VASP on NEC Vector Engine

07/15/2023
ACES Workshop
Log into ACES Using the HPRC Portal

- HPRC webpage: [https://hprc.tamu.edu/](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.
Shell access via the HPRC Portal

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isses Shell Access

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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
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

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

```bash
#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_AB
# 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
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.