

VASP on NEC Vector Engine

07/15/2023

ACES Workshop



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

TEXAS A&M UNIVERSITY TO ACQUIRE A

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 text "Powered By CILogon" with the CILogon logo. Below the header is a teal bar with the text "Consent to Attribute Release" and a dropdown arrow. Underneath is a white box containing the text "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 this is a teal bar with the text "Select an Identity Provider". Underneath is a white box with a dropdown menu showing "ACCESS CI (XSEDE)" and a question mark icon. Below the dropdown is a checkbox labeled "Remember this selection" and a teal "Log On" button. At the bottom of the white box is the text "By selecting 'Log On', you agree to the [privacy policy](#)". At the bottom of the teal bar is the text "For questions about this site, please see [FAQs](#) or send email to help@cilogon.org. Know your responsibilities using the CILogon Service. See <https://www.cilogon.org/support> for support for this site."

The screenshot shows the ACCESS portal login page. At the top left is the ACCESS logo, and at the top right is the CILogon logo. Below the header is the text "Login to CILogon". Underneath are two input fields: "ACCESS Username" and "ACCESS Password". Below the password field is a checkbox labeled "Don't Remember Login". At the bottom of the form is a teal "Login" button. To the right of the form is the CILogon logo and the text "CILogon facilitates secure access to CyberInfrastructure (CI)". Below this are several 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?". At the bottom of the teal bar is the text "Click Here for Assistance".

This is a close-up of the "Select an Identity Provider" dropdown menu. The dropdown is highlighted with a yellow border and shows the text "ACCESS CI (XSEDE)" followed by a question mark icon.

Select the Identity Provider appropriate for your account.

Shell access via the HPRC Portal



ACES Vector Engine Node

- From the ACES login node, ssh into the dss
 - `ssh dss`
- 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

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>

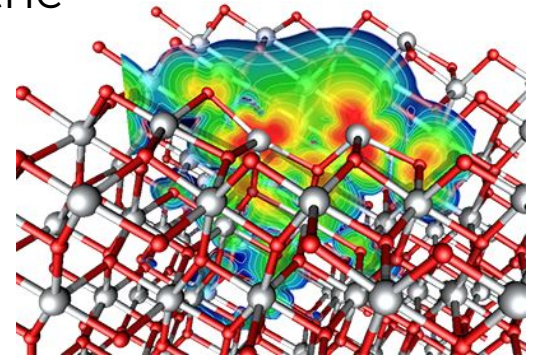


Image Credit: <https://www.nec.com/en/global/solutions/hpc/articles/tech24.html>

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)
cp /scratch/training/nec/vasp/MD/e01_solid-cd-Si/POSCAR .
```

Setup Your Environment and Run VASP

```
#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
```


Run VASP using the 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
```



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

<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), 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.

