HIGH PERFORMANCE RESEARCH COMPUTING

Ab initio Molecular Dynamics on NEC VE

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High Performance
Research Computing
DIVISION OF RESEARCH

Molecular Dynamics

- Computer simulation technique used to analyze the physical movements of atoms and molecules over time:
  Newton's laws of motion

- Calculate the forces acting on each atom and update their positions and velocities over each time step:
  ***Ab initio*, semi-empirical, classical**

Ab initio Simulation

- Uses first principles through quantum mechanics to simulate the motion of atoms in a system:
  Density Functional Theory

- Does not rely on empirical potentials or force fields:
  Plane waves & pseudopotentials

Ab initio Molecular Dynamics

- Structure stability
- Diffusion processes
- Phase transitions
- Surface and interface dynamics
- Reaction mechanism and pathways
- Thermal properties
- Solvation dynamics
- ……

Ab initio Molecular Dynamics

- AIMD exercise for VASP and Quantum ESPRESSO
  - 64-atom silicon supercell
  - finite-temperature (2000K)
  - 90 fs (30 steps, 3.0 fs time step)
  - NVT ensemble

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.

https://vasp.at

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

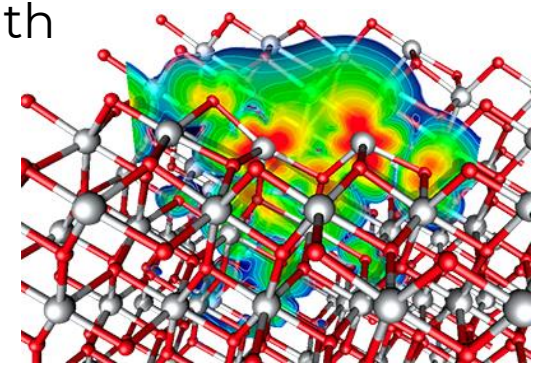


Image Credit: https://www.nec.com/en/global/solutions/hpc/articles/tech24.html

Quantum ESPRESSO

Quantum ESPRESSO is an integrated suite of open-source computer codes for electronic-structure calculations and materials modeling at the nanoscale.

- Completely free
- Highly customizable
- Strong community

https://www.quantum-espresso.org/

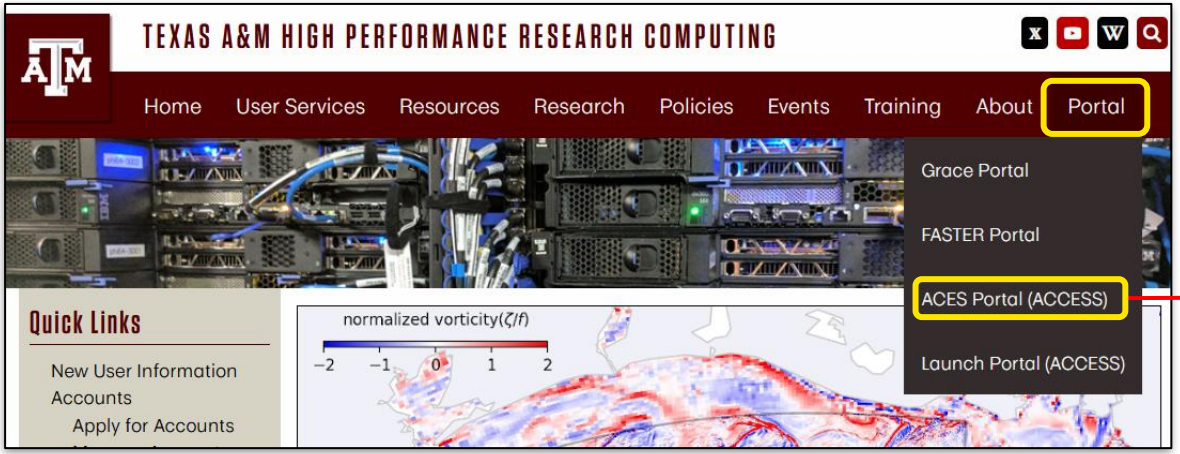
NEC Vector Engine Card

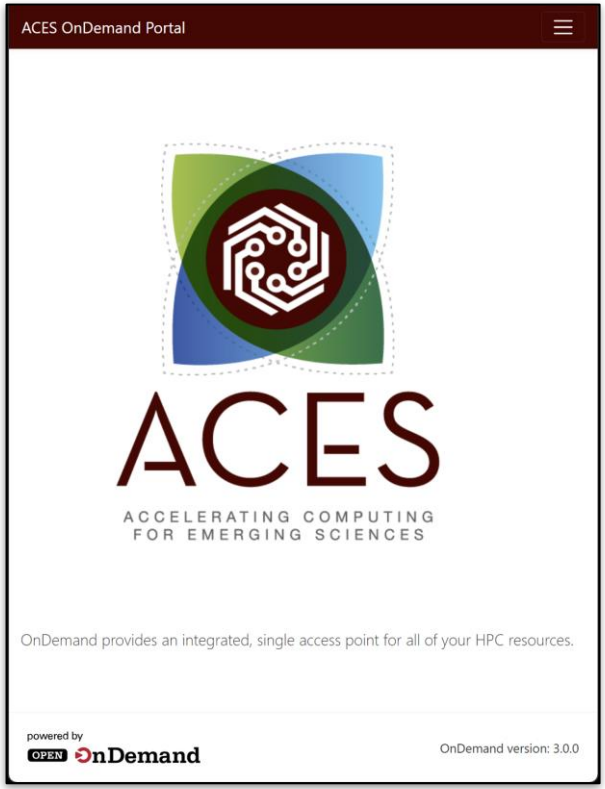
- 8 cores per processor
- 48GB on-chip memory
- Double precision
- Low power consumption

ACES Vector Engine Node

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

ACES Portal

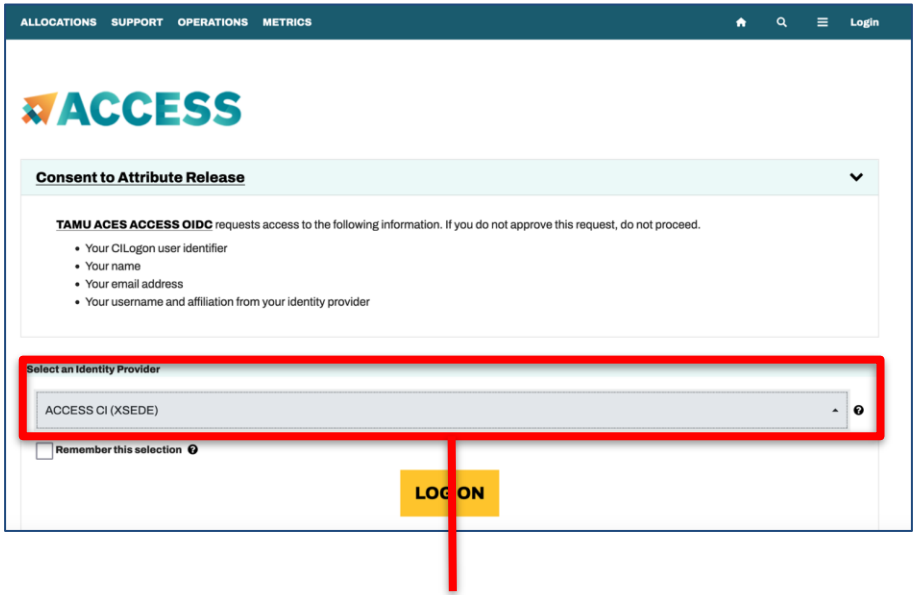




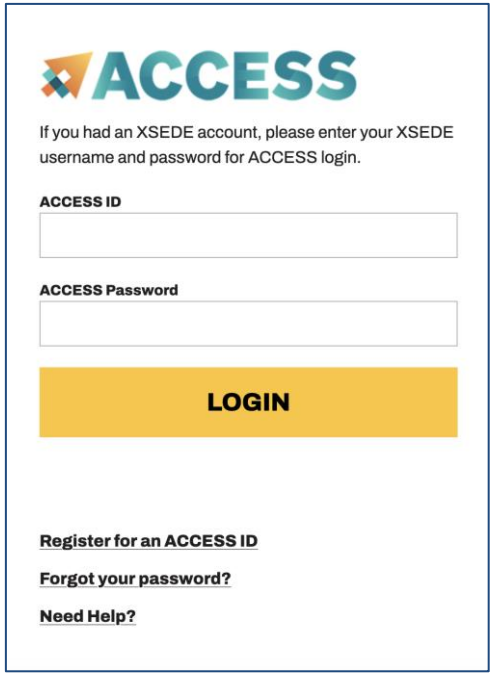
ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

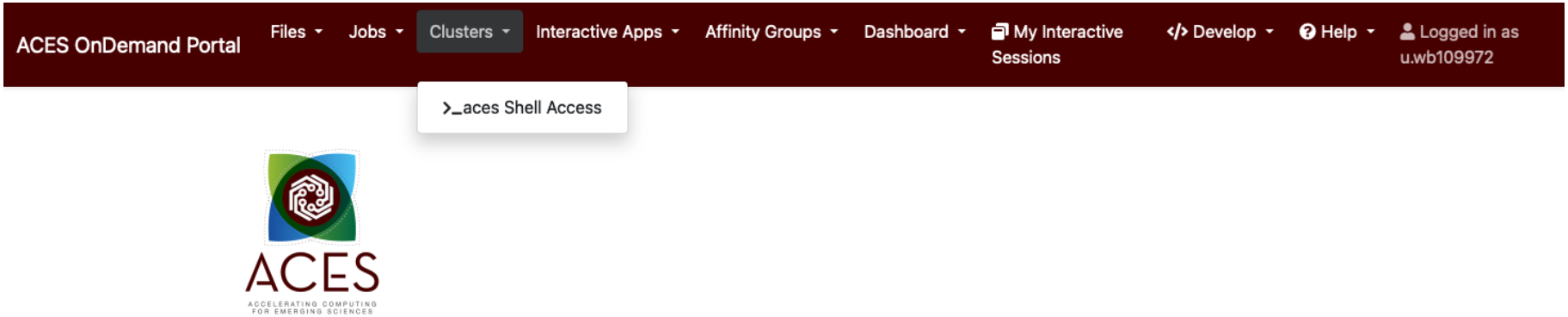
Open OnDemand (OOD) is an advanced web-based graphical interface framework for HPC users

Accessing ACES via the Portal (ACCESS)



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. !!

Tutorial Setup

Change to your scratch space
cd $SCRATCH

Download the tutorial files:
cp /scratch/training/nec/short_course/ve.zip .

Unzip the file
unzip ve.zip

Change directory
cd ./ve/vasp

Submit the VASP job to queue
sbatch ve-vasp.job

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

Running VASP on NEC VE

Run the job using 1 VE card and 2 vector engine processes
mpirun -ve 0 -vennp 2 $VASPHOME/bin/vasp_gam >& 1ve_02vep_out.log

Run the job using 1 VE card and 4 vector engine processes
mpirun -ve 0 -vennp 4 $VASPHOME/bin/vasp_gam >& 1ve_04vep_out.log

Run the job using 4 VE cards and 2 vector engine processes per card
mpirun -ve 0-3 -vennp 2 $VASPHOME/bin/vasp_gam >& 4ve_08vep_out.log

Run the job using 8 VE cards and 2 vector engine processes per card
mpirun -ve 0-7 -vennp 2 $VASPHOME/bin/vasp_gam >& 8ve_16vep_out.log

View time information from VASP results
grep -H "Real Time" *.log | awk '{a[$1]=$0} END{for(i in a) print a[i]}' | sort

Submitting QE Job on NEC VE

Change directory
cd $SCRATCH/ve/qe

Submit the QE job to queue
sbatch ve-qe.job

View wall time of each calculations
grep “PWSCF “ *out

Running QE on NEC VE

VE setup for QE
source /opt/nec/ve/mpi/3.4.0/bin/necmpivars-runtime.sh
export OMP_NUM_THREADS=1

Quantum ESPRESSO setup
EXE="-v /opt/nec/ve/bin/mpisep.sh /sw/hprc/sw/ve/QE/7.1/bin/pw.x"

Run the job using 1 VE cards and 2 vector engine processes per card
mpirun -nve 1 -vennp 8 $EXE -in $PWD/large-test.in &> $PWD/large-test_1ve_08vep.out

Run the job using 4 VE cards and 2 vector engine processes per card
mpirun -nve 4 -vennp 8 $EXE -in $PWD/large-test.in &> $PWD/large-test_4ve_32vep.out

Run the job using 8 VE cards and 2 vector engine processes per card
mpirun -nve 8 -vennp 8 $EXE -in $PWD/large-test.in &> $PWD/large-test_8ve_64vep.out

More MPI Options

mpirun -ve 0-3 -np 16 -vennp 4

- **-nve <N>:** Number of VEs to use (shortcut for -ve 0-<N-1>)
- **-ve <list>:** Explicitly select VE numbers (e.g., -ve 0-7, -ve 3, -ve 0,2,4)
- **-np <N>:** Total number of MPI processes
- **-vennp <N> or -ve_nnp <N>:** Number of MPI processes per VE (useful with -np)

Vector Engine Knowledge Base

- HPRC knowledge base Vector Engine page
  - https://hprc.tamu.edu/kb/User-Guides/ACES/vectorengine/
- NEC Compiler User's manuals
  - https://sxauroratsubasa.sakura.ne.jp/Documentation
- Detailed turning guide for the Vector Engine
  - https://sxauroratsubasa.sakura.ne.jp/wiki/images/6/6c/AuroraVE_TuningGuide.pdf

Need Help?

First check the FAQ

- Knowledge Base
- Send us a ticket using the dashboard tab on our web portal
- Email further questions to help@hprc.tamu.edu

Help us help you -- when you contact us, tell us:

- Which cluster you're using
- Your username
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used, if any
- Module(s) loaded, if any
- Error messages
- Steps you have taken, so we can reproduce the problem

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TEXAS A&M UNIVERSITY

https://hprc.tamu.edu

HPRC Helpdesk:

help@hprc.tamu.edu
Phone: 979-845-0219

Take our short course survey!

HPRC Survey

https://u.tamu.edu/hprc_shortcourse_survey

Help us help you. Please include details in your request for support, such as, **Cluster** (ACES, FASTER, Grace, Launch), NetID (UserID), Job information (**JobID**(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.

Acknowledgements

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- the National Science Foundation (NSF), award numbers:
  - 2112356 - ACES - Accelerating Computing for Emerging Sciences
  - 1925764 - SWEETER - SouthWest Expertise in Expanding, Training, Education and Research
  - 2019129 - FASTER - Fostering Accelerated Scientific Transformations, Education, and Research
- Staff and students at Texas A&M High-Performance Research Computing.
- ACCESS CCEP pilot program, Tier-II