

HPC Workflow on Shaheen

(Chemistry, Physics & Materials Science)

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Outline

- Workflow
 - Use VASP as an example to show the steps to run
 - The Vienna Ab-initio 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>).

Workflow

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

Login Shaheen

- Login
 - ssh -X <UserName>@shaheen.hpc.kaust.edu.sa

```
zhuz — ssh -X zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[zhuz:~]$ ssh -X zhuz@shaheen.hpc.kaust.edu.sa
Use of this system is limited to users who have been properly authorised by
the KAUST Supercomputing Laboratory. Unauthorised users must disconnect
immediately.

For support, see http://www.hpc.kaust.edu.sa/
or email help@hpc.kaust.edu.sa
zhuz@shaheen.hpc.kaust.edu.sa's password:
(zhuz@shaheen.hpc.kaust.edu.sa) One-time password (OATH) for `zhuz':
-----
[zhuz@login2:~]$
```

Code Availability

- On Shaheen login node:
 - module avail
- In /sw/ex111genoa software stack:
 - ls /sw/ex111genoa
- From our website:
 - <https://docs.hpc.kaust.edu.sa>

Code Availability

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

```
[[ zhuz@login3:~] $module avail
----- /sw/ex111genoa/modulefiles -----
abinit/9.10.3          mpibench/20241001
adf/2019.301           mpibench/cpe2309
airss/0.9.4            mpifileutils/0.11.1
alamode/1.4.2          mrcc/2023-08-28_mpi
almabte/1.3.2          mrcc/2023-08-28_omp
[[ zhuz@login3:~] $module avail vasp/6.4.2
----- /sw/ex111genoa/modulefiles -----
vasp/6.4.2              vasp/6.4.2_optaxis  vasp/6.4.2_vaspSol
vasp/6.4.2_dftd4        vasp/6.4.2_scpc      vasp/6.4.2_vtst198
[[ zhuz@login3:~] $
```

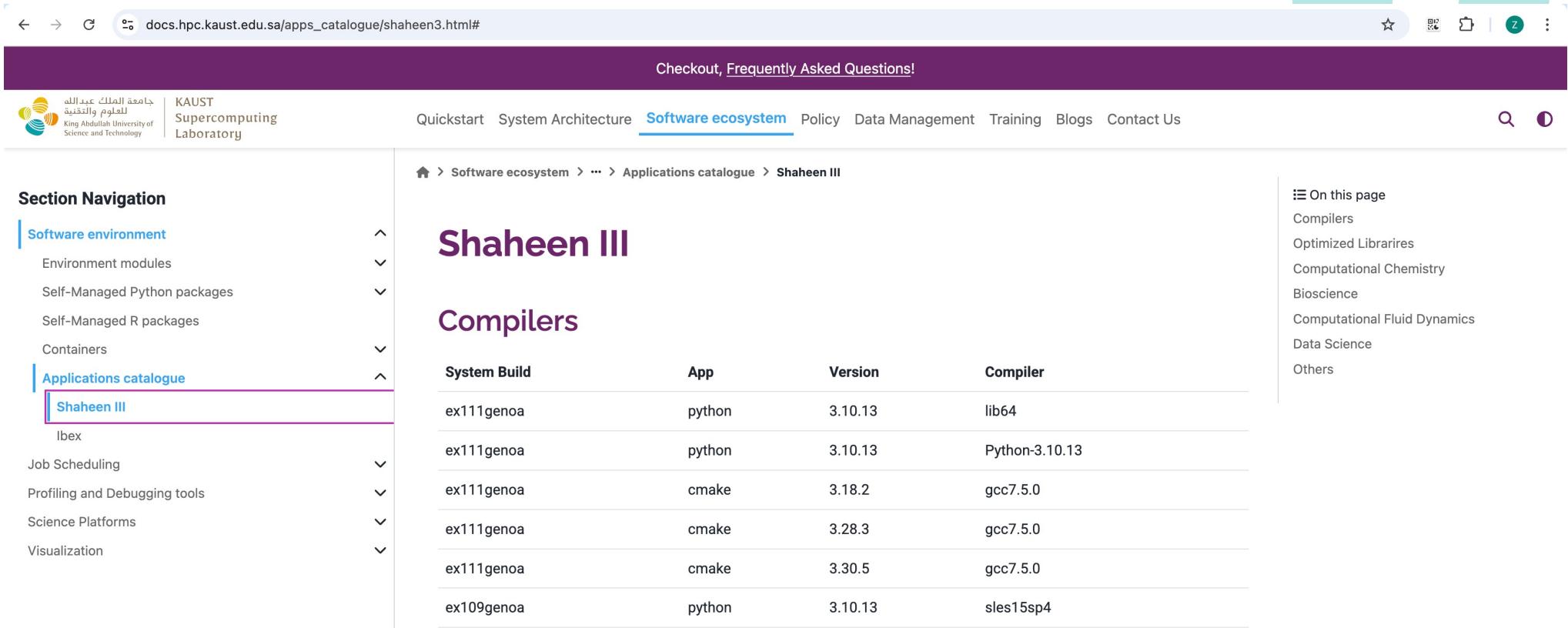
Code Availability

- ls /sw/ex11genoa

```
[[ zhuz@login3:~]$ ls /sw/ex11genoa
abinit      crystal14    jmol          openfoam          sod
adf         cuby4        koopmans      openmolcas      softbv
airss       dftbplus    kwant         openmx          spack
alamode     dftd4        lammps       orca           sumo
almabte     dlpoly       lev00        osu-microbenchmarks tbmodels
amber       dpcode       libxc        ovito          tdep
amd         dssp         libxml2      p4vasp         thirdorder
ams         eddp         lobster      pacchem        totalview
amset       edmftf      materstudio packmol        towhee
ansys      egsnrc      matlab       periodic_nbo turbomole
arm-forge   eigen        milo        perturbo      uspex
ase         elk         mkl         phono3py      vampire
atk         elpa         modulefiles phonopy      vasp
atompaw    espresso     mohid       plumed       vaspkit
```

Code Availability

- <https://docs.hpc.kaust.edu.sa>
 - Software ecosystem -> Software environment -> Applications catalogue -> Shaheen III



The screenshot shows a web browser displaying the KAUST Supercomputing Laboratory's software ecosystem page. The URL in the address bar is docs.hpc.kaust.edu.sa/apps_catalogue/shaheen3.html#. The page has a purple header with the text "Checkout, Frequently Asked Questions!". The navigation bar includes links for Quickstart, System Architecture, Software ecosystem (which is underlined), Policy, Data Management, Training, Blogs, and Contact Us. A search bar and a "On this page" sidebar are also present. The main content area shows the "Shaheen III" section, which includes a "Compilers" table with the following data:

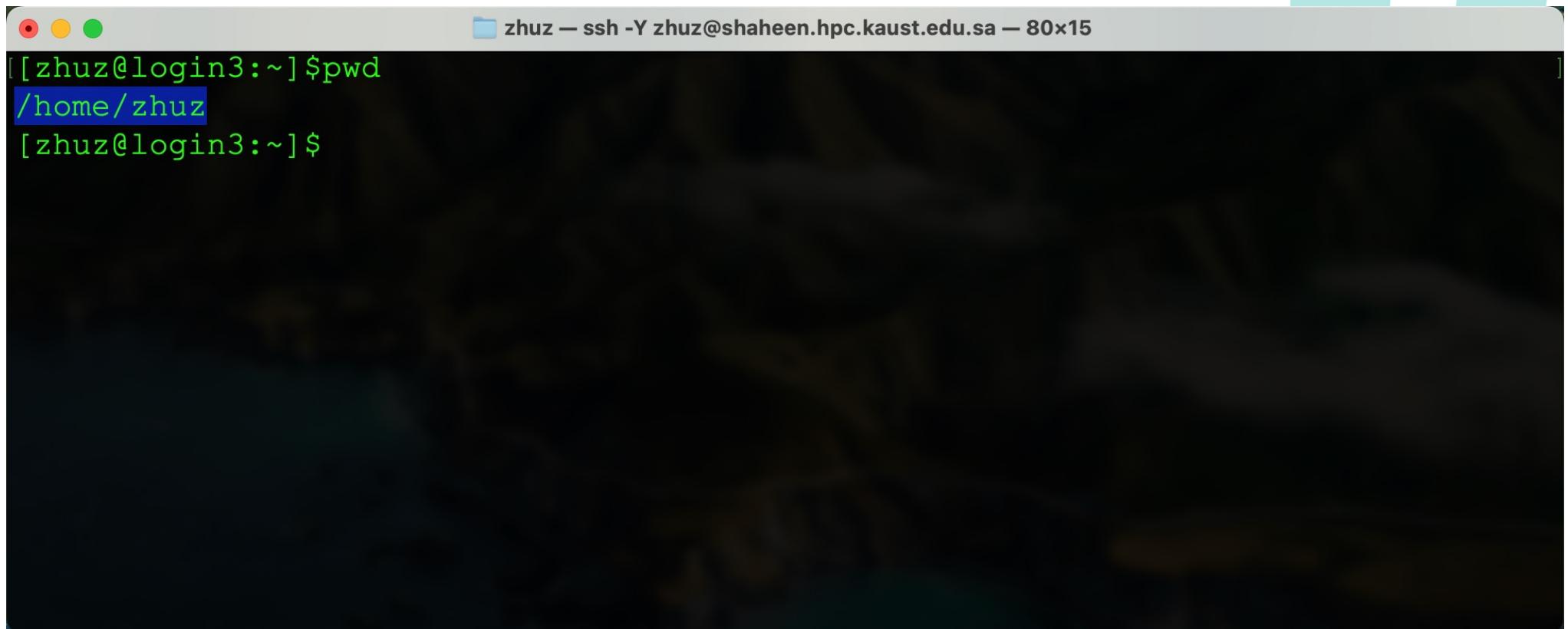
System Build	App	Version	Compiler
ex111genoa	python	3.10.13	lib64
ex111genoa	python	3.10.13	Python-3.10.13
ex111genoa	cmake	3.18.2	gcc7.5.0
ex111genoa	cmake	3.28.3	gcc7.5.0
ex111genoa	cmake	3.30.5	gcc7.5.0
ex109genoa	python	3.10.13	sles15sp4

Code Availability

- On Shaheen login node:
 - module avail
- In `/sw/ex11genoa` software stack:
 - `ls -l /sw/ex11genoa`
- From our website:
 - <https://docs.hpc.kaust.edu.sa>
- Not found?
 - help@hpc.kaust.edu.sa

3 Different Working Directories

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

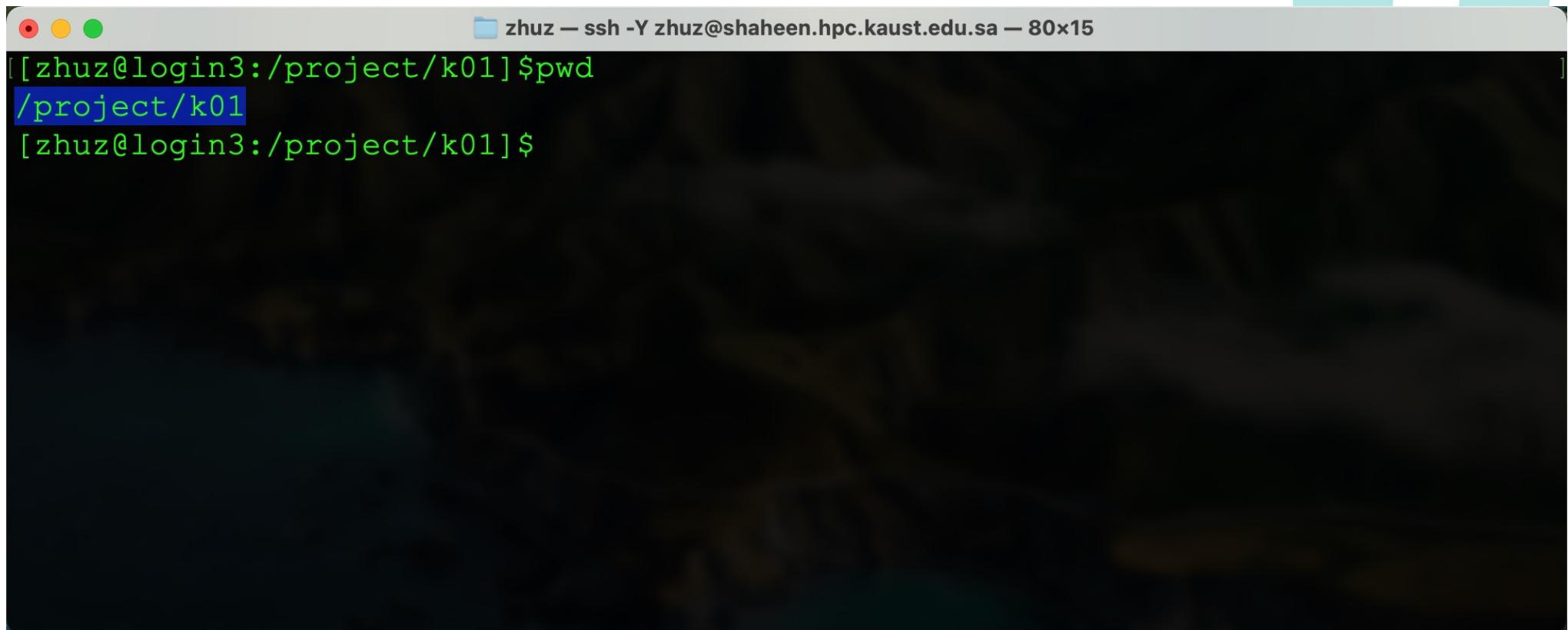


A screenshot of a terminal window on a Mac OS X desktop. The window title is "zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15". The terminal shows the following command and output:

```
[[ zhuz@login3:~] $pwd  
/home/zhuz  
[ zhuz@login3:~] $
```

3 Different Working Directories

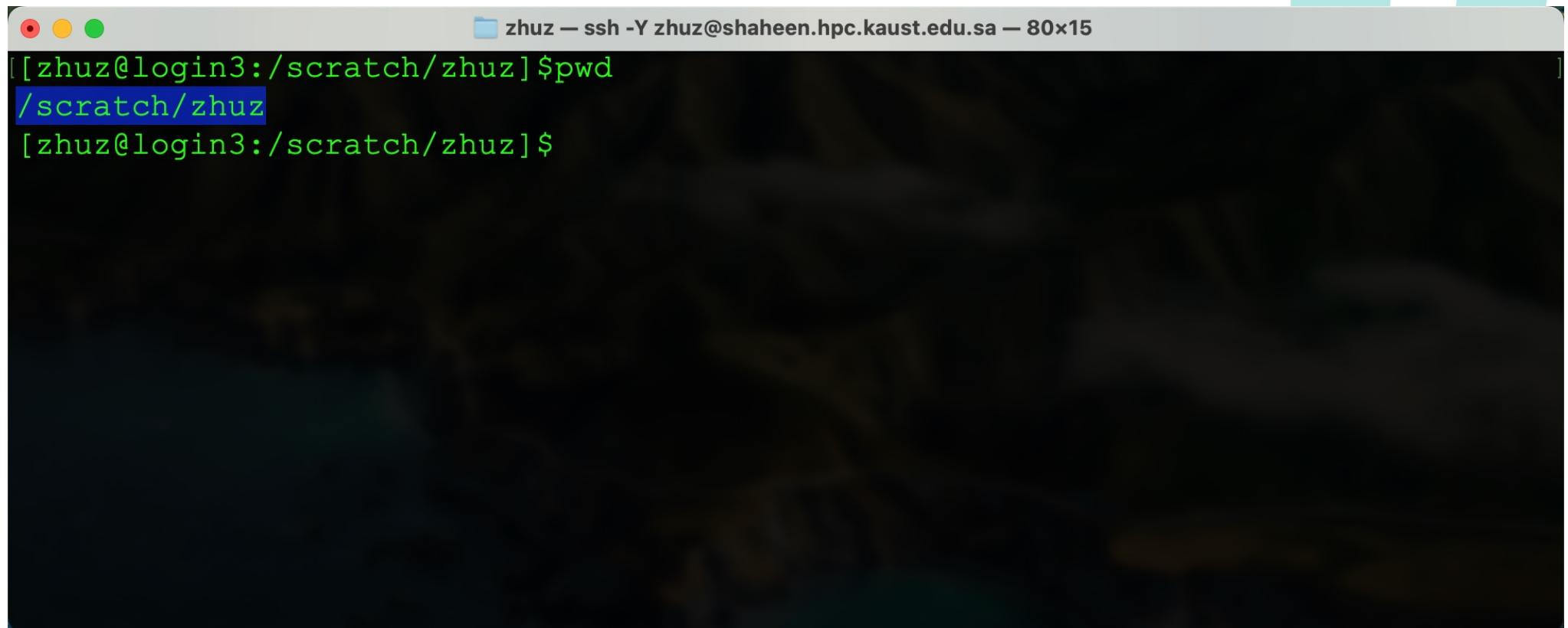
- `/project/<projectname>`
 - Read-only for compute nodes (job submission will fail); Used for data backup and data sharing



```
zhuz - ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 80x15
[[ zhuz@login3:/project/k01]$pwd
/project/k01
[zhuz@login3:/project/k01]$
```

3 Different Working Directories

- `/scratch/<username>`
 - Almost unlimited space

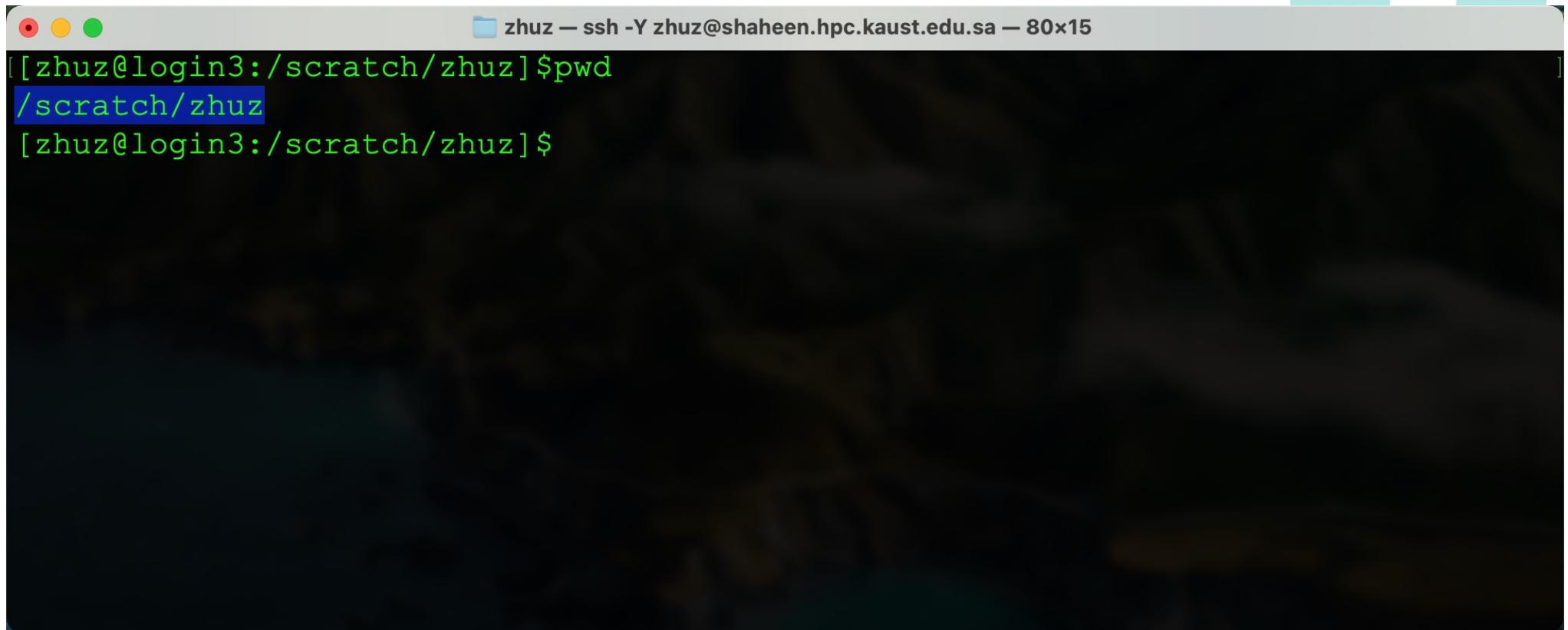


A screenshot of a macOS terminal window. The window title is "zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15". The terminal prompt shows the user is in their scratch directory: "[zhuz@login3:/scratch/zhuz] \$". The user then runs the command `pwd`, which outputs the path `/scratch/zhuz`. The terminal window has a dark background and a light gray header bar. The text in the terminal is green.

```
[[ zhuz@login3:/scratch/zhuz] $pwd  
/scratch/zhuz  
[zhuz@login3:/scratch/zhuz] $
```

3 Different Working Directories

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



A screenshot of a terminal window with a dark background. The window title is "zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15". The terminal prompt is "[zhuz@login3:/scratch/zhuz] \$". The user types "pwd" and the output is "/scratch/zhuz". The user then types a new command, starting with "[zhuz@login3:/scratch/zhuz] \$".

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[ zhuz@login3:/scratch/zhuz] $pwd
/scratch/zhuz
[zhuz@login3:/scratch/zhuz] $
```

3 Different Working Directories

- `/scratch/<username>` - 3 tiers
 - capacity, bandwidth, iops

```
[[ zhuz@login3:/scratch/zhuz] $pwd
/scratch/zhuz

[[ zhuz@login3:/scratch/zhuz/bandwidth] $pwd
/scratch/zhuz/bandwidth

[[ zhuz@login3:/scratch/zhuz/iops] $pwd
/scratch/zhuz/iops
[zhuz@login3:/scratch/zhuz/iops] $
```

3 Different Working Directories

- `/scratch/<username>`
 - Tier “capacity”
 - Large capacity (10T per user by default)
 - Low performance in terms of bandwidth and iops
 - Used for calculations that are not sensitive to IO performance
 - Data purged after 60 days of no access

3 Different Working Directories

- `/scratch/<username>/bandwidth`
 - tier “bandwidth”
 - Low capacity (1T per user by default)
 - High performance in terms of IO bandwidth
 - Used for calculations that read/write a large amount of data
 - Data purged after 60 days of no access

3 Different Working Directories

- `/scratch/<username>/iops`
 - Tier “iops”
 - Low capacity (50G per user by default)
 - High performance in terms of # IO operations
 - Used for calculations that read/write large number of files, and software installation (conda, python, etc)
 - No data purging

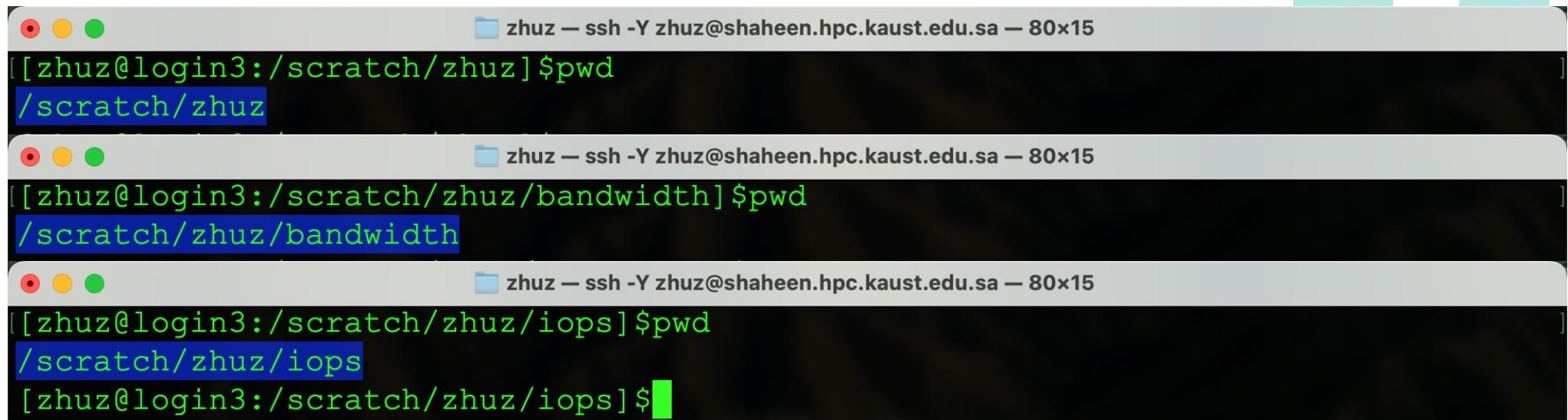
3 Different Working Directories

- Quota limits
 - `kuq`

```
zhuz@ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 100x20
[zhuz@login3:~]$ kuq
-----
Filesystem quota limits for user zhuz
Tier      Filesystem  used  quota  limit  grace  files  quota  limit  grace
-----
scratch      /scratch  678.3G  0k    11T    -    242181  0 1024000  -
capacity     /scratch  667.1G  0k    10T    -    242181  0      0  -
bandwidth    /scratch  458.2M  0k    1T     -    242181  0      0  -
iops         /scratch  10.89G  0k    50G    -    242181  0      0  -
project      /project  3.491T  0k    0k     -   2211833  0 3000000  -
[zhuz@login3:~]$
```

3 Different Working Directories

- Which tier to use? It depends!
 - Do your own tests



The image shows three separate terminal windows, each with a dark background and light-colored text. The windows are arranged vertically and have the standard Mac OS X window controls (red, yellow, green buttons) in the top-left corner. Each window has a title bar indicating the user is ssh'd into a host named 'zhuz'.

- Top Window:** The title bar says "zhuz - ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 80x15". The command entered is "[zhuz@login3:/scratch/zhuz]\$pwd", and the output is "/scratch/zhuz".
- Middle Window:** The title bar says "zhuz - ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 80x15". The command entered is "[zhuz@login3:/scratch/zhuz/bandwidth]\$pwd", and the output is "/scratch/zhuz/bandwidth".
- Bottom Window:** The title bar says "zhuz - ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 80x15". The command entered is "[zhuz@login3:/scratch/zhuz/iops]\$pwd", and the output is "/scratch/zhuz/iops".

Prepare Input Files

- Examples under Installation Folder
 - /sw/ex111genoa/code/ver/compilation/example
 - Inputs for application; Jobscrip for Slurm

```
[[ zhuz@login3:~]$cd /scratch/zhuz
[[ zhuz@login3:/scratch/zhuz]$mkdir vasp
[[ zhuz@login3:/scratch/zhuz]$cd vasp
[[ zhuz@login3:/scratch/zhuz/vasp]$cp /sw/ex111genoa/vasp/6.4.2/intel19.0.5/exampl
e/02/* .
[[ zhuz@login3:/scratch/zhuz/vasp]$ls -l
total 696
-rw-r--r-- 1 zhuz g-zhuz      421 Jan 29 10:24 INCAR
-rw-r--r-- 1 zhuz g-zhuz      36 Jan 29 10:24 KPOINTS
-rw-r--r-- 1 zhuz g-zhuz  29531 Jan 29 10:24 POSCAR
-rw-r--r-- 1 zhuz g-zhuz 664880 Jan 29 10:24 POTCAR
-rw-r--r-- 1 zhuz g-zhuz    1137 Jan 29 10:24 z_jobs_shaheen
[zhuz@login3:/scratch/zhuz/vasp]$
```

Prepare Input Files

- VASP Input Files
 - Upload from your own personal workstations
 - Modifying existing input files

```
zhuz@zhuz:~$ ssh -Y zhuz@shaheen.hpc.kaust.edu.sa - 80x15
[[zhuz@login3:/scratch/zhuz/vasp]$ls -l
total 696
-rw-r--r-- 1 zhuz g-zhuz 421 Jan 29 10:24 INCAR
-rw-r--r-- 1 zhuz g-zhuz 36 Jan 29 10:24 KPOINTS
-rw-r--r-- 1 zhuz g-zhuz 29531 Jan 29 10:24 POSCAR
-rw-r--r-- 1 zhuz g-zhuz 664880 Jan 29 10:24 POTCAR
-rw-r--r-- 1 zhuz g-zhuz 1137 Jan 29 10:24 z_jobs_shaheen
[zhuz@login3:/scratch/zhuz/vasp]$
```

Prepare Input Files

- Slurm Jobsript
 - SLURM directives

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15

#!/bin/bash
#SBATCH --partition=workq
#SBATCH --job-name=vasp
#SBATCH --nodes=8
#SBATCH --time=4:00:00
#SBATCH --exclusive
#SBATCH --err=std.err
#SBATCH --output=std.out
#-----#
module switch PrgEnv-cray PrgEnv-intel
module switch intel intel/19.0.5.281
module load vasp/6.4.2
#module load vasp/6.4.4_dftd4 # https://github.com/dftd4/dftd4_vasp
#module load vasp/6.4.2_optaxis # https://github.com/Chengcheng-Xiao/VASP_OPT_AX
z_jobs_shaheen lines 1-14/25 42%
```

Prepare Input Files

- Slurm Jobsript
 - Environments settings

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
module switch PrgEnv-cray PrgEnv-intel
module switch intel intel/19.0.5.281
module load vasp/6.4.2
#module load vasp/6.4.4_dftd4 # https://github.com/dftd4/dftd4_vasp
#module load vasp/6.4.2_optaxis # https://github.com/Chengcheng-Xiao/VASP_OPT_AX
IS (Fixing specific stress tensor element(s))
#module load vasp/6.4.2_scpc # https://github.com/aradi/SCPC-Method/tree/main
#module load vasp/6.4.2_vaspsol # https://github.com/henniggroup/VASPsol/tree/ma
ster
#module load vasp/6.4.2_vtst198 # http://theory.cm.utexas.edu/vtsttools
export FI_CXI_RX_MATCH_MODE=software
export MKL_DEBUG_CPU_TYPE=5
export MKL_CBWR=auto
export OMP_NUM_THREADS=1
z_jobs_shaheen lines 10-21/25 77%
```

Prepare Input Files

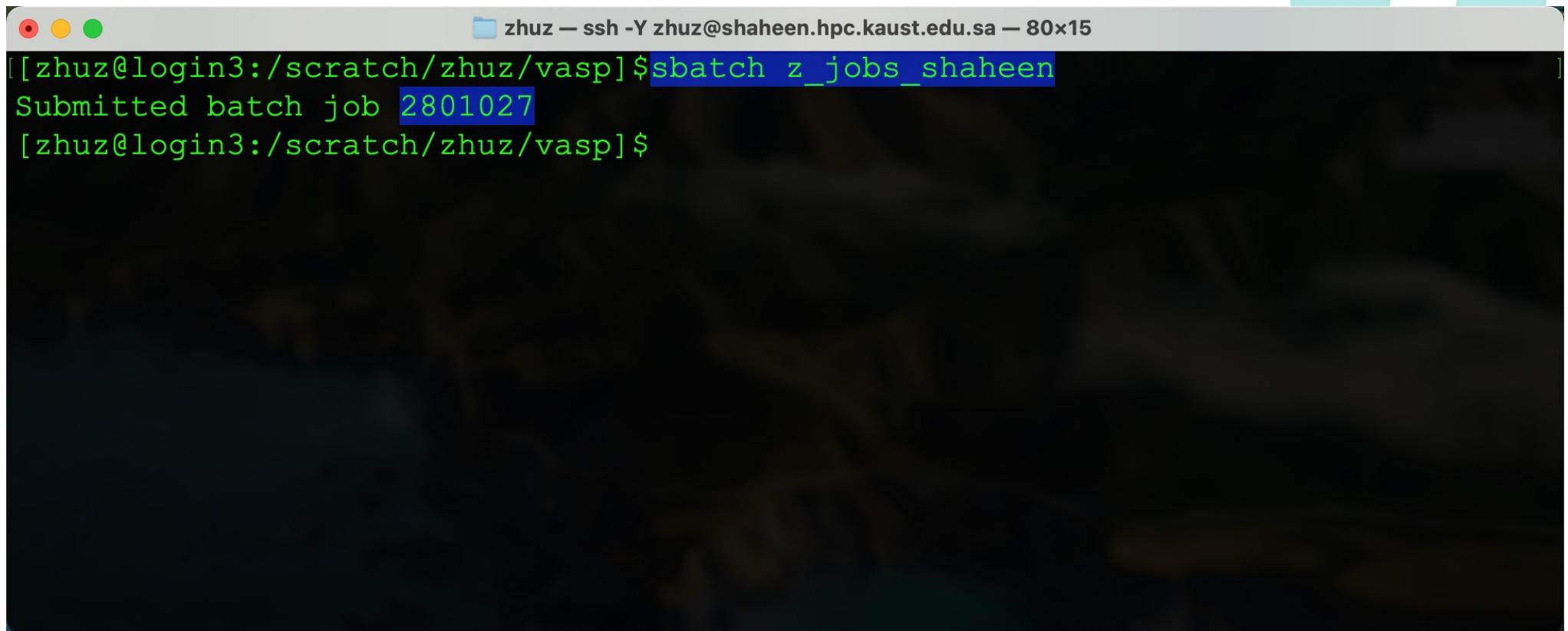
- Slurm Jobsript
 - Commands to run

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15

#module load vasp/6.4.2_optaxis # https://github.com/Chengcheng-Xiao/VASP_OPT_AX
IS (Fixing specific stress tensor element(s))
#module load vasp/6.4.2_scpc # https://github.com/aradi/SCPC-Method/tree/main
#module load vasp/6.4.2_vaspsol # https://github.com/henniggroup/VASPsol/tree/ma
ster
#module load vasp/6.4.2_vtst198 # http://theory.cm.utexas.edu/vtsttools
export FI_CXI_RX_MATCH_MODE=software
export MKL_DEBUG_CPU_TYPE=5
export MKL_CBWR=auto
export OMP_NUM_THREADS=1
#-----
echo "The job "${SLURM_JOB_ID}" is running on "${SLURM_JOB_NODELIST}
#-----
srun --ntasks=1536 --map-by-numa --hint=nomultithread ${VASP_HOME}/vasp_std
z_jobs_shaheen lines 14-25/25 (END)
```

Job Submission

- **sbatch**
 - Submit jobs



```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[ zhuz@login3:/scratch/zhuz/vasp] $sbatch z_jobs_shaheen
Submitted batch job 2801027
[zhuz@login3:/scratch/zhuz/vasp] $
```

Job Submission

- **squeue**
 - Check job status

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 120x24
[zhuz@login3:/scratch/zhuz/vasp]$squeue --me
  JOBID      USER ACCOUNT      NAME  ST REASON      START_TIME      TIME  TIME_LEFT  NODES
 2795375      zhuz      k01      vasp  R  None  2025-01-29T09:10:46  1:27:08  2:32:52      4
 2801027      zhuz      k01      vasp  R  None  2025-01-29T10:36:57  0:57   3:59:03      8
[zhuz@login3:/scratch/zhuz/vasp]$
```

Job Submission

- **scancel**
 - Cancel jobs

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 120x24
[zhuz@login3:/scratch/zhuz/vasp]$squeue --me
  JOBID      USER ACCOUNT      NAME  ST REASON      START_TIME      TIME  TIME_LEFT  NODES
  2795375    zhuz      k01      vasp  R  None  2025-01-29T09:10:46  1:27:08  2:32:52      4
  2801027    zhuz      k01      vasp  R  None  2025-01-29T10:36:57  0:57    3:59:03      8
[zhuz@login3:/scratch/zhuz/vasp]$scancel 2801027
[zhuz@login3:/scratch/zhuz/vasp]$squeue --me
  JOBID      USER ACCOUNT      NAME  ST REASON      START_TIME      TIME  TIME_LEFT  NODES
  2795375    zhuz      k01      vasp  R  None  2025-01-29T09:10:46  1:28:26  2:31:34      4
[zhuz@login3:/scratch/zhuz/vasp]$
```

Check Output Files

- Successful or Not? If yes, Analyze Results
 - Standard output/error files: std.out/std.err)
 - Application output files: OUTCAR

```
zhuz@zhuz:~$ ssh -Y zhuz@shaheen.hpc.kaust.edu.sa -t ls -l std.*  
-rw-r--r-- 1 zhuz g-zhuz 132500 Jan 29 10:41 std.err  
-rw-r--r-- 1 zhuz g-zhuz 5653 Jan 29 10:49 std.out  
zhuz@zhuz:~$ grep "free energy TOTEN" OUTCAR  
  free energy TOTEN = -3042.35709769 eV  
zhuz@zhuz:~$
```

Tips

- Do not run directly on the login nodes
 - login nodes are shared
- It won't work to submit jobs from /home
 - /home is not seen 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

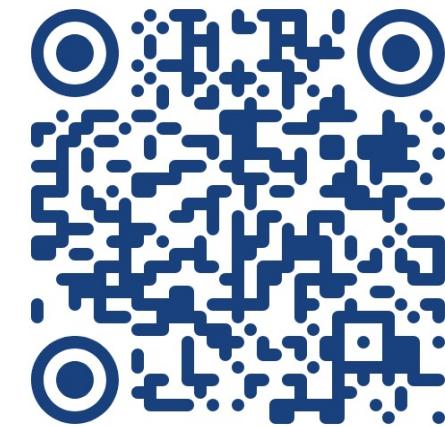
- Licensed software
 - Need license for commercial software
 - Different software have different license terms
 - VASP: You can use it on Shaheen, as long as you have your own license
 - Gaussian: For external users, you cannot use it on Shaheen, even if you have your own license
 - Contact us if you have any questions

Thank You!

help@hpc.kaust.edu.sa

Agenda

- 8:30am Welcome
- 8:35am Shaheen III Overview
- 8:55am How to apply on Shaheen III
- 9:05am Getting Started on Shaheen III
- 9:15am Software Environment
- 9:35am Job Scheduling
- 10:00am Coffee Break
- 10:15am Storage overview & Best practices
- 10:30am Applications software example: VASP workflow
- **10:50 am Applications software example: CFD applications**
- 11:10 am Applications software example: Bio informatics
- **11:20-11.30am Q&A and Open Discussion**



Shaheen III Survey