Each screenshot also includes a 'Connect to Jupyter' button in the 'Starting' and 'Running' states.

If you need to troubleshoot,
find logs at the link next to
“Session ID”

Outline

- ACES System Overview
- Basic Usage
 - Open OnDemand Portal
 - File Systems and Quotas
 - Software Infrastructure
- Interactive Jobs
- **Setting up workshop files**

Get the Notebooks

- The notebook files for this workshop are on ACES already
–you just need to make your own copies of them
- Start an ACES terminal and enter these two commands:

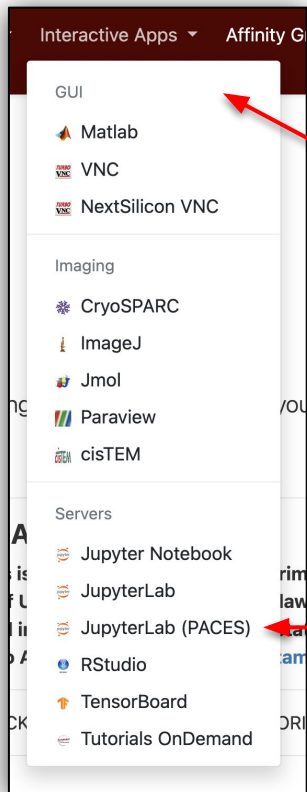
```
cd $SCRATCH
```

```
cp -r /scratch/training/paces_Feb2025/ .
```



Make sure you have this period
with a space before it!

Launch the Interactive App



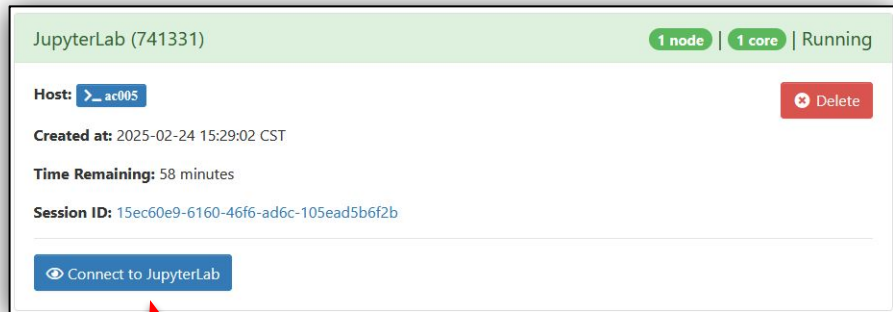
Close the terminal

Launch a JupyterLab session from the portal with these criteria:

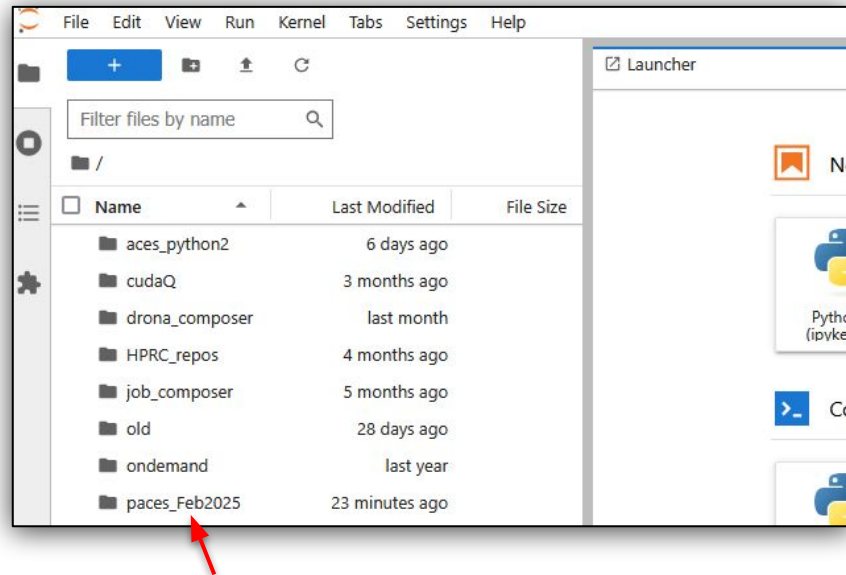
- CPU only (for today)
- (time depending on where we are in the day)
- 1 core
- 5 GB
- (leave the rest blank)

A screenshot of the 'JupyterLab (PACES)' configuration form. The form has a title 'JupyterLab (PACES)' and a subtitle 'This app will launch a JupyterLab server on the ACES cluster.' It contains several sections: 'Module' with a dropdown menu set to 'Anaconda3/2024.02-1'; 'Optional Environment to be activated' with a text input field containing '/sw/hprc/sw/Anaconda3/2024.02-1/envs/ai-labs'; 'Node type' with a dropdown menu set to 'CPU only' and a note 'Select a GPU node for software that supports GPU processing.'; 'Number of hours (max 168)' with a text input field set to '1'; 'Number of cores (max 3)' with a text input field set to '1'; 'Total GB memory (max 5)' with a text input field set to '5'; 'Account' with a text input field; 'Email' with a text input field; and a 'Launch' button. There are also checkboxes for 'I would like to receive an email when the session starts' and a note about session data access.

Find Your Notebooks



Wait for the job to start, then hit
“Connect to Jupyter”



Find and open the directory you copied
(you won't have all the directories in this screenshot)

Advanced Topics

Status of Composability

Composability is currently handled by sysadmins

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

Accelerator Access Summary

Component	Access	node or partition
BittWare IA-840F FPGA	Slurm	--partition=bittware
Intel PAC D5005 FPGA	Slurm	--partition=d5005
Intel GPU Max 1100 (PVC)	Slurm	--partition=pvc
Intel Optane SSD	Slurm	--partition=memverge
NextSilicon Coprocessor	Slurm	--partition=nextsilicon
NVIDIA A30 GPUs	Slurm	--partition=gpu
NVIDIA H100 GPUs	Slurm	--partition=gpu
Graphcore Bow IPU	Interactive	ssh poplar2
Graphcore Colossus IPU	Interactive	ssh poplar1
NEC Vector Engine	Interactive	ssh dss

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>

Hands-on Exercise: Python Software Install

1. `ml purge`
`ml GCCcore/13.2.0 Python/3.11.5`

2. `create_venv myEnv`

3. `source activate_venv myEnv`

4. `python -c "import pytime"`

5. `pip install python-time`

6. `python -c "import pytime; print(pytime)"`

7. `deactivate`

-Set up the underlying Python module

-Use HPRC's "create_venv" tool.
Creates a virtual environment in
\$SCRATCH/virtual_envs

-Activate virtual environment.

-Check if python-time is installed (it is not).

-Install python-time.

-Where is python-time installed?

-Close virtual environment.

Data Transfers Using Globus

The screenshot displays the Globus File Manager interface. On the left, a sidebar contains navigation icons for File Manager, Bookmarks, Activity, Collections, Groups, Console, Flows, Compute, Settings, Logout, and Help & Support. The main area is titled 'File Manager' and shows two collections: 'ACCESS TAMU ACES DTN' and 'TAMU grace-dtn'. The 'ACCESS TAMU ACES DTN' collection is selected, showing a list of files and folders. The 'TAMU grace-dtn' collection is also visible, showing a list of files and folders. A 'Start' button is present for each collection. Below the file lists, a 'Transfer & Timer Options' section is visible. On the right, a panel titled 'TAMU grace-dtn to ACCESS TAMU ACES DTN' shows the transfer status as 'transfer completed'. It includes an 'Overview' tab and an 'Event Log' tab. The 'Overview' tab displays the following information:

Task Label	TAMU grace-dtn to ACCESS TAMU ACES DTN
Source	TAMU grace-dtn
Destination	ACCESS TAMU ACES DTN
Task ID	52fa3c22-4362-11ee-a06d-eb83daae1adf
Owner	Wesley Brashear (wbrashear@tamu.edu)
Condition	SUCCEEDED
Requested	8/25/2023, 11:13 AM
Completed	8/25/2023, 11:13 AM
Duration	15 seconds
Transfer Settings	- verify file integrity after transfer - transfer encrypted - overwriting all files on destination

On the right side of the 'Overview' tab, a summary of the transfer is shown:

2	Files
7	Directories
2	Files Transferred
7.60 GB	Bytes Transferred
505.76 MB/s	Effective Speed
0	Skipped files on sync
0	Skipped files on error

A 'View debug data' link is located at the bottom right of the transfer summary.

Log in at <https://www.globus.org/>