
# Intro to HPC Workshop

# CODE OF CONDUCT

**Any form or behaviour to exclude, intimidate, or cause discomfort is a violation of the Code of Conduct. In order to foster a positive and professional learning environment we encourage the following kinds of behaviours throughout this workshop:**

- **Use welcoming and inclusive language**
- **Be respectful of different viewpoints and experiences**
- **Gracefully accept constructive criticism**
- **Focus on what is best for the workshop**
- **Show courtesy and respect towards other course participants**

# SCHEDULE

| | |
|---|---|
| [20m] | What is a HPC and what is Apollo2? |
| [10m] | Basic Exercise #1 |
| [ 5m] | Interactive Jobs |
| [10m] | Basic Exercise #2 |
| | Break |
| [10m] | Batch and Array System |
| [15m] | Basic Exercise #3 |
| [15m] | Basic Exercise #4 |
| [10m] | Wrap Up |

# WORKSHOP STRUCTURE

- Each Session will typically initially be led by the Instructor with some information slides. Questions Welcome.

- Then there will be time to work through some problems/examples where the instructor will be available to help and answer questions for those problems.

- You are not expected to always complete all the examples in the time provided. It is expected you will complete those after, if needed.

# WORKSHOP STRUCTURE

- Please Join the RC Slack channel using your sussex email:

  https://www.tinyurl.com/SussexRCSlackInvite

- Join the Channel **#IntroToHPC** and feel free to chat there, share questions and answers during and after the course.

- At the end of the session, there will be a pinned comment for you to leave feedback.

# OVERVIEW

**The A Team**
Who are we?
01

**What is a HPC?**
Overview of Apollo2
02

**Interactive Jobs**
SGE Qlogin, rules, Login nodes
03

04
**Batch, Array Jobs**
Job submission, Batch, Arrays

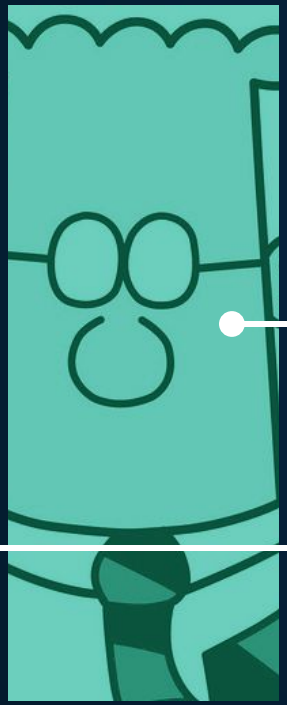
05
**Exercise Hints**
Hints and Tips

06
**Wrap Up**
Summary and Goodbye


# Our Mission

**Platforms - Research** supports multi-million pound research facilities and projects at the University and world-wide. The goal of the team is to enable, accelerate and support research for all at the University. Big or Small!

# THE TEAM



**Reese Wilkinson**
Systems Engineer

**Simon Davis**
Senior Infrastructure Engineer

**Leo Rojas**
Platform Owner

# THE TEAM

**Benjamin Donnachie**
Systems Engineer
MPS

**Luke Ingerson**
Systems Analyst

**Haruna Adoga**
Systems Engineer
MPS

# THE TEAM

**Platform Owner: Leo Rojas**

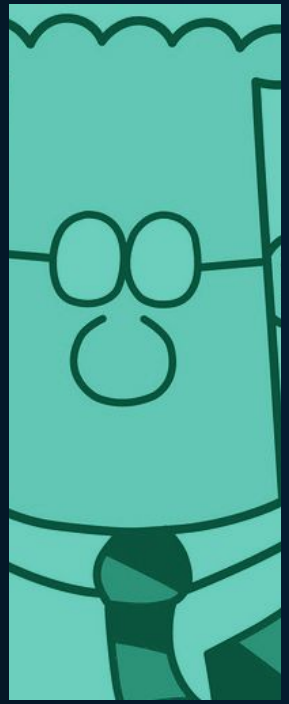
**Hobbies and Interests:** Asterix and Obelix

**Years at Sussex:** 7

**Key Responsibilities:**

- Platform Owner - Research
- Team Lead
- HPC, Research Storage, Research Backups, Research Servers and VMs.
- HPC Steering Group, HPC Users Group

# THE TEAM



**Senior Infrastructure Engineer: Simon Davis**

**Hobbies and Interests:** Raspberry Pi's

**Years at Sussex:** 20+

**Key Responsibilities:**

- Research Data Management
- Research Storage Servers
- Backups, Recovery, Repair for Research Data Services

# THE TEAM

**Systems Engineer: Reese Wilkinson**

**Hobbies and Interests:** Warhammer 40k, Astronomy, Video Games

**Years at Sussex:** 11

**Key Responsibilities:**

- Research Software Stack
- VM's and Web Services
- User Training
- HPC Health, Queues, Services

# THE TEAM

**Systems Engineer: Haruna Adoga**

**Hobbies and Interests:**

**Years at Sussex:** <1

**Key Responsibilities:**

- Networks
- GridPP
- General HPC Workloads

# THE TEAM

**Systems Analyst: Luke Ingerson**

**Hobbies and Interests:** BH Albion, Art Galleries & Museums

**Years at Sussex:** 17

**Key Responsibilities:**

- Accounts, Access, Users
- Ticket Triage
- Filesystems
- Usage and Incident Reports

# THE TEAM

**Systems Engineer:** Benjamin Donnachie

**Hobbies and Interests:** His Doggo, Running

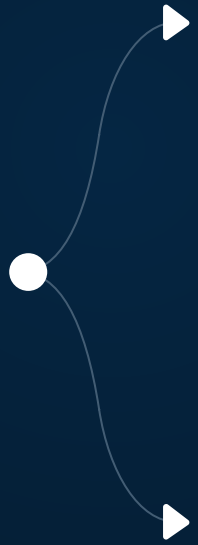
**Years at Sussex:** <1

**Key Responsibilities:**

- MPS
- Cybersecurity
- GridPP

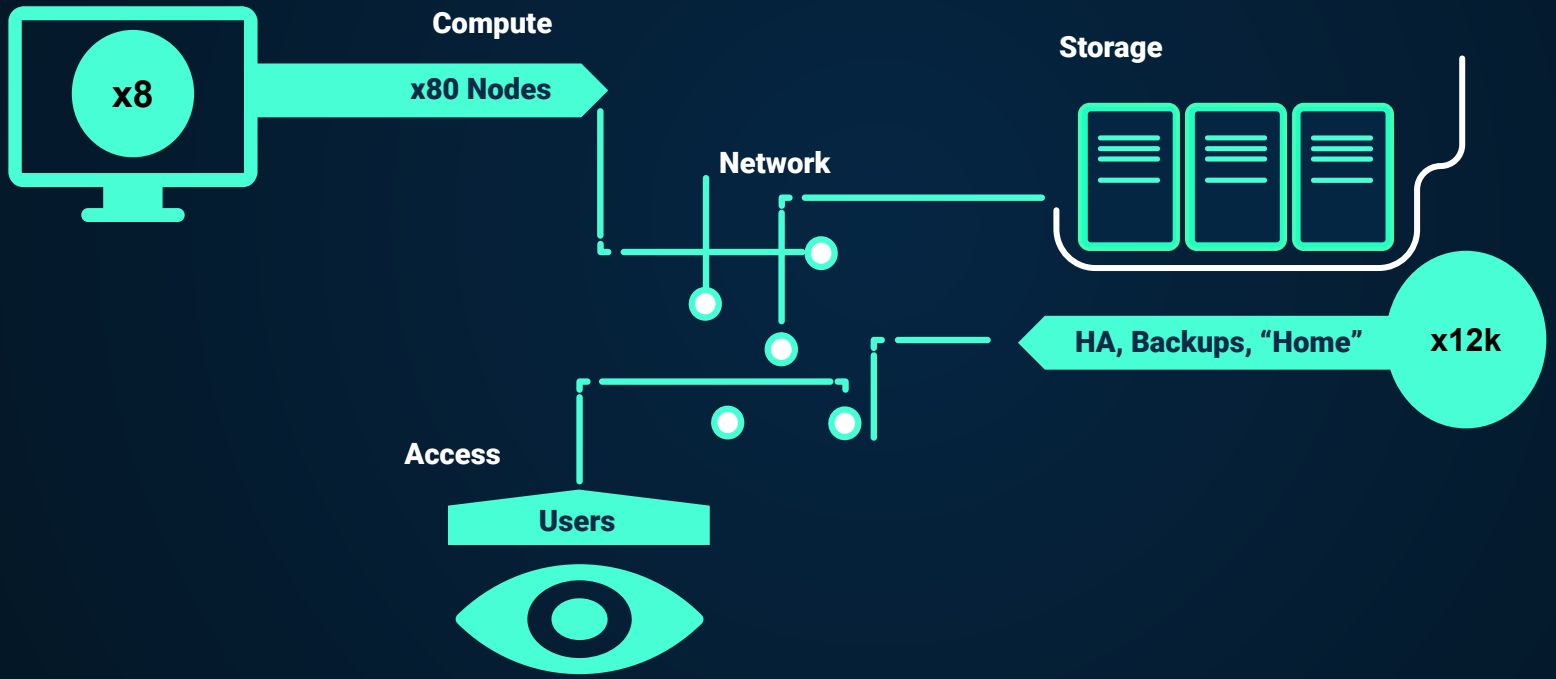
# When Is It Us?

- HPC or Computing Cluster
- ".hpc.sussex.ac.uk" Subdomain
- Omero, Huygens, DICOM
- Research Storage



- Research ✓
- Computing (or HPC) ✓
- Desktop/Laptop ✗
- Licensing ✗

# Apollo2 HPC


Compute
x8
x80 Nodes
Storage
Network
HA, Backups, “Home”
x12k
Access
Users

# Apollo2 HPC

- ~2.4k CPU Cores
- ~4PB Storage
- ~1k Users
- >2k Software Stack
- HA Computing Cluster
- Requisition Provision Support


# Basic Exercise 1

# Interactive Jobs

**Login Nodes**

**Compute Nodes**



**Apollo2 Basic Interactive Session Command:**

```
qlogin
```

| | |
|---|---|
| `-q smp.q` | Queue |
| `-l h_vmem=2G` | Hard RAM Limit |
| `-l m_mem_free=2G` | Force RAM Reserve |
| `-pe openmp 1` | Number of CPUs |

```
$ qlogin -q smp.q -l h_vmem=2G -l m_mem_free=2G -pe openmp 1
```

# Modules and Software

**Apollo2 Software:**

```
module avail
module spider
module list
module load <software>/<version>-<toolchain>-<suffix>
module purge
module save <name>
module restore <name>
```

**Mixing Toolchains**

**Mixing Libs**

```
------------------------------------------------------ /mnt/ebinstall/modules/all -------------------------------------------------------
   AFNI/21.3.10-foss-2020a-R-3.6.3-Python-3.8.2                    Python/3.6.2-foss-2017b
   ANTs/2.3.2-foss-2019b-Python-3.7.4                              Python/3.6.4-foss-2018a
   BeautifulSoup/4.9.1-GCCcore-9.3.0-Python-3.8.2                  Python/3.6.4-fosscuda-2018a
   Biopython/1.73-foss-2018b-Python-3.6.6                          Python/3.6.4-intel-2018a
   Biopython/1.78-foss-2020b                                       Python/3.6.4-iomkl-2018a
   Biopython/1.79-foss-2022a                                (D)    Python/3.6.6-foss-2018b
   Boost.Python/1.66.0-foss-2018a-Python-3.6.4                     Python/3.6.6-intel-2018b
   Boost/1.63.0-foss-2016b-Python-2.7.12                           Python/3.6.8-GCCcore-8.2.0
   Boost/1.63.0-foss-2016b-Python-3.5.2                            Python/3.7.0-foss-2018b
   Boost/1.63.0-foss-2018a-Python-2.7.14                           Python/3.7.2-GCCcore-8.2.0
   Boost/1.63.0-intel-2017a-Python-2.7.13                          Python/3.7.4-GCCcore-8.3.0
   Boost/1.65.1-foss-2017b-Python-2.7.14                           Python/3.8.2-GCCcore-9.3.0
   CGAL/4.9-intel-2017a-Python-2.7.13                              Python/3.8.6-GCCcore-10.2.0
   CGAL/4.11.1-foss-2018a-Python-3.6.4                      (D)    Python/3.9.5-GCCcore-10.3.0-bare
   EMAN2/2.21a-foss-2018a-Python-2.7.14-Boost-1.63.0               Python/3.9.5-GCCcore-10.3.0
   FFC/2018.1.0-foss-2018a-Python-3.6.4                            Python/3.9.6-GCCcore-11.2.0-bare
   FIAT/2018.1.0-foss-2018a-Python-3.6.4                           Python/3.9.6-GCCcore-11.2.0
   FSL/5.0.11-foss-2018b-Python-3.6.6                              Python/3.10.4-GCCcore-11.3.0-bare
```


# Basic Exercise 2

# Batch Jobs

**Batch file:**

```
#!/bin/sh
#$ -N  test
#$ -cwd
#$ -j y
#$ -S /bin/bash
#$ -m eas
#$ -M <username>@sussex.ac.uk
#$ -jc test.short

# # This is where you script normally
```

**Submit:**

```
module load sge
qsub <args> <jobfile>
```

Command Line args overwrite anything set in a job file

**Plaintext secrets**

**Submit with loops**

**100k file outputs**

# Array Jobs

**Batch file:**

```
#!/bin/sh
#$ -N  test
#$ -q smp.q
#$ -pe openmp 1
#$ -cwd
#$ -o /path/to/file_or_folder
#$ -j y
#$ -S /bin/bash
#$ -m eas
#$ -M <username>@sussex.ac.uk
#$ -jc test.short
#$ -t start:stop:step
#$ -tc 25

# # This is where you script normally
```

**Submit:**

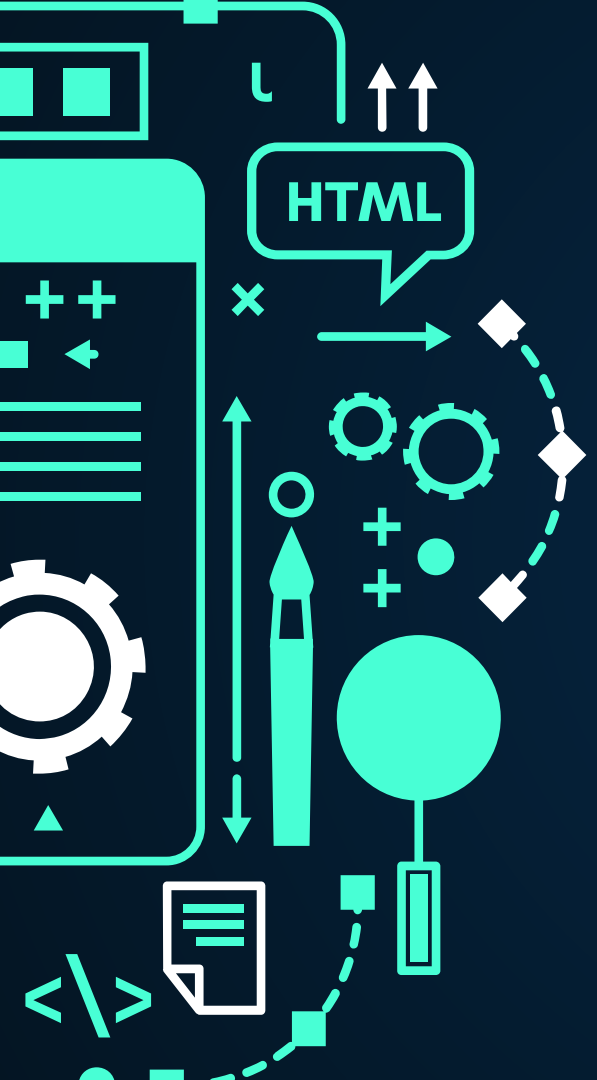
```
module load sge
qsub <args> <jobfile>
```

Command Line args overwrite anything set in a job file

| All Jobs | Array Jobs Only |
|---|---|
| $JOB_ID | $SGE_TASK_ID |
| $SGE_O_WORKDIR | $SGE_TASK_FIRST |
| $SGE_O_HOME | $SGE_TASK_LAST |
| $SGE_O_HOST | $SGE_TASK_STEPSIZE |


# Basic Exercise 3


# Basic Exercise 4




# THANKS!

Does anyone have any thworts, kwoments, kwestions, konzerns?

ITS Office: Shawcross E1-1-08

Slack: UoS-Research-Computing

Teams: ITS Research Support