Ab initio Molecuar Dynamics on NEC VE

2025 ACES Workshop

Lisa Perez

July 20, 2025

High Performance
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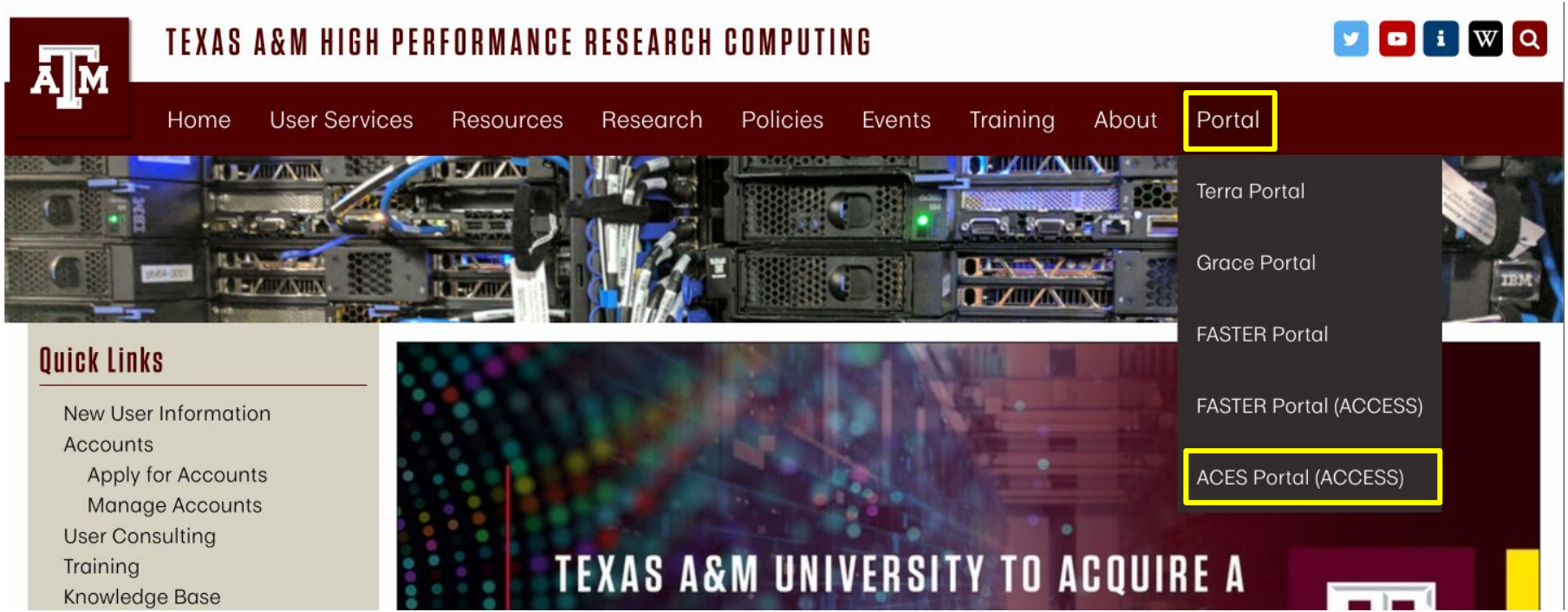
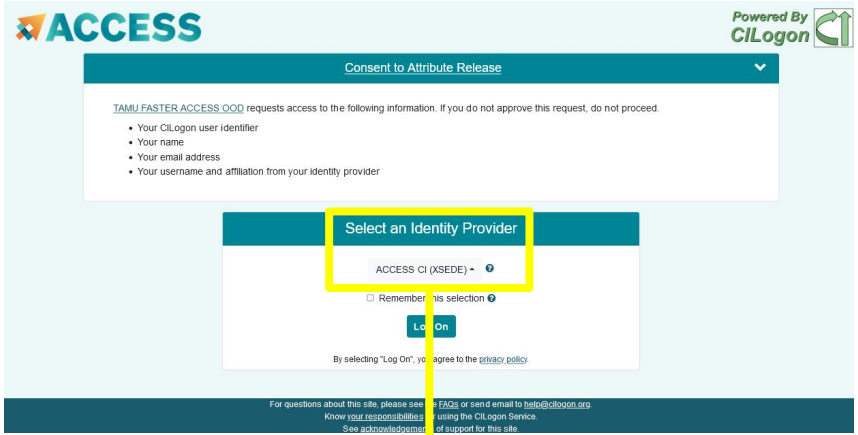
Log into ACES Using the HPRC Portal

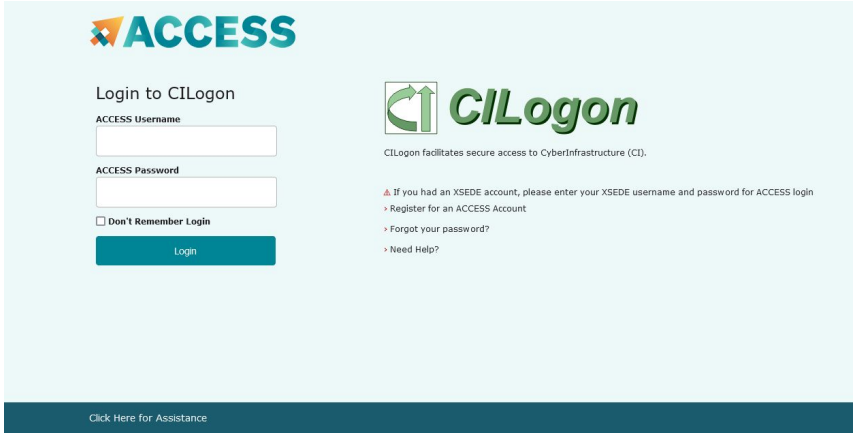
- HPRC webpage: https://hprc.tamu.edu/, Portal dropdown menu

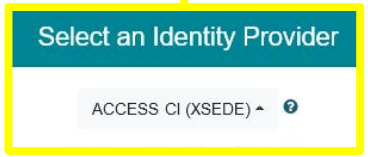


Accessing ACES via the ACES Portal (ACCESS)

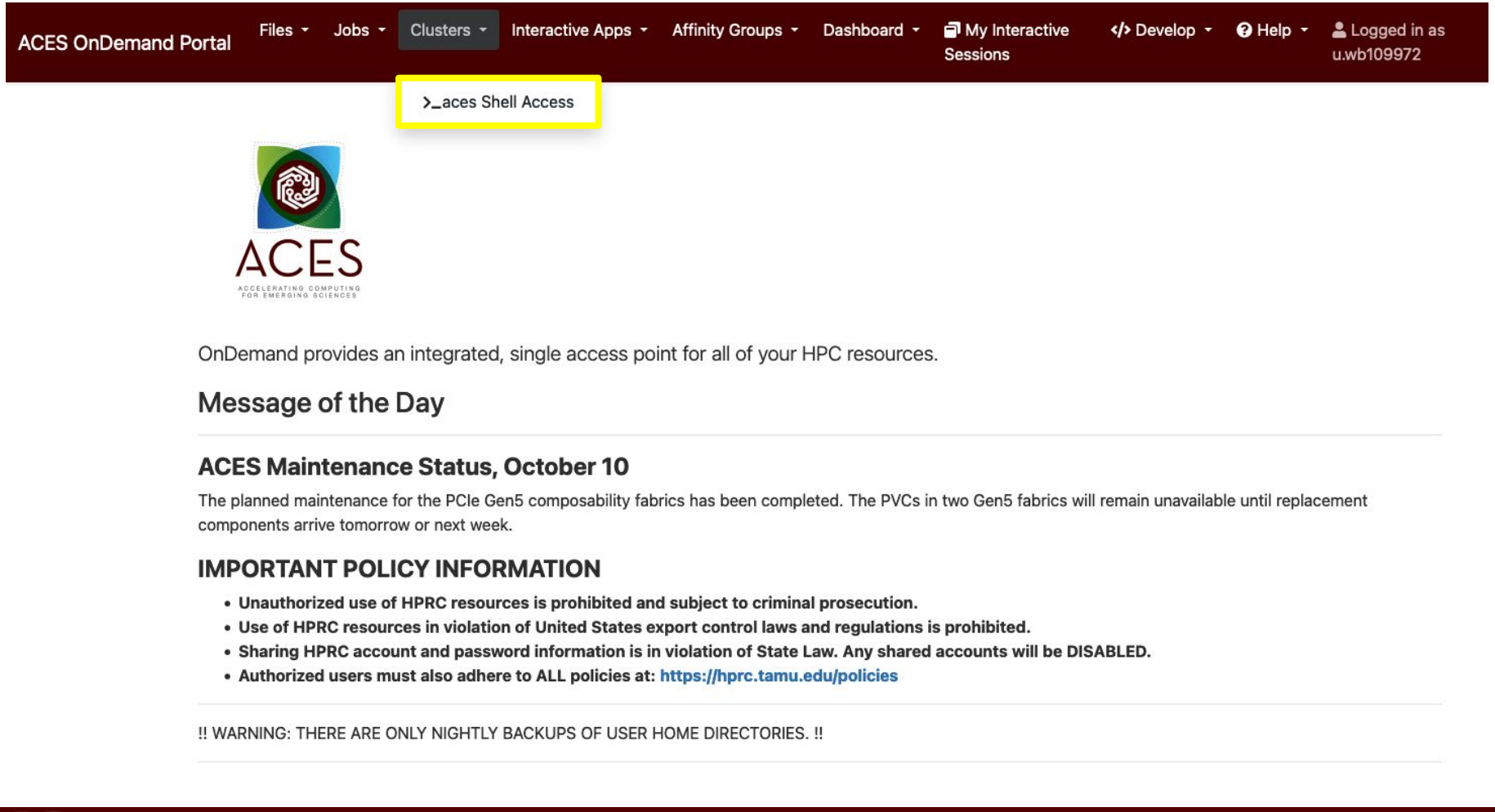
Log-in using your ACCESS credentials.







Select the Identity Provider appropriate for your account.


ACES OnDemand Portal
Files
Jobs
Clusters
Interactive Apps
Affinity Groups
Dashboard
My Interactive Sessions
Develop
Help
Logged in as u.wb109972
>_aces Shell Access
ACES
ACCELERATING COMPUTING FOR EMERGING SCIENCES
OnDemand provides an integrated, single access point for all of your HPC resources.
Message of the Day
ACES Maintenance Status, October 10
The planned maintenance for the PCIe Gen5 composability fabrics has been completed. The PVCs in two Gen5 fabrics will remain unavailable until replacement components arrive tomorrow or next week.
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. !!

VASP - Vienna Ab initio Simulation Package

The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling from first principles.

Licensed Software

For VASP License holders, to access the VASP install on ACES, send a request to help@hprc.tamu.edu with the following information:

- Name
- E-mail
- License Holder Name
- License Holder E-mail
- License Number

https://vasp.at

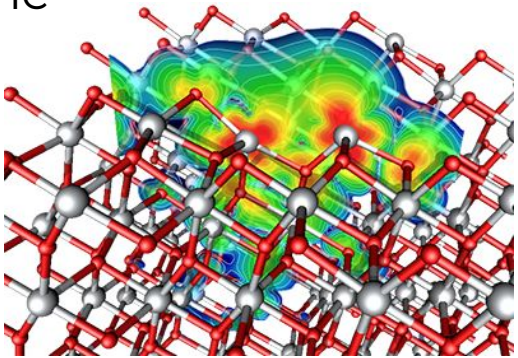


Image Credit: https://www.nec.com/en/global/solutions/hpc/articles/tech24.html

VASP Tutorial Setup

```
# change to your scratch space
cd $SCRATCH

# Download the tutorial files from the VASP website:
curl -O https://www.vasp.at/tutorials/latest/md-part1.zip

# Unzip the file
unzip md-part1.zip

# Change directory
cd MD/e01_solid-cd-Si

#Copy POSCAR (also available on the VASP tutorial page)& ve.job
cp /scratch/training/nec/vasp/MD/e01_solid-cd-Si/POSCAR  .
cp /scratch/training/nec/vasp/ve.job .
```

ACES Vector Engine Node

```
sbatch ve.job
```

- dss node:
  - Dell DSS8440
  - 8 NEC Vector Engine Cards
  - 48 core (2 sockets with 24-core per socket)
    - Intel Xeon 8268 (Cascade Lake)
  - 768 GB DDR4 Memory

Environment to run VASP on NEC VE

```
#setup your environment for NEC VE compiler libraries
export PATH=/opt/nec/ve/bin/:$PATH
source /opt/nec/ve/mpi/3.4.0/bin64/necmpivars.sh

#setup environment for vasp
export VASPHOME=/sw/restricted/vasp/sw/6.3.2/nec_5.0.1/

#Turn on printing details about VE card usage
export VE_PROGINF=DETAIL

#create an alias or bash script named vasp_rm for the following command:
# rm -f CHG CHGCAR CONTCAR STOPCAR DOSCAR DYNMAT EIGENVAL IBZKPT OPTIC
OSZICAR OUTCAR PROCAR PCDAT WAVECAR XDATCAR PARCHG vasprun.xml REPORT
wannier90.win wannier90_band.gnu wannier90_band.kpt wannier90.chk
wannier90.wout vaspout.h5 PENALTYPOT HILLSPOT ML_LOGFILE ML_ABN ML_FFN
ML_HIS ML_REG
```

Runing VASP using the NEC VE card

```
#Run the job using 1 VE card and 2 vector engine processes
mpirun -ve 0 -vennp 2 $VASPHOME/bin/vasp_gam >& 1ve_2vep_out.log

#clean up using the vasp_rm command
vasp_rm

#Run the job using 1 VE card and 8 vector engine processes
mpirun -ve 0 -vennp 8 $VASPHOME/bin/vasp_gam >& 1ve_8vep_out.log

#Run the job using 4 VE cards and 2 vector engine processes per card
vasp_rm;mpirun -ve 0-3 -vennp 2 $VASPHOME/bin/vasp_gam >&
4ve_8vep_out.log

#Run the job using 8 VE cards and 2 vector engine processes per card
vasp_rm;mpirun -ve 0-7 -vennp 2 $VASPHOME/bin/vasp_gam >& 8ve_16_out.log
```

Texas A&M HPRC at PEARC25

Tutorials and Workshop	Date/Time	Room
Tutorial: ACES Tutorial for using Graphcore Intelligence Processing Units (IPUs) for AI/ML Workflows	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room A213
Tutorial: Open OnDemand Overview, Customization, and App Development	Mon, July 21, 2025 1:30 AM-5:00 PM ET	Room A226
Workshop: Collaborating with K12 Schools: Supporting Secondary Students and Teachers in Computing	Mon, July 21, 2025 1:30 PM-5:00 PM ET	Room B132

Texas A&M HPRC at PEARC25

Presentations and BoF	Date/Time	Room
WFT&E-2-3: ByteBoost: An advanced cybertraining program designed to enhance research on testbed systems	Tue, July 22, 2025 11:50 AM-12:05 PM ET	Room A216
A&SW-2-5: Generating Scientific Workflows With Drona Environments	Tue, July 22, 2025 12:00 PM-12:15 PM ET	Room A220-A221
WFT&E-3-2: Empowering NAIRR "Pilots" of all skill levels to become "ACES" with HPC	Tue, July 22, 2025 2:15 PM-2:30 PM ET	Room A114-A115
WFT&E-5-4: Exploring the Role of Academics, Research and Workforce Development in Establishing Research Computing Collaborations	Wed, July 23, 2025 11:55 AM-12:10 PM ET	Room A114-A115
A&SW-6-2: Comparison of GPU Performance Scaling for Molecular Dynamics	Wed, July 23, 2025 2:15 PM-2:30 PM ET	Room A212-A213
BOF-18: Node to Joy: Finding the Right Compute Resources	Wed, July 23, 2025 4:15 PM-5:15 PM ET	Room A213-A215

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Thank you

- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES), #2019129 (FASTER) and #19257614 (SWEETER)

- Please visit our talks and BoF at PEARC25
- Helpdesk: help@hprc.tamu.edu