

# *Ab initio* Molecular Dynamics on NEC VE

2025 ACES Workshop

Lisa Perez  
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High Performance  
Research Computing  
DIVISION OF RESEARCH



# Log into ACES Using the HPRC Portal

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

**ATM** TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING

Home User Services Resources Research Policies Events Training About **Portal**

Terra Portal  
Grace Portal  
FASTER Portal  
FASTER Portal (ACCESS)  
**ACES Portal (ACCESS)**

**Quick Links**

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

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# Accessing ACES via the ACES Portal (ACCESS)

Log-in using your ACCESS credentials.

The screenshot shows the ACCESS portal interface. At the top left is the ACCESS logo, and at the top right is the 'Powered By CILogon' logo. Below the logo is a 'Consent to Attribute Release' section with a dropdown arrow. The consent text states: 'TAMU FASTER ACCESS OOD requests access to the following information. If you do not approve this request, do not proceed.' followed by a bulleted list: 'Your CILogon user identifier', 'Your name', 'Your email address', and 'Your username and affiliation from your identity provider'. Below the consent section is a 'Select an Identity Provider' dropdown menu. The selected option is 'ACCESS CI (XSEDE)' with a question mark icon. Below the dropdown is a 'Log On' button. At the bottom, there is a footer with links for 'For questions about this site, please see the FAQs or send email to help@cilogon.org', 'Know your responsibilities using the CILogon Services', and 'See acknowledgements of support for this site'.

The screenshot shows the ACCESS portal login interface. At the top left is the ACCESS logo, and at the top right is the CILogon logo. Below the logo is a 'Login to CILogon' section with two input fields: 'ACCESS Username' and 'ACCESS Password'. Below the password field is a checkbox labeled 'Don't Remember Login'. A 'Login' button is at the bottom. To the right of the login form, there is a note: 'CILogon facilitates secure access to CyberInfrastructure (CI).'. Below this note are three links: 'If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login', 'Register for an ACCESS Account', 'Forgot your password?', and 'Need Help?'.

This is a close-up of the 'Select an Identity Provider' dropdown menu. The selected option is 'ACCESS CI (XSEDE)' with a question mark icon.

Select the Identity Provider appropriate for your account.



[>\\_aces Shell Access](#)

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](mailto:help@hprc.tamu.edu) with the following information:

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



<https://vasp.at>

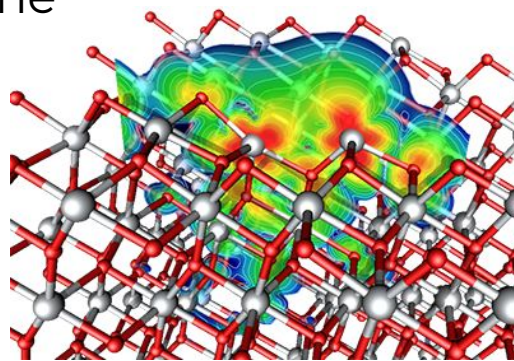


Image Credit: <https://www.nec.com/en/global/solutions/hpc/articles/tech24.html>



# 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

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

