

Getting Started on Shaheen

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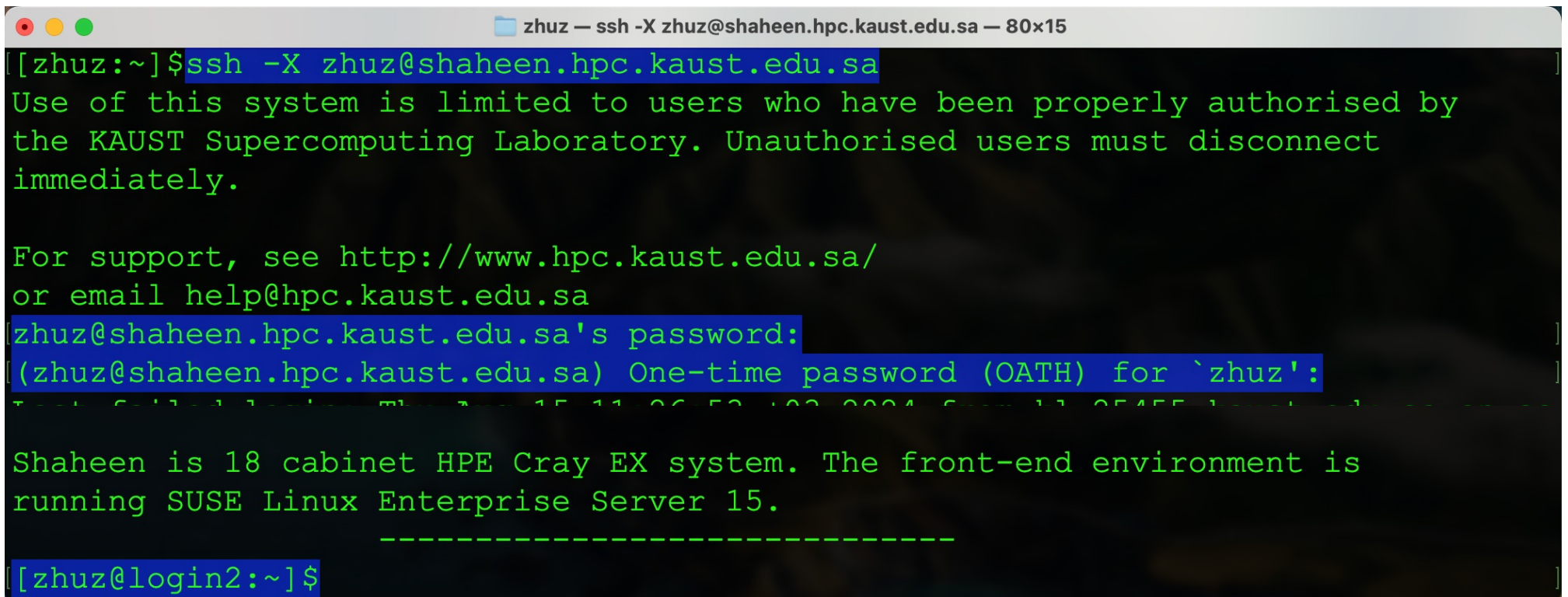
KAUST Supercomputing Core Lab

Outline

- Login Shaheen
- Module Environments
- Working Directories
- Compilation
- Slurm Job Scheduler
- Check Results
- Help

Login Shaheen

- Login (Linux and Mac OS)
 - User “terminal”
 - `ssh -X <UserName>@shaheen.hpc.kaust.edu.sa`



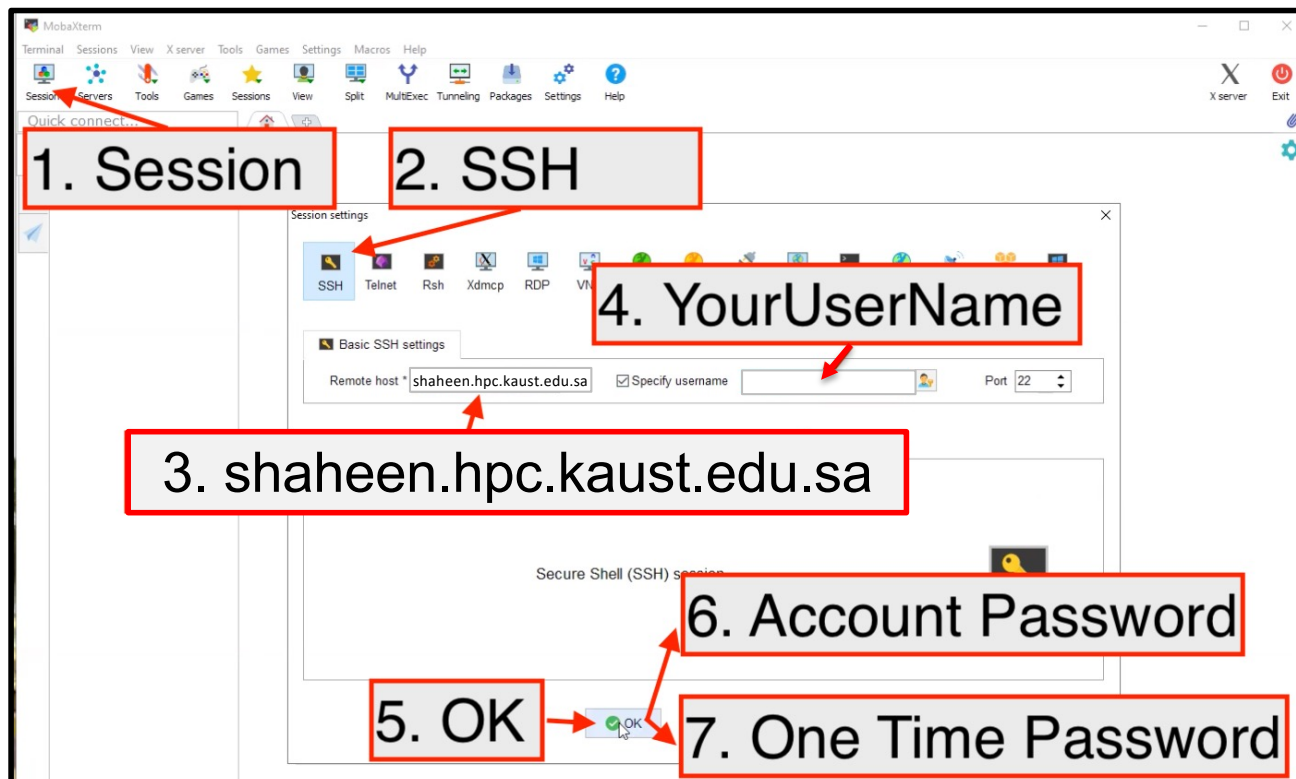
```
zhuz — ssh -X zhuz@shaheen.hpc.kaust.edu.sa — 80x15
[zhuz:~]$ ssh -X zhuz@shaheen.hpc.kaust.edu.sa
Use of this system is limited to users who have been properly authorised by
the KAUST Supercomputing Laboratory. Unauthorised users must disconnect
immediately.

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':
-----
Shaheen is 18 cabinet HPE Cray EX system. The front-end environment is
running SUSE Linux Enterprise Server 15.

-----
[zhuz@login2:~]$
```

Login Shaheen

- Login (Windows)
 - Use “MobaXterm” (or other tools)
 - <https://mobaxterm.mobatek.net/download.html>



Module Environments

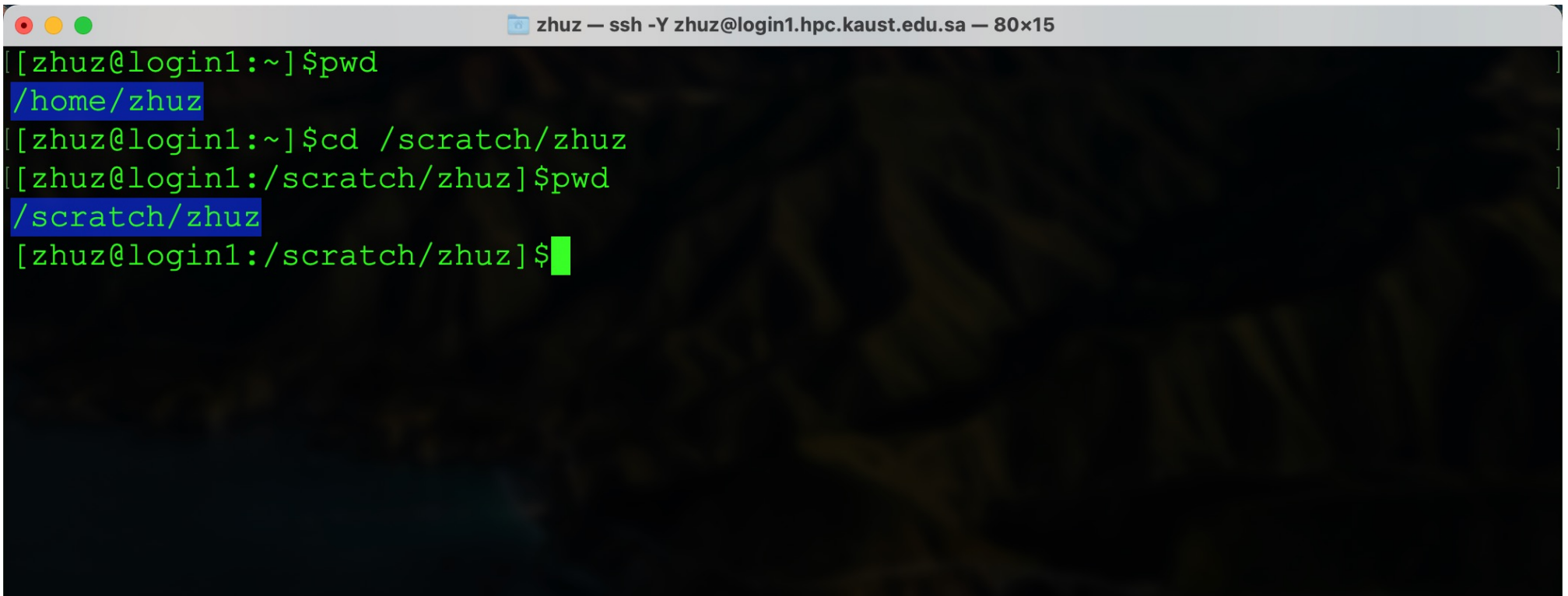
- What is Available
 - module avail, module load, module list
 - module help

```
zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 80x15
[zhuz@login1:~]$ module avail
----- /opt/cray/pe/perftools/23.09.0/modulefiles -----
perftools          perftools-lite-gpu    perftools-preload
perftools-lite     perftools-lite-hbm
perftools-lite-events perftools-lite-loops

----- /opt/cray/pe/modulefiles -----
PrgEnv-aocc/8.4.0 (default)
PrgEnv-aocc/8.5.0
PrgEnv-cray/8.4.0 (default)
PrgEnv-cray/8.5.0
PrgEnv-gnu/8.4.0 (default)
PrgEnv-gnu/8.5.0
PrgEnv-intel/8.4.0 (default)
```

Working Directories

- Where to Run
 - /scratch/<username>

A terminal window with a grey title bar containing the text "zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 80x15". The terminal content shows a sequence of commands and their outputs: the user runs "pwd" and the output is "/home/zhuz"; then the user runs "cd /scratch/zhuz" and the prompt changes to "[zhuz@login1:/scratch/zhuz]"; finally, the user runs "pwd" and the output is "/scratch/zhuz". The prompt is currently "[zhuz@login1:/scratch/zhuz]\$".

```
[zhuz@login1:~]$pwd
/home/zhuz
[zhuz@login1:~]$cd /scratch/zhuz
[zhuz@login1:/scratch/zhuz]$pwd
/scratch/zhuz
[zhuz@login1:/scratch/zhuz]$
```


Compilation

- Programming Environments
 - aocc, cray, intel, gnu

```
zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 80x15
[zhuz@login1:/scratch/zhuz/mytest]$cat welcome.c
#include <stdio.h>
int main() {
    printf(" ---- Welcome to Shaheen III! ---- \n");
    return 0;
}

[zhuz@login1:/scratch/zhuz/mytest]$module switch PrgEnv-cray/8.4.0 PrgEnv-intel
[zhuz@login1:/scratch/zhuz/mytest]$cc welcome.c -o welcome
[zhuz@login1:/scratch/zhuz/mytest]$ls -l
total 16
-rwxr-xr-x 1 zhuz g-zhuz 11632 Mar 26 14:16 welcome
-rw-r--r-- 1 zhuz g-zhuz 101 Mar 26 14:15 welcome.c
[zhuz@login1:/scratch/zhuz/mytest]$
```

Slurm Job Scheduler

- Jobscript to Run on the Compute Nodes
 - #SBATCH directives; Environment settings;
Command lines

```
zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 80x15
[zhuz@login1:/scratch/zhuz/mytest]$cat submit
#!/bin/bash
#SBATCH --partition=workq
#SBATCH --job-name=welcome
#SBATCH --nodes=1
#SBATCH --time=4:00:00
#SBATCH --err=std.err
#SBATCH --output=std.out
#-----#
module switch PrgEnv-cray/8.4.0 PrgEnv-intel
#-----#
echo "The job "${SLURM_JOB_ID}" is running on "${SLURM_JOB_NODELIST}"
#-----#
srun --ntasks=1 --hint=nomultithread ./welcome
[zhuz@login1:/scratch/zhuz/mytest]$
```

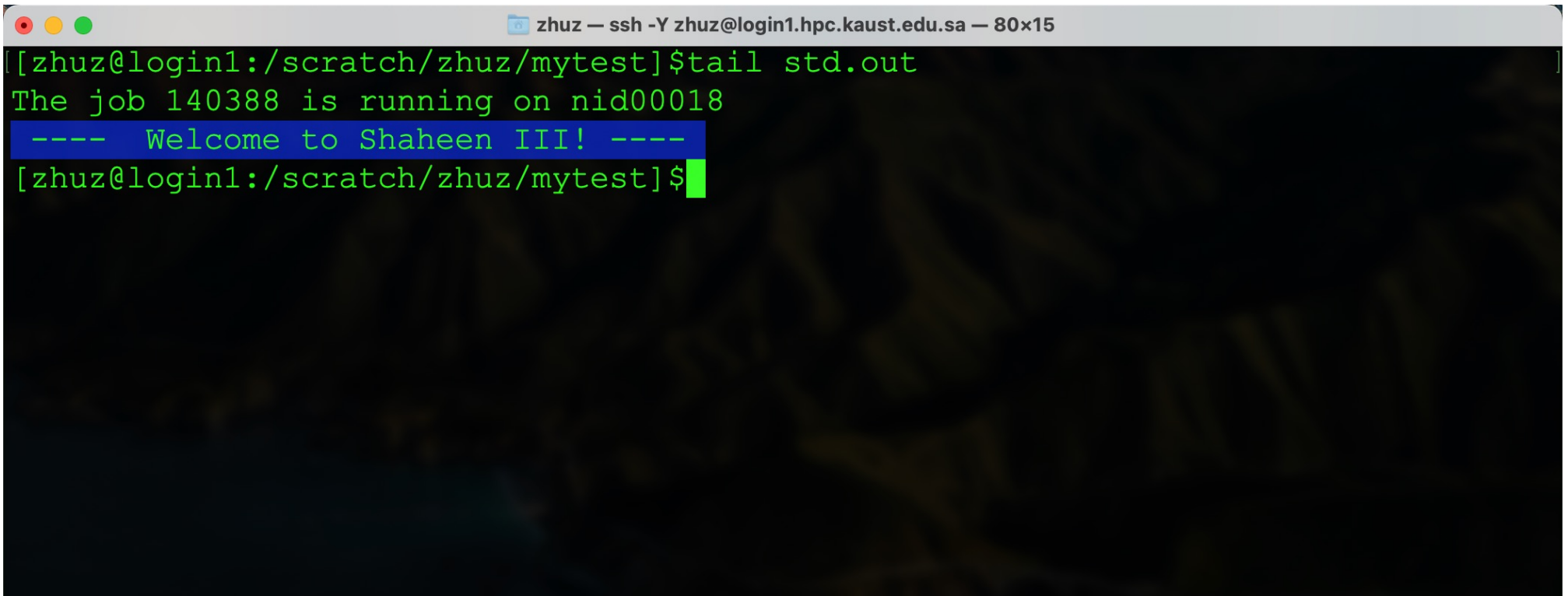

Slurm Job Scheduler

- Submit/Check/Cancel jobs
 - sbatch, squeue, scancel

```
zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 108x23
[[zhuz@login1:/scratch/zhuz/mytest]$ sbatch submit
Submitted batch job 140388
[[zhuz@login1:/scratch/zhuz/mytest]$ squeue --me
   JOBID      USER ACCOUNT      NAME  ST REASON      START_TIME      TIME  TIME_LEFT  NODES
   140388      zhuz   k01         welcome  R None      2024-03-26T14:19:13  0:00   4:00:00    1
[[zhuz@login1:/scratch/zhuz/mytest]$ scancel 140388
[[zhuz@login1:/scratch/zhuz/mytest]$ squeue --me
   JOBID      USER ACCOUNT      NAME  ST REASON      START_TIME      TIME  TIME_LEFT  NODES
[[zhuz@login1:/scratch/zhuz/mytest]$
```

Check Results

- Output files
 - std.out, std.err
 - Application specific output files

A terminal window with a grey title bar containing the text "zhuz — ssh -Y zhuz@login1.hpc.kaust.edu.sa — 80x15". The terminal content shows a green prompt "[zhuz@login1:/scratch/zhuz/mytest]\$" followed by the command "tail std.out". The output is "The job 140388 is running on nid00018" followed by a blue highlighted line containing "---- Welcome to Shaheen III! ----". The prompt returns to "[zhuz@login1:/scratch/zhuz/mytest]\$" with a green cursor.

```
[zhuz@login1:/scratch/zhuz/mytest]$tail std.out
The job 140388 is running on nid00018
---- Welcome to Shaheen III! ----
[zhuz@login1:/scratch/zhuz/mytest]$
```

Help

- Open a Ticket for any Issues/Questions
 - help@hpc.kaust.edu.sa
 - One issue one ticket

Agenda

- 8:30am Welcome
- 8:35am Shaheen III Hardware 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



Shaheen III Survey