

# HPC Workflow on Shaheen

## (Chemistry, Physics & Materials Science)

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# Outline

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- 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>).

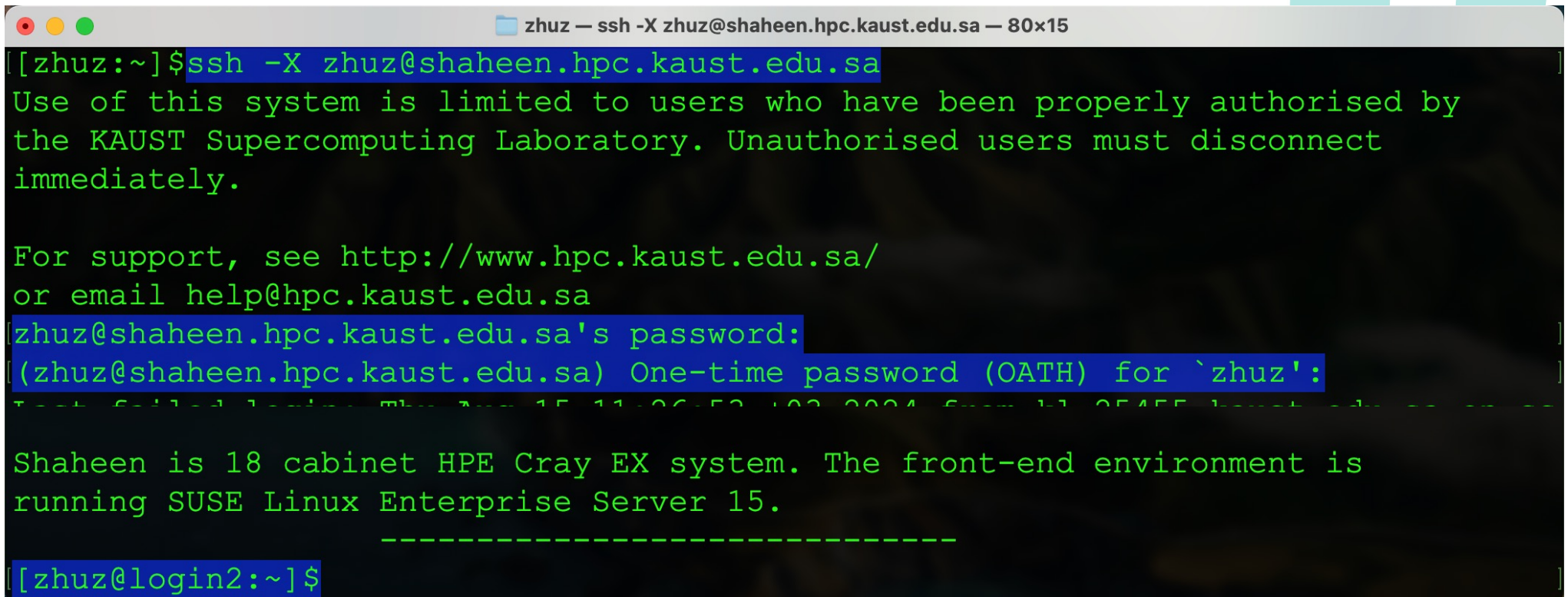
# Workflow

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- 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 <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':
Test failed! Please check your OATH device.
Shaheen is 18 cabinet HPE Cray EX system. The front-end environment is
running SUSE Linux Enterprise Server 15.
-----
[zhuz@login2:~]$
```

# Code Availability

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- 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 — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[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 — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[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           egsrc          matlab          periodic_nbo    turbomole
arm-forge       eigen          milo            perturbo        uspex
ase             elk            mk1             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](#)

← → ↺ docs.hpc.kaust.edu.sa/apps\_catalogue/shaheen3.html# ☆

Checkout, [Frequently Asked Questions!](#)

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🔍 ⓘ

🏠 > Software ecosystem > ... > Applications catalogue > Shaheen III

## Shaheen III

### Compilers

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

📄 On this page

- Compilers
- Optimized Libraries
- Computational Chemistry
- Bioscience
- Computational Fluid Dynamics
- Data Science
- Others

**Section Navigation**

- Software environment
  - Environment modules
  - Self-Managed Python packages
  - Self-Managed R packages
  - Containers
- Applications catalogue
  - Shaheen III**
  - Ibex
- Job Scheduling
- Profiling and Debugging tools
- Science Platforms
- Visualization



# Code Availability

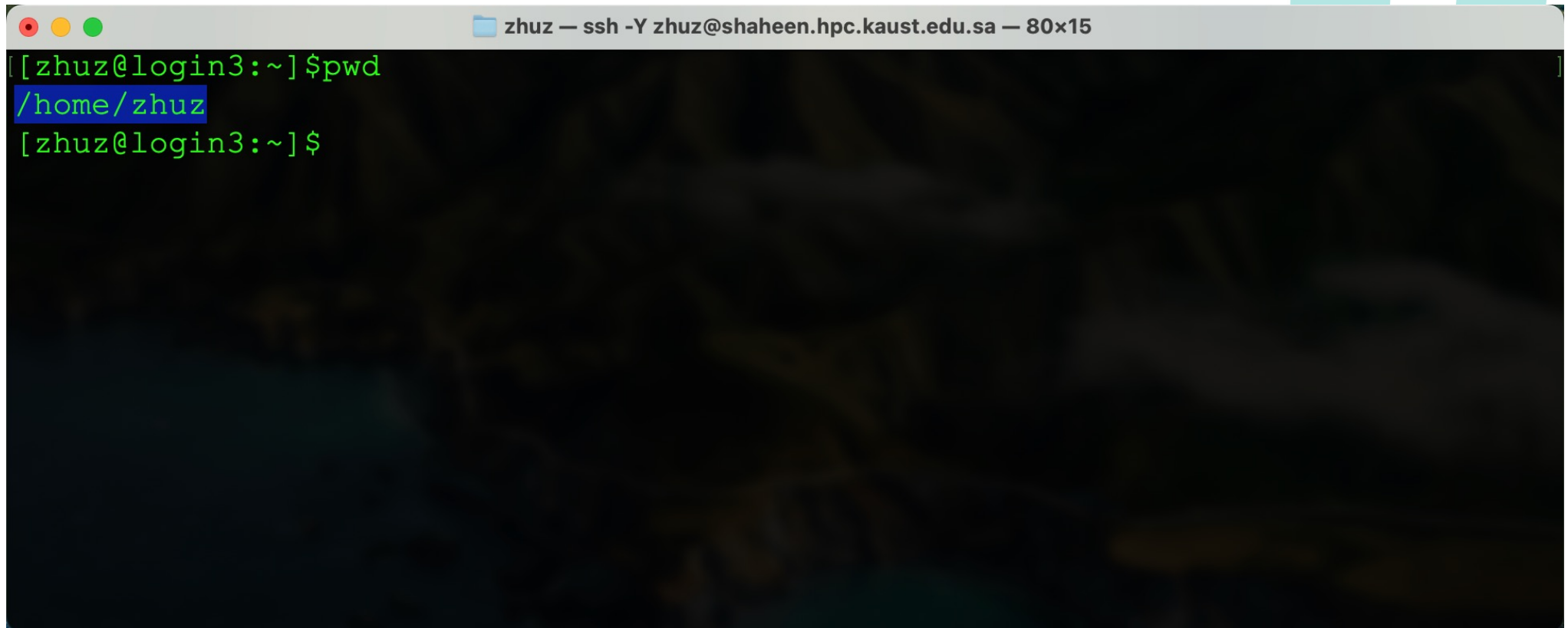
---

- On Shaheen login node:
  - module avail
- In /sw/ex111genoa software stack:
  - ls -l /sw/ex111genoa
- From our website:
  - <https://docs.hpc.kaust.edu.sa>
- Not found?
  - [help@hpc.kaust.edu.sa](mailto:help@hpc.kaust.edu.sa)



# 3 Different Working Directories

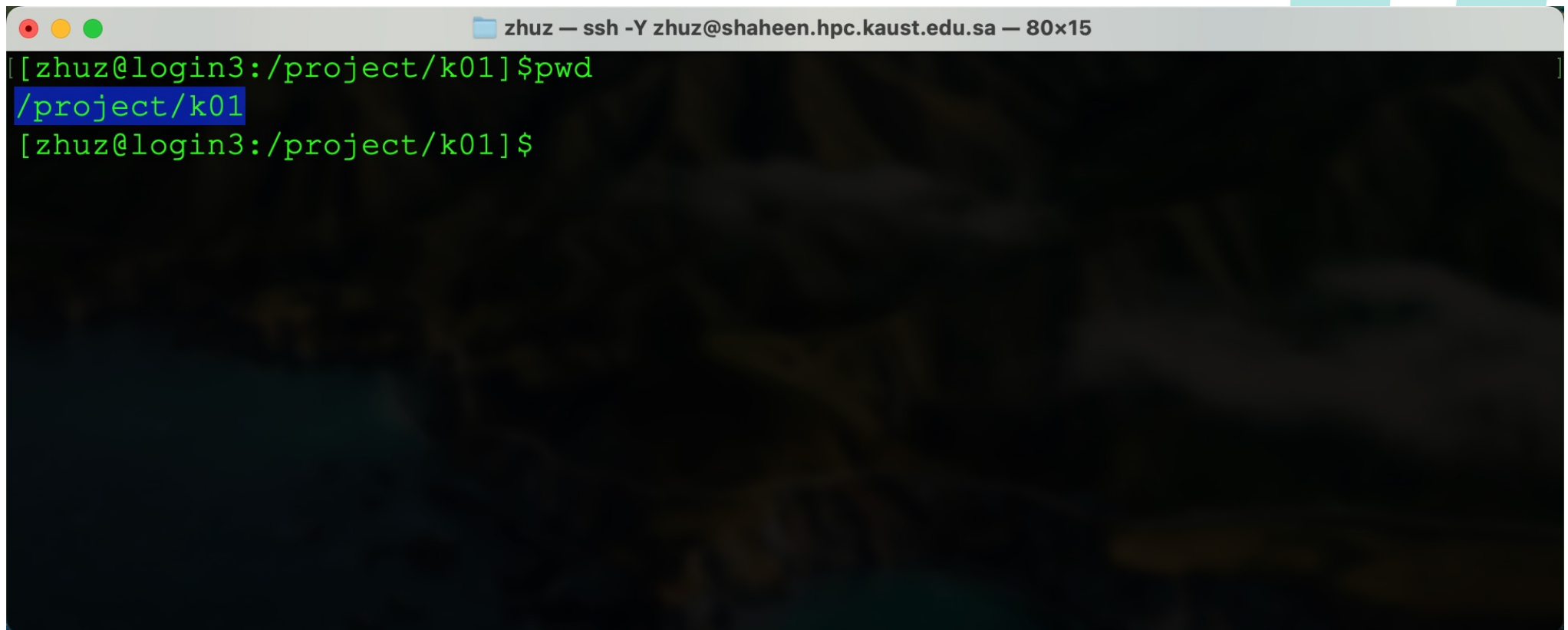
- /home
  - Very limited space; Not mounted on compute nodes (job submission will fail)



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

# 3 Different Working Directories

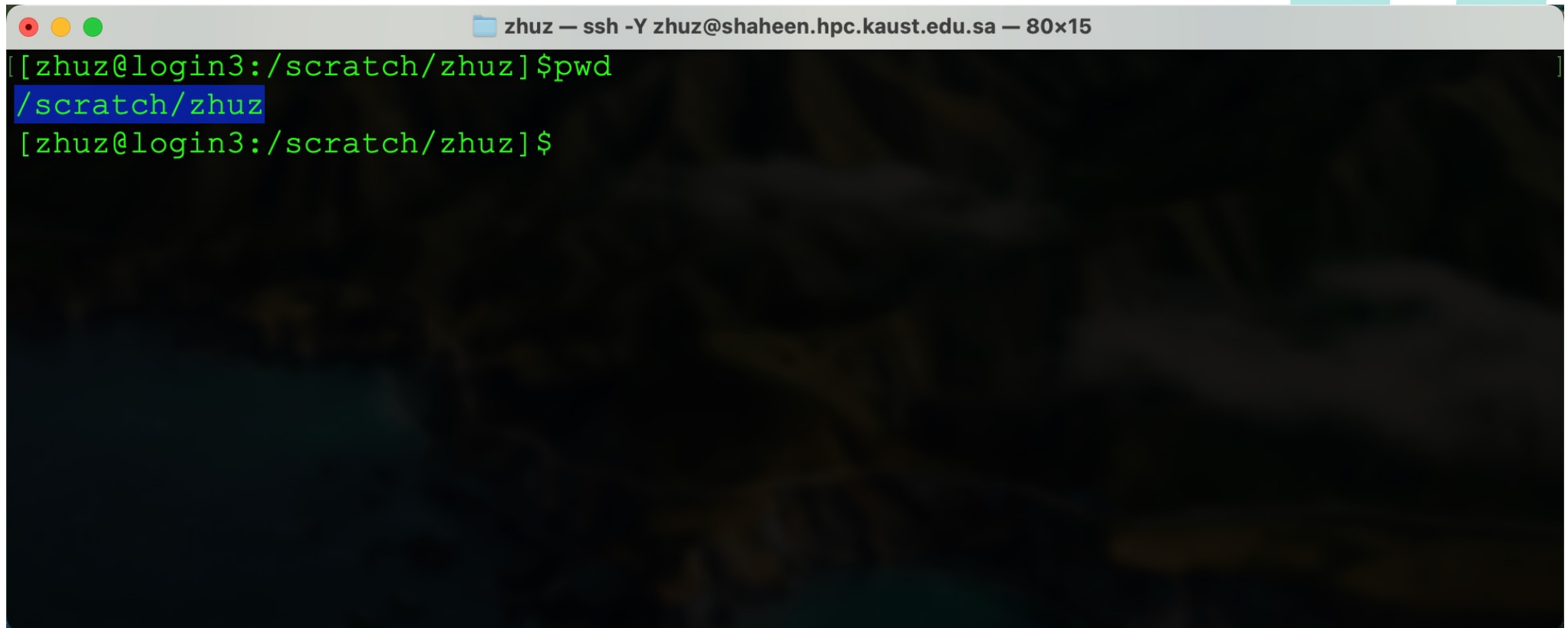
- /project/<projectname>
  - Read-only for compute nodes (job submission will fail); Used for data backup and data sharing



```
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

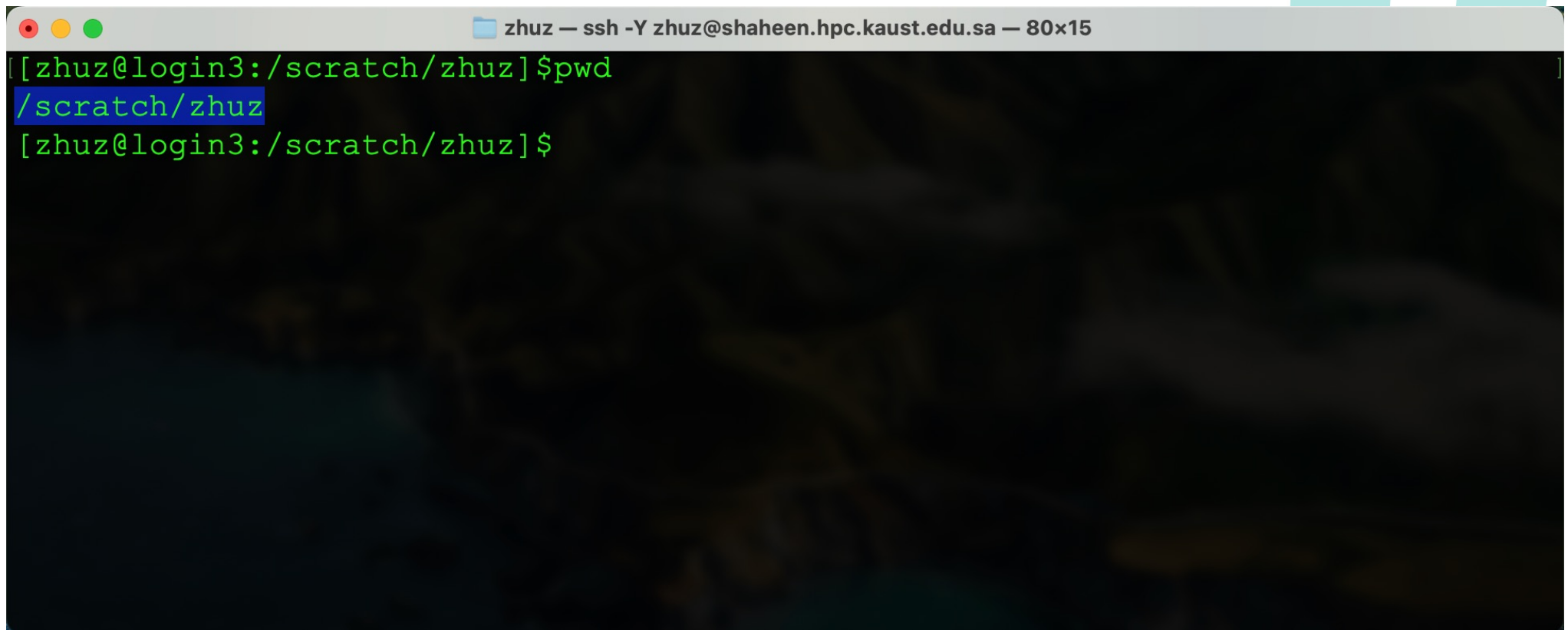
- /scratch/<username>
  - Almost unlimited space



```
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

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

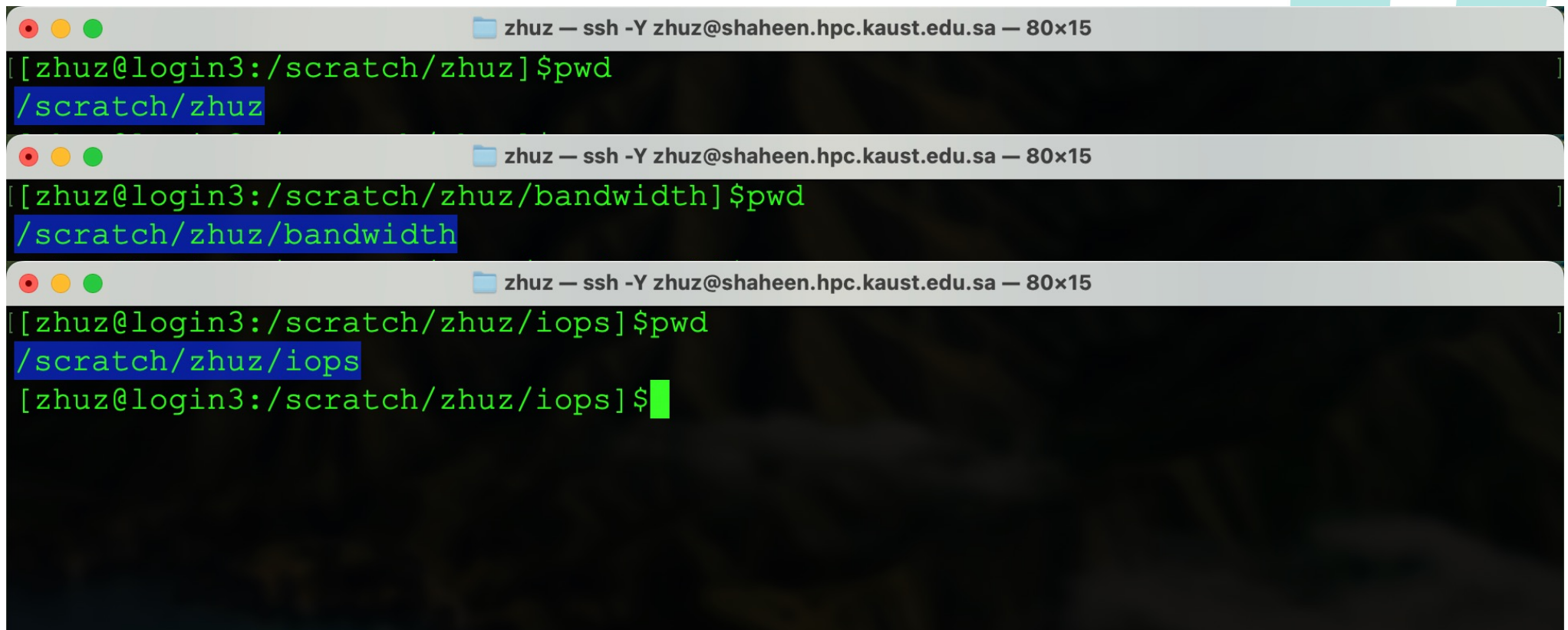


```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[zhuz@login3:/scratch/zhuz] $pwd
/scratch/zhuz
[zhuz@login3:/scratch/zhuz] $
```



# 3 Different Working Directories

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



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

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

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

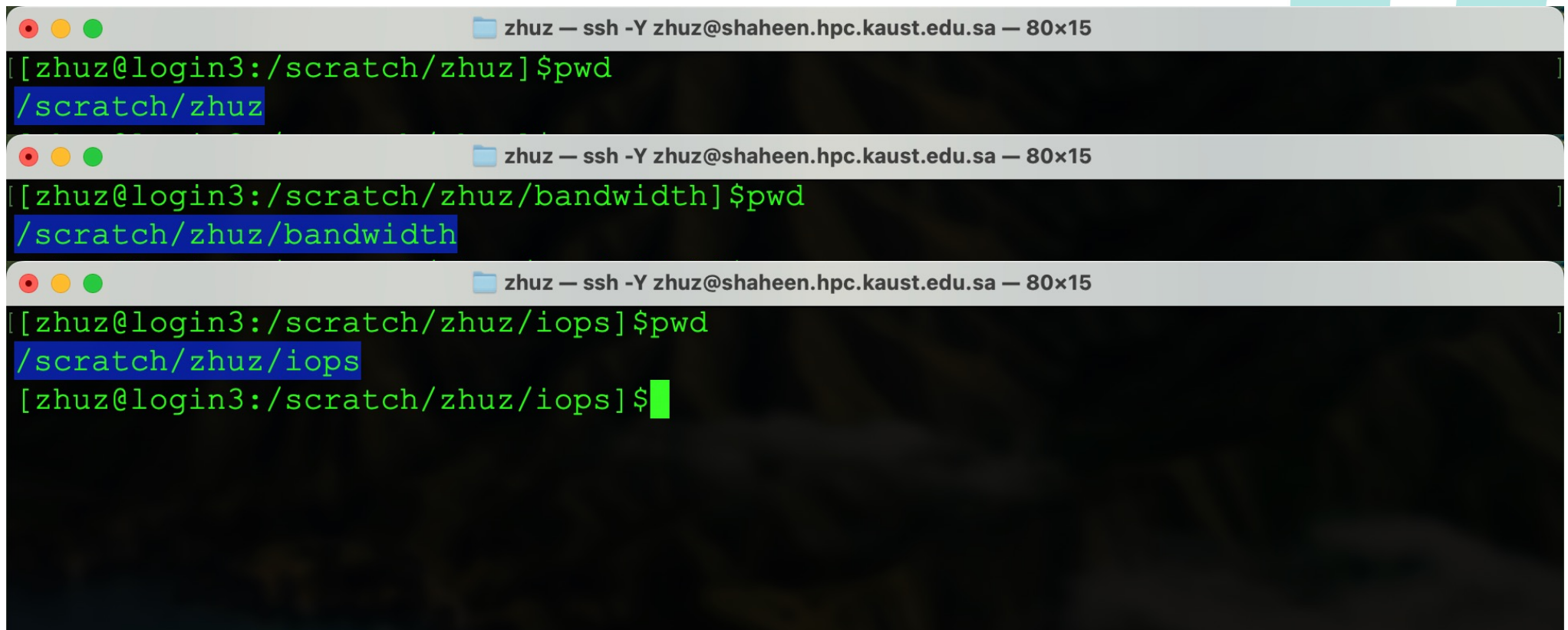
- Quota limits
  - kuq

```
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



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

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

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

# Prepare Input Files

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

```
zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[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/example/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 — 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 Jobscrip  
– 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 Jobscrip  
– 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/master
#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%
```



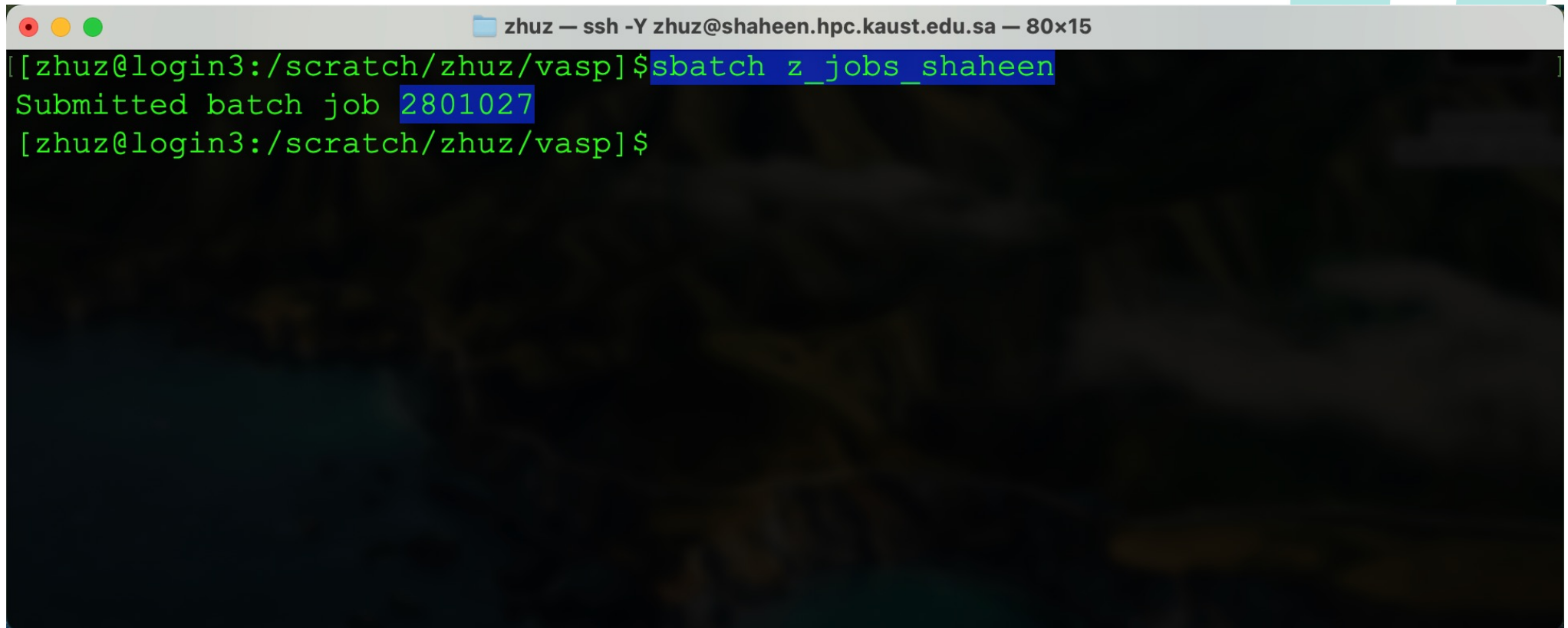
# Prepare Input Files

- Slurm Jobscrip  
– 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

A terminal window with a grey title bar containing three colored window control buttons (red, yellow, green) on the left and a title text 'zhuz — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15' on the right. The terminal has a black background with green text. The first line shows a prompt '[zhuz@login3:/scratch/zhuz/vasp]\$' followed by the command 'sbatch z\_jobs\_shaheen'. The second line shows the output 'Submitted batch job 2801027'. The third line shows the prompt '[zhuz@login3:/scratch/zhuz/vasp]\$' followed by a dollar sign '\$'.

```
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 — ssh -Y zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[[zhuz@login3:/scratch/zhuz/vasp]$ls -l std.*
-rw-r--r-- 1 zhuz g-zhuz 132500 Jan 29 10:41 std.err
-rw-r--r-- 1 zhuz g-zhuz   5653 Jan 29 10:49 std.out
[[zhuz@login3:/scratch/zhuz/vasp]$grep "free energy TOTEN" OUTCAR
  free energy TOTEN  =    -3042.35709769 eV
[[zhuz@login3:/scratch/zhuz/vasp]$
```



# 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

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- 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

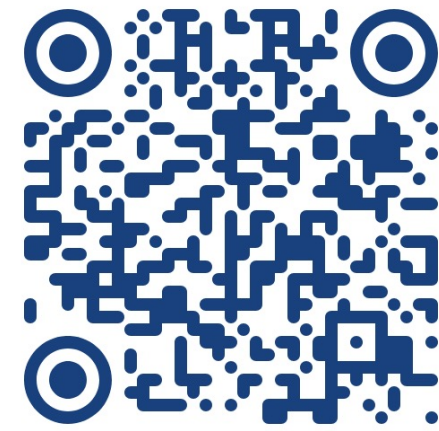
# Thank You!

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[help@hpc.kaust.edu.sa](mailto:help@hpc.kaust.edu.sa)



# Agenda



Shaheen III Survey

- 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 workflow
- 11:20-11.30am Q&A and Open Discussion