Introduction to Gadi — Part I
Get Full Access to All Resources on Gadi

NCI Training

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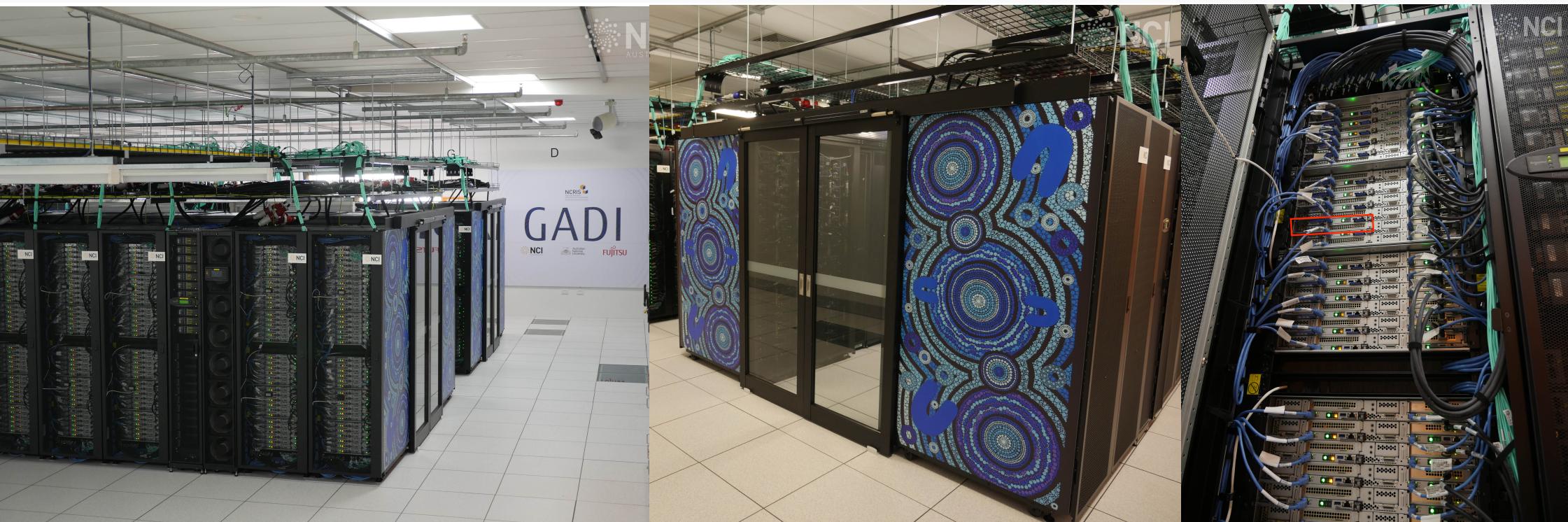
Agenda

- First half of [Welcome to Gadi](#) opus page
- Three sections
    - Login
    - Storage and data transfer
    - Jobs
- Exercise + Key points + Q&A
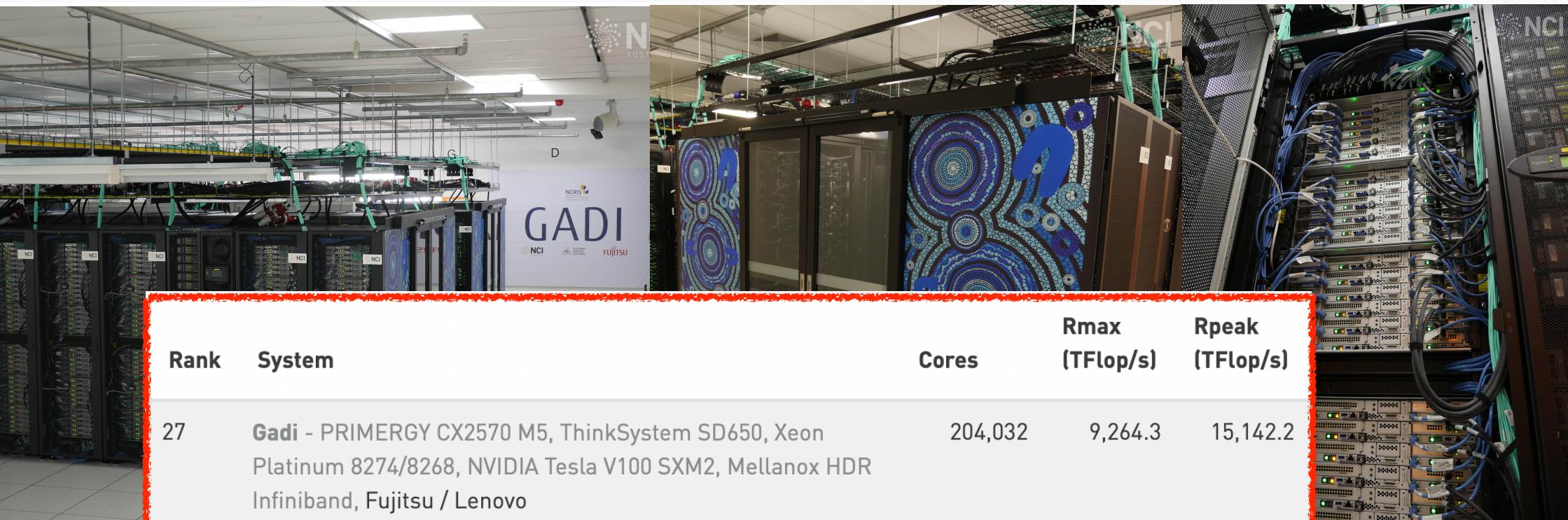
What is Gadi

- High Performance Computing System operated by NCI
- Supercomputer
  - 10 login nodes
  - 6 data mover nodes
  - 4000+ compute nodes, including 160 GPU ones
  - Mellanox HDR InfiniBand interconnect network
  - 22 PiB storage available on the parallel Lustre filesystems
  - Application software available through environment module
 - PBSPro server handles 3-4M jobs per quarter

Gadi
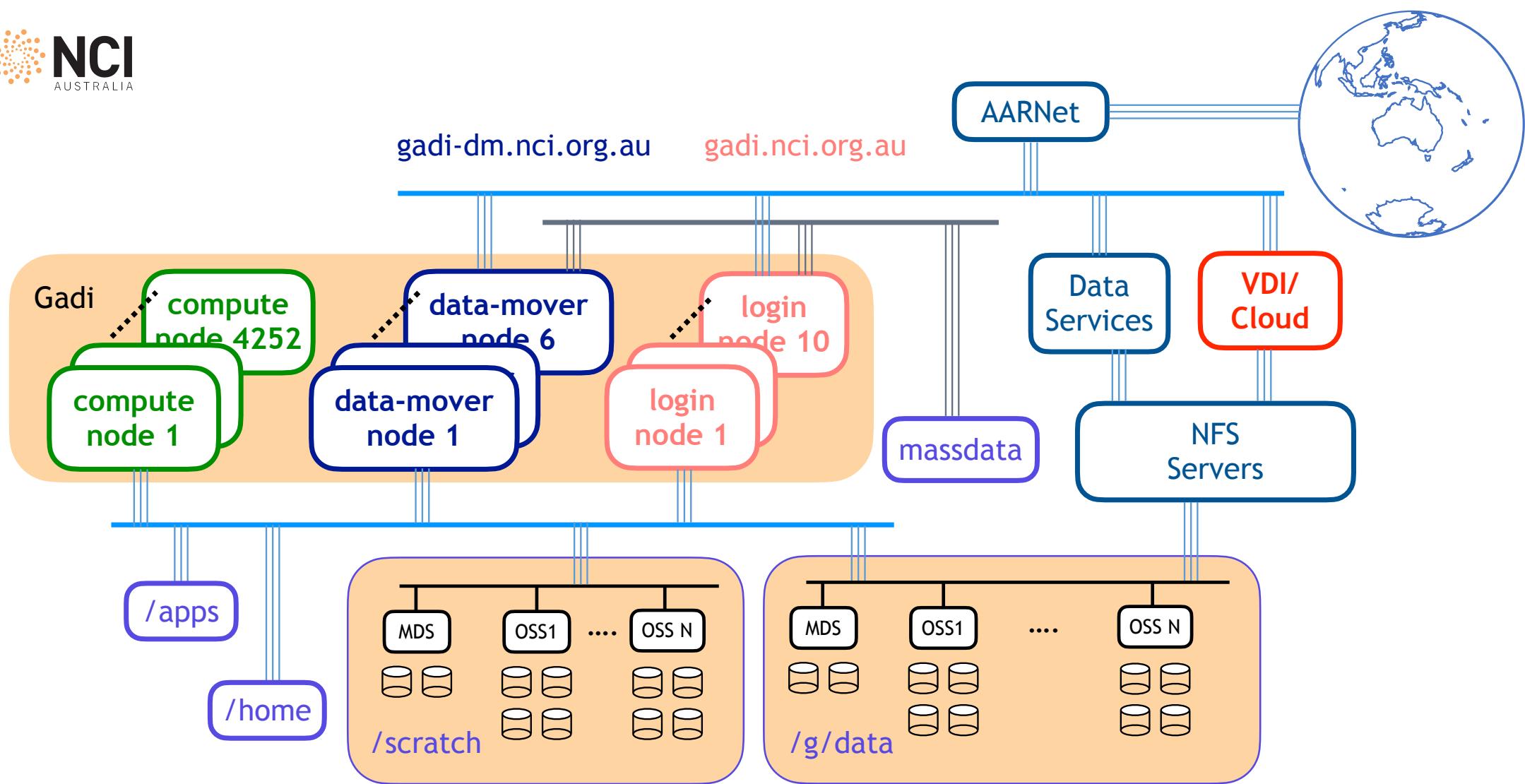
Gadi

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)
27	**Gadi** - PRIMERGY CX2570 M5, ThinkSystem SD650, Xeon Platinum 8274/8268, NVIDIA Tesla V100 SXM2, Mellanox HDR Infiniband, Fujitsu / Lenovo National Computational Infrastructure (NCI Australia) Australia	204,032	9,264.3	15,142.2

https://www.top500.org/lists/top500/list/2020/11/

Login and Login Environment

User, Project, and Shell

Login to Gadi
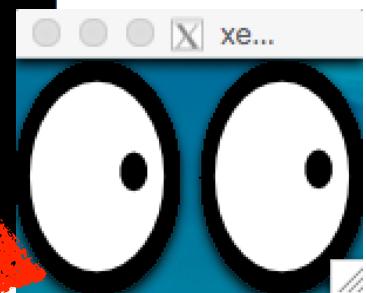
a. Open a terminal and login to one of the ten login nodes by doing

ssh <jjj777>@gadi.nci.org.au

Your username goes here

b. X forwarding enabled login and test with xeyes

```
Sue@local:~ $ ssh -Y jjj777@gadi.nci.org.au
jjj777@gadi.nci.org.au's password:
[jjj777@gadi-login-05 ~]$ xeyes
[jjj777@gadi-login-05 ~]$ exit
Sue@local:~ $
```

Explore Login Environment

- shell: echo $SHELL

- who you are

  - user: echo $USER

  - default project: echo $PROJECT

- where you are

  - gadi-login-xx where xx=[01…10]: hostname
  - directory path: pwd, echo $HOME

Edit Login Environment

- To define your own login environment, edit the following two files
    - ~/.config/gadi-login.conf
    - ~/.bashrc for SHELL=/bin/bash, or ~/.cshrc for SHELL=/bin/csh etc.

- Be careful when making changes because bad edit can lock you out

Q&A
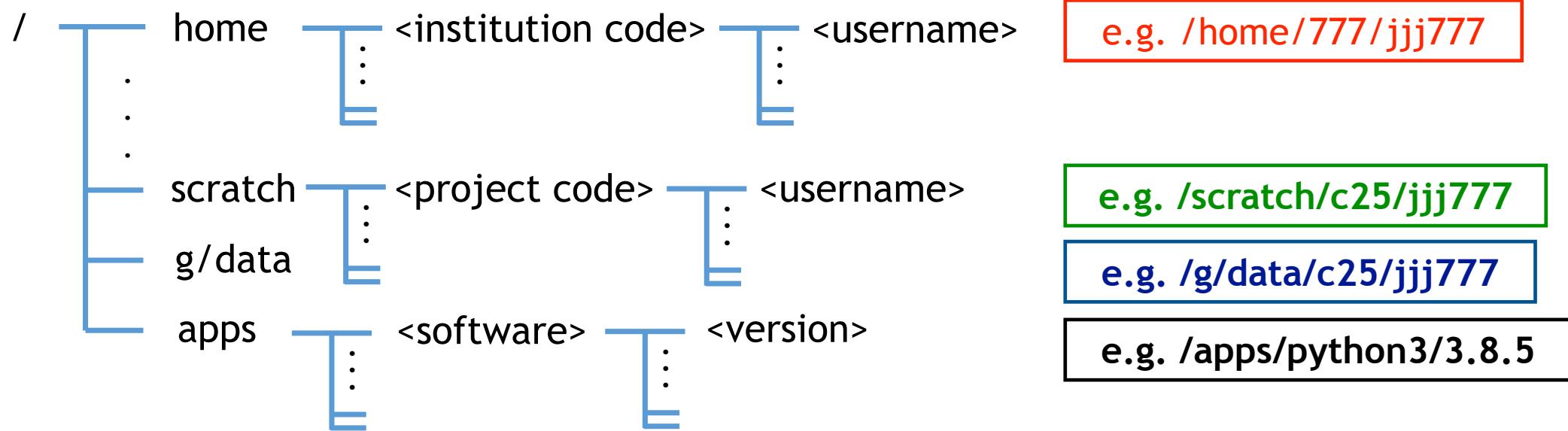
- MOTD
  - login
  - cat /etc/motd
- Usage limit on login node
  - 57 users and 64 login processes on gadi-login-01 at 9:18am this morning
  - Any processes on the login nodes will be terminated immediately if exceeding 30-minute CPU cumulative time limit and/or 4GB memory usage limit.
- Round-robin login
- Other questions?

Storage and Data Transfer
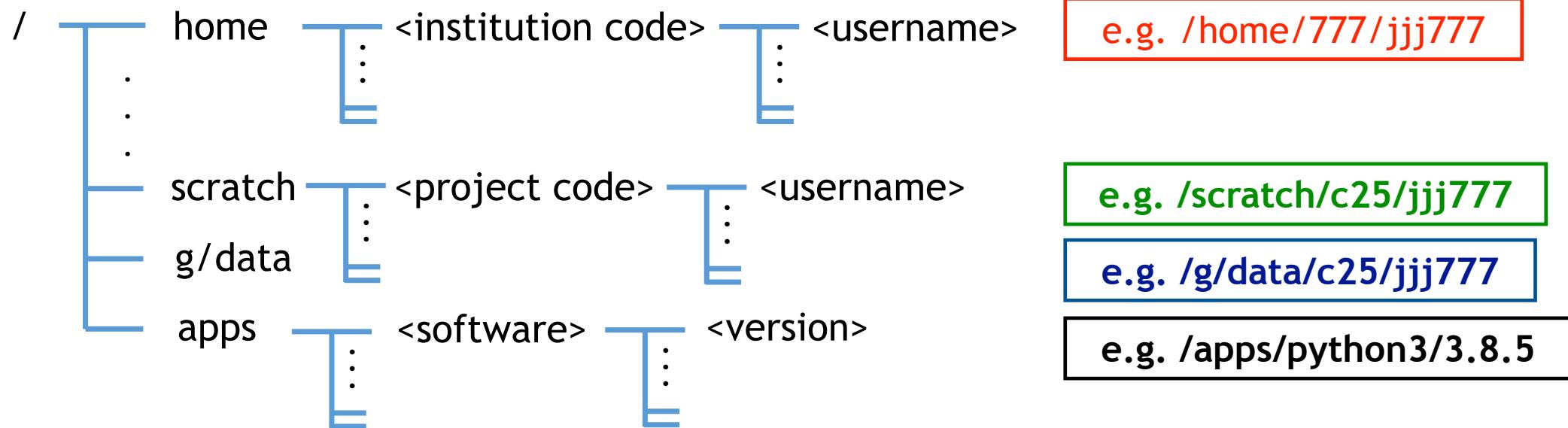
Accessible Directories and their Limits

Navigating through directories on login nodes

/ ── home ── <institution code> ── <username>

e.g. /home/777/jjj777

── scratch ── <project code> ── <username>

e.g. /scratch/c25/jjj777

── g/data

e.g. /g/data/c25/jjj777

── apps ── <software> ── <version>

e.g. /apps/python3/3.8.5

- Does your project have storage allocation on /g/data/? : lquota
- What's your data footprint on Lustre filesystems? : nci-files-report -u $USER

Navigating through directories on login nodes

```
/ ──┬── home ──┬── <institution code> ──┬── <username>      e.g. /home/777/jjj777
    ┊          ┊                          ┊
    ┊          └─                         └─
    ┊
    ├── scratch ──┬── <project code> ──┬── <username>        e.g. /scratch/c25/jjj777
    ┊            ┊                      ┊
    ├── g/data   └─                     └─                   e.g. /g/data/c25/jjj777
    ┊
    └── apps ──┬── <software> ──┬── <version>                e.g. /apps/python3/3.8.5
               ┊                ┊
               └─               └─
```

e.g. /home/777/jjj777

e.g. /scratch/c25/jjj777

e.g. /g/data/c25/jjj777

e.g. /apps/python3/3.8.5

- Where are massdata and $PBS_JOBFS

Remote Transfer through Data-mover Node

Upload data to Gadi from local PC

```
Sue@local:~ $ scp test.hdf5 jjj777@gadi-dm.nci.org.au:/scratch/c25/jjj777/input.hdf5
```

    from/source   **to/destination**

Download data from Gadi to local PC

```
Sue@local:~ $ scp jjj777@gadi-dm.nci.org.au:/scratch/public/IntroToGadi.pdf ./
```

              from/source   **to/destination**

- You can also transfer data through gadi-dm.nci.org.au using
  - commands such as sftp, rsync,...
  - applications such as FileZilla, WinSCP,....
- No interactive sessions on any of the data-mover nodes, try interactive copyq jobs

Q&A

- Shared filesystem vs compute node local disk $PBS_JOBFS
  - Shared access at all time vs 'exclusive' access during the running job
  - Size: 22 PiB vs ~400GB
- Home vs project directories vs massdata
  - Access frequency and inodes limit
  - Ownership
- Data located inside the project directory vs data owned by the project
- Apply for more storage space
  - on /scratch from NCI
  - on /g/data and massdata from scheme managers
- Other questions?

Jobs

Submission and Monitoring

Submit Jobs

```
cp /scratch/public/yxs900/gutentag.sh ./
qsub gutentag.sh
```

Any Errors?

```
$ qsub gutentag.sh
qsub: Error: You are not a member of project c25.
You must be a member of a project to submit a job
under that project.
```

- User has to join a project to use its resources
- Use the -P flag in the command line to overwrite the job submission script

> qsub -P $PROJECT gutentag.sh

Monitor Jobs

- After submission, query the job status by running
  - qstat -u $USER
  - qstat -sw <jobID>
  - qstat -f <jobID>
- Delete submitted jobs
  - qdel <jobID1> <jobID2> …
- After the job finishes, look up the jobs by running
  - qstat -fx <jobID> with the first 24 hours
  - cat gutentag.sh.o<jobID>
  - cat gutentag.sh.e<jobID>

Q&A

- How much does the gutentag job cost
  - Queue—> charge rate
  - CPU and memory request, walltime usage —> resource hour
  - Reserved SU
- qsub, qstat, qdel all launch requests to PBS server
  - run with frequency < 0.1Hz
- Other questions?

Any More Questions?

help@nci.org.au

![NCI Australia logo]

Thank you

Part 2 is coming next week on 18 March 2021