Cambridge Pathology
Introduction to High-Performance Computing

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Outline

We will cover:

1. how to create an account,
2. logging in,
3. types of data storage,
4. types of compute nodes,
5. running jobs,
6. how to check on the status of jobs,
7. how to set up environments.

Account Creation

Link for account creation:
www.hpc.cam.ac.uk/applications-access-research-computing-services

Workflow:

1. Have your PI create an account first (if they haven't already).
2. Students/postdocs/staff apply for their own account.
3. PI gets an Email to approve student/postdoc/staff account creation, linking to lab's account.
4. Set up multifactor authentication.

Resources Available Per Account

Computing Resources Per Lab Account

- 200,000 CPU hours per PI per quarter.
- 3,000 GPU hours per PI per quarter.
- Refreshes on first of: Nov, Feb, May, Aug.

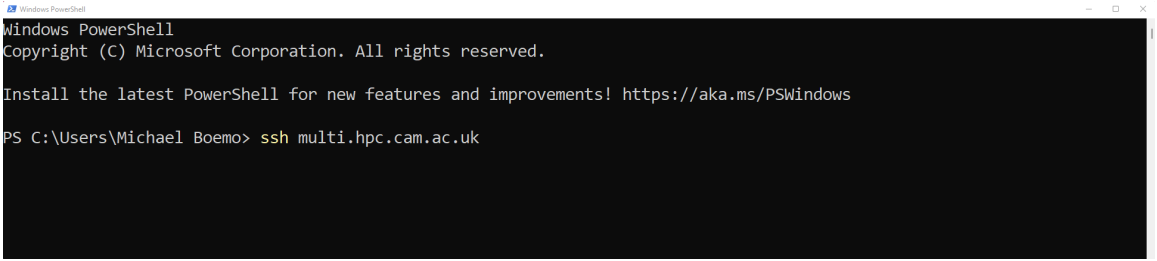
Data Storage Per User Account

1 TB in rds/hpc-work (hot storage; not backed up).

Setting up Multifactor Authentication

Download and install Microsoft Authenticator app on your phone:
https://www.microsoft.com/en-us/security/mobile-authenticator-app
(You probably already have this for Outlook login.)

Open PowerShell (Windows) or a terminal (OSX or Linux).
Type: `ssh multi.hpc.cam.ac.uk`

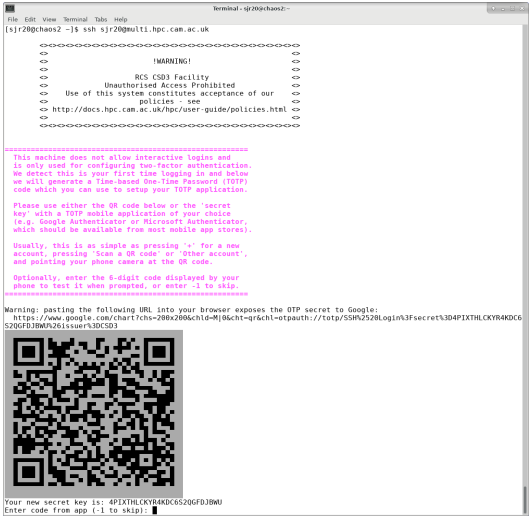


Setting up Multifactor Authentication

Enter your username and password.
Username: CRSid
Password: Raven password

From phone app: tap “+” in the right corner.
Scan the QR code that appears in the terminal.
Phone app will show a 6-digit TOTP code.
(Code changes every 30 seconds.)
Enter TOTP code in terminal.

Connection should terminate.



Ways to Log In

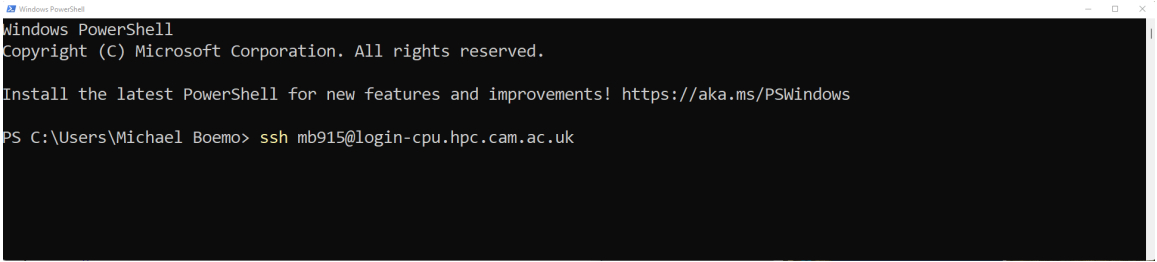
Command Line

- submit jobs,
- move files around,
- ftp files between servers,
- PowerShell or PuTTY (Windows) or terminal (OSX or Linux).

FTP Client

- move files between your computer and the server,
- graphical user interface,
- FileZilla (Windows, OSX), CyberDuck (Windows, OSX), Nautilus (Ubuntu).

Logging In (Command Line)

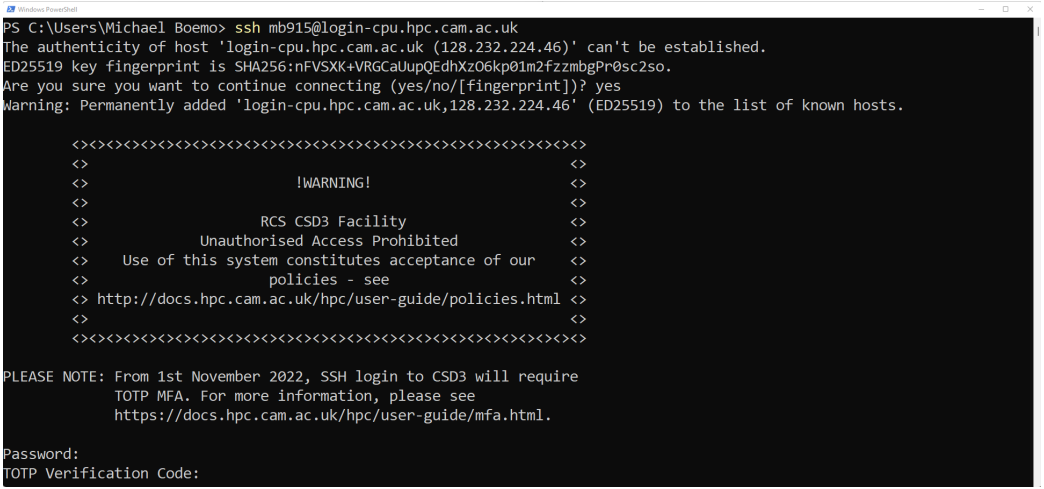


Logging In (Command Line)

Windows PowerShell

```
PS C:\Users\Michael Boemo> ssh mb915@login-cpu.hpc.cam.ac.uk
The authenticity of host 'login-cpu.hpc.cam.ac.uk (128.232.224.46)' can't be established.
ED25519 key fingerprint is SHA256:nFVSXK+VRGCaUupQEdhXzO6kp01m2fzzmbgPr0sc2so.
Are you sure you want to continue connecting (yes/no/[fingerprint])? yes
Warning: Permanently added 'login-cpu.hpc.cam.ac.uk,128.232.224.46' (ED25519) to the list of known hosts.

        <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
        <>                                                          <>
        <>                        !WARNING!                         <>
        <>                                                          <>
        <>                    RCS CSD3 Facility                     <>
        <>             Unauthorised Access Prohibited               <>
        <>    Use of this system constitutes acceptance of our     <>
        <>                     policies - see                       <>
        <> http://docs.hpc.cam.ac.uk/hpc/user-guide/policies.html <>
        <>                                                          <>
        <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>

PLEASE NOTE: From 1st November 2022, SSH login to CSD3 will require
             TOTP MFA. For more information, please see
             https://docs.hpc.cam.ac.uk/hpc/user-guide/mfa.html.

Password:
```

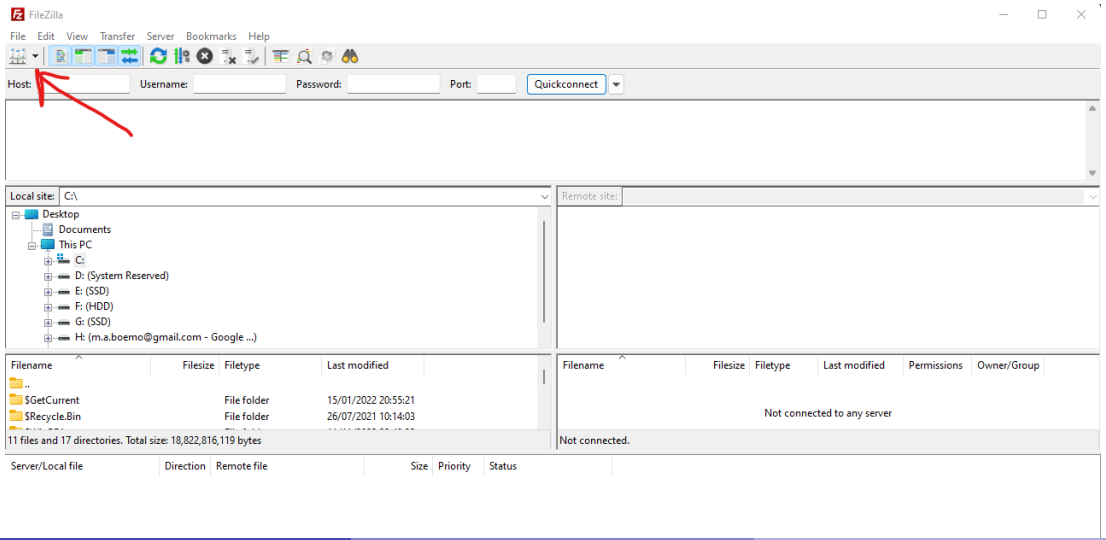
Logging In (Command Line)



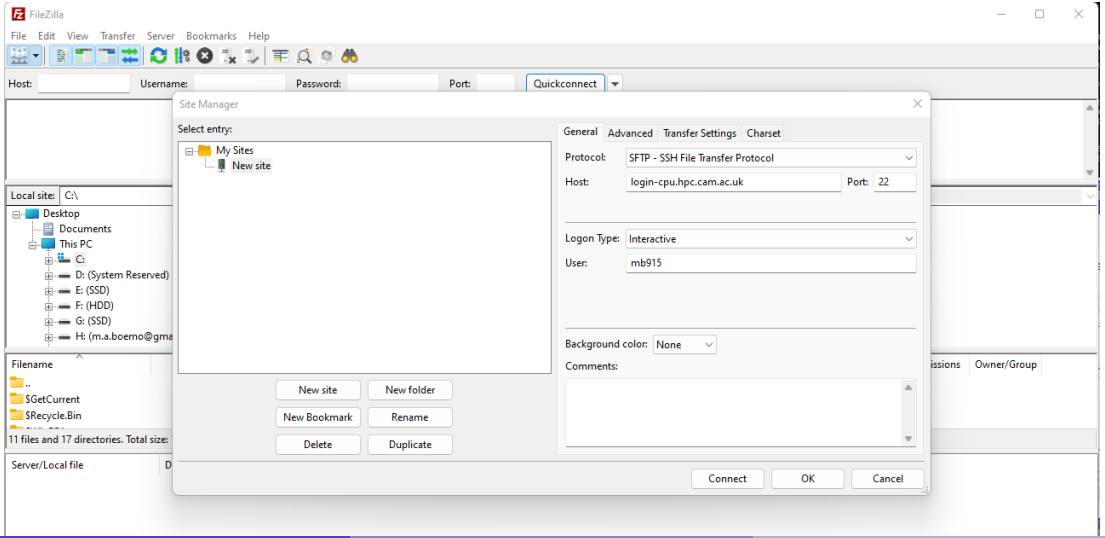
Logging In (Command Line)

```
mb915@login-e-9:~
PS C:\Users\Michael Boemo> ssh mb915@login-cpu.hpc.cam.ac.uk
The authenticity of host 'login-cpu.hpc.cam.ac.uk (128.232.224.46)' can't be established.
ED25519 key fingerprint is SHA256:nFVSXK+VRGCaUupQEdhXzO6kp01m2fzzmbgPr0sc2so.
Are you sure you want to continue connecting (yes/no/[fingerprint])? yes
Warning: Permanently added 'login-cpu.hpc.cam.ac.uk,128.232.224.46' (ED25519) to the list of known hosts.

        <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>
        <>                                                          <>
        <>                        !WARNING!                         <>
        <>                                                          <>
        <>                    RCS CSD3 Facility                     <>
        <>             Unauthorised Access Prohibited               <>
        <>     Use of this system constitutes acceptance of our     <>
        <>                       policies - see                     <>
        <> http://docs.hpc.cam.ac.uk/hpc/user-guide/policies.html <>
        <>                                                          <>
        <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>

PLEASE NOTE: From 1st November 2022, SSH login to CSD3 will require
             TOTP MFA. For more information, please see
             https://docs.hpc.cam.ac.uk/hpc/user-guide/mfa.html.

Password:
TOTP Verification Code: 055513
Last login: Fri Nov  4 17:39:33 2022 from 10.249.26.95
(base) [mb915@login-e-9 ~]$
```

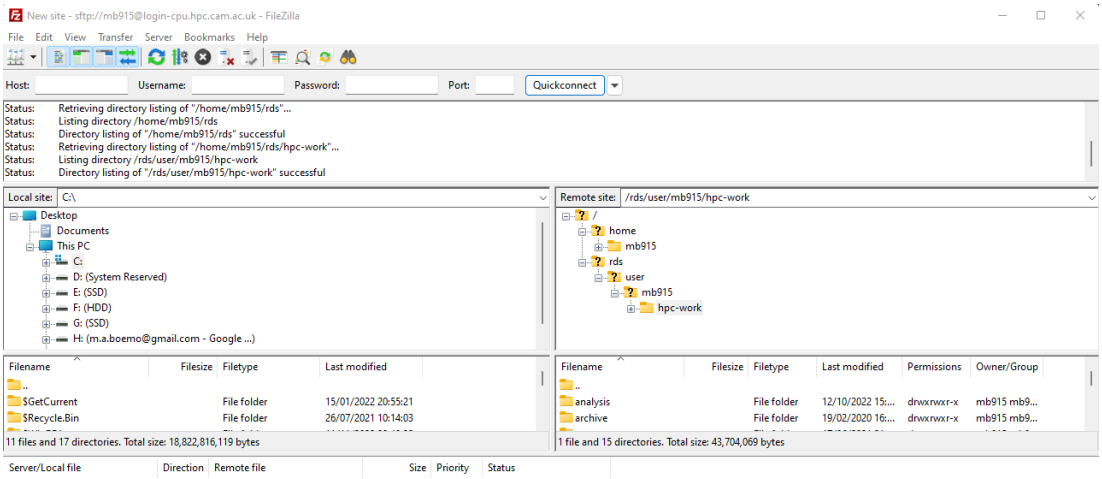
Logging In (FTP Client)



Logging In (FTP Client)



Logging In (FTP Client)



Data Services

Research Data Storage (RDS)

- high-performance, hot storage mounted on HPC platforms,
- not redundant,
- £54 per TB per year.

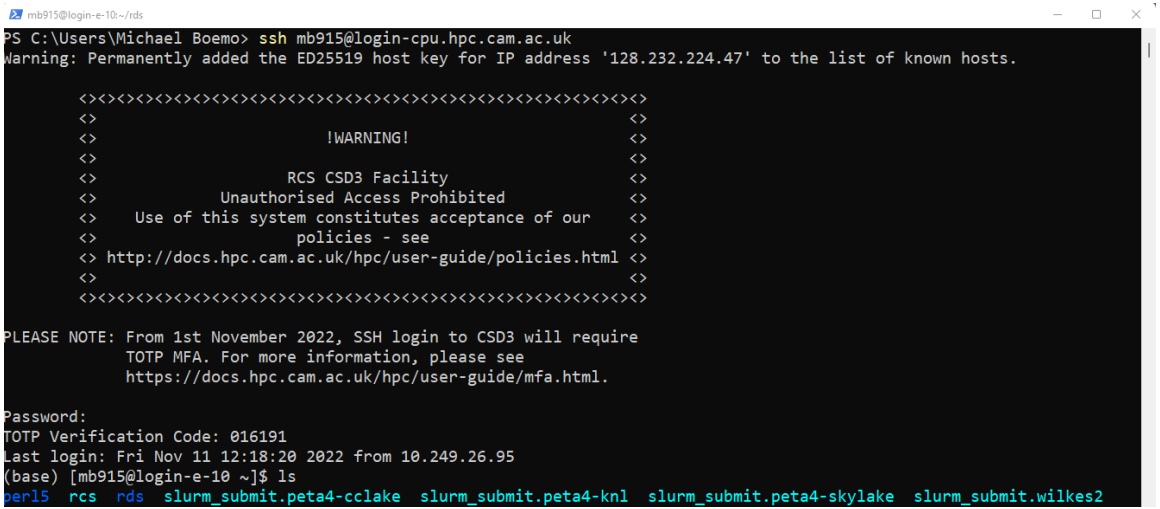
Research Cold Storage (RCS)

- slow, redundant cold storage on two tape libraries,
- £30.72 per TB per year.

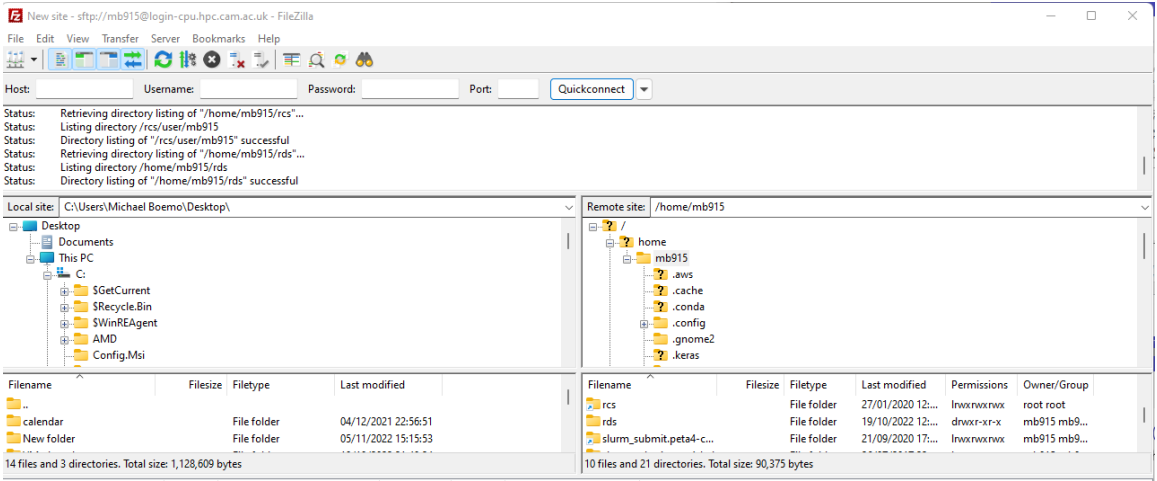
Research File Share (RFS)

- not mounted on HPC platforms, but resilient with frequent snapshots for backups,
- £116.10 per TB per year.

Accessing Data Services (Command Line)



Accessing Data Services (FTP Client)



Data Services Working Together

Consider the following lab:

- protocols, spreadsheets, and documents shared and edited between a number of people (Research File Share),
- data and files from lab members that have left (Research Cold Storage),
- backups of all raw sequencing datasets (Research Cold Storage),
- sequencing datasets actively being used for omics analyses (Research Data Storage).

Backup and Data Handling Practices

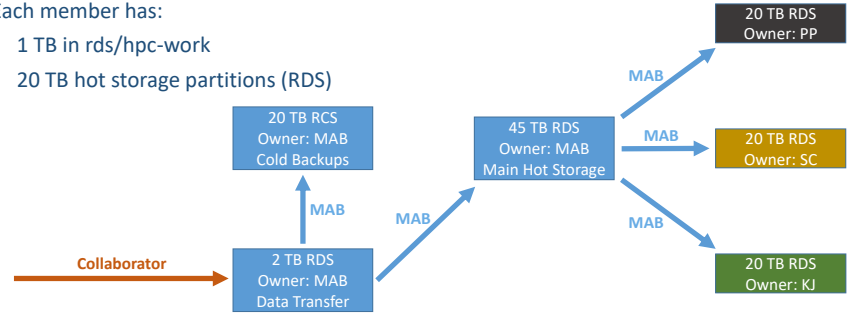
- at least one data copy should be completely raw,
- good naming conventions and record keeping for datasets,
  - `2021_08_12_VM_ONT_EdU_HU_BrdU_ULR_fast5`
- think through how data is moving and any weak points,
- accidents should never cause permanent damage,
- clear and agreed upon backup strategies.

Backup Strategies

Data Storage

Each member has:

- 1 TB in rds/hpc-work
- 20 TB hot storage partitions (RDS)



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Tracking the Flow of Data

	A	B	C	D	E	F	G	H	I	J	K
1	**Collaborator**	**Institution**	**Date Received**	**Cold Storage c/o**	**Cold Storage Location**	**Hot Storage c/o**	**Hot Storage Location**	**Sequencing Platform**	**Organism**	**Cell Line**	**Protocol/Description**
2	XXXXX	XXXXX	26/10/2022	MAB	rcs/rcs-mb915-rawdataar	PLP	rds/rds-pfuderer-G2yvlif	MinION (R9.4.1)	XXXXX	XXXXX	XXXXX
3	XXXXX	XXXXX	26/10/2022	MAB	rcs/rcs-mb915-rawdataar	PLP	rds/rds-pfuderer-G2yvlif	MinION (R9.4.1)	XXXXX	XXXXX	XXXXX
4	XXXXX	XXXXX	26/10/2022	MAB	rcs/rcs-mb915-rawdataar	PLP	rds/rds-pfuderer-G2yvlif	MinION (R9.4.1)	XXXXX	XXXXX	XXXXX
5	XXXXX	XXXXX	24/10/2022	MAB	rcs/rcs-mb915-rawdataar	SY	rds/rds-ye_shutong-xcyv	MinION (R9.4.1)	XXXXX	XXXXX	XXXXX
6	XXXXX	XXXXX	24/10/2022	MAB	rcs/rcs-mb915-rawdataar	SY	rds/rds-ye_shutong-xcyv	MinION (R9.4.1)	XXXXX	XXXXX	XXXXX

CPU Compute Nodes Available

Cascade Lake Nodes

- 56 CPUs (112 threads) per node,
- 192 GB of RAM per node,
- high memory nodes with 384 GB of RAM.

Ice Lake Nodes

- 76 CPUs (152 threads) per node,
- 192 GB of RAM per node,
- high memory nodes with 384 GB of RAM.

GPU Compute Nodes Available

A100 Nodes

- four NVIDIA Amphere A100 80 GB GPUs per node,
- 128 AMD CPUs per node.

At-Once Usage Caps

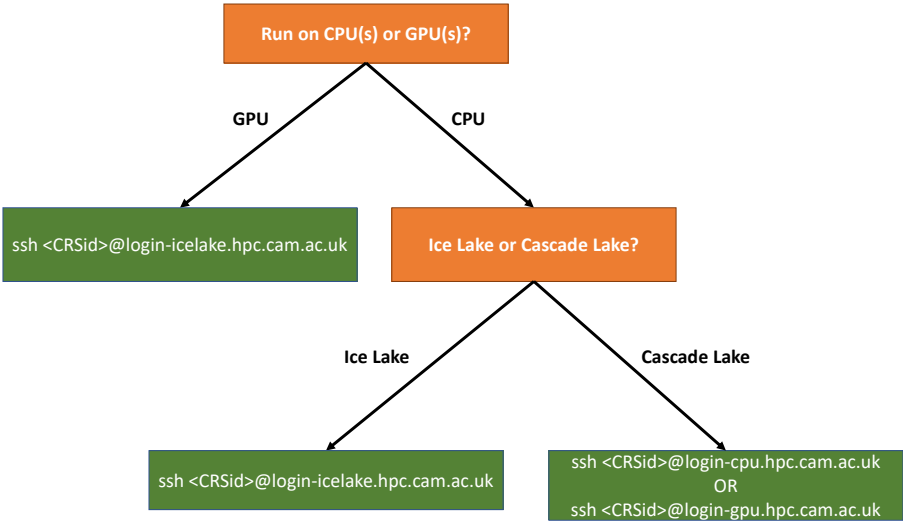
SL3

- 320 CPUs,
- 32 GPUs,
- 12-hour maximum job time.

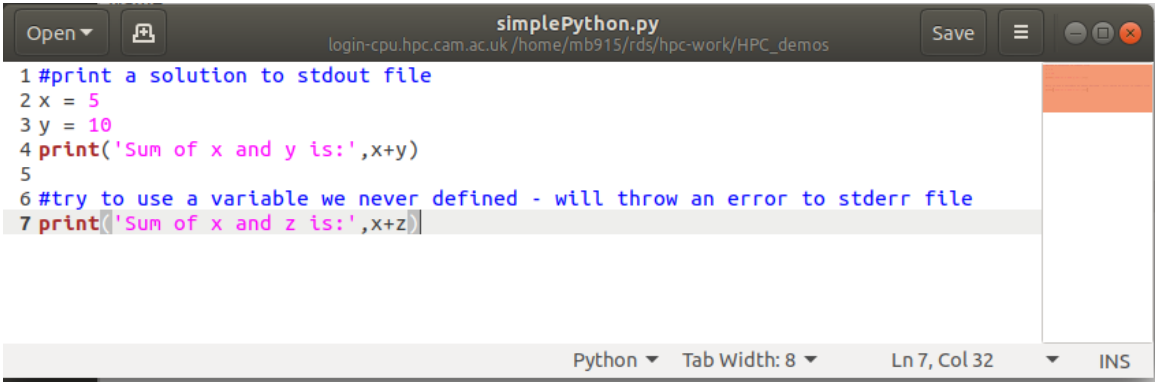
SL1/2

- 1280 CPUs,
- 64 GPUs,
- 36-hour maximum job time.

Which Login Node to Use?



Create a Simple Python Script



Creating an sbatch Script

Open | HPCtraining1.sh | Save

login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_demos

```
1 #!/bin/bash
2 #
3 #SBATCH -p icelake
4 #SBATCH -A BOEMO-SL3-CPU
5 #SBATCH --job-name=simplePy
6 #SBATCH --nodes=1
7 #SBATCH --ntasks=1
8 #SBATCH --cpus-per-task=1
9 #SBATCH --output="/home/mb915/rds/hpc-work/HPC_demos/2021_10_15_simplePython.stdout"
10 #SBATCH --error="/home/mb915/rds/hpc-work/HPC_demos/2021_10_15_simplePython.stderr"
11 #SBATCH --time=0:01:00
12
13 SCRIPT="/home/mb915/rds/hpc-work/HPC_demos/simplePython.py"
14
15 srun python $SCRIPT
```

Submitting Jobs to Compute Nodes

```
(base) [mb915@login-e-8 HPC_demos]$ sbatch HPCtraining1.sh
Submitted batch job 47460048
(base) [mb915@login-e-8 HPC_demos]$ squeue -u mb915
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
          47455220    cclake      bcs    mb915 PD       0:00      1 (Priority)
          47455255    cclake      bcs    mb915 PD       0:00      1 (Priority)
          47460048    cclake simplePy    mb915 PD       0:00      1 (Priority)
(base) [mb915@login-e-8 HPC_demos]$
```

Submitting Jobs to Compute Nodes

simplePython.py
login-gpu.hpc.cam.ac.uk /home/mb915/rds/hpc-work/HPC_demos

```
1 #print a solution to stdout file
2 x = 5
3 y = 10
4 print('Sum of x and y is:',x+y)
5
6 #try to use a variable we never defined - will throw an error to stderr file
7 print('Sum of x and z is:',x+z)
```

Python Tab Width: 8 Ln 7, Col 32 INS

2021_10_15_simplePython.stdout
login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_demos

```
1 Sum of x and y is: 15
```

Plain Text Tab Width: 8 Ln 1, Col 1 INS

2021_10_15_simplePython.stderr
login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_demos

```
1 Traceback (most recent call last):
2   File "/home/mb915/rds/hpc-work/HPC_demos/simplePython.py", line 7, in <module>
3     print('Sum of x and z is:',x+z)
4 NameError: name 'z' is not defined
5 srun: error: cpu-q-235: task 0: Exited with exit code 1
```

Multicore Processing

Open | minimap2.sh | Save

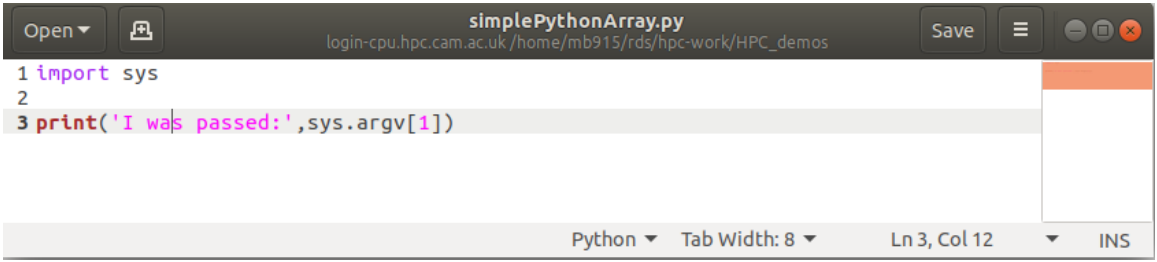
login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_demos

```
#!/bin/bash
#
#SBATCH -p icelake
#SBATCH -A BOEMO-SL3-CPU
#SBATCH --job-name=align
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=76
#SBATCH --output="/home/mb915/rds/hpc-work/HPC_demos/alignment.stdout"
#SBATCH --error="/home/mb915/rds/hpc-work/HPC_demos/alignment.stderr"
#SBATCH --time=6:00:00

MINIMAP2="/home/mb915/rds/hpc-work/software/minimap2-2.17_x64-linux/minimap2"
OUTSAM="/home/mb915/rds/hpc-work/HPC_demos/alignments.sam"
GENOME="/home/mb915/rds/hpc-work/reference.fasta"
QUERY="/home/mb915/rds/hpc-work/HPC_demos/reads.fastq"

srun $MINIMAP2 -ax map-ont -t 76 -a -o $OUTSAM $GENOME $QUERY
```

Job Arrays

We have:

- one Python script that will do some analysis,
- lots of data files (called `input0`, `input1`, ..., `input6`) that we want to run this same script on.



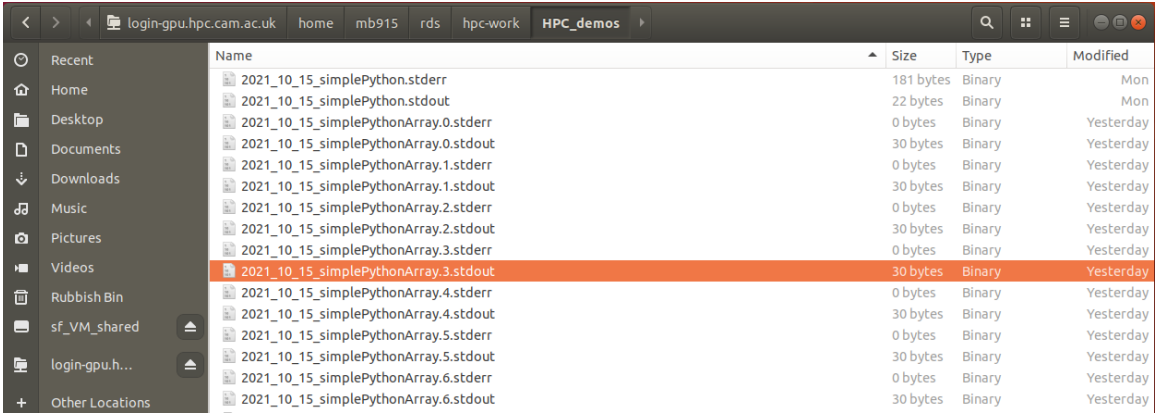
Job Arrays

Open ▾ *HPCtraining3.sh Save

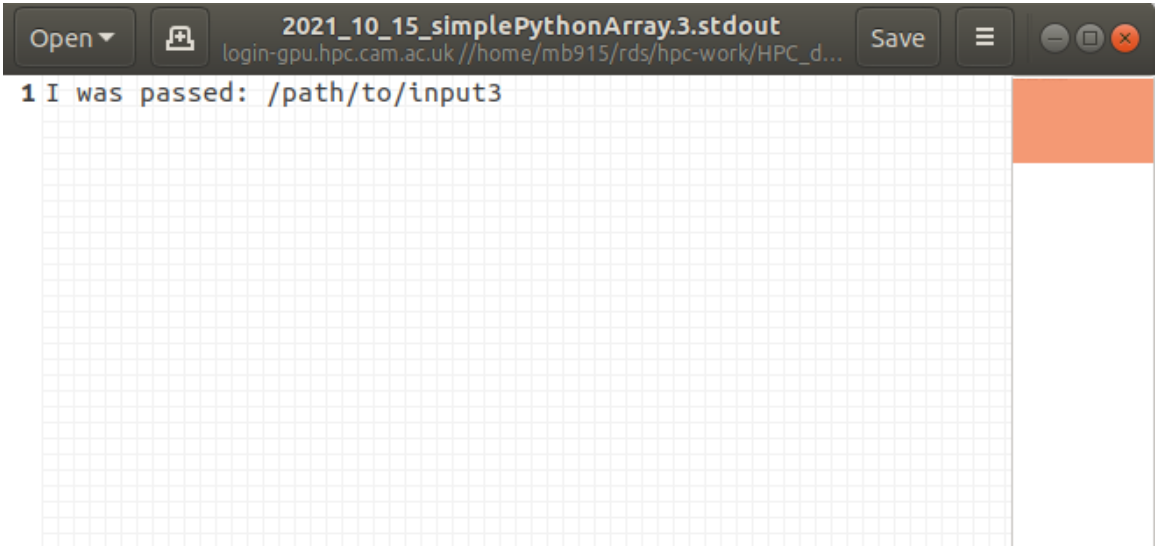
login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_demos

```
#!/bin/bash
#
#SBATCH -p cclake
#SBATCH -A BOEMO-SL3-CPU
#SBATCH --job-name=simplePyArr
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --output="/home/mb915/rds/hpc-work/HPC_demos/2021_10_15_simplePythonArray.%a.stdout"
#SBATCH --error="/home/mb915/rds/hpc-work/HPC_demos/2021_10_15_simplePythonArray.%a.stderr"
#SBATCH --time=0:01:00
#SBATCH --array=0-6

SCRIPT="/home/mb915/rds/hpc-work/HPC_demos/simplePythonArray.py"
INPUTDATA="/path/to/input${SLURM_ARRAY_TASK_ID}"

srun python $SCRIPT $INPUTDATA
```

Job Arrays


login-gpu.hpc.cam.ac.uk
home
mb915
rds
hpc-work
HPC_demos
Recent
Home
Desktop
Documents
Downloads
Music
Pictures
Videos
Rubbish Bin
sf_VM_shared
login-gpu.h...
Other Locations
Name
Size
Type
Modified
2021_10_15_simplePython.stderr 181 bytes Binary Mon
2021_10_15_simplePython.stdout 22 bytes Binary Mon
2021_10_15_simplePythonArray.0.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.0.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.1.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.1.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.2.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.2.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.3.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.3.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.4.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.4.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.5.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.5.stdout 30 bytes Binary Yesterday
2021_10_15_simplePythonArray.6.stderr 0 bytes Binary Yesterday
2021_10_15_simplePythonArray.6.stdout 30 bytes Binary Yesterday

Job Arrays


Open
2021_10_15_simplePythonArray.3.stdout
login-gpu.hpc.cam.ac.uk //home/mb915/rds/hpc-work/HPC_d...
Save
1 I was passed: /path/to/input3

Modules

All modules currently loaded:
`module list`

List all modules available to load:
`module avail`

Search for an available module (samtools, for example):
`module avail samtools`

Virtual Environments

We have:

- at least one Python package we want to install.

We could do:

- `pip3 install --user tensorflow=2.4.1`

Better:

- use virtual environments!

Virtual Environments

Making a new virtual environment:

- `virtualenv HPC_TRAINING`

Activate it:

- `source /path/to/HPC_TRAINING/bin/activate`

Deactivate it:

- `deactivate`

Putting It All Together: Run on GPUs

Open ▾ HPCtraining2.sh
login-gpu.hpc.cam.ac.uk//home/mb915/rds/hpc-work/HPC_demos Save

```
#!/bin/bash
#
#SBATCH -p pascal
#SBATCH -A BOEMO-SL3-GPU
#SBATCH --job-name=gpuJob
#SBATCH --gres=gpu:1
#SBATCH --ntasks=1
#SBATCH --nodes=1
#SBATCH --cpus-per-task=3
#SBATCH --output="/home/mb915/rds/hpc-work/output/2021_10_15_gpuJob.stdout"
#SBATCH --error="/home/mb915/rds/hpc-work/output/2021_10_15_gpuJob.stderr"
#SBATCH --time=4:00:00

module purge
module load rhel7/default-gpu
module unload cuda/8.0
module load python/3.6 cuda/11.0 cuda/11.1 cudnn/8.0_cuda-11.1

source /home/mb915/rds/hpc-work/tensorflow-env/bin/activate

SCRIPT="/home/mb915/rds/hpc-work/trainLargeDNN.py"

srun python $SCRIPT
```

Seeing Past Jobs and Statuses

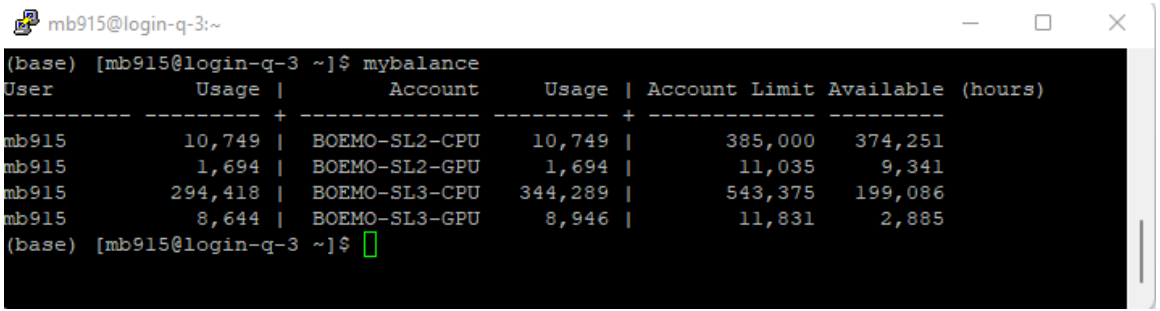
```
(base) [mb915@login-e-5 HPC_demos]$ sacct --starttime 2021-10-14
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
47654390_0   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_0.+      batch            boemo-sl3+          1  COMPLETED      0:0
47654390_0.+     extern            boemo-sl3+          1  COMPLETED      0:0
47654390_1   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_1.+      batch            boemo-sl3+          1  COMPLETED      0:0
47654390_1.+     extern            boemo-sl3+          1  COMPLETED      0:0
47654390_2   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_2.+      batch            boemo-sl3+          1  COMPLETED      0:0
47654390_2.+     extern            boemo-sl3+          1  COMPLETED      0:0
47654390_3   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_3.+      batch            boemo-sl3+          1  COMPLETED      0:0
47654390_3.+     extern            boemo-sl3+          1  COMPLETED      0:0
47654390_4   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_4.+      batch            boemo-sl3+          1  COMPLETED      0:0
47654390_4.+     extern            boemo-sl3+          1  COMPLETED      0:0
47654390_5   simplePyA+     cclake boemo-sl3+          1  COMPLETED      0:0
47654390_5.+      batch            boemo-sl3+          1  COMPLETED      0:0
```

Checking Used Diskspace

mb915@login-q-3:~

```
(base) [mb915@login-q-3 ~]$ quota
Filesystem/Project    GB         quota     limit          grace           files    quota    limit
ser/Grp/Proj
/home                 16.4        50.0      55.0                        ------- No File Quotas
:mb915
/rds-d4              754.5      1099.5    1209.5                      -  715031  1048576  1048576
:mb915
/rcs2               6152.7     21990.2   21990.2                      -  588937  2000000  2000000
rds-6m653hlCD3A       13.3      1000.0    1000.0                      -      35   512000   512000
/rds-d2                0.0         0.0       0.0                      -       1        0        0
/rds-d4             1114.8      2199.0    2199.0                      -    5082  1048576  1048576
/rds-d4            48311.7     48378.5   48378.5                      - 15564252 23068672 23068672
/rds-d5                0.0         0.0       0.0                      -       1        0        0
rds-e89MpZIlFKg     6000.3      6000.0    6000.0                      -  198691  3072000  3072000
rds-G2yvliM05O4     3174.8     20000.0   20000.0                      -  387968 10240000 10240000
rds-KxAwp6sTNTA    11795.3     20000.0   20000.0                      -   41396 10240000 10240000
rds-lbo2YIBtMG4      223.0      1000.0    1000.0                      -    2580   512000   512000
rds-llQYKINinB8      877.8     20000.0   20000.0                      -    9592 10240000 10240000
rds-povrOiKbCCA        0.0      1000.0    1000.0                      -       1   512000   512000
rds-PwZwSmUxXag      570.5     10000.0   10000.0                      -  112705  5120000  5120000
rds-X7FJV3IVilA       91.2      1000.0    1000.0                      -     799   512000   512000
rds-xcywAxU6Kd0       384.3     20000.0   20000.0                      -   22586 10240000 10240000
(base) [mb915@login-q-3 ~]$
```

Checking Number of CPU/GPU Hours Remaining



Where to Find Resources

- These slides and Slurm scripts: https://github.com/MBoemo/HPC-resources
- HPC computing documentation: https://docs.hpc.cam.ac.uk/hpc/
- HPC storage documentation: https://docs.hpc.cam.ac.uk/storage/
- Purchasing storage: https://selfservice.uis.cam.ac.uk/
- SBS bioinformatics Slack channel: https://www.bio.cam.ac.uk/facilities/bioinformatics-computing