

ACES: AI/ML on Intel PVC GPUs

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High Performance
Research Computing
DIVISION OF RESEARCH



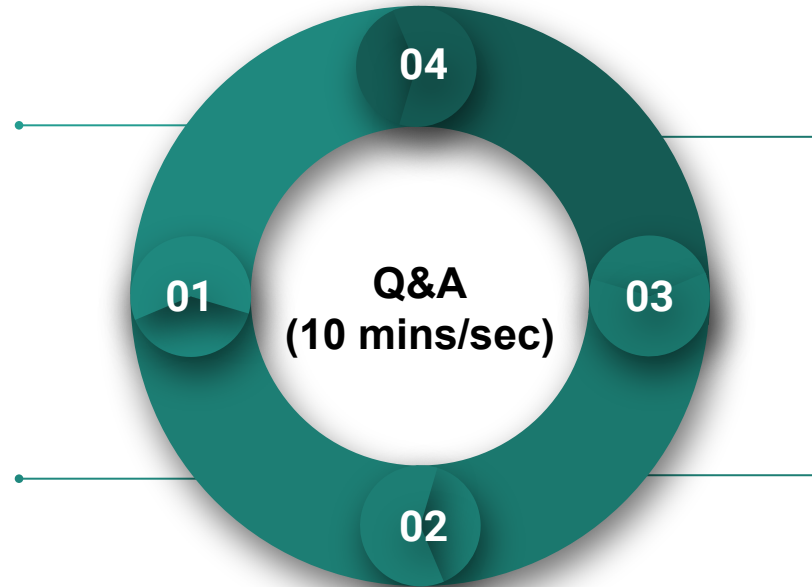
Outline

Section I. Intro to PVCs

We will introduce Intel's PVC, its architecture, and the PVC GPUs on the TAMU ACES platform.

Section II. Demo on ACES

We will demonstrate how to run models of different frameworks with PVC GPUs on the ACES system.



Section IV. TensorFlow on PVC

Students will learn how to convert a TensorFlow image classification model to run on a PVC GPU.

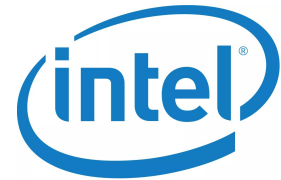
Section III PyTorch on PVC

Students will learn how to convert a PyTorch image classification model to run on a PVC GPU.

Lab I. Introducing Intel PVC GPUs on ACES



Intel Data Center GPU Max Series PCIe Card



NSF ACES

Accelerating Computing for Emerging Sciences

Our Mission:

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

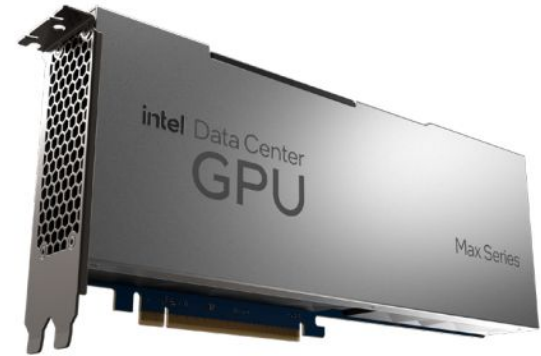


ACES Accelerators

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
Intel PAC D5005 FPGA	2	Accelerator with Intel Stratix 10 GX FPGA and 32 GB DDR4
BittWare IA-840F FPGA	2	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 Intel Optane SSDs addressable as memory w/ MemVerge Memory Machine.
NVIDIA H100 + A30	30 + 4	NVIDIA GPUs for HPC, DL Training, AI Inference
Intel GPU Max 1100 (PVC)	120	Intel GPUs for HPC, DL Training, AI Inference

Intel Max GPU 1100

- 1 tile/stack per card
- 56 X^e cores, 448 execution units (8 per core)
- 300W PCIe Gen5 x16 card
- 48GB HBM2e memory
- 1.2 TB/s memory bandwidth
- 22 TF FP64 peak performance



Intel Data Center GPU Max Series PCIe Card

Intel® oneAPI Toolkits

Intel® oneAPI Base Toolkit

A core set of high-performance libraries and tools for building C++, SYCL and Python applications



Add-on Domain-specific Toolkits



Intel® oneAPI Tools for HPC

Deliver fast Fortran, OpenMP & MPI applications that scale



Intel® oneAPI Tools for IoT

Build efficient, reliable solutions that run at network's edge



Intel® oneAPI Rendering Toolkit

Create performant, high-fidelity visualization applications

Toolkits powered by oneAPI



Intel® AI Analytics Toolkit

Accelerate machine learning & data science pipelines end-to-end with optimized DL frameworks & high-performing Python libraries



Intel® Distribution of OpenVINO™ Toolkit

Deploy high performance inference & applications from edge to cloud

(Source: Intel)

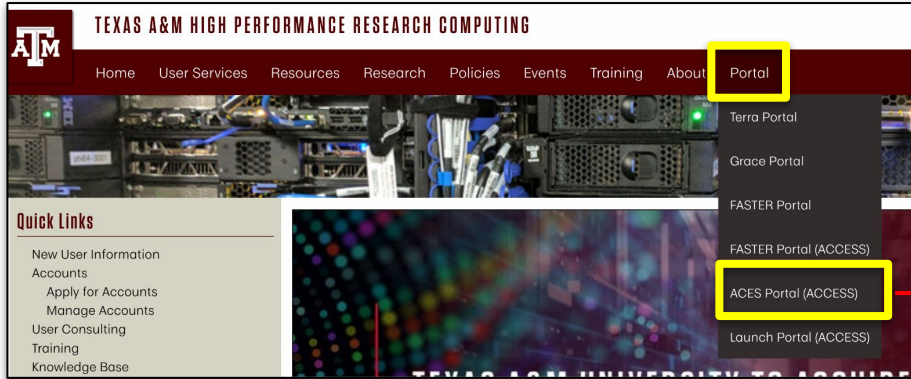
Shared Data Directories on ACES

- Datasets: ImageNet datasets for PyTorch and TensorFlow
/scratch/data/pytorch-computer-vision-datasets
/scratch/data/tensorflow-computer-vision-datasets
- Models: Intel AI models
/scratch/data/intel-ai-models
- Containers
/scratch/data/containers/intel-deep-learning-2023.2-py3.10-perms.sif

Resources

- [Texas A&M High Performance Research Computing \(HPRC\)](#)
- [ACES Quick Start Guide](#)
- [ACES Portal \(ACCESS\)](#)
- [ACCESS Documentation](#)
- [HPRC YouTube Channel](#)
- help@hprc.tamu.edu

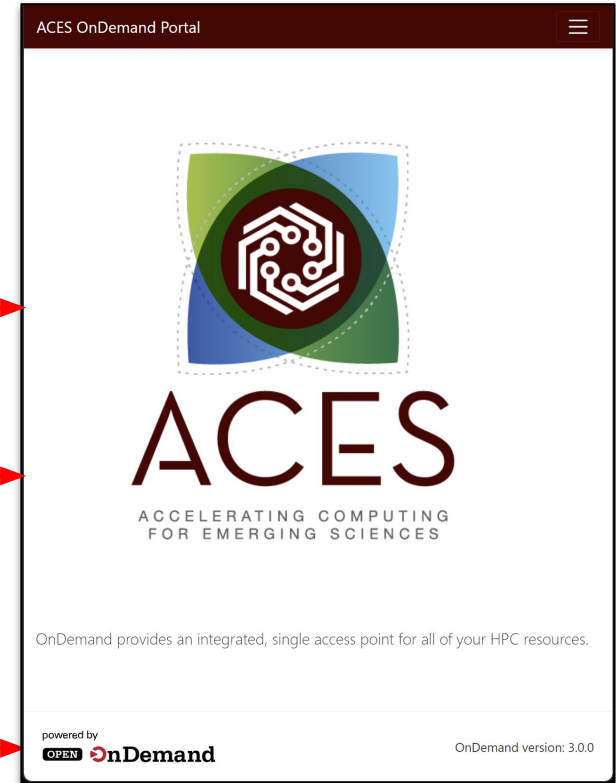
ACES Portal



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

[HPRC Portal YouTube tutorials](#)

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



Accessing via ACCESS

Log-in using your ACCESS CI credentials.

ACCESS Powered By **CILogon**

Consent to Attribute Release

TAMU FASTER ACCESS OOD requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

Select an Identity Provider

ACCESS CI (XSEDE)

Remember this Selection

Log On

By selecting "Log On", you agree to the [privacy policy](#).

For questions about this site, please see [FAQs](#) or send email to help@cilogon.org.
Know your [responsibilities](#) using the CILogon Service.
See [acknowledgments](#) of support for this site.

ACCESS

Login to CILogon

ACCESS Username

ACCESS Password

Don't Remember Login

Login

CILogon

CILogon facilitates secure access to CyberInfrastructure (CI).

- If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login
- Register for an ACCESS Account
- Forgot your password?
- Need Help?

[Click Here for Assistance](#)

Select an Identity Provider

ACCESS CI (XSEDE)

Select the Identity Provider appropriate for your account.

Shell Access via the Portal

ACES OnDemand Portal Files Jobs Clusters Interactive Apps Affinity Groups Dashboard

>_aces Shell Access

Get a shell terminal right in your browser

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```
Host: login.aces Theme: Default
*****
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: Wed Mar 13 09:55:42 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 Update, March 7 ****

The pvc queue has been updated with a new set of nodes with 2x, 4x, and 8x 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 mo!d command.
Your current disk quotas are:
Disk          Disk Usage  Limit  File Usage  Limit
/home/u.zh108696 5.4G      10.0G  3148       10000
/scratch/user/u.zh108696 439.2G   1.0T   1169787    2000000
Type 'showquota' to view these quotas again.
[u.zh108696@aces-login2 ~]$
```

PVC Slurm Nodes Status Check

- View the pvc nodes and number of GPUs

```
$ pstat -p pvc -G
```

- View more details of the pvc node features

```
$ sinfo -N -p pvc -o "%8n %10f %G"
```

Copy the Materials to Personal Directory

- Navigate to your personal scratch directory

```
$ cd $SCRATCH
```

- Files for this course are located at

```
/scratch/training/aces_pvc_course_24s
```

Make a copy in your personal scratch directory

```
$ cp -r /scratch/training/aces_pvc_course_24s $SCRATCH
```

- Enter this directory (your local copy)

```
$ cd $SCRATCH/aces_pvc_course_24s
```

Lab II. Using PVCs on ACES



Environment Setup for PyTorch Models

Use Intel AI Analytics Toolkit

```
# load all the necessary modules
module purge
module load intel/AIKit/2023.2.0
module load intel/2023.07

ENV_NAME=aikit-pt-gpu-clone

# If it doesn't exist, create the environment
if ! conda env list | grep -q "$ENV_NAME"; then
    conda create -n $ENV_NAME --clone aikit-pt-gpu
fi

# activate the conda environment
source activate $ENV_NAME
```

in pt_demo.slurm

Environment Setup for PyTorch Models

Use Python Virtual Environment (Alternative for reference)

```
# Change to pytorch directory
cd $SCRATCH/aces_pvc_course_24s/pytorch

# Load modules
module load WebProxy
module load intel/2023.03
module load Python/3.10.8

# Create and activate a Python virtual environment
python -m venv pt-pvc-labs
source pt-pvc-labs/bin/activate
```

Please do not type

Environment Setup for PyTorch Models

Use Python Virtual Environment (Alternative for reference)

```
# Install torch, torchvision and oneccl_bindings_for_pytorch
python -m pip install torch==1.13.0a0+git6c9b55e
torchvision==0.14.1a0 intel_extension_for_pytorch==1.13.120+xpu -f
https://developer.intel.com/ipex-whl-stable-xpu

python -m pip install oneccl_bind_pt==1.13.200+gpu -f
https://developer.intel.com/ipex-whl-stable-xpu

# Install tensorboard
python -m pip install tensorboard
```

Run PyTorch ResNet50 model

- We have prepared a Slurm job file (*pt_demo.slurm*) to run the PyTorch ResNet50 model. Submit the job using the command
- `$ cd pytorch/`
- `$ sbatch pt_demo.slurm`

Environment Setup for TensorFlow Models

Using the Intel AI Analytics Toolkit

```
# load all the necessary modules
module purge
module load WebProxy
module load intel/2023.07
module load intel/AIKit/2023.1.0

ENV_NAME=aikit-tf-gpu-clone

# If it doesn't exist, create the environment
if ! conda env list | grep -q "$ENV_NAME"; then

    conda create -n $ENV_NAME --clone aikit-tf-gpu
fi

# activate the conda environment
source activate $ENV_NAME
```

in tf_demo.slurm

Run Tensorflow ResNet50 Model

- We have prepared a Slurm job file (*tf_demo.slurm*) to run the Tensorflow ResNet50 model. Submit the job using the command

```
$ cd ..
```

```
$ cd tensorflow/
```

```
$ sbatch tf_demo.slurm
```

Lab III. PyTorch on PVC



1. Import Intel Extension for PyTorch

Intel Extension for PyTorch is a Python package for extending PyTorch models to run on an Intel platform.

Add the following import statement to the beginning of your script:

```
import intel_extension_for_pytorch as ipex
```

2. Move the Model and Criterion to “xpu”

```
model = model.to("xpu")
```

```
criterion = criterion.to("xpu")
```


3. Apply the “ipex optimize” Function

Apply the ipex optimize function against the model and optimizer objects.

```
model, optimizer = ipex.optimize(model, optimizer=optimizer,  
dtype=torch.bfloat16)
```

4. Move the Data and Target to “xpu”

In the training loop,

```
data = data.to("xpu")
```

```
target = target.to("xpu")
```

5. Use Auto Mixed Precision (AMP)

Use automatic mixed-precision (AMP) with BFloat16 data type with the *torch.xpu.amp.autocast* context manager

```
with torch.xpu.amp.autocast(enabled=True, dtype=torch.bfloat16):
```

Hands-on Session

- Navigate to the PyTorch exercises directory

```
$ cd $SCRATCH/aces_pvc_course_24s/pytorch/exercises
```

- Open the exercise file (*cifar10_pvc_todo.py*) with your preferred editor (e.g. vim) or the file editor of the OnDemand portal.
- Complete the **#Todos** in the *cifar10_pvc_todo.py* file.
- Modify the Slurm job file (*pt_cifar10_pvc.slurm*) and submit your job.

```
$ sbatch pt_cifar10_pvc.slurm
```

Lab IV. TensorFlow on PVC



Install Intel Extension for Tensorflow

The Intel Extension for Tensorflow is based the on Tensorflow PluggableDevice interface to bring Intel XPU (GPU, CPU, etc) devices into Tensorflow.

To check the version, add import statement to the beginning of your script:

```
import intel_extension_for_tensorflow as itex
print(itex.__version__)
```

The default device will be Intel GPU after installing `intel-extension-for-tensorflow`

Source: Intel presentation at ACES Workshop

No Code Changes are Needed!



Credit: Bing Chat Enterprise

Hands-on Session

- Navigate to the TensorFlow exercises directory

```
$ cd $SCRATCH/aces_pvc_course_24s/tensorflow/exercises
```

- Open the exercise file (*cifar10_pvc.py*) with your preferred editor (e.g. vim) or the file editor of the OnDemand portal.
- Read through the code to verify that there are no code changes
- Modify the Slurm job file (*tf_cifar10_pvc.slurm*) and submit your job.

```
$ sbatch tf_cifar10_pvc.slurm
```

```
##### TODO #####  
#uncomment below lines to run the cifar-10 exercise  
# cd $SCRATCH/aces_pvc_labs_24s/tensorflow/exercises  
# python cifar10_pvc.py  
##### END TODO #####
```


PVC Monitoring Tools

- View the pvc nodes and number of GPUs

```
$ pstat -p pvc -G
```

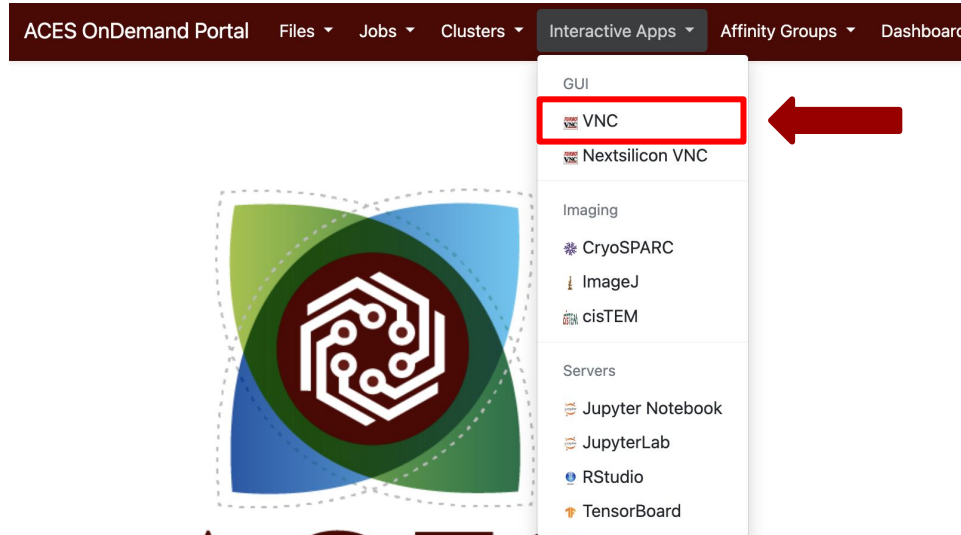
- Monitor the system activity

```
$ watch -n 5 sysmon
```

- Intel XPU manager

```
$ watch -n 5 xpumcli stats -d <device index>
```

Start a VNC job



The screenshot shows the ACES OnDemand Portal navigation bar with the following items: ACES OnDemand Portal, Files, Jobs, Clusters, Interactive Apps, Affinity Groups, and Dashboard. The 'Interactive Apps' dropdown menu is open, listing the following categories and items:

- GUI
 - VNC (highlighted with a red box and a red arrow pointing to it)
 - Nextsilicon VNC
- Imaging
 - CryoSPARC
 - ImageJ
 - cisTEM
- Servers
 - Jupyter Notebook
 - JupyterLab
 - RStudio
 - TensorBoard

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VNC Form

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

Home / My Interactive Sessions / VNC

Interactive Apps

- GUI
- VNC**
- Nextsilicon VNC
- Imaging
- CryoSPARC
- ImageJ
- cisTEM
- Servers
- Jupyter Notebook
- JupyterLab
- RStudio
- TensorBoard

VNC

This app will launch a [VNC](#) job on [ACES](#) for remote visualization.

Node type

Intel GPU Max (PVC) ▾

- select a non-CPU node type only if your software supports the Accelerator

Number of GPUs

1

- Current GPU Node Configuration
 - 13 x H100:2
 - 6 x PVC:4
 - 1 x H100:4
- Current GPU Node Availability
 - 5 x PVC:4
 - 1 x H100:1*
 - 1 x PVC:3*

Number of hours (max 48)

1

Number of cores (max 96)

3

Interactive Apps [Sandbox]

- Servers

Fields:

Node Type: Intel GPU Max (PVC)

Number of GPUs: 1

Number of hours: 1

Number of cores: 3

Total memory (GB): 5

Launch VNC

ACES OnDemand Portal Files Jobs Clusters Interactive Apps Affinity Groups Dashboard

Session was successfully deleted. X

Home / My Interactive Sessions

Interactive Apps

- GUI
- VNC
- Nextsilicon VNC
- Imaging
 - CryoSPARC
- ImageJ
- cisTEM
- Servers
 - Jupyter Notebook
 - JupyterLab
 - RStudio
 - TensorBoard

VNC (28902) 1 node | 3 cores | Running

Host: >_ac026 Delete


Created at: 2023-11-06 15:49:00 CST

Time Remaining: 56 minutes

Session ID: 83fc469d-4f99-4b4e-a8b1-39e6a343ba80

Compression Image Quality
0 (low) to 9 (high) 0 (low) to 9 (high)

Launch VNC View Only (Share-able Link)



```
My Interactive Sessions - ACE x TurboVNC: ac026:2 (u.zh1086 x +
portal-aces.hprc.tamu.edu/pun/sys/dashboard/noVNC-1.3.0/...
@ac026:/scratch/user/ /aces_pvc_course/pytorch/exercises
ses]$ pwd
/aces_pvc_course/pytorch/exercises
ses]$ ml purge
ses]$ ml intel/AIKit/2023.2.0
ses]$ ml intel/2023.07
ses]$ source activate aikit-pt-gpu-clone
(aikit-pt-gpu-clone) @ac026 exercises]$ python cifar10_pvc_solution.py > out.txt 2>&1 &
[1] 275895
(aikit-pt-gpu-clone) @ac026 exercises]$ watch sysmon

Every 2.0s: sysmon

-----
GPU 0: Intel(R) Data Center GPU Max 1100   PCI Bus: 0000:21:00.0
Vendor: Intel(R) Corporation   Driver Version: 1.3.26516   Subdevices: 0
EU Count: 448   Threads Per EU: 8   EU SIMD Width: 16   Total Memory(MB): 46679.2
Core Frequency(MHz): 200.0 of 1550.0   Core Temperature(C): unknown
-----

Running Processes: 3
  PID, Device Memory Used(MB), Shared Memory Used(MB), GPU Engines, Executable
  4793,          5.1,          0.0, COMPUTE, /usr/bin/xpumd
 279895,      6888.2,          0.0, COMPUTE;DMA, python ←
 280095,          1.8,          0.0, UNKNOWN, sysmon
```

Acknowledgement

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- NSF award number 2112356 ACES - Accelerating Computing for Emerging Sciences,
- NSF award number 1925764 SWEETER - SouthWest Expertise in Expanding, Training, Education and Research,
- NSF award number 2019129 FASTER - Fostering Accelerated Scientific Transformations, Education, and Research,
- Dumni Aribuki from Intel,
- Staff and students at Texas A&M High Performance Research Computing.



High Performance Research Computing

DIVISION OF RESEARCH

<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

Help us help you. Please include details in your request for support, such as, Cluster (ACES, Faster, Grace, Terra, ViDaL), UserID, Job information (Job id(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.