# Cambridge Pathology Introduction to High-Performance Computing

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#### Outline

#### We will cover:

- how to create an account,
- logging in,
- types of data storage,
- types of compute nodes,
- for running jobs,
- 6 how to check on the status of jobs,
- how to set up environments.

#### **Account Creation**

Link for account creation:

www.hpc.cam.ac.uk/applications-access-research-computing-services

#### Workflow:

- Have your PI create an account first (if they haven't already).
- Students/postdocs/staff apply for their own account.
- Opening PI gets an Email to approve student/postdoc/staff account creation, linking to lab's account.
- 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

```
Windows PowerShell
Copyright (C) Microsoft Corporation. All rights reserved.

Install the latest PowerShell for new features and improvements! https://aka.ms/PSWindows
PS C:\Users\Michael Boemo> 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).

```
Windows PowerShell
Copyright (C) Microsoft Corporation. All rights reserved.

Install the latest PowerShell for new features and improvements! https://aka.ms/PSWindows

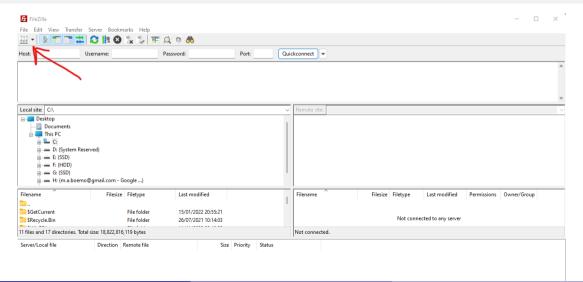
PS C:\Users\Michael Boemo> ssh mb915@login-cpu.hpc.cam.ac.uk
```

```
North Decomposited
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+VRGCaUupOEdhXzO6kp01m2fzzmbgPr0sc2so.
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.
       IMARNITNGI
                            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:
```

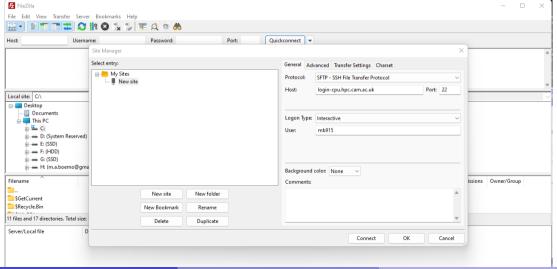
```
Windows PowerShell
PS C:\Users\Michael Boemo> ssh mb915@login-cpu.hpc.cam.ac.uk
The authenticity of host 'login-cpu.hpc.cam.ac.uk (128.232.224.46)' can't be established.
ED25519 key fingerprint is SHA256:nFVSXK+VRGCaUupOEdhXzO6kp01m2fzzmbgPr0sc2so.
Are you sure you want to continue connecting (ves/no/[fingerprint])?          ves
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
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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:
```

```
M mb915@looin-e-9t-
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 kev fingerprint is SHA256:nFVSXK+VRGCaUupOEdhXzO6kp01m2fzzmbgPr0sc2so.
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.
                                !WARNTNG!
                            RCS CSD3 Facility
                     Unauthorised Access Prohibited
             Use of this system constitutes acceptance of our
                             nolicies - 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 ~]$
```

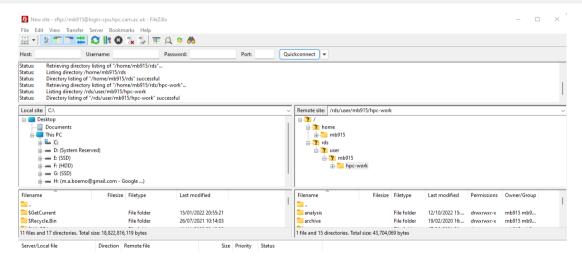
# Logging In (FTP Client)



# 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.

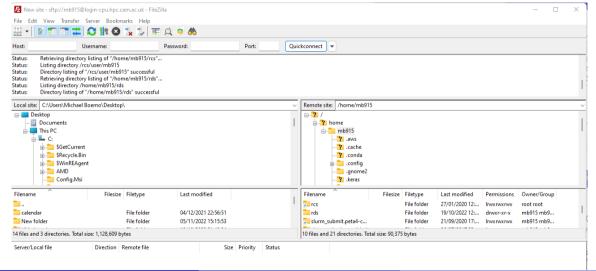
#### Research File Share (RFS)

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

# Accessing Data Services (Command Line)

```
M mb915@login-e-10:~/rds
PS C:\Users\Michael Boemo> ssh mb915@login-cpu.hpc.cam.ac.uk
warning: Permanently added the ED25519 host key for IP address '128.232.224.47' 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 <>
                                                           25
      <del>^^^</del>
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: 016191
Last login: Fri Nov 11 12:18:20 2022 from 10.249.26.95
(base) [mb915@login-e-10 ~1$ ls
er15 rcs rds slurm submit.peta4-cclake slurm submit.peta4-knl slurm submit.peta4-<u>skvlake slurm submit.wilkes2</u>
```

# 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

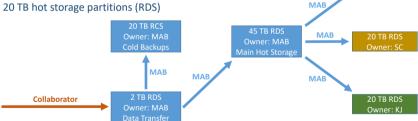
- at least one data copy should be completely raw,
- good naming conventions and record keeping for datasets,
  - 2021\_08\_12\_VM\_ONT\_EdU\_HU\_BrdU\_ULR\_fast5
- think through how data is moving and any weak points,
- accidents should never cause permanent damage,
- clear and agreed upon backup strategies.

#### Backup Strategies

#### **Data Storage**

#### Each member has:

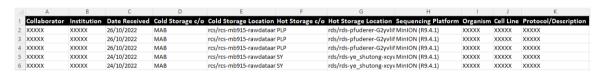
- 1 TB in rds/hpc-work
- 20 TB hot storage partitions (RDS)





20 TB RDS Owner: PP

### Tracking the Flow of Data



### **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

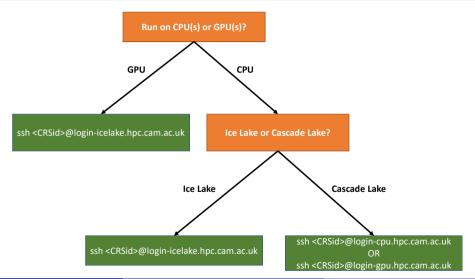
#### SL3

- 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



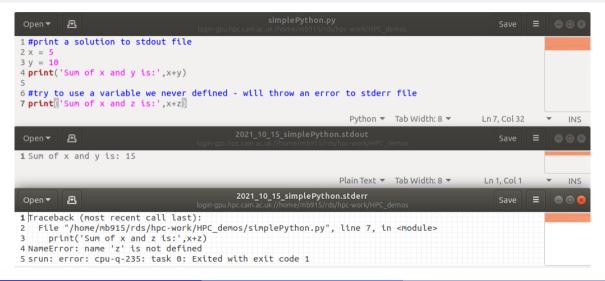
# Creating an sbatch Script

```
HPCtraining1.sh
          Д
 1 #!/bin/bash
 2 #
 3 #SBATCH -p icelake
 4 #SBATCH - A BOEMO-SL3-CPU
 5 #SBATCH -- iob-name=simplePv
 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 SSCRIPT
```

# Submitting Jobs to Compute Nodes

```
(base) [mb915@login-e-8 HPC demos]$ sbatch HPCtrainingl.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



### Cancelling Queued or Running Jobs

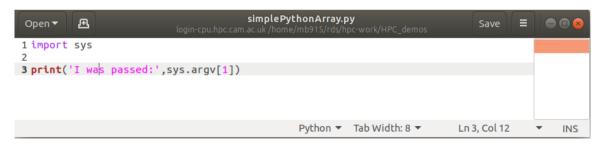
- Find jobIDs of each job using: squeue -u <YOUR CRSID>
- Cancel one job using its jobID: scancel <JOBID>
- Cancel all jobs you have queued or running: scancel -u <YOUR CRSID>

### Multicore Processing

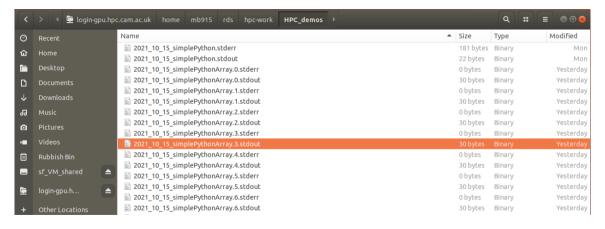
```
minimap2.sh
          Æ
 Open ▼
 1 #!/bin/bash
 3 #SBATCH -p icelake
 4 #SBATCH - A BOFMO-SL3-CPU
 5 #SBATCH --iob-name=align
 6 #SBATCH --nodes=1
 7 #SBATCH --ntasks=1
 8 #SBATCH --cpus-per-task=76
 9 #SBATCH --output="/home/mb915/rds/hpc-work/HPC demos/alignment.stdout"
10 #SBATCH --error="/home/mb915/rds/hpc-work/HPC demos/alignment.stderr"
11 #SBATCH --time=6:00:00
12
13 MINIMAP2="/home/mb915/rds/hpc-work/software/minimap2-2.17 x64-linux/minimap2"
14 OUTSAM="/home/mb915/rds/hpc-work/HPC demos/alignments.sam"
15 GENOME="/home/mb915/rds/hpc-work/reference.fasta"
16 OUERY="/home/mb915/rds/hpc-work/HPC demos/reads.fastg"
17
18 SCUD SMINIMAP2 -ax map-ont -t 76 -a -o SOUTSAM SGENOME SOUERY
```

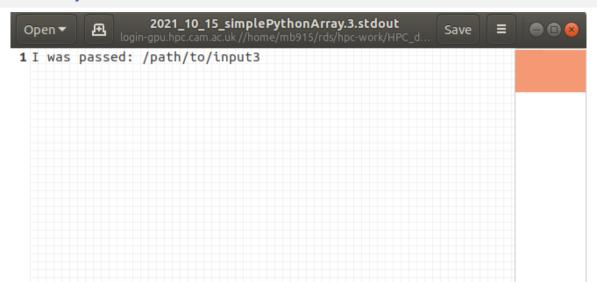
#### We have:

- 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.



```
*HPCtraining3.sh
          Щ
 Open ▼
 1 #!/bin/bash
 3 #SBATCH -p cclake
 4 #SBATCH - A BOEMO-SL3-CPU
 5 #SBATCH -- iob-name=simplePvArr
 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_simplePythonArray.%a.stdout"
10 #SBATCH --error="/home/mb915/rds/hpc-work/HPC demos/2021 10 15 simplePythonArray.%a.stderr"
11 #SBATCH --time=0:01:00
12 #SBATCH --array=0-6
13
14 SCRIPT="/home/mb915/rds/hpc-work/HPC demos/simplePythonArray.py"
15 INPUTDATA="/path/to/input${SLURM ARRAY TASK ID}
16
17 srun bython SSCRIPT SINPUTDATA
```





#### Modules

```
module list

List all modules available to load:

module avail

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

module avail samtools
```

All modules currently loaded:

#### 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

```
HPCtraining2.sh
  Open
                                                                                 Save
                                login-cpu.hpc.cam.ac.uk/home/mb915/rds/hpc-work/HPC_demos
 1#!/bin/bash
 2 #
 3 #SBATCH -p ampere
 4 #SBATCH - A BOFMO-SI 3-GPII
 5 #SBATCH -- iob-name=gpuJob
 6 #SBATCH --gres=gpu:1
 7 #SBATCH --ntasks=1
 8 #SBATCH --nodes=1
 9 #SBATCH --cpus-per-task=3
10 #SBATCH --output="/home/mb915/rds/hpc-work/output/2021 10 15 gpuJob.stdout"
11 #SBATCH --error="/home/mb915/rds/hpc-work/output/2021 10 15 gpuJob.stderr"
12 #SBATCH --time=4:00:00
13
14 module purge
15 module load rhel7/default-gpu
16 module unload cuda/8.0
17 module load cuda/11.0 cuda/11.1 cudnn/8.0 cuda-11.1
18
19 source /home/mb915/rds/hpc-work/tensorflow-env/bin/activate
20
21 SCRIPT="/home/mb915/rds/hpc-work/trainLargeDNN.py"
22
23 srun python SSCRIPT
```

### 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 simplePvA+ cclake boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 0.+ batch boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 0.+ extern boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 l simplePyA+ cclake boemo-sl3+ l COMPLETED
                                                 0:0
47654390 1.+ batch boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 1.+ extern boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 2 simplePvA+ cclake boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 2.+ batch boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 2.+ extern boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 3 simplePyA+ cclake boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 3.+ batch
                  boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 3.+ extern boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 4 simplePvA+ cclake boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 4.+ batch boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 4.+ extern boemo-s13+ 1 COMPLETED
                                                 0:0
47654390 5 simplePyA+ cclake boemo-sl3+ 1 COMPLETED
                                                 0:0
47654390 5.+ batch boemo-s13+ 1 COMPLETED
                                                 0:0
```

# Checking Used Diskspace

<b>№</b> mb915@login-q-3:~						_	
(base) [mb915@login-q-3 ~]\$ quota							
Filesystem/Projec	t GB	quota	limit	grace	files	quota	limit
ser/Grp/Proj							
/home	16.4	50.0	55.0			No File	e Quotas
:mb915							
rds-d4	754.5	1099.5	1209.5		715031	1048576	1048576
mb915							
rcs2	6152.7	21990.2	21990.2		588937	2000000	2000000
ds-6m653h1CD3A	13.3	1000.0	1000.0		- 35	512000	512000
rds-d2	0.0	0.0	0.0				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				0
ds-e89MpZI1FKg	6000.3	6000.0	6000.0		198691	3072000	3072000
ds-G2yvliM0504	3174.8	20000.0	20000.0		387968	10240000	10240000
ds-KxAwp6sTNTA	11795.3	20000.0	20000.0		41396	10240000	10240000
ds-1bo2YIBtMG4	223.0	1000.0	1000.0		2580	512000	512000
ds-11QYKINinB8	877.8	20000.0	20000.0		9592	10240000	10240000
ds-povr0iKbCCA	0.0	1000.0	1000.0			512000	512000
ds-PwZwSmU <b>xX</b> ag	570.5	10000.0	10000.0		112705	5120000	5120000
ds-X7FJV3IVilA	91.2	1000.0	1000.0		799	512000	512000
ds-xcywAxU6Kd0	384.3	20000.0	20000.0		22586	10240000	10240000
base) [mb915@log	in-q-3 ~]\$						

# Checking Number of CPU/GPU Hours Remaining

```
mb915@login-g-3:~
       [mb915@login-g-3 ~]$ mybalance
(base)
User
               Usage
                               Account
                                            Usage | Account Limit Available (hours)
mb915
              10.749 |
                         BOEMO-SL2-CPU
                                           10,749 |
                                                           385,000
                                                                      374,251
mb915
                         BOEMO-SL2-GPU
                                            1.694 I
                                                            11,035
                                                                        9.341
               1.694 I
mb915
             294.418 I
                         BOEMO-SL3-CPU
                                          344,289 I
                                                           543,375
                                                                     199.086
                         BOEMO-SL3-GPU
mb915
               8.644 I
                                            8.946 I
                                                            11,831
                                                                        2,885
       [mb915@login-q-3 ~]$ ☐
(base)
```

#### 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