Getting Started on Shaheen

Zhiyong Zhu

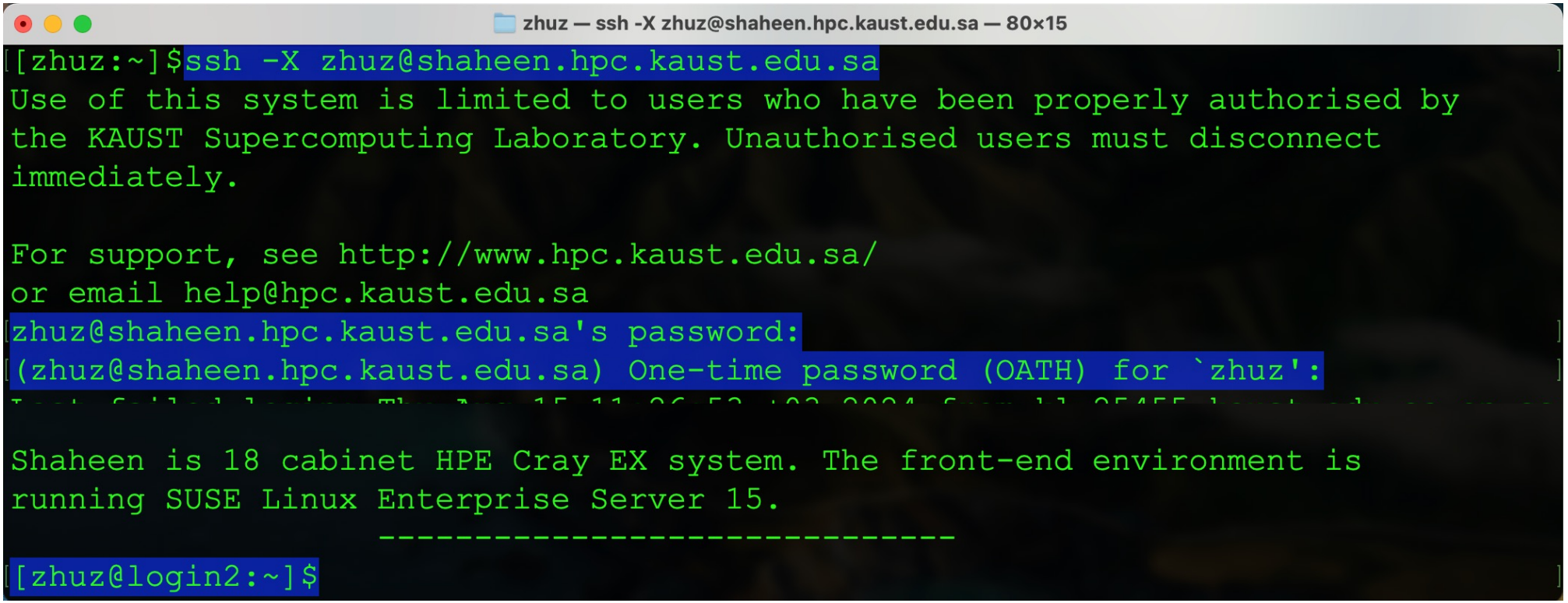
KAUST Supercomputing Core Lab

Outline

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

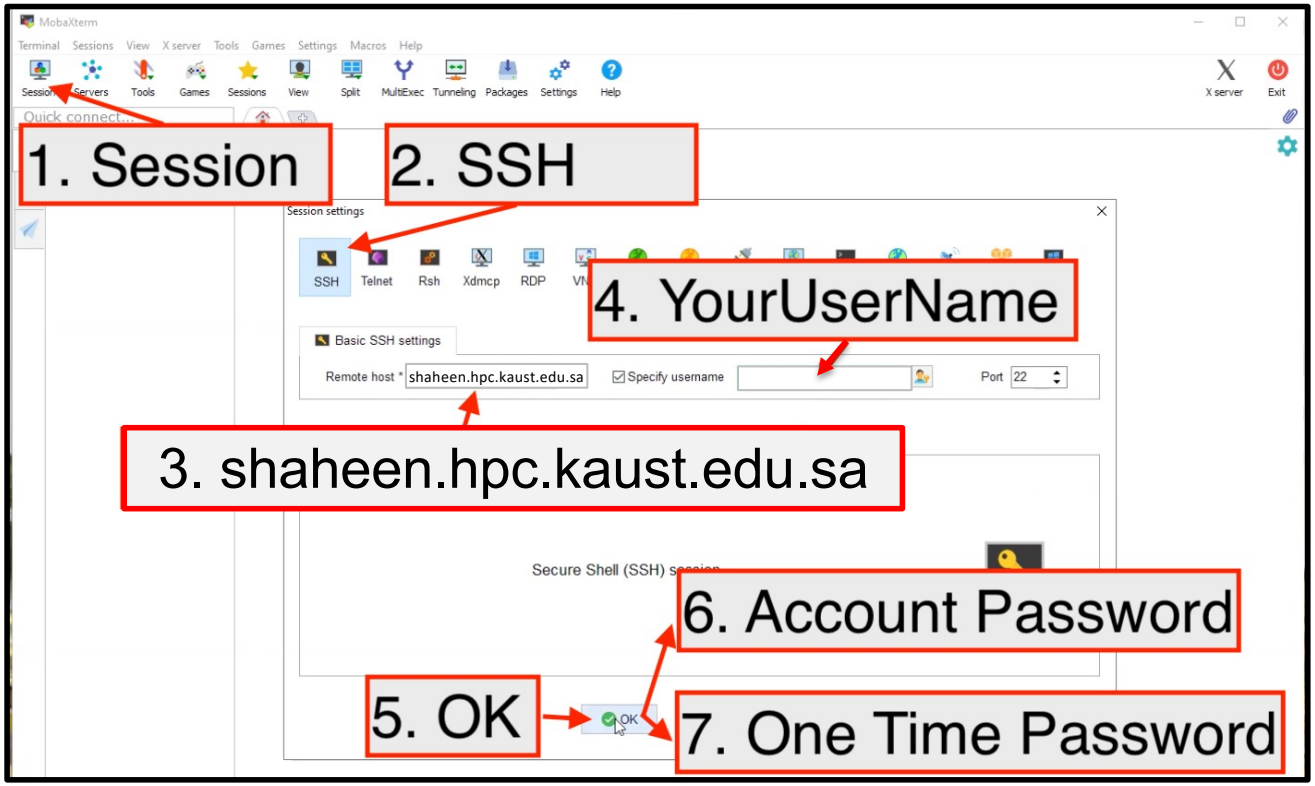
Login Shaheen

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



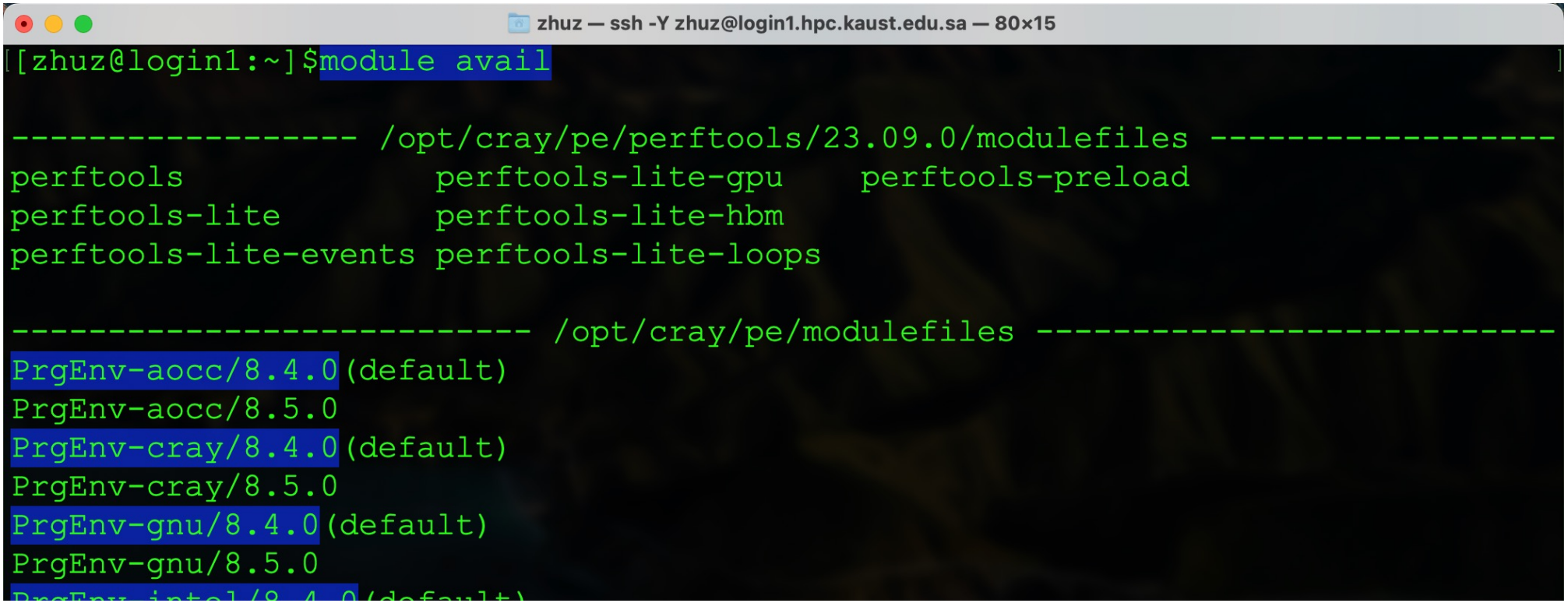
Login Shaheen

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



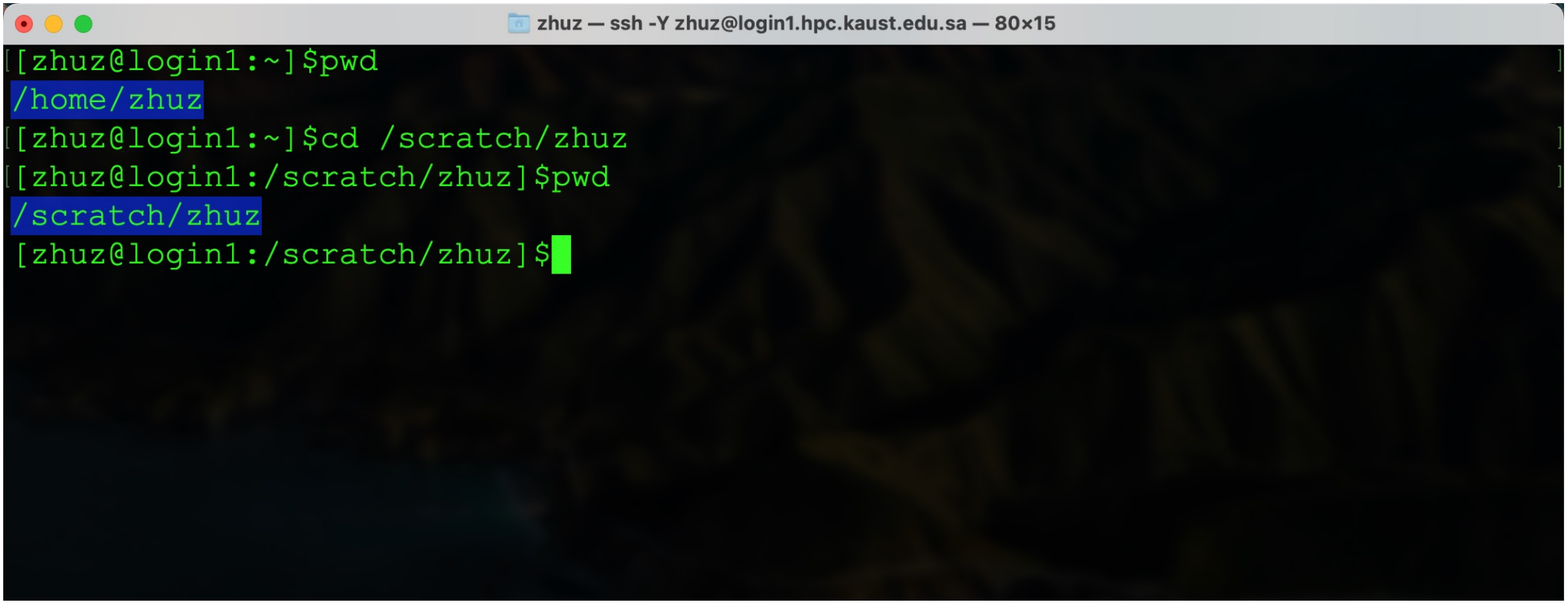
Module Environments

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



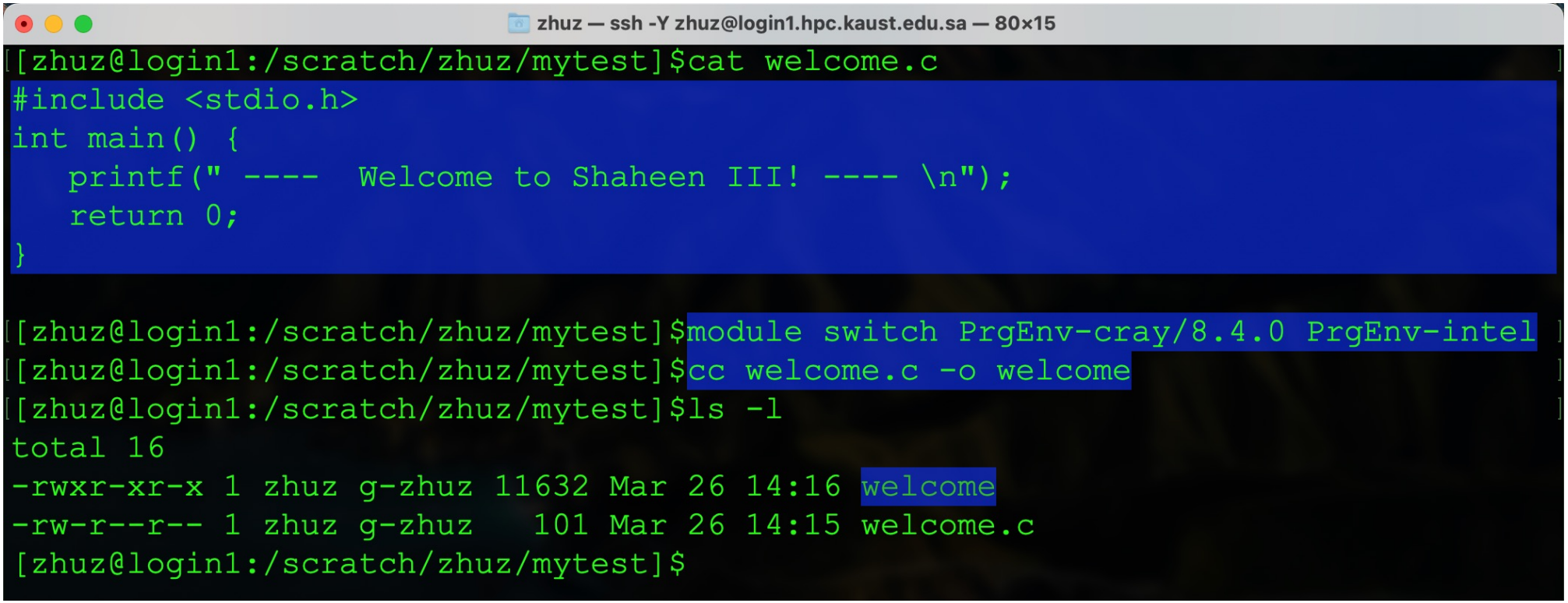
Working Directories

- Where to Run
  - /scratch/<username>



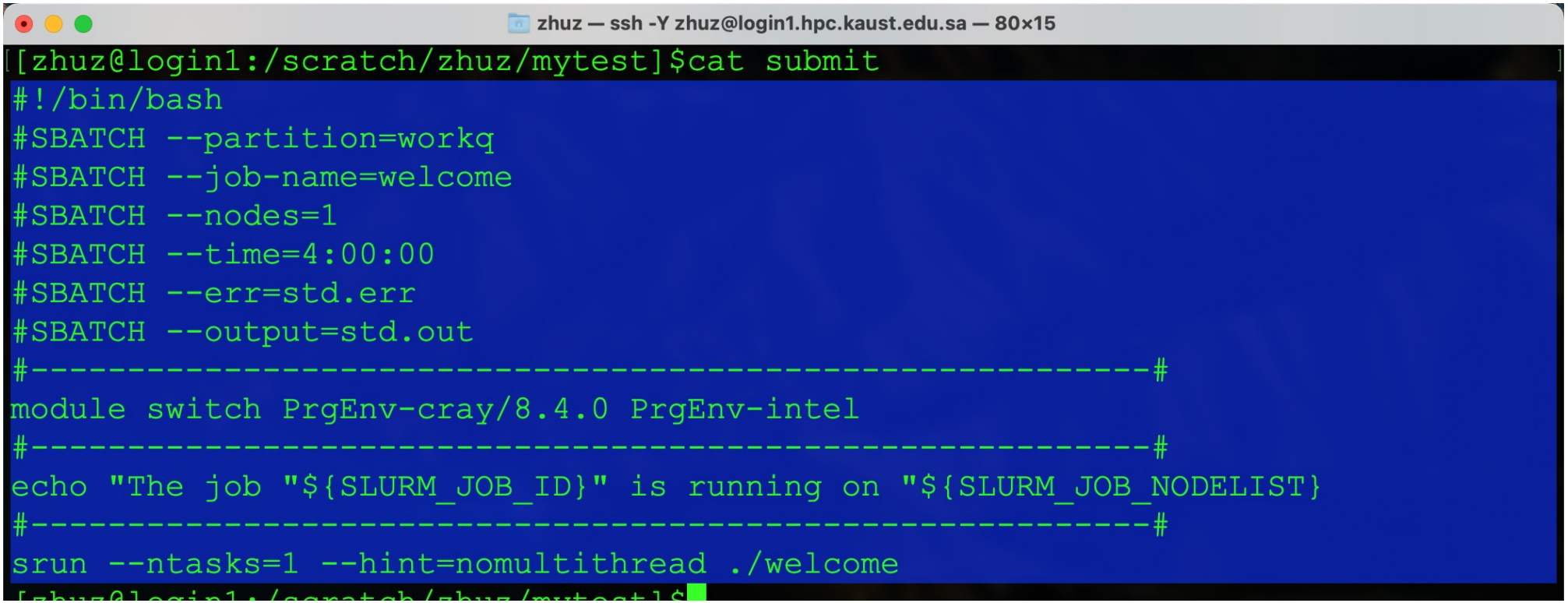
Compilation

- Programming Environments
  - aocc, cray, intel, gnu



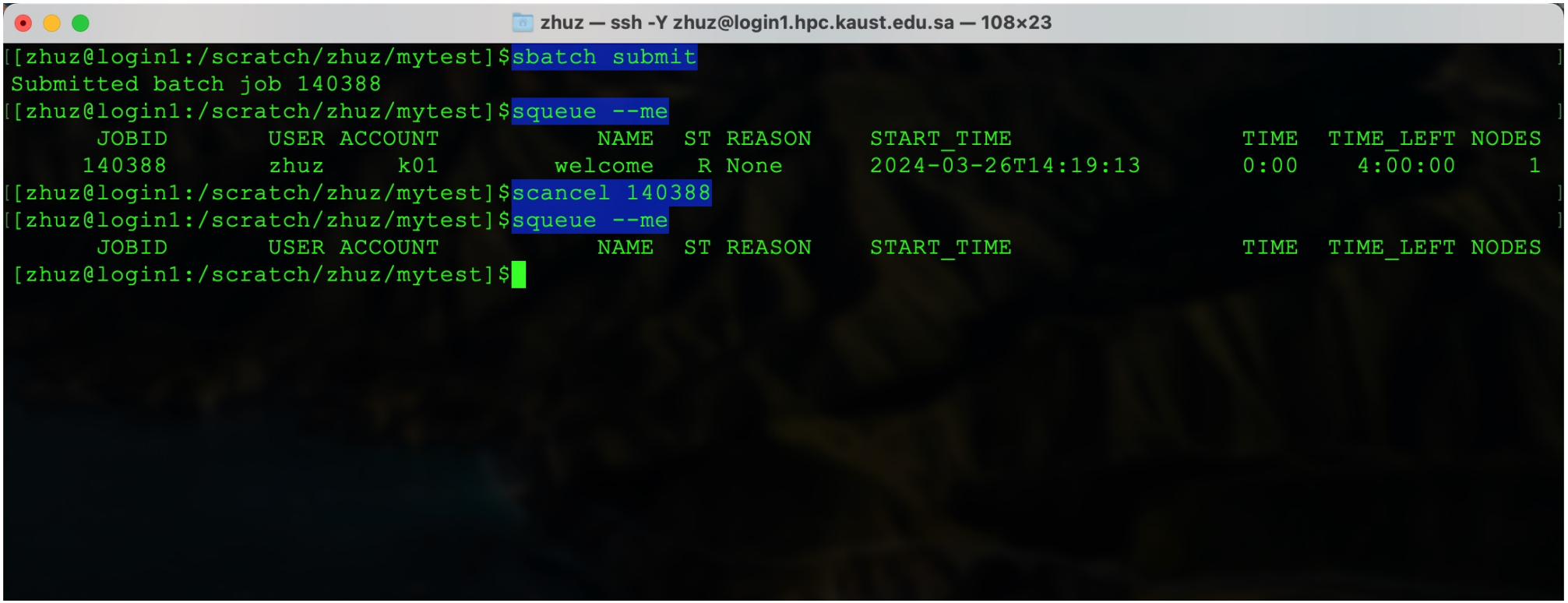
Slurm Job Schedular

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



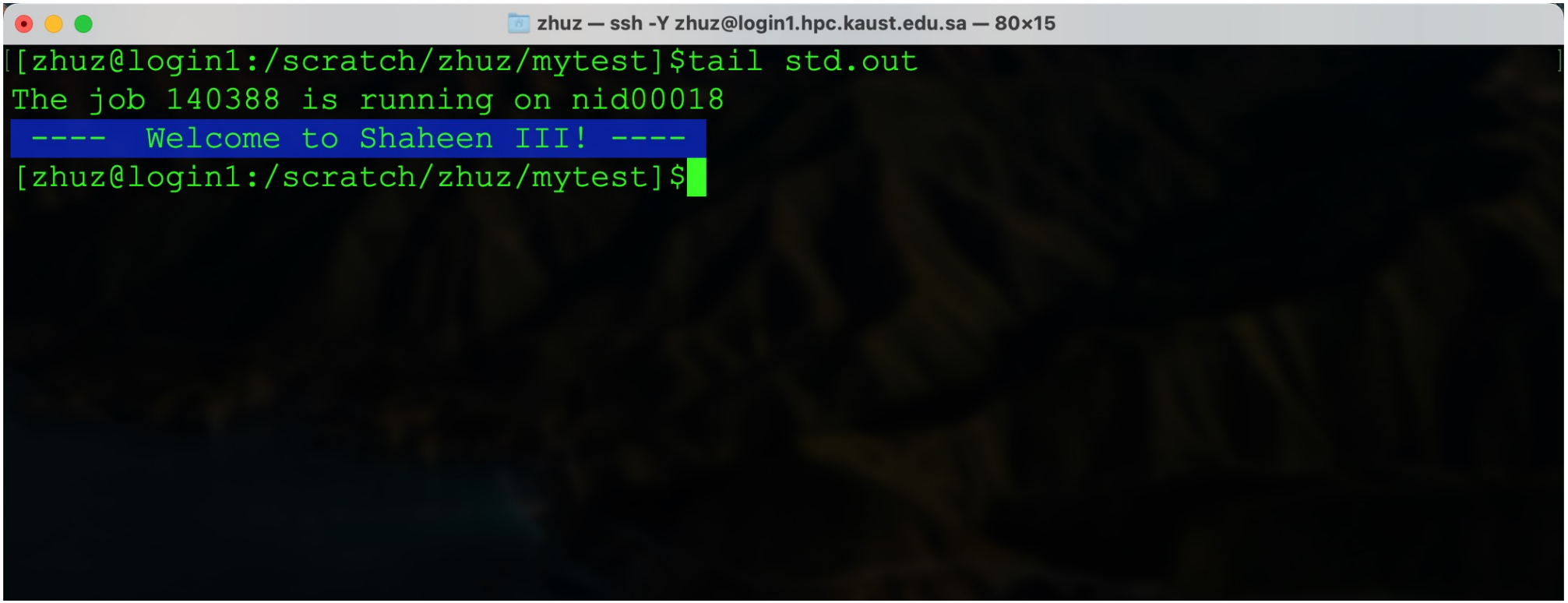
Slurm Job Schedular

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



Check Results

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



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