

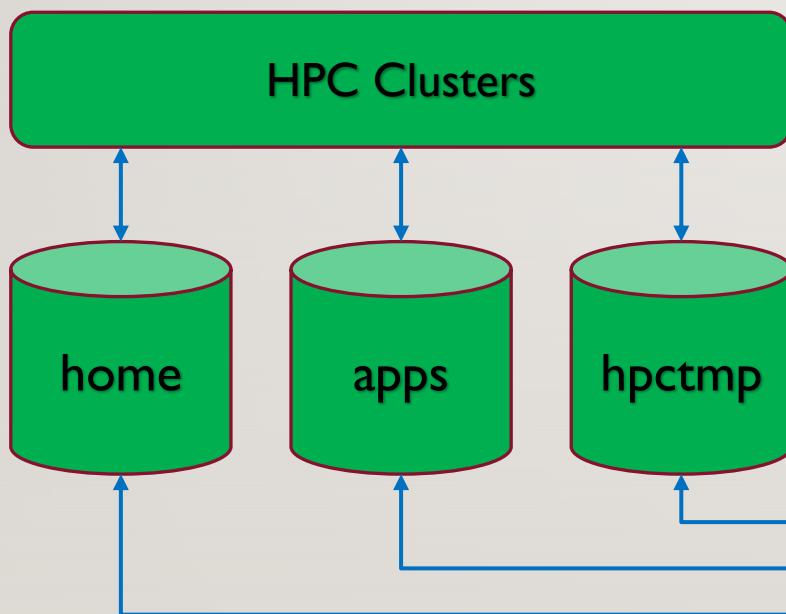
HPC CLOUD BRIEFING

6 AUGUST 2020

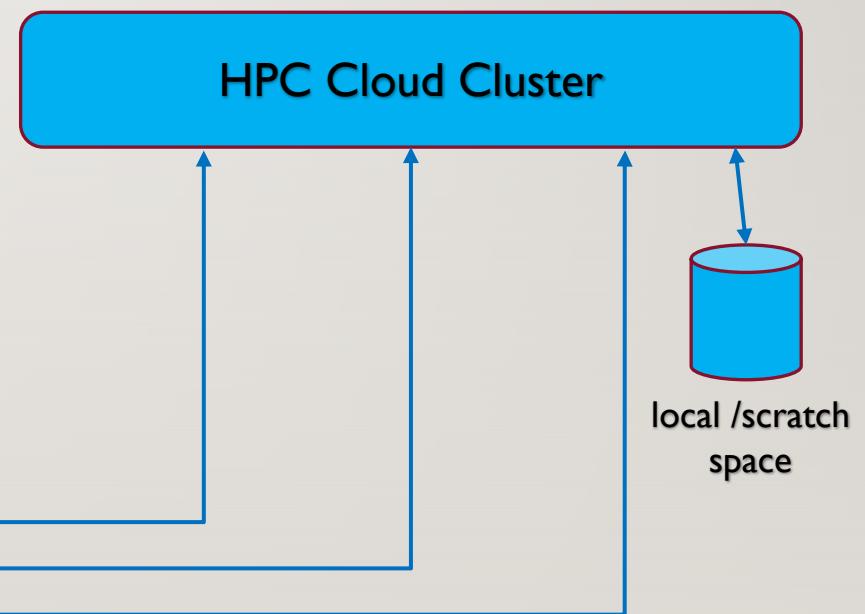
10:30AM

OVERVIEW OF HPC CLOUD

On Campus



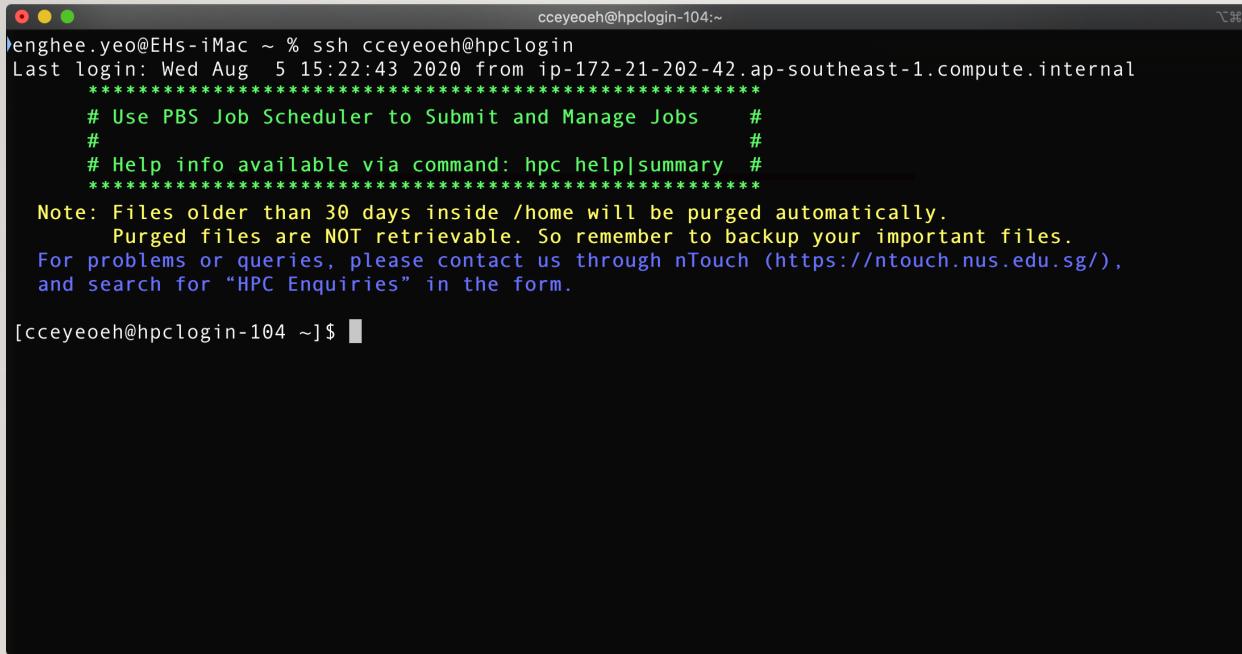
In the Cloud



WHY CLOUD

- Scalability
- Flexibility
- Access to the latest hardware
- Better HPC experience for all users
- Cost savings in bulk

LOGIN TO HPC CLOUD LOGIN HOST

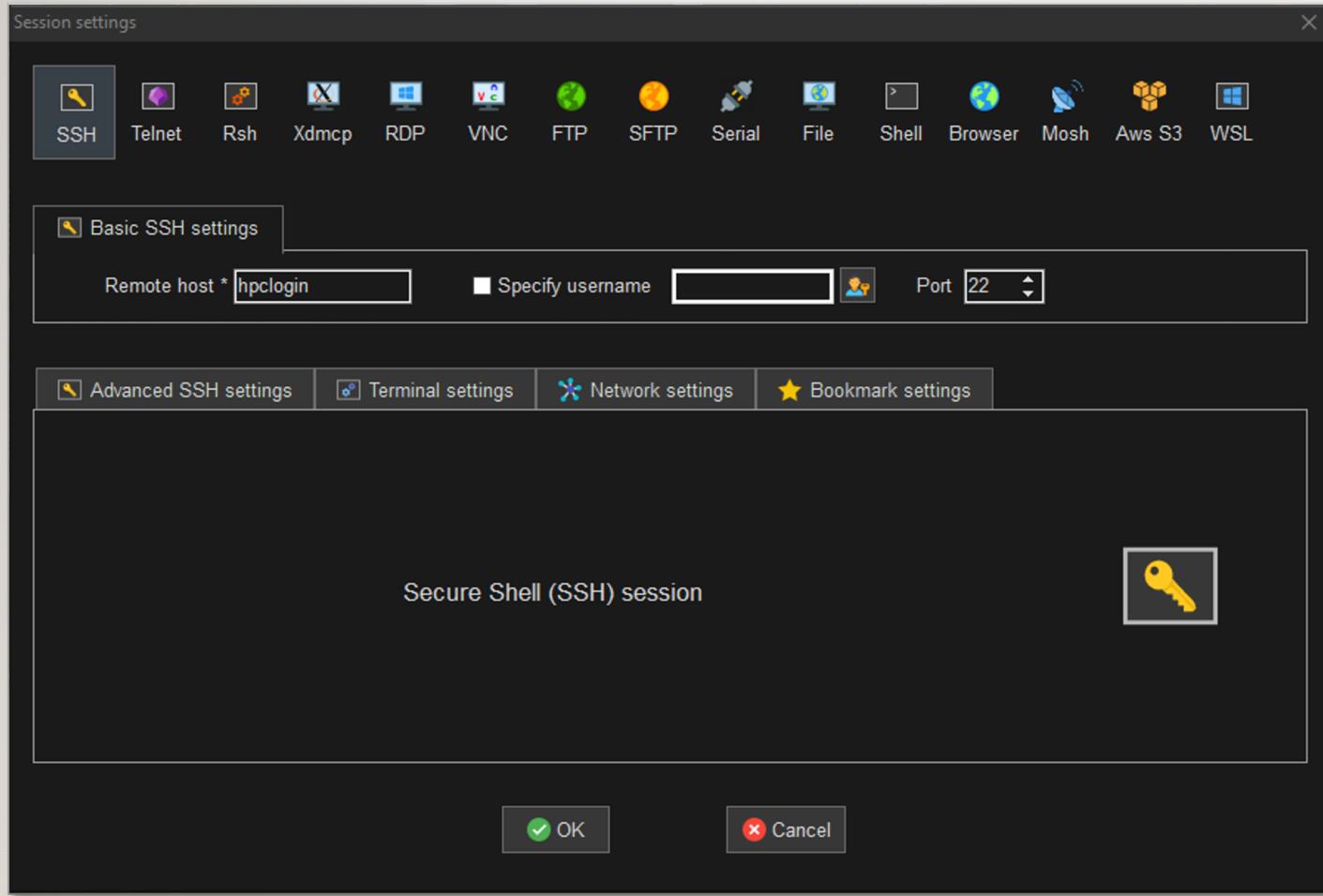


A screenshot of a macOS terminal window titled "cceyeoeh@hpclogin-104:~". The window shows the following text output:

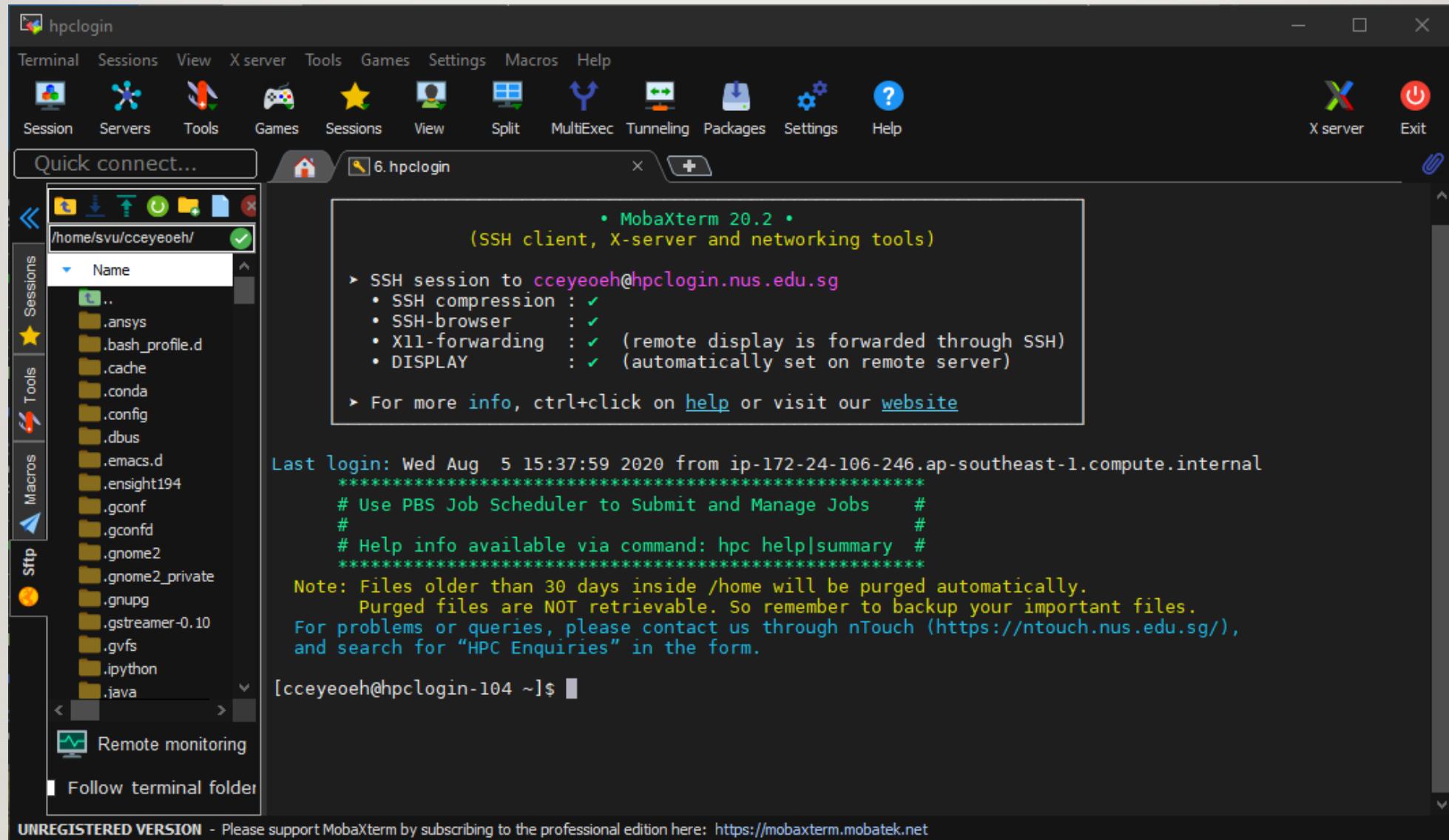
```
cceyeoeh@EHs-iMac ~ % ssh cceyeoeh@hpclogin
Last login: Wed Aug  5 15:22:43 2020 from ip-172-21-202-42.ap-southeast-1.compute.internal
*****# Use PBS Job Scheduler to Submit and Manage Jobs  #
##
# Help info available via command: hpc help|summary  #
*****Note: Files older than 30 days inside /home will be purged automatically.
Purged files are NOT retrievable. So remember to backup your important files.
For problems or queries, please contact us through nTouch (https://ntouch.nus.edu.sg/), and search for "HPC Enquiries" in the form.

[cceyeoeh@hpclogin-104 ~]$
```

- SSH from your desktop, after you login to Pulse Secure VPN
- Login using NUS account and password
- SSH to the login host:
 - **ssh [userid]@hpclogin**



USING MOBAXTERM



TRANSFERRING JOB FILES

- Transfer your files to your home directory or /hpctmp
- Same quotas as HPC Clusters on campus
- Same file aging policies as in /hpctmp on campus

PBS PRO JOB SUBMISSION

- PBS Pro job scheduler
- Same commands as the HPC clusters on campus
- Only one queue: flexi queue

PBS PRO JOB SUBMISSION

- Sample job script:

```
## HEADER ##

#!/bin/bash

#PBS -P [PROJECT_NAME]
#PBS -j oe
#PBS -N [JOB_NAME]
```

PBS PRO JOB SUBMISSION

- Sample job script:

```
## QUEUE DIRECTIVES ##

#PBS -l select=16:ncpus=1

# opt for -l place=free to run on any idle cpu within the cluster
#PBS -l place=free
# opt for -l place=pack to keep your analysis within the same node
###PBS -l place=pack
```

PBS PRO JOB SUBMISSION

- Sample job script:

```
## MISC DIRECTIVES ##

## Automatically calculate the number of processors
cd ${PBS_O_WORKDIR}; ### this line is needed, do not delete.
np=$( cat ${PBS_NODEFILE} | wc -l ); ### get number of CPUs
```

PBS PRO JOB SUBMISSION

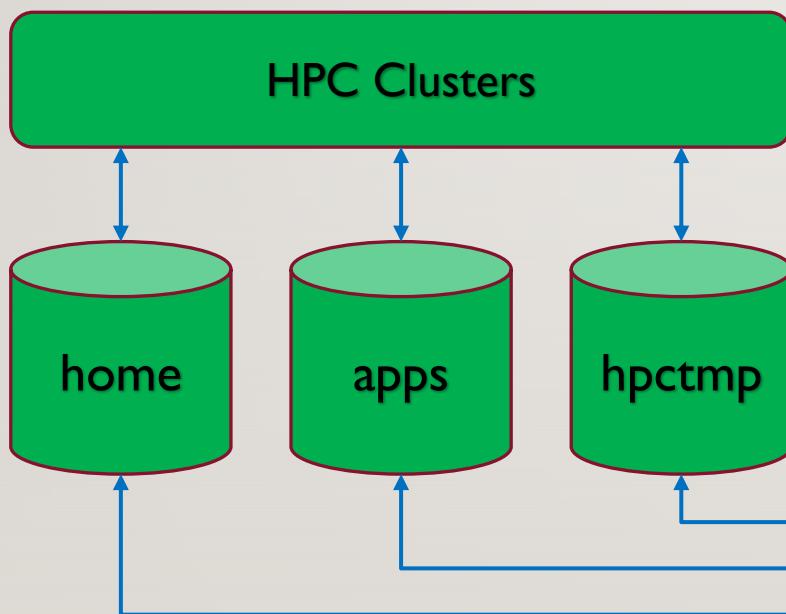
- Sample job script: (Note: /scratch versus /hpctmp)

```
## SCRATCH SPACE DIRECTIVES ##

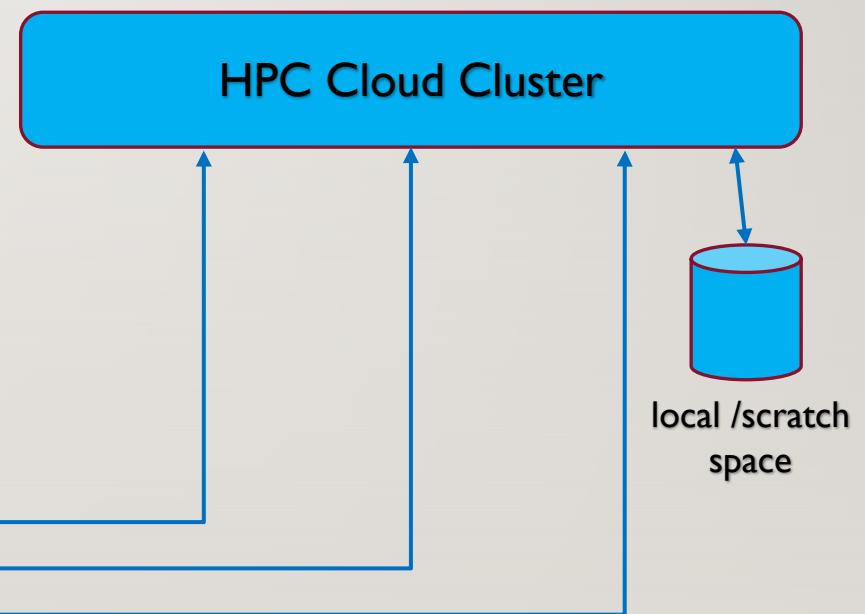
## Make a temporary scratch space (this should be on /scratch/)
scratch=/scratch/${USER}/${PBS_JOBID}
export TMPDIR=${scratch}
mkdir -p ${scratch}
```

OVERVIEW OF HPC CLOUD

On Campus



In the Cloud



PBS PRO JOB SUBMISSION

- Sample job script:

```
## JOB DIRECTIVES ##

##--- Put your exec/application commands below ---
module load Abaqus/cmd
module load Intel/xe_2018
abaqus scratch=${scratch} input=rigmultimech_std job=abaqus_job \
    cpus=${np} double interactive
wait;
## Remove scratch space
rm -rf ${scratch}
exit 0
```

APPLICATION SOFTWARE

- Same set of application software as in HPC Cluster on-campus
- Use the same modules commands to access the software, example:
 - `module avail`
 - `module list`
 - `module load Intel/xe_2018`

REMINDERS

- Only one queue: flexi
- Request for resources in chunks:
 - `#PBS -l select=1:ncpus=1:mem=1950mb`
 - `#PBS -l select=1:ncpus=1`
- Use home directory (20GB quota) and /hpctmp (500GB quota) for jobs files
- /scratch is a fast local storage for jobs within a single server (not for distributed parallel jobs) or some MPI jobs that can make use of the local fast storage.

WHAT TO EXPECT IN HPC CLOUD?

- shorter queueing / waiting time
- access to newer hardware technology
- better user experience – caveat: not for interactive graphical apps
- Coming soon (end August): New HPC Cloud Portal - watch for the announcements!

DEMOS
