HPC Workflow on Shaheen

(VASP as an Example)

Zhiyong Zhu
KAUST Supercomputing Core Lab
2022/09/13

Outline

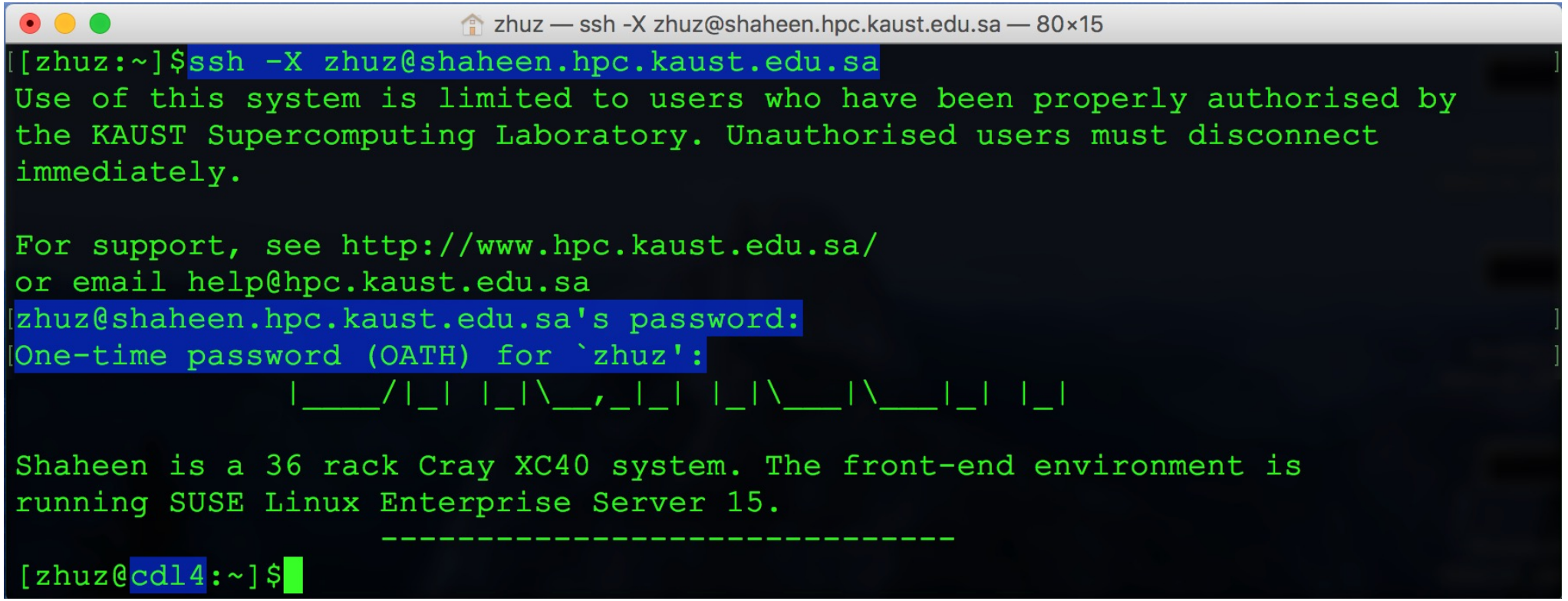
- Steps to Run
  - Use VASP as an example
    - The Vienna Ab-initial Simulation Package (VASP) is a computer program for atomic scale materials modeling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics from first-principles (https://www.vasp.at).
- Tips

Steps to Run

- Login Shaheen
- Check Code Availability
- Working Directory
- Prepare Input Files for VASP
- Prepare Jobscript for Slurm Job Scheduler
- Job Submission using Slurm Commands
- Check Output Files

Login Shaheen

- Login
  - ssh -X zhuz@shaheen.hpc.kaust.edu.sa

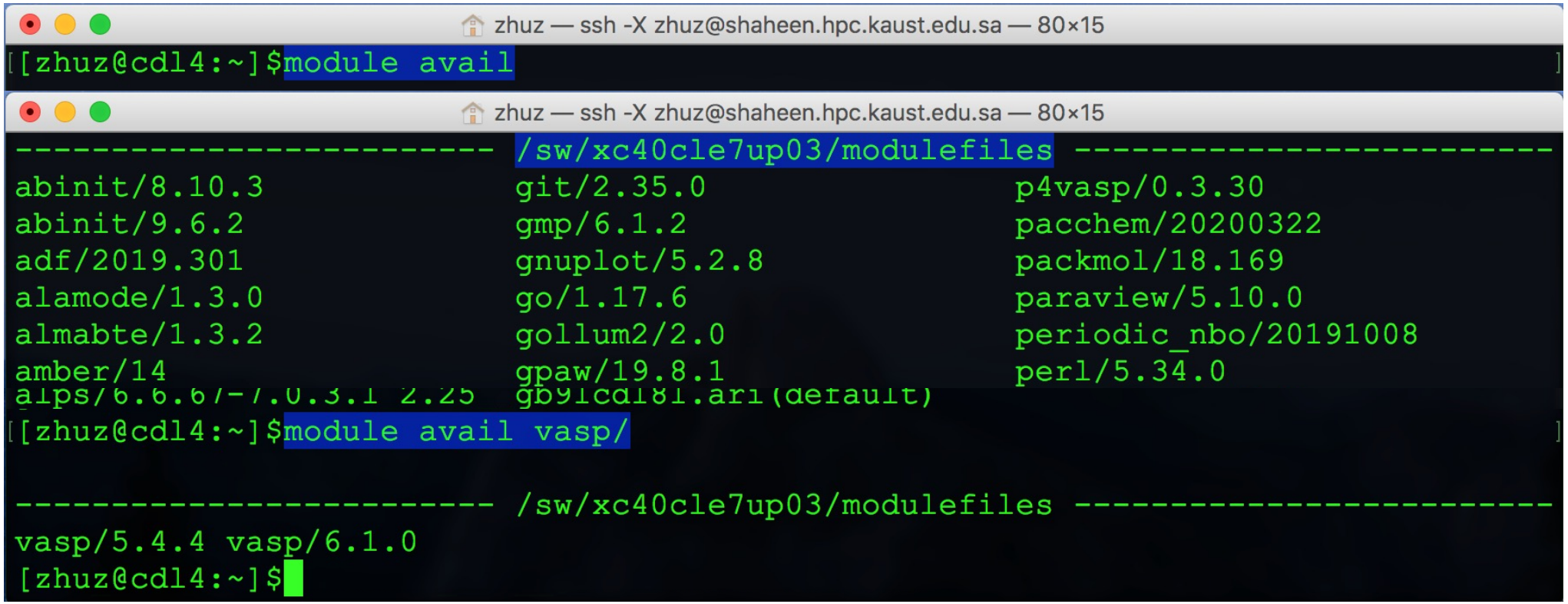


Code Availability

- On Shaheen login node:
  - module avail
- In /sw/xc40cle7up03 software stack:
  - ls -l /sw/xc40cle7up03
- From our website:
  - www.hpc.kaust.edu.sa/app7up03

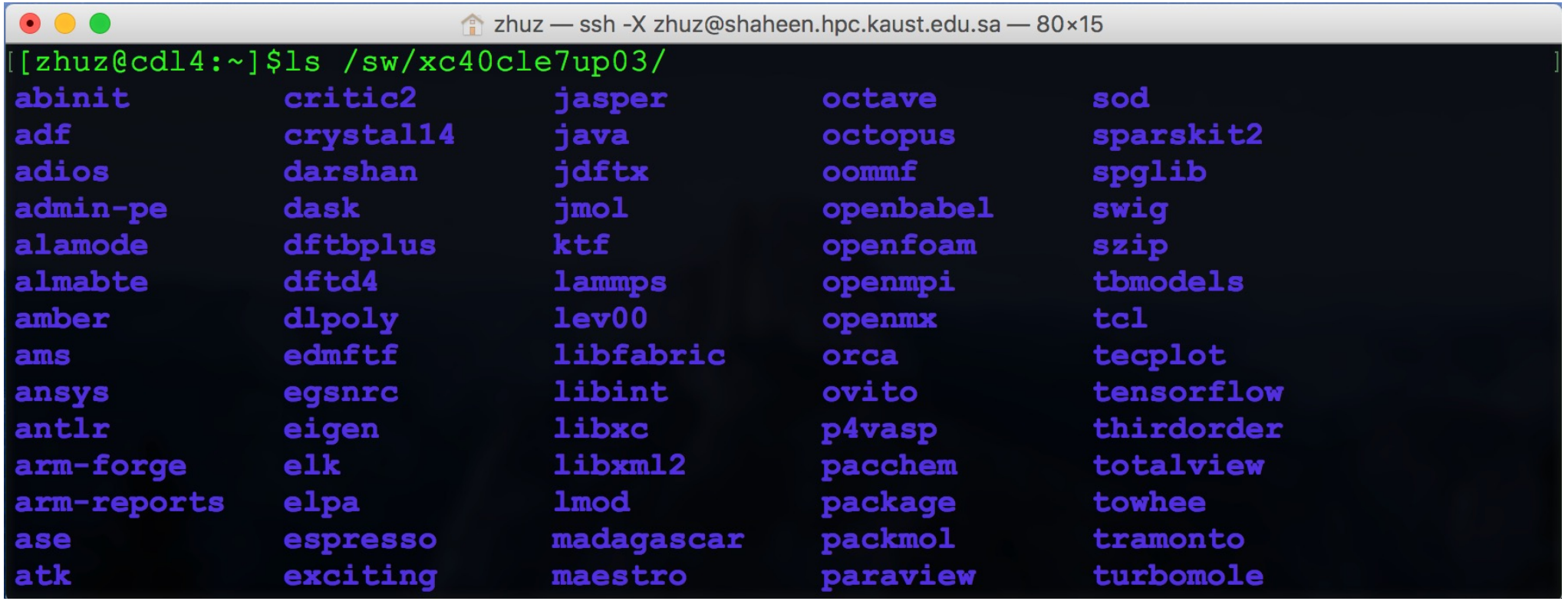
Code Availability

- module avail
  - module avail
  - module avail <code>/<version>



Code Availability

- ls -l /sw/xc40cle7up03



Code Availability

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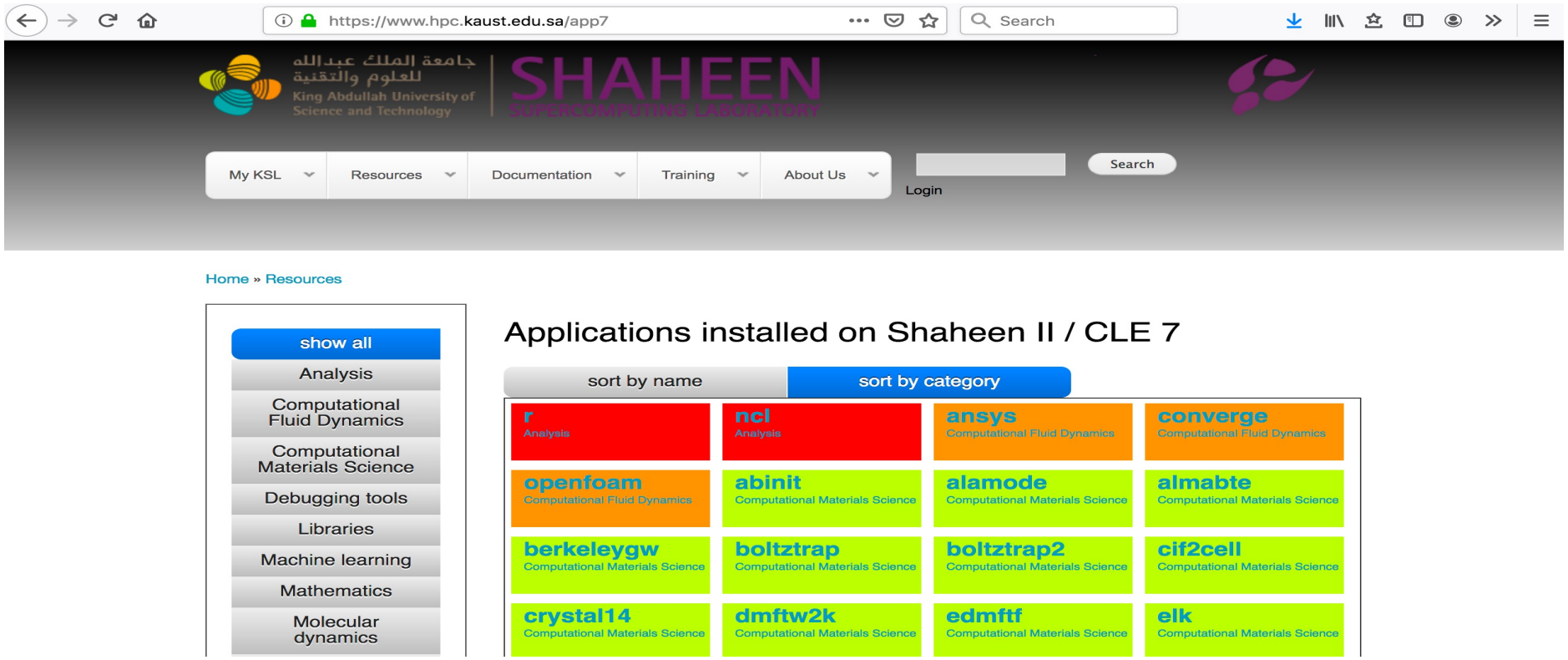
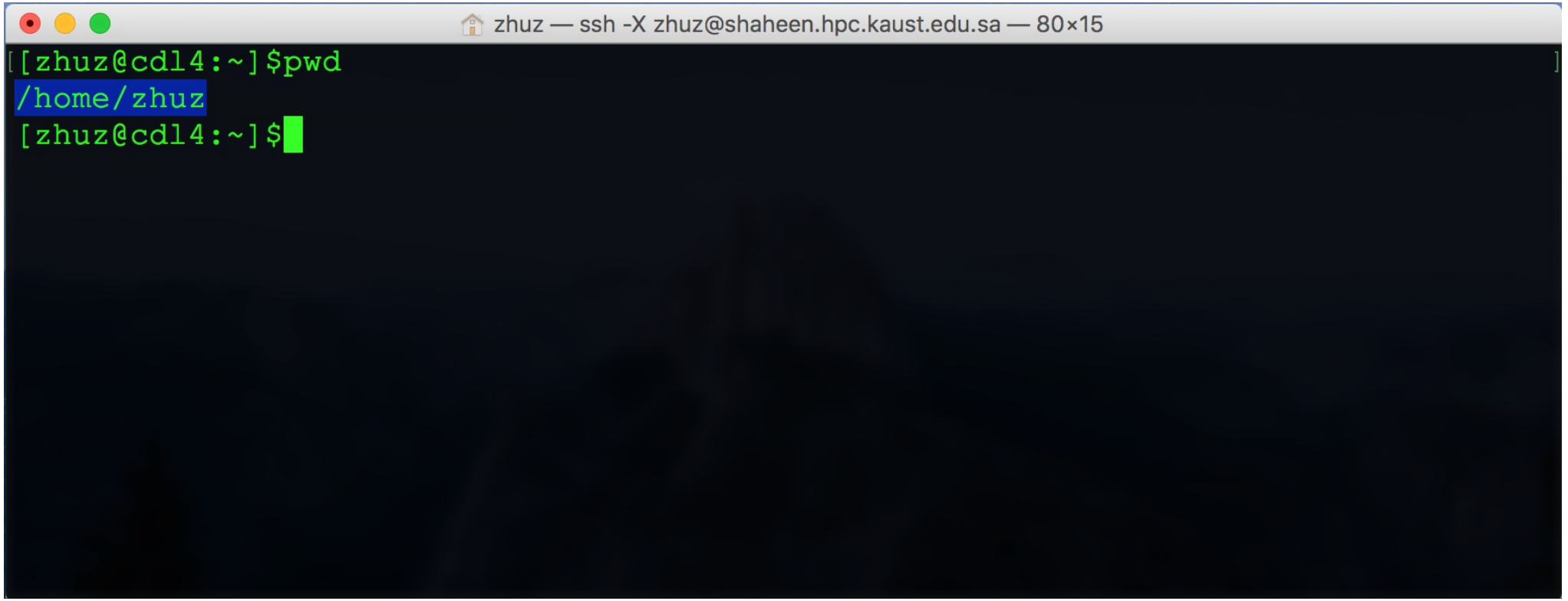


Code Availability

- From our website:
  - www.hpc.kaust.edu.sa/app7
- On Shaheen login node:
  - module avail
- In /sw/xc40cle7 software stack:
  - ls -l /sw/xc40cle7
- Not found?
  - help@hpc.kaust.edu.sa

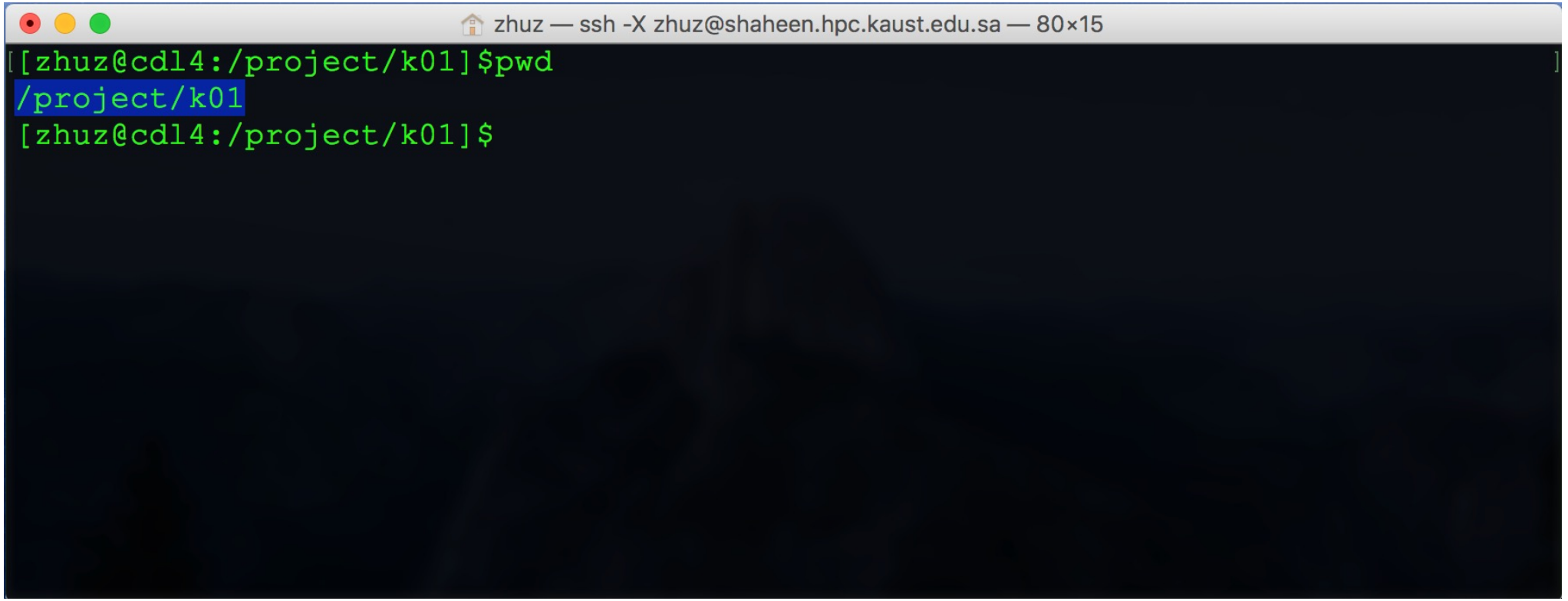
3 Different Working Directories

- /home
  - Very limited space; Not mounted on compute nodes (job submission will fail)



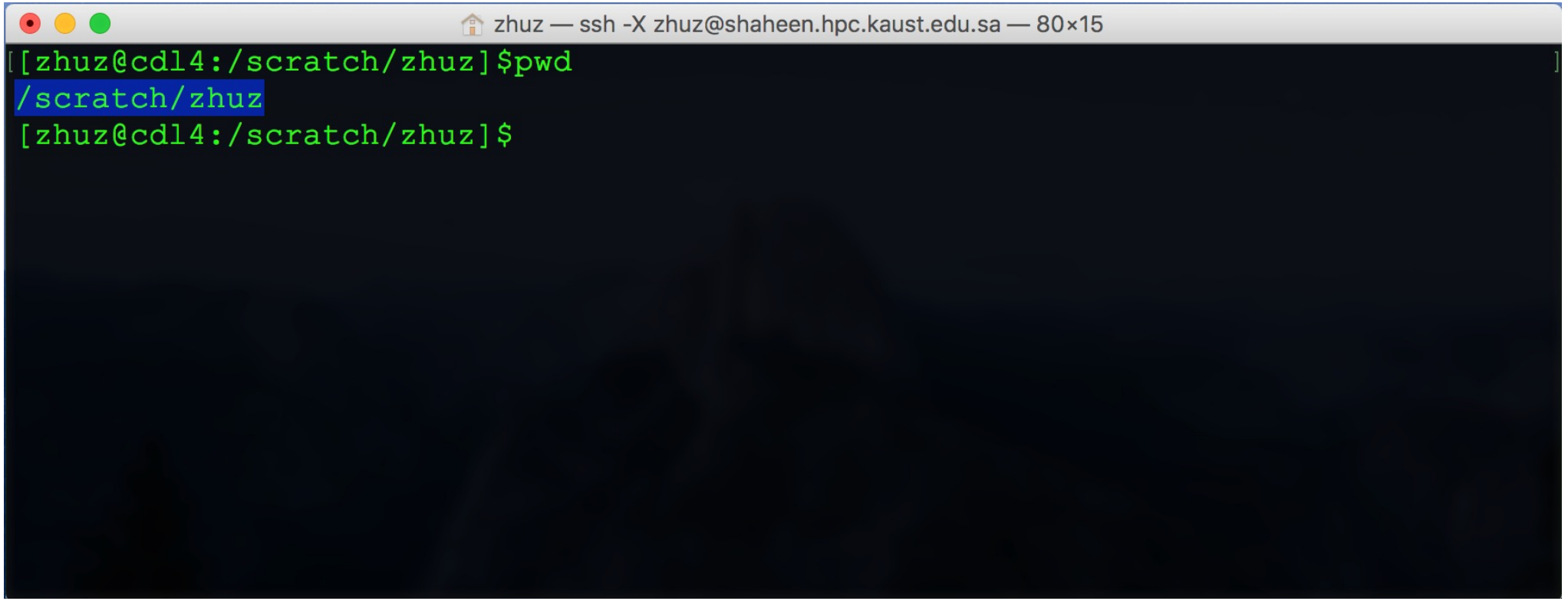
3 Different Working Directories

- /project/<projectname>
  - Read-only for compute nodes (job submission will fail); Used for data backup and data sharing



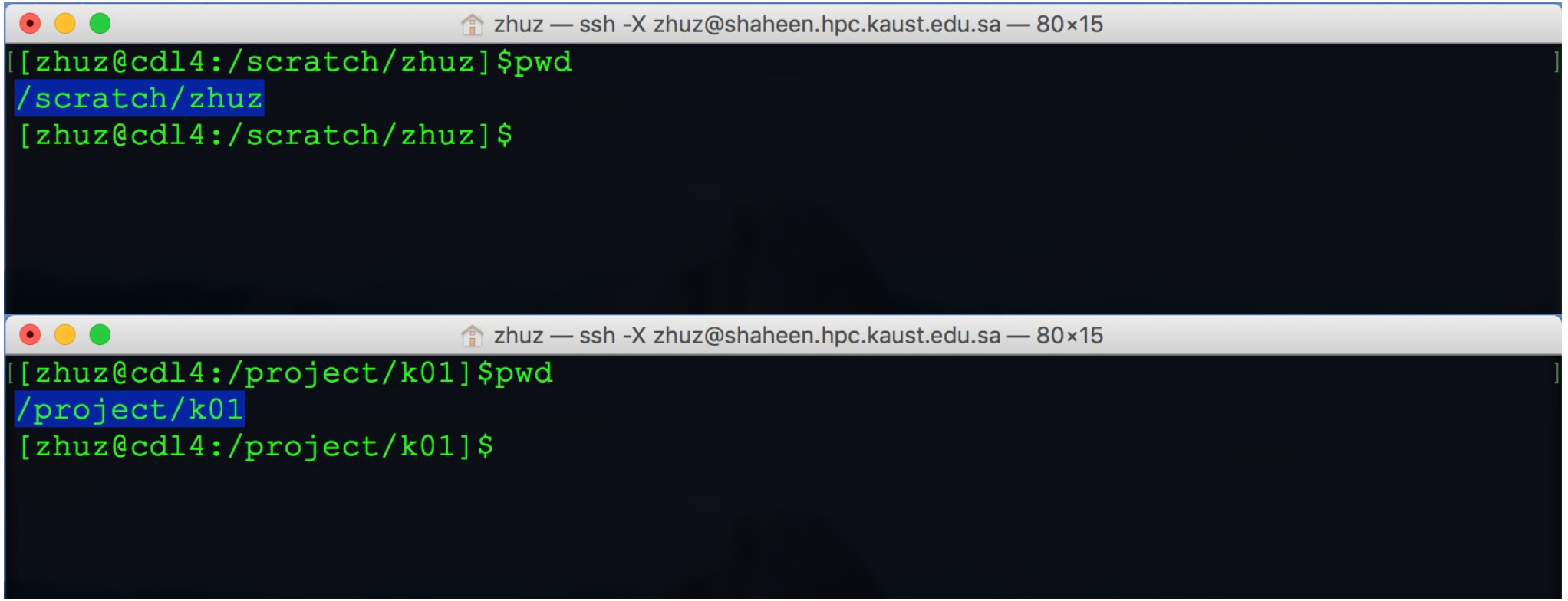
3 Different Working Directories

- /scratch/<username>
  - Almost unlimited space; Files older than 60 days are deleted automatically without warning



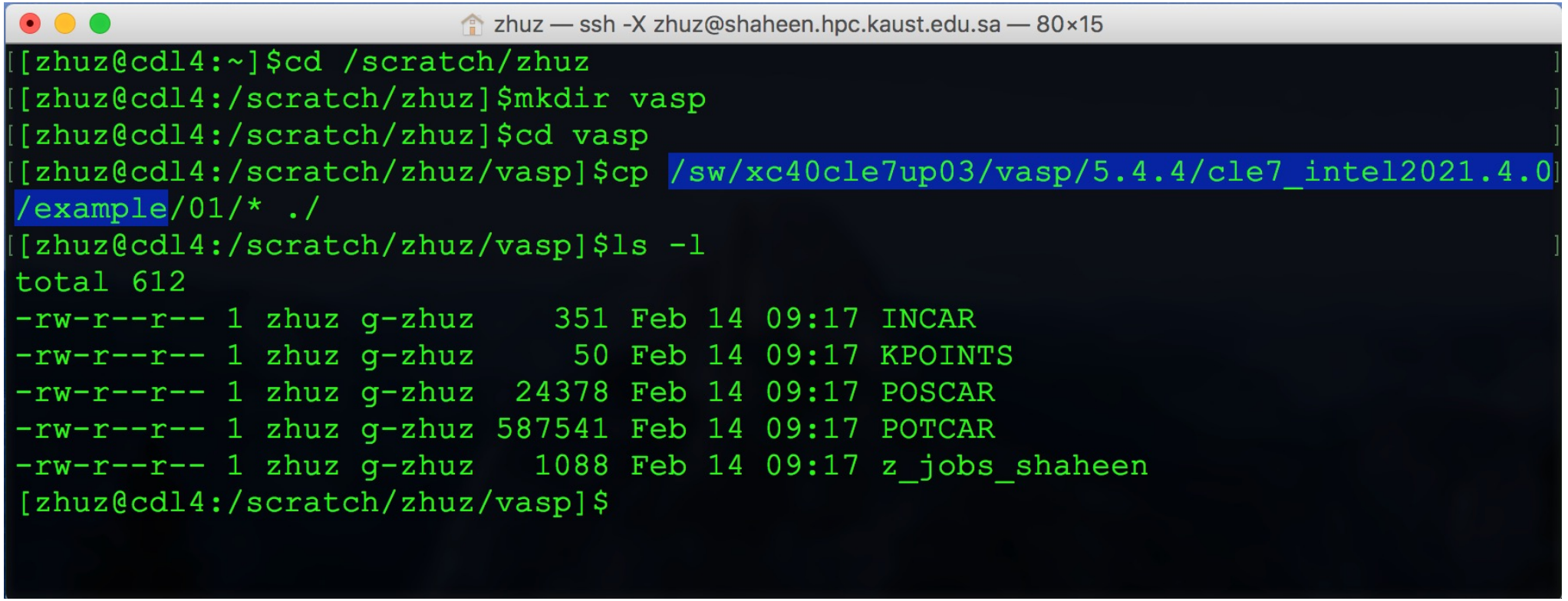
3 Different Working Directories

- Where to run? /scratch!
  - The only place to run
  - Remember to backup important data to /project



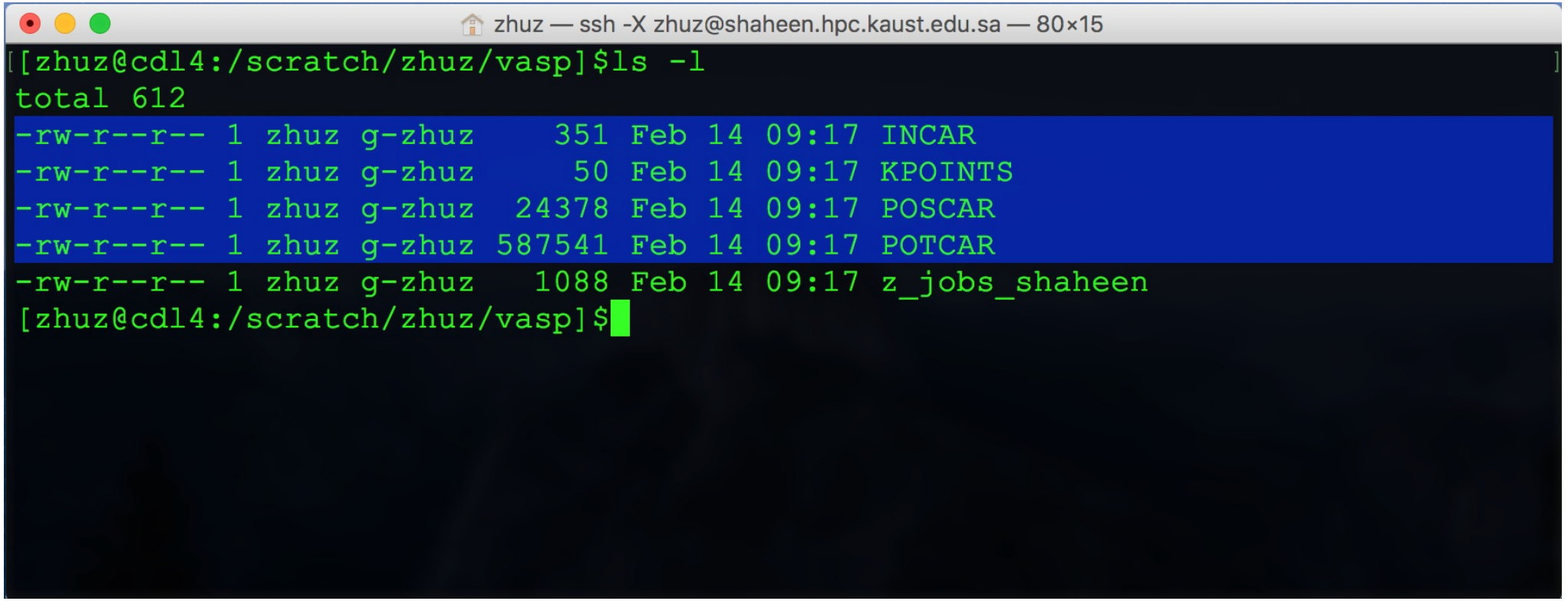
Prepare Input Files

- Examples under Installation Folder
  - /sw/xc40cle7up03/*code*/*ver*/*compilation*/example
  - Inputs for application; Jobscript for Slurm



Prepare Input Files

- VASP Input Files
  - Upload from local workstations (scp)
  - Modifying existing input files



Prepare Input Files

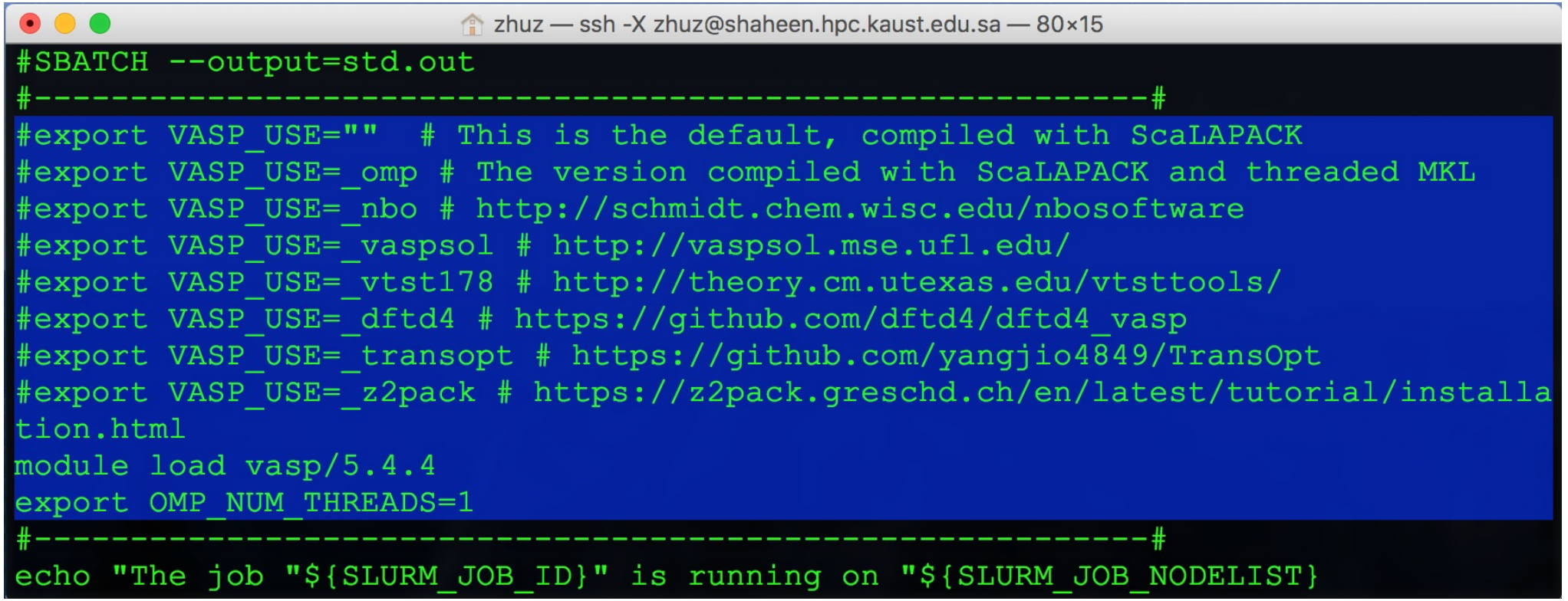
- Slurm Jobscript
  - SLURM directives

zhuz — ssh -X zhuz@shaheen.hpc.kaust.edu.sa — 80×15

```
[zhuz@cdl4:/scratch/zhuz/vasp]$more z_jobs_shaheen
#!/bin/bash
#SBATCH --partition=workq
#SBATCH --job-name="vasp"
#SBATCH --nodes=16
#SBATCH --time=4:00:00
#SBATCH --exclusive
#SBATCH --err=std.err
#SBATCH --output=std.out
#-----------------------------------------------------------#
#export VASP_USE=""  # This is the default, compiled with ScaLAPACK
#export VASP_USE=_omp # The version compiled with ScaLAPACK and threaded MKL
#export VASP_USE=_nbo # http://schmidt.chem.wisc.edu/nbosoftware
#export VASP_USE=_vaspsol # http://vaspsol.mse.ufl.edu/
#export VASP_USE=_vtst178 # http://theory.cm.utexas.edu/vtsttools/
```

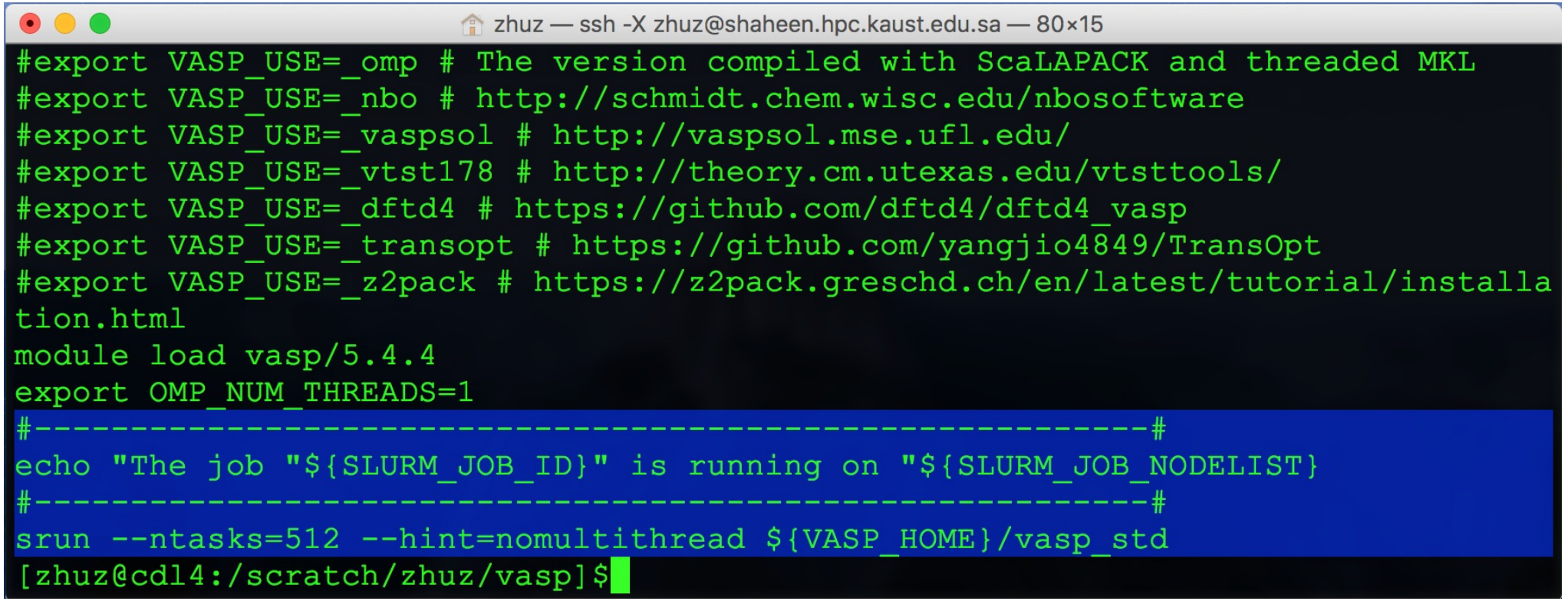
Prepare Input Files

- Slurm Jobscript
  - Environments settings



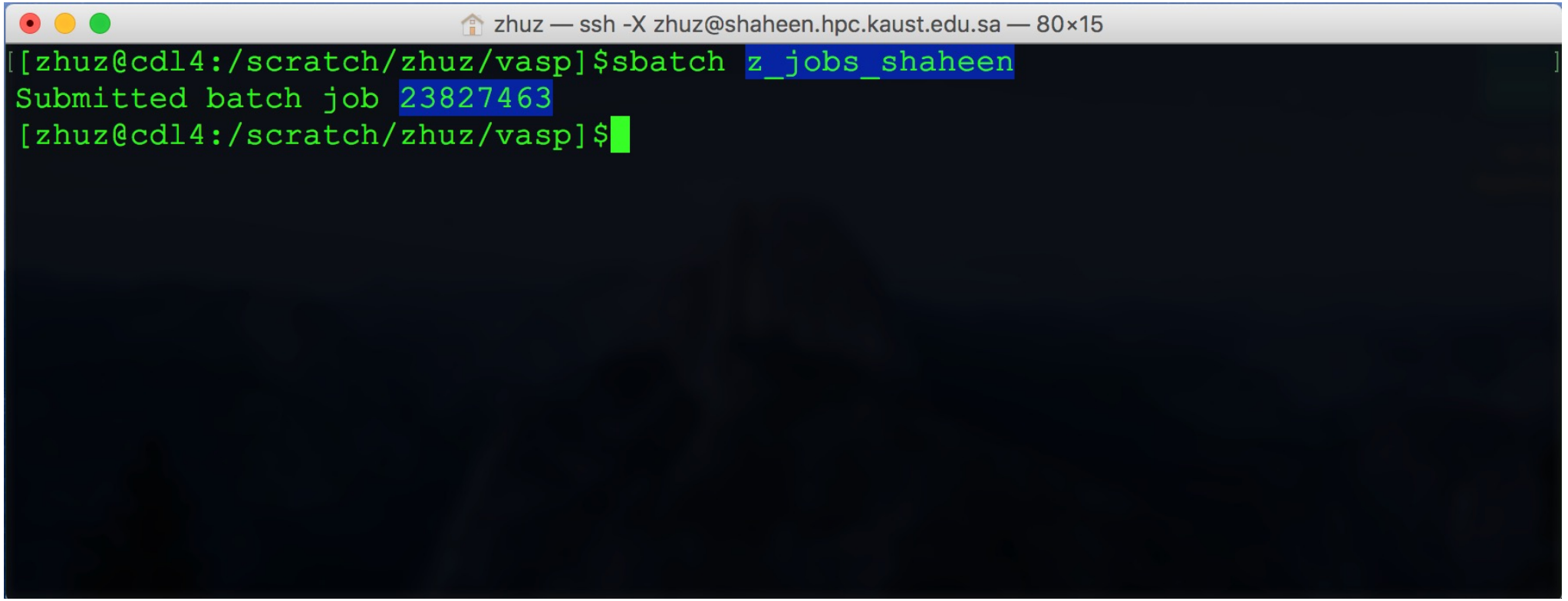
Prepare Input Files

- Slurm Jobscript
  - Commands to run



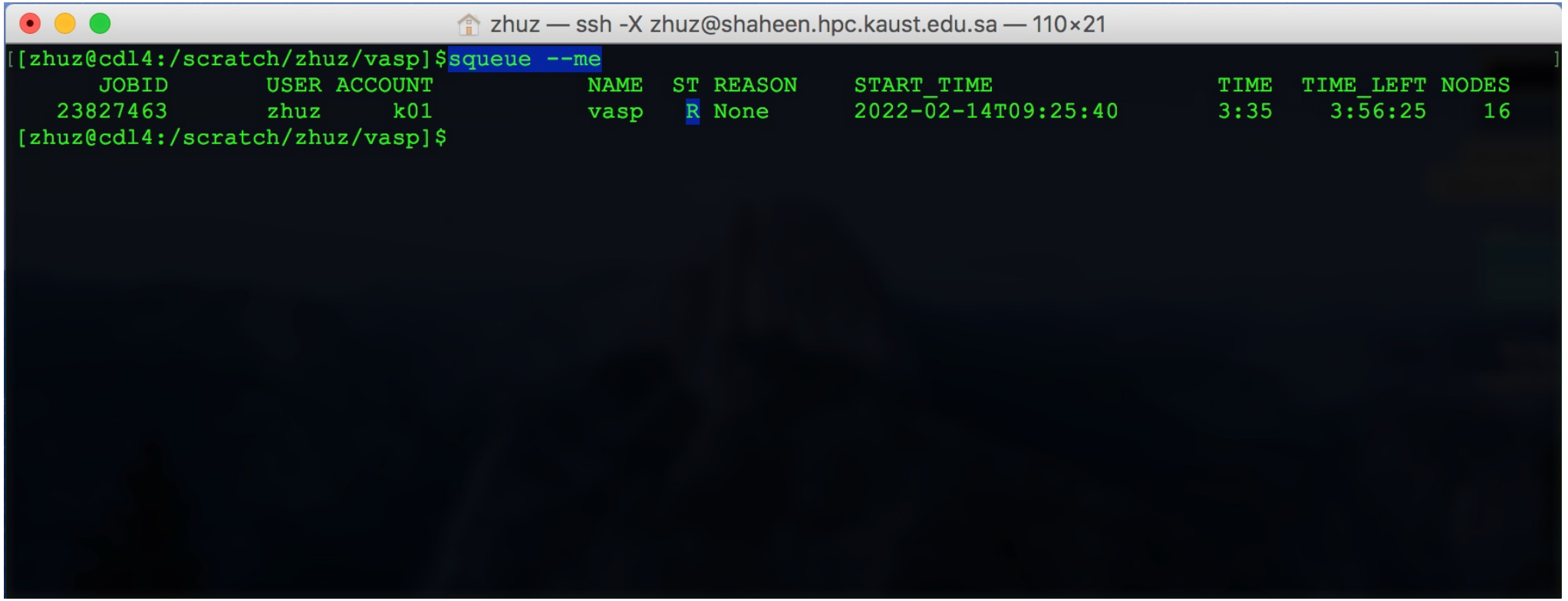
Job Submission

- sbatch
  - Submit jobs



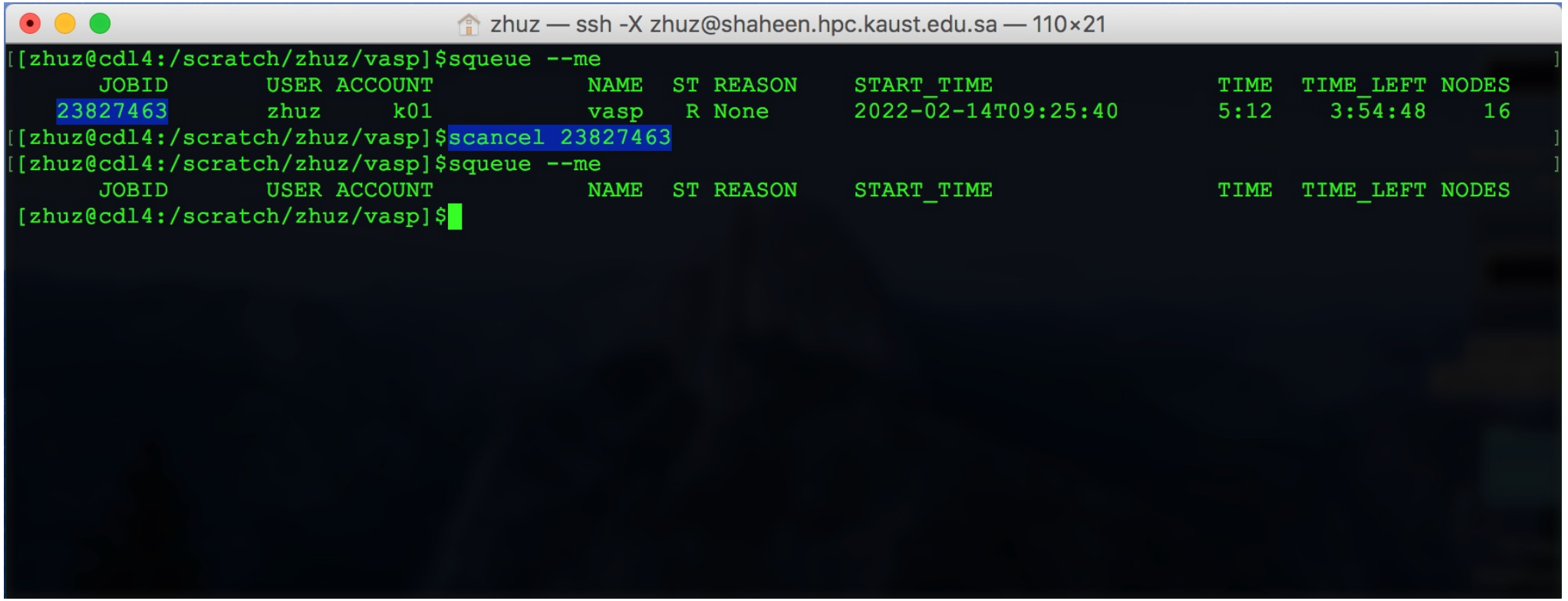
Job Submission

- squeue
  - Check job status



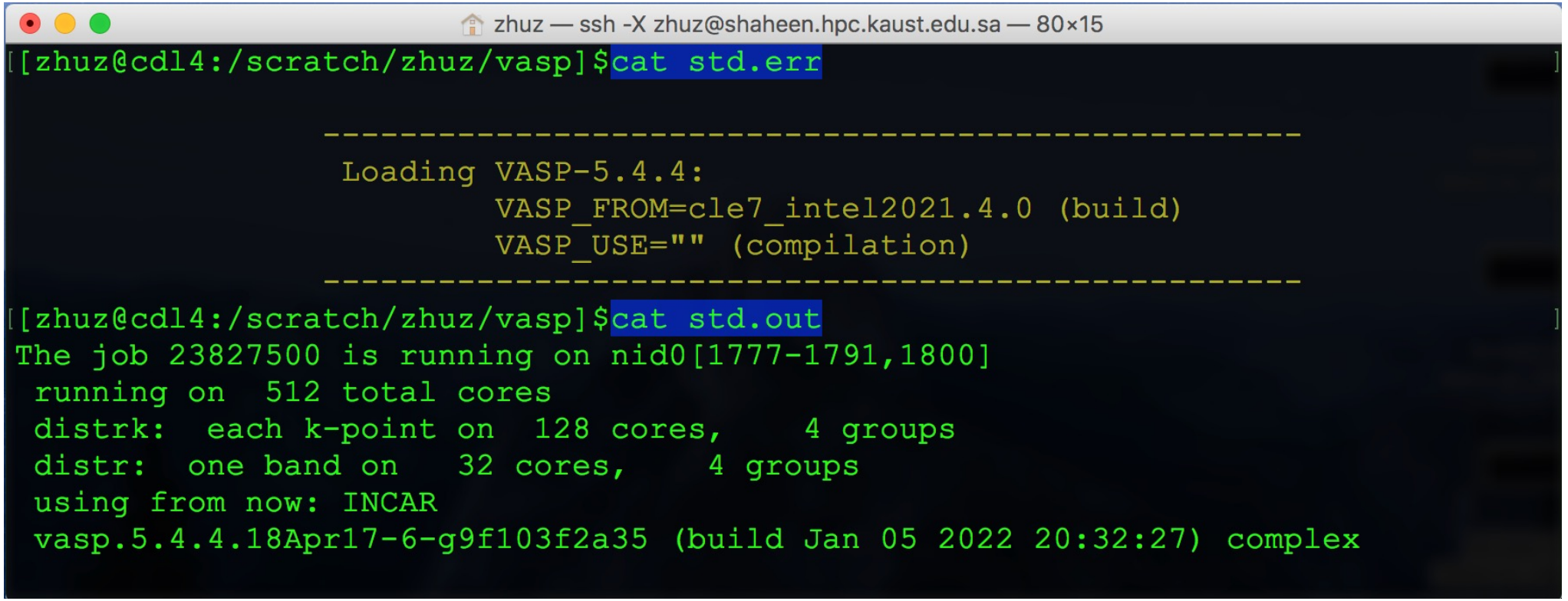
Job Submission

- scancel
  - Cancel jobs



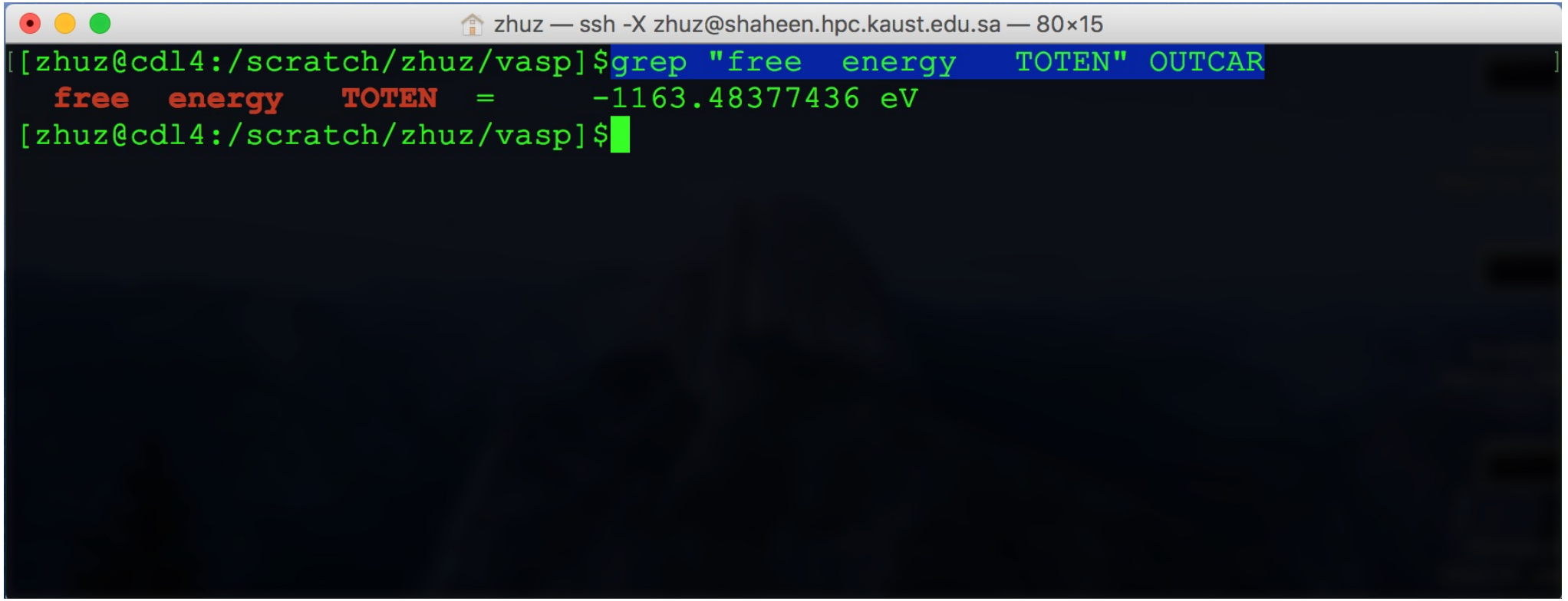
Check Output Files

- Errors or Not?
  - Standard outputs (std.out)
  - Standard errors (std.err)



Check Output Files

- Results Analysis
  - Download to local workstations (scp)
  - Check it on-site



Tips

- Do not run directly on CDL login nodes
  - CDL login nodes are shared
- It won't work to submit jobs from /home and /project
  - /home is not seen on the compute nodes
  - /project is read-only on the compute nodes
- Backup important data from /scratch to /project (or /home, or your local computers)
  - Files in /scratch are not backed up, and are deleted automatically after 60 days
  - Do not confuse /scratch/project and /project

Tips

- Download and Upload (Mac & Linux)
  - scp -r LocalFiles zhuz@shaheen.hpc.kaust.edu.sa:RemoteFolder
  - scp -r zhuz@shaheen.hpc.kaust.edu.sa:RemoteFiles LocalFolder
- Download and Upload (Windows)
  - MobaXterm
    - https://mobaxterm.mobatek.net
  - Bitvise SSH Client
    - https://www.bitvise.com/ssh-client-download

Thank You!

help@hpc.kaust.edu.sa