

An Introduction to High Performance Computing on the CSD3 Cluster

Paul Sumption

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Research Computing Services (<http://www.hpc.cam.ac.uk/>)
University Information Services (<http://www.uis.cam.ac.uk/>)

Welcome

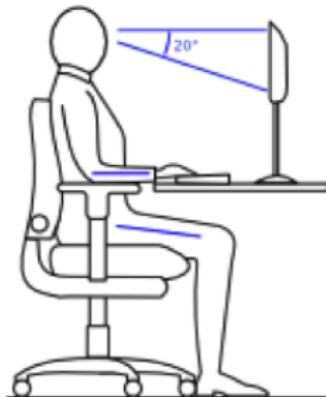
- ▶ Please sign in on the **attendance sheet**.
- ▶ Please fill in the **online feedback** at the end of the course: There is a link to this on your desktop.
- ▶ Keep your belongings with you.
- ▶ Course files can be downloaded from: www.cs3.cam.ac.uk

Plan of the Course

- 10:00 Part 1: Course Introduction
- 10:15 Part 2: HPC - Basic Concepts
- 11:00 BREAK
- 11.20 Part 3: HPC - Facilities
- 12:00 Part 4: HPC - Connecting
- 13:00 LUNCH
- 14:00 Part 5: HPC - User Environment
- 15:00 Part 6: HPC - Submission scripts
- 16:30 FEEDBACK and CLOSE

Part I: Introduction

Health and Safety



Your trainer for today will be:

- ▶ Paul Sumption — Research Computing Technical Liaison
- ▶ Please ask questions and let us know if you need assistance.

Introduction: Training accounts

- ▶ For our practical exercise's we will use HPC training accounts.
- ▶ You will find a piece of paper on your desk.
- ▶ 1: Your training account details.
- ▶ Your training account will only be valid for today.

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- ▶ Boring but very, very important...
- ▶ Cambridge IT is under constant attack by would-be intruders.
- ▶ Your data and research career is threatened by intruders.
- ▶ Cambridge systems are high profile and popular targets.
- ▶ Don't let intruders in.

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2. Always choose strong passwords.
3. Your UIS password is used for multiple systems so keep it secure!
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Pre-requisites

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- ▶ Suggested Courses:
- ▶ Unix: Introduction to the Command Line Interface (Self-paced)
<https://www.training.cam.ac.uk/ucs/Course/ucs-unixintro1>
- ▶ Shell scripting experience is desirable:
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Navigating your terminal

Useful commands for navigating your terminal.

- ▶ `cd <dirname>` - change into a directory
- ▶ `ls <dirname>` - list the contents of a directory
- ▶ `cd` or `cd ~` - change into your home folder
- ▶ `cd ..` - change back one folder
- ▶ `man ls` - will bring up the manual page for the ls command
- ▶ `pwd` - print working directory

Part II: Basics

Basics: Why Buy a Big Computer?

What types of big problem might require a “Big Computer”?

Compute Intensive: A single problem requiring a large amount of computation.

Memory Intensive: A single problem requiring a large amount of memory.

Data Intensive: A single problem operating on a large amount of data.

High Throughput: Many unrelated problems to be executed in bulk.

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Basics: Compute Intensive Problems

- ▶ Distribute the **work** for a **single problem** across multiple CPUs to reduce the execution time as far as possible.
- ▶ Program workload must be *parallelised*:
 - Parallel programs split into copies (processes or threads).
 - Each process/thread performs a part of the work on its own CPU, concurrently with the others.
 - A well-parallelised program will fully exercise as many CPUs as there are processes/threads.
- ▶ The CPUs typically need to exchange information rapidly, requiring specialized communication hardware.
- ▶ Many use cases from Physics, Chemistry, Engineering, Astronomy, Biology...
- ▶ The traditional domain of **HPC** and the **Supercomputer**.

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Basics: Scaling & Amdahl's Law

- ▶ Using more CPUs is not necessarily faster.
- ▶ Typically parallel codes have a scaling limit.
- ▶ Partly due to the system overhead of managing more copies, but also to more basic constraints;
- ▶ Amdahl's Law (idealized):

$$S(N) = \frac{1}{(1 - p + \frac{p}{N})}$$

where

$S(N)$ is the fraction by which the program has sped up
relative to $N = 1$

p is the fraction of the program which can be parallelized
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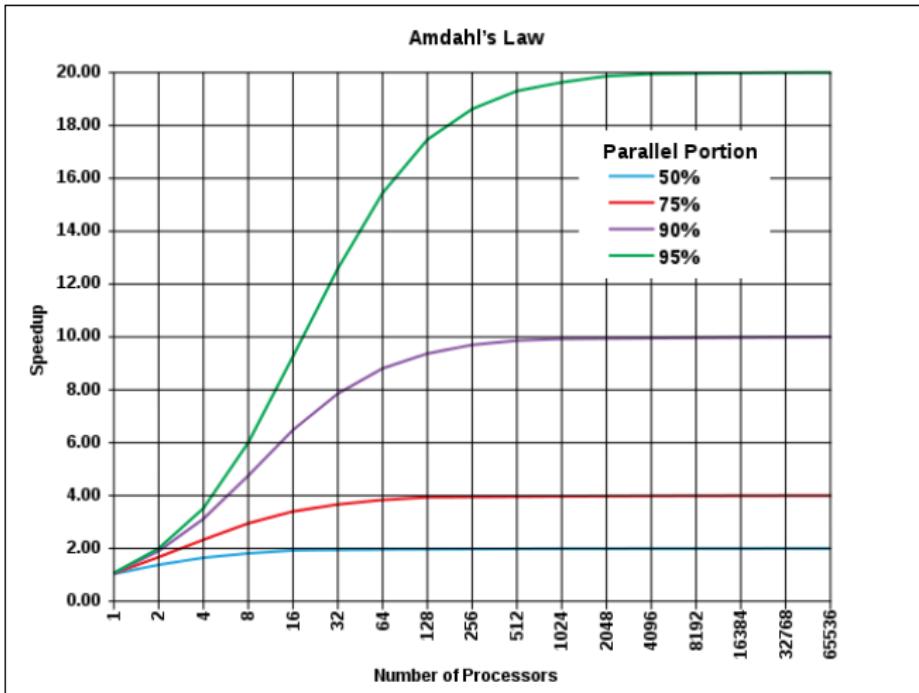
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The Bottom Line

- ▶ Parallelisation requires effort:
 - ▶ There are libraries to help (e.g. [OpenMP](#), [MPI](#)).
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- ▶ The *same* work may be done on each data segment.
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- ▶ Workload is trivially (or *embarrassingly*) parallel:
 - * Workload breaks up naturally into *independent* pieces.
 - * Each piece is performed by a separate process/thread on a separate CPU (concurrently).
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- ▶ Require aggregation of large memory into a **single system image** (i.e. a single computer running Linux).
- ▶ Technically more challenging to build machines (very fast, low latency interconnection between **all** CPUs and **all** memory).
- ▶ Coding/porting easier (memory appears seamless).
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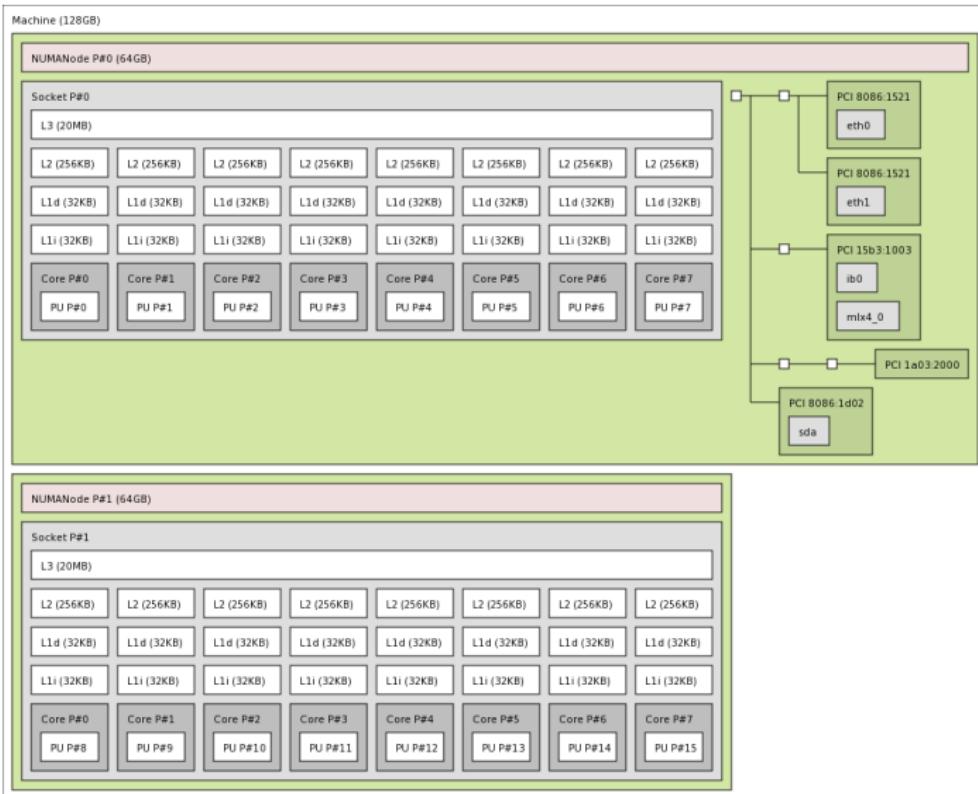
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 but users still see a single computer (**single system image**).

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1. Take some (multicore) CPUs plus some memory.

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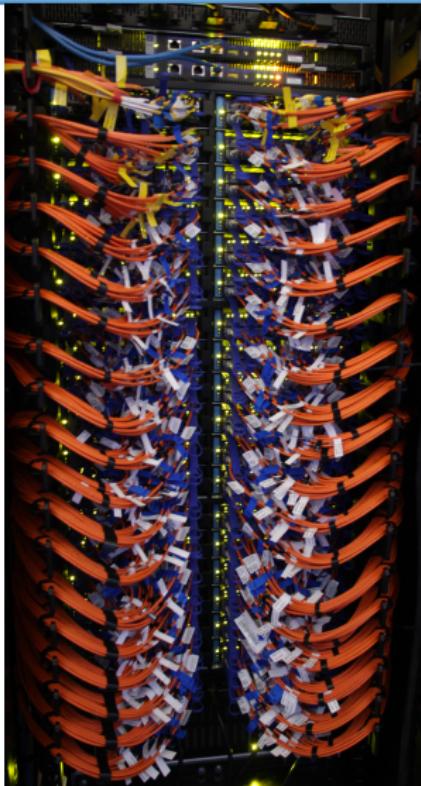
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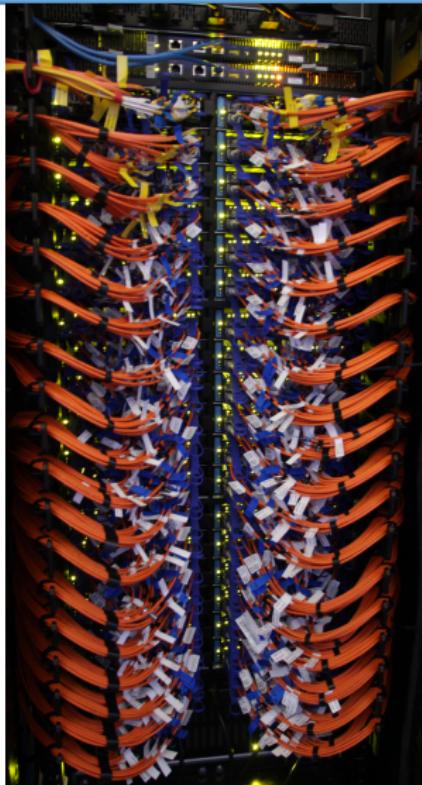
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Basics: How to Build a Supercomputer

3. Logically bind the nodes

- ▶ Clusters consist of distinct nodes (i.e. separate Linux computers) on common private network(s) and controlled centrally.
 - * Private networks allow CPUs in different nodes to communicate.
 - * Clusters are *distributed memory* machines:
Each process/thread sees only its local node's CPUs and memory (without help).
 - * Each process/thread must fit within a single node's memory.

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- ▶ Non-parallel (serial) code
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► Parallel code

- * Shared memory methods within a node.
E.g. pthreads, OpenMP.
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- ▶ Why have a supercomputer?
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Part III: HPC Facilities

- ▶ Cambridge Service for Data Driven Discovery
 - ▶ Peta4 — Intel CPU cluster
 - ▶ Wilkes2 — NVIDIA GPU cluster
 - ▶ Hadoop-based data analytic platform
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Peta4-Skylake

- ▶ Each compute node:
 - * 2x16 cores, Intel Skylake 2.6 GHz
 - * 192 GB or 384 GB RAM
 - * 100 Gb/sec Omni-Path
- ▶ 768 compute nodes, 384 are 192GB RAM nodes and 384 are 384GB RAM nodes
- ▶ 8 login nodes (login-cpu.hpc.cam.ac.uk)

Peta4-Skylake

- ▶ Each compute node:
 - * 32 CPUs
 - * 6 GB or 12 GB per CPU
 - * 10 GB/sec (for MPI and storage)
- ▶ 768 compute nodes, 384 are 192GB RAM nodes and 384 are 384GB RAM nodes
- ▶ 8 login nodes (login-cpu.hpc.cam.ac.uk)

- ▶ Each compute node:
 - * 4 × NVIDIA P100 GPU
 - * 1x12 cores, Intel Broadwell 2.2 GHz
 - * 96 GB RAM
 - * 100 Gb/sec (4X EDR) Infiniband.
- ▶ 90 compute nodes.
- ▶ 8 login nodes (login-gpu.hpc.cam.ac.uk).

Wilkes2-GPU

- ▶ Each compute node:
 - * 4 GPUs
 - * 12 CPUs
 - * 96 GB RAM
 - * 10 GB/sec (for MPI and storage)
- ▶ 90 compute nodes.
- ▶ 8 login nodes (login-gpu.hpc.cam.ac.uk).

Peta4-KNL (Intel Phi)

- ▶ Each compute node:
 - * 64 cores, Intel Phi 7210
 - * 96 GB RAM
 - * 100 Gb/sec Omni-Path
- ▶ 342 compute nodes
- ▶ Shared login nodes with Peta4-Skylake

Peta4-KNL (Intel Phi)

- ▶ Each compute node:
 - * 256 CPUs
 - * 96 GB RAM
 - * 10 GB/sec (for MPI and storage)
- ▶ 342 compute nodes
- ▶ Shared login nodes with Peta4-Skylake

HPCS: Storage

- ▶ Multi-petabytes split across multiple filesystems with tape.
- ▶ Lustre cluster filesystem:
 - * Multiple RAID6 back-end disk volumes.
 - * Multiple object storage servers.
 - * Single metadata server.
 - * Tape-backed HSM on newest filesystems.
 - * 4 GB/sec overall read or write.
 - * Prefers big read/writes over small.
- ▶ For active HPC work only.

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Obtaining an Account and Support

- ▶ To apply for an account, complete our online form:
- ▶ <https://www.cs3.cam.ac.uk/services/applying-for-resources>
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Obtaining an Account and Support

- ▶ For support enquiries please email our Service Desk:
- ▶ support@hpc.cam.ac.uk
- ▶ Please try to give plenty of detail:
- ▶ Which nodes are you using? job id? modules loaded? etc

Part IV: Using HPC

Basics: Connecting

- ▶ When connecting to the cluster will we use the SSH secure protocol only.
- ▶ We will use the Linux workstations during this course
- ▶ Please check your workstation is booted into Ubuntu Linux, ask if you need help with this.
- ▶ You are welcome to use your own laptop, however you may need to install some software in order to connect.
- ▶ Later in this section of the slides we will cover the software you may need to install on your own computer.

Basics: Connecting

- ▶ SSH secure protocol only.
- ▶ HPCS now allows direct access from outside of the CUDN.

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It is still worth configuring the UIS VPN service
<http://www.ucs.cam.ac.uk/vpn>
Useful for other CUDN only services.

Basics: Connecting

- ▶ To access the Peta4-Skylake (CPU cluster) nodes:
ssh <username>@login-cpu.hpc.cam.ac.uk
- ▶ To access the Peta4-KNL (KNL cluster) nodes:
ssh <username>@login-knl.hpc.cam.ac.uk
- ▶ To access the Wilkes2-GPU (GPU cluster) nodes:
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Connecting: Linux Clients

- ▶ ssh, scp, sftp, rsync
Installed (or installable), in Ubuntu we will use 'Terminal'.
- ▶ X Windows, for using graphical applications remotely *This is already installed on your desktop.*

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Connecting: Login

- ▶ From Linux/MacOSX/UNIX (or Cygwin):
`ssh -Y abc123@login-cpu.hpc.cam.ac.uk`

- ▶ From graphical clients:

Host: `login-cpu.hpc.cam.ac.uk`

Username: `abc123` (your UCAM account name)

- ▶ `login-cpu.hpc` will map to a random login node
i.e. one of `login-e-9, ..., login-e-16`

NB you'll never connect to the head node.

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Connecting: First time login

- ▶ The first connection to a particular hostname produces the following:

```
The authenticity of host 'login-e-10.hpc.cam.ac.uk (128.232.224.47)'  
can't be established.
```

RSA key fingerprint is

```
0b:ef:59:90:fb:13:4a:c9:56:82:7b:cd:4b:2b:e1:3b.
```

Are you sure you want to continue connecting (yes/no)? yes

Warning: Permanently added 'login-sand2.hpc.cam.ac.uk' (RSA) to the
list of known hosts.

- ▶ One should always check the fingerprint before typing “yes”.
- ▶ Graphical SSH clients *should* ask a similar question.
- ▶ Designed to detect fraudulent servers.

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- ▶ You may be presented with any of the following fingerprints (depending on your client):

MD5:0b:ef:59:90:fb:13:4a:c9:56:82:7b:cd:4b:2b:e1:3b

SHA256:sSkVfzpwpjwiFvxLcdPoDpN8IsN3kt0ZSywhDhPKZPAG

MD5:34:9b:f2:d2:c6:b3:5c:63:99:b7:27:da:5b:c8:16:fe

SHA256:HsiY10e0M8tS6JwR76PeQQA/VB7r8675BzG50YQ4h34

MD5:64:7c:7c:ff:05:9d:0e:dc:06:fe:f1:c2:10:37:7a:85

SHA256:wq91jBfPa71XXpQq+rk5JTBXLJ0/kXj0c5A7rp4ENzA

Connecting: File Transfer

- ▶ From Linux/MacOSX/UNIX (or Cygwin):

`rsync -av old_directory/`

`abc123@login-cpu.hpc.cam.ac.uk:/home/abc123/new_directory`

copies contents of old_directory to `~/home/abc123/new_directory`.

`rsync -av old_directory`

`abc123@login-cpu.hpc.cam.ac.uk:/home/abc123/new_directory`

copies old_directory (and contents) to

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- * For transfers in the opposite direction, place the remote machine as the first argument.

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Basics: Connecting from other clients

- ▶ When using your own computer you may need to install some software in order to connect.
- ▶ There are quite a few choices of software packages for this, we will just cover a few.
- ▶ Our website
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Connecting: MacOSX/UNIX Clients

- ▶ ssh, scp, sftp, rsync

Installed (or installable) OS X has a native terminal package. This can be launched by clicking Apple >Go >Utilities and then clicking the Terminal icon.

- ▶ TurboVNC (for remote desktop, 3D optional)

<http://sourceforge.net/projects/turbovnc/files/>

- ▶ On MacOSX, install XQuartz to display remote graphical applications.

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Connecting: Windows Clients

- ▶ putty, pscp, psftp

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- ▶ WinSCP

<http://winscp.net/eng/download.php>

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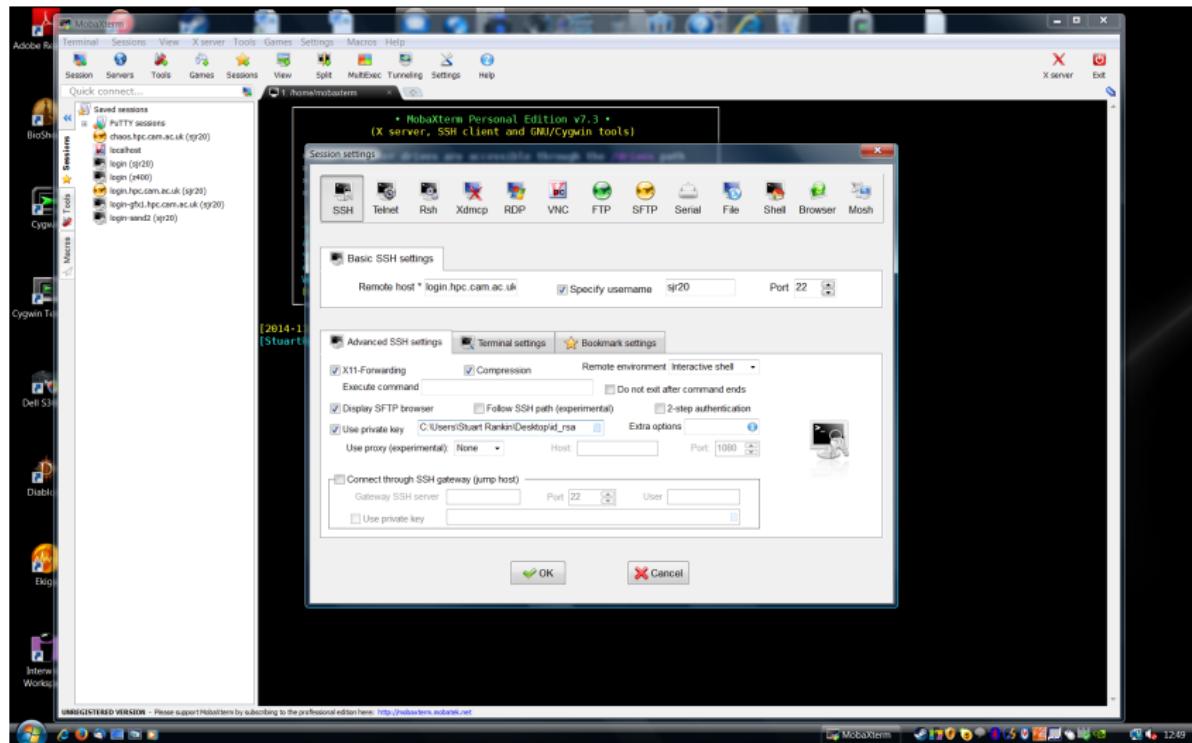
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- ▶ TurboVNC (remote desktop, 3D optional)
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- ▶ Cygwin (provides an application environment similar to Linux)
<http://cygwin.com/install.html>
Includes X server for displaying graphical applications running remotely.
- ▶ MobaXterm
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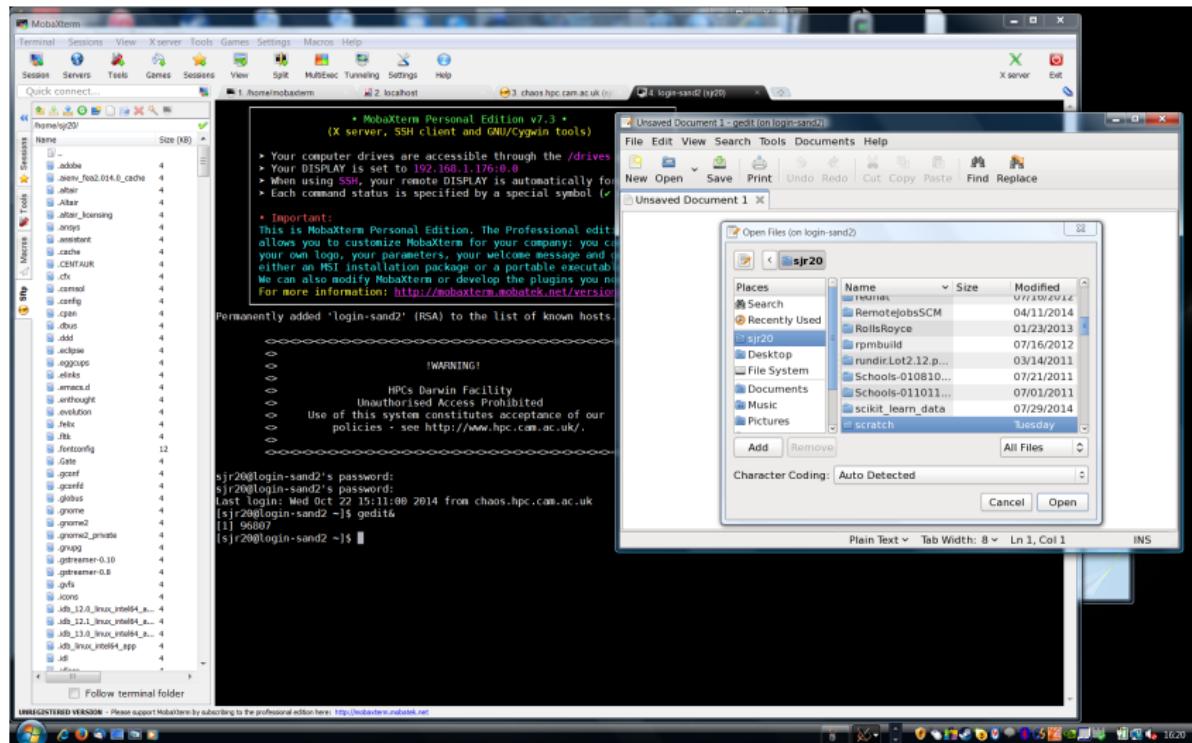
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MobaXterm SSH (Windows)



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Simple command line operations

- ▶ Some simple exercises will help us gauge your experience.
- ▶ Exercise 1: Login with SSH
- ▶ Exercise 2: SFTP file transfer
- ▶ Exercise 3: Unzip the excercises.tar file
- ▶ Exercise 4: Navigating the command line
- ▶ Exercise 5: Learn more about a command

Exercise 1: Login

Using a Linux terminal you will login to the cluster with your HPC training account.

- ▶ Start the terminal by double clicking on the terminal icon
- ▶ In your terminal enter:
 - ▶ ssh -Y **abc123**@login-cpu.hpc.cam.ac.uk
Replace abc123 with your training account username
- ▶ Enter your password as supplied on the sheet
- ▶ Leave this terminal open, you will need it for exercise 3,4 and 5!

Exercise 2: Transfer some files

You will need to transfer the exercise files to the cluster.

- ▶ Open a new Linux terminal on your training computer.
- ▶ Enter this command: `cd ~\Course_material`
- ▶ Check the file 'exercises.tar' is in your directory listing
- ▶ Hint: `ls`

Exercise 2: Transfer some files

Transfer the exercises.tar to your HPC home folder.

- ▶ In the local terminal on your training computer enter the command:
- ▶ `sftp abc123@login-cpu.hpc.cam.ac.uk`
Change abc123 to your training account username
- ▶ The command: `put exercises.tar` will transfer the file from your local computer to the remote one
- ▶ Check the file 'exercises.tar' is in your directory listing
- ▶ Hint: `ls`
- ▶ Type 'exit' to close the local terminal

Exercise 3: Unzip the excercises.tar file

- ▶ In a terminal logged into the cluster: (see exercise 1.)
 - (a) Use the `ls` to list your home folder contents — you should see the copy of exercises.tar.
 - (b) Unpack the tar archive to create an exercise subdirectory.
 - (c) Move the exercise subdirectory to a new directory.

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Hints: Do `cd ~` then `ls -al`. Note that `cd ~` will take you back to your home directory.
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 - (a) Use the `ls` to list your home folder contents — you should see the copy of exercises.tar.

Hints: Do `cd ~` then `ls -al`. Note that `cd ~` will take you back to your home directory.
 - (b) Unpack the tar archive to create an exercise subdirectory.

Hints: Do `tar -xvf exercises.tar`
 - (c) Move the exercise subdirectory to a new directory.

Hints: Do `mv exercises myexercises`

Exercise 4: File listings

- ▶ In a terminal logged into the cluster: (see exercise 1.)
 - ▶ [(a)] List the contents of your current directory `ls`. This won't show everything — use `ls -al` for a long listing showing all files. Initially you will start in your home directory — use `pwd` to print the name of your current working directory. If you get lost, you can always do `cd` without arguments to return to your home directory.
- (b) Focus your long listing on **all files with names beginning "myexercises"**.
- (c) Print a long listing of the subdirectory **myexercises**.

Exercise 4: File listings

- ▶ In a terminal logged into the cluster: (see exercise 1.)
 - ▶ [(a)] List the contents of your current directory `ls`. This won't show everything — use `ls -al` for a long listing showing all files. Initially you will start in your home directory — use `pwd` to print the name of your current working directory. If you get lost, you can always do `cd` without arguments to return to your home directory.
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- Hints:* Do `ls -al myexercises*`
- (c) Print a long listing of the subdirectory `myexercises`.

Exercise 4: File listings

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- (b) Focus your long listing on all files with names beginning "myexercises".

Hints: Do `ls -al myexercises*`

- (c) Print a long listing of the subdirectory `myexercises`.

Hints: Do `ls -al myexercises/`.

Exercise 5: Learn more about a command

- ▶ In a terminal logged into the cluster: (see exercise 1.)
 - (a) View the man page for the `cp` command by doing `man cp`. Use **SPACE** to page down and **b** to page up. Press **q** to exit the manual page command.
 - (b) View the man pages for the `mkdir` and `mv` commands.

Part V: Using HPC

Using HPC: User Environment

- ▶ Scientific Linux 7.4 ([Red Hat Enterprise Linux 7.4 rebuild](#))
 - ▶ bash shell
 - ▶ Gnome or XFCE4 desktop ([if you want](#))
 - ▶ GCC compilers and other development software.
- ▶ But you don't need to know that.

Using HPC: User Environment

Red Hat Enterprise Linux 7

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Using HPC: User Environment

Red Hat Enterprise Linux 7

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User Environment: Filesystems

When you apply for an HPC account a home directory is created for you.

- ▶ [/home/abc123](#)

- ▶ 40GB quota.
- ▶ Visible equally from all nodes.
- ▶ Single storage server.
- ▶ Hourly, daily, weekly snapshots copied to tape.
- ▶ Not intended for job outputs or large/many input files.

- ▶ [/rds/user/abc123/hpc-work](#)

- ▶ Visible equally from all nodes.
- ▶ Larger and faster (1TB initial quota).
- ▶ Intended for job inputs and outputs.
- ▶ **Not backed up.**

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Our storage services

- ▶ We have several storage services for users that need to exceed 1TB.
- ▶ <http://www.uis.cam.ac.uk/initiatives/storage-strategy/storage-services>
- ▶ The most relevant services to HPC are RCS and RDS.
- ▶ RCS - Research Cold Store is for data that isn't changing, data goes to disk then two sets of tapes.
- ▶ RDS - Research Data Store, non backed up high performance storage for projects.

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Filesystems: Snapshots

- ▶ ZFS snapshots on /home are taken hourly, daily and weekly
- ▶ No backups are made of data in the RDS directories - take care when deleting.
- ▶ Snapshots are not backups, they are retained for two weeks
- ▶ Very short lived files are unlikely to get written to snapshots
- ▶ The file needs exist long enough to get into a snapshot.
- ▶ It is possible to search /home/.zfs/snapshot and browse the snapshots
- ▶ Locate the most recent version of the file then copy it back to your home folder

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Filesystems: Quotas

- ▶ quota

```
[ps459@login-e-13 hpc-work]$ quota
Filesystem  GiBytes   quota   limit   grace   files   quota   limit   grace User/group
/home        12.4     40.0    40.0    0       ---- No ZFS File Quotas  ----- U:ps459
/rds-d1      89.2    1024.0  1126.4  -       757345  1048576  1048576  -       G:ps459
/rds-d1      22.1    1024.0  1024.0  -       113475  1048576  1048576  -       G:rds-ps459-test
```

- ▶ Aim to stay below the soft limit (*quota*).
- ▶ Once over the soft limit, you have 7 days grace to return below.
- ▶ When the grace period expires, or you reach the hard limit (*limit*), no more data can be written.
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- ▶ When the grace period expires, or you reach the hard limit (*limit*), no more data can be written.
- ▶ It is important to rectify an out of quota condition ASAP.

Filesystems: Permissions

- ▶ Be careful and if unsure, please ask support.
 - ▶ Can lead to accidental destruction of your data or account compromise.
- ▶ Avoid changing the permissions on your home directory.
 - ▶ Files under /home are particularly security sensitive.
 - ▶ Easy to break passwordless communication between nodes.

Using HPC: Software

- ▶ Free software accompanying Red Hat Enterprise is (or can be) provided.
- ▶ Other software (free and non-free) is available via modules.
- ▶ Some proprietary software may not be generally accessible.
- ▶ See <http://www.hpc.cam.ac.uk/using-clusters/software>.
- ▶ New software may be possible to provide on request.
- ▶ Self-installed software must be properly licensed.
- ▶ *sudo will not work. (You should be worried if it did.)*

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User Environment: Environment Modules

- ▶ Modules load or unload additional software packages.
- ▶ Some are **required** and automatically loaded on login.
- ▶ Others are optional extras, or possible replacements for other modules.
- ▶ **Beware** unloading default modules in `~/.bashrc`.
- ▶ **Beware** overwriting environment variables such as `PATH` and `LD_LIBRARY_PATH` in `~/.bashrc`. If necessary append or prepend.

User Environment: Environment Modules

- ▶ Currently loaded:

```
module list
Currently Loaded Modulefiles:
  1) dot                               2) singularity/current
  ....plus several more default modules
                                              2) intel
```

- ▶ Available:

```
module av
```

User Environment: Environment Modules

- ▶ What is:

```
module whatis openmpi-3.0.0-gcc-4.8.5-n2hvjgm
openmpi-3.0.0-gcc-4.8.5-n2hvjgm: The Open MPI Project is an open source...
```

- ▶ Load:

```
module load openmpi-3.0.0-gcc-5.4.0-4ryklvu
```

- ▶ Unload:

```
module unload openmpi-3.0.0-gcc-5.4.0-4ryklvu
```

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2017b
```

- ▶ Invoking matlab in batch mode:

```
matlab -nodisplay -nojvm -nosplash command
```

where the file `command.m` contains your matlab code.

- ▶ The current site license contains the Parallel Computing Toolbox.

User Environment: Environment Modules

- ▶ Matlab

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module load matlab/r2017b
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where the file `command.m` contains your matlab code.

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User Environment: Environment Modules

- ▶ Purge and Load Defaults:

```
module purge
module load rhel7/default-peta4
```

- ▶ sbatch scripts, purge modules, load default modules, load modules you specify
- ▶ This gives you a clean environment when running a job

User Environment: Compilers

- ▶ Load a newer GCC

```
module show gcc-7.2.0-gcc-4.8.5-pqn7o2k
module load gcc-7.2.0-gcc-4.8.5-pqn7o2k
Your commands to compile your software....
```

- ▶ If you have compiled software yourself your run time environment must match compile time environment!

```
gcc -O3 -mtune=native code.c -o prog
gfortran -O3 -mtune=native code.f90 -o prog
```

```
module load openmpi-3.0.0-gcc-4.8.5-n2hvjgm
mpicc -O3 -mtune=native mpi_code.c -o mpi_prog
mpif90 -O3 -mtune=native mpi_code.f90 -o mpi_prog
```

User Environment: Compilers

- ▶ Load a newer GCC

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module show gcc-7.2.0-gcc-4.8.5-pqn7o2k
module load gcc-7.2.0-gcc-4.8.5-pqn7o2k
Your commands to compile your software....
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```
module load openmpi-3.0.0-gcc-4.8.5-n2hvjgm
mpicc -O3 -mtune=native mpi_code.c -o mpi_prog
mpif90 -O3 -mtune=native mpi_code.f90 -o mpi_prog
```

Excercise 6: Environment Modules

- ▶ Connect to the cluster using your training account: See excercise 1 if you have closed your terminal.
- ▶ Get a list of modules that are currently loaded

Hints: [module list](#)

- ▶ Get a list of available R modules

Hints: [module av r](#)

Excercise 7: Run an Rscript

- ▶ Connect to the cluster using your training account: See exercise 1 if you have closed your terminal.
- ▶ In the exercises folder you transferred earlier there is a file called test.r
- ▶ Run this script using: Rscript hello.r
- ▶ Load the module for: r-3.4.3-gcc-5.4.0-rbvhnga

Hints: `module load r-3.4.3-gcc-5.4.0-rbvhnga`

- ▶ Run the script again: Rscript hello.r
- ▶ What happens? what changes?

Exercise 8: Install the R library locally

As a user you can create a local R library directory for packages that you want to install.

- ▶ Load an R module: `module load r-3.4.3-gcc-5.4.0-rbvhnge`
- ▶ Create a folder in your home for your own R package installs:
`mkdir ~/my-R-libs`
- ▶ Make R aware of the new library location:
`echo "R_LIBS_USER=~/my-R-libs" > ~/.Renviron`
- ▶ Start R: `R`
- ▶ Display your library paths: `.libPaths()`
- ▶ Try loading a library: `require(pander)`
- ▶ Its not installed, lets install it: `install.packages("pander")`
- ▶ Try loading a library: `require(pander)`
- ▶ Library is now installed, lets quit R: `quit()`

Excercise 8: Explained

- ▶ To load one of our R modules: `module load r/(version)`
- ▶ `echo " "` outputs the text between the quotes, `>`redirects the text into the `.Renvironment` file.
- ▶ When we start R the `.Renvironment` file is read and R will now be aware of our local library directory.
- ▶ `.libPaths()` is how to check your library locations

Exercise 9: Modules and Compilers

- ▶ Connect to the cluster using your training account: See exercise 1 if you have closed your terminal.
- ▶ Go to the `myexercises` directory.

Try to compile the `hello.c` program using the default `gcc` compiler (it will fail because there is a deliberate bug).
- ▶ To fix the problem, open the `hello.c` file in the `gedit` editor.
- ▶ If you get this error:

WARNING **: cannot open display:
then you have missed the '-Y' in your SSH command

Exercise 9: Modules and Compilers

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Try to compile the `hello.c` program using the default `gcc` compiler (it will fail because there is a deliberate bug).

Hints: `gcc hello.c -o hello`

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- ▶ If you get this error:
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Exercise 9: Modules and Compilers

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- ▶ Go to the `myexercises` directory.
Try to compile the `hello.c` program using the default `gcc` compiler (it will fail because there is a deliberate bug).

Hints: `gcc hello.c -o hello`

- ▶ To fix the problem, open the `hello.c` file in the `gedit` editor.
Hints: Launch gedit in the background by doing `gedit&`. A gedit window should appear. Remove the word `BUG`, save the file and recompile. Do `./hello` to run the program.
- ▶ If you get this error:

WARNING **: cannot open display:

then you have missed the '`-Y`' in your SSH command

Exercise 10: Modules and Compilers

- ▶ The default version of gcc is 4.8.5. Compile hello.c again with [gcc 5.4.0](#).

Hints: module av, module load gcc-5.4.0-gcc-4.8.5-fis24gg, then
[gcc hello.c -o hello2](#)

Part VI: HPC Job Submission

Using HPC: Job Submission



Using HPC: Job Submission

- ▶ Compute resources are managed by a scheduler:
[SLURM](#)/PBS/SGE/LSF/...
- ▶ Jobs are submitted to the scheduler
 - analogous to submitting jobs to a print queue
 - a file (*submission script*) is copied and queued for processing.

Using HPC: Job Submission

- ▶ Jobs are submitted from the **login node**
 - not itself managed by the scheduler.
- ▶ Jobs may be either **non-interactive** (**batch**) or **interactive**.
- ▶ **Batch** jobs run a shell script on the first of a list of allocated nodes.
- ▶ **Interactive** jobs provide a command line on the first of a list of allocated nodes.

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Using HPC: Job Submission

- ▶ Jobs may use **part** or **all** of one or more nodes
 - the owner can specify `--exclusive` to force exclusive node access.
- ▶ Template submission scripts are available under
[`/usr/local/Cluster-Docs/SLURM`](#).

Job Submission: Using SLURM

- ▶ Prepare a shell script and submit it to SLURM:

```
[abc123@login-a-1]$ sbatch slurm_submission_script  
Submitted batch job 790299
```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

```
[abc123@login-a-1]$ squeue -u abc123
      JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
    790299    skylake   Test3  abc123 PD      0:00      2 (Priority)
    790290    skylake   Test2  abc123 R  27:56:10      2 cpu-a-[1,10]
```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

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      JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
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```

Job Submission: Show Queue

- Submitted job scripts are copied and stored in a queue:

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     JOBID PARTITION      NAME      USER ST          TIME  NODES NODELIST(REASON)
 790299    skylake    Test3  abc123 PD          0:00      2 (AssocGrpCPUMinsLimit)
 790290    skylake    Test2  abc123 R  27:56:10      2 cpu-a-[1,10]
```

Job Submission: Monitor Job

- ▶ Examine a particular job:

```
[abc123@login-a-1]$ scontrol show job=790290
```

Job Submission: Cancel Job

- ▶ Cancel a particular job:

```
[abc123@login-a-1]$ scancel 790290
```

Job Submission: Scripts

► SLURM

In [`/job_templates`](#), see examples: [`slurm_submit.skylake.generic`](#), [`slurm_submit.skylake.matlab`](#).

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A TRAINING-CPU
#! How many whole nodes should be allocated?
#SBATCH --nodes=1
#! How many tasks will there be in total? (<= nodes*32)
#SBATCH --ntasks=1
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

► **#SBATCH** lines are *structured comments*

— correspond to sbatch command line options.

► The above job will be given 1 cpu on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

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#! Name of the job:
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#! Which project should be charged:
#SBATCH -A TRAINING-CPU
#! How many whole nodes should be allocated?
#SBATCH --nodes=1
#! How many tasks will there be in total? (<= nodes*32)
#SBATCH --ntasks=16
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

► **#SBATCH** lines are *structured comments*

— correspond to sbatch command line options.

► The above job will be given **16 cpus** on **1 node** for **2 hours** (by default there is 1 task per node, and 1 cpu per task).

Job Submission: Accounting Commands

- ▶ How many core hours available do I have?

```
mybalance
```

User	Usage	Account	Usage	Account Limit	Available (hours)
sjr20	3	SUPPORT-CPU	2,929	22,425,600	22,422,671
sjr20	0	SUPPORT-GPU	0	87,600	87,600

- ▶ How many core hours does some other project or user have?

```
gbalance -p SUPPORT-CPU
```

User	Usage	Account	Usage	Account Limit	Available (hours)
pfb29	2,925	SUPPORT-CPU	2,929	22,425,600	22,422,671
sjr20 *	3	SUPPORT-CPU	2,929	22,425,600	22,422,671
...					

(Use -u for user.)

- ▶ List all jobs charged to a project/user between certain times:

JobID	User	Account	JobName	Partition	End	ExitCode	State	CompHrs
263	xyz10	support-c+ _interact+		skylake	2018-04-18T19:44:40	0:0	TIMEOUT	1.0
264	xyz10	support-c+ _interact+		skylake	2018-04-18T19:48:07	0:0	CANCELLED+	0.1
275	xyz10	support-c+ _interact+		skylake	Unknown	0:0	RUNNING	0.3
...								

Job Submission: Single Node Jobs

- ▶ Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=
#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS= # For OpenMP across cores
$application $options
...
```

Job Submission: Single Node Jobs

- ▶ Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=
#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
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$application $options
...
```

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```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=1
# Default is 1 cpu (core) per task
#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS= # For OpenMP across cores
$application $options
...
```

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```
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...
#SBATCH --nodes=1
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# Default is 1 cpu (core) per task
#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
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```
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...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=1
# Default is 1 cpu (core) per task
#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS= # For OpenMP across cores
$application $options
...
```

Job Submission: Single Node Jobs

- ▶ Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=32 # Whole node

#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=32 # For OpenMP across 32 cores
$application $options
...
```

Job Submission: Single Node Jobs

- ▶ Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=16 # Half node

#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=16 # For OpenMP across 16 cores
$application $options
...
```

Job Submission: Single Node Jobs

- ▶ Serial jobs requiring large memory, or OpenMP codes.

```
#!/bin/bash
...
#SBATCH --nodes=1
#SBATCH --ntasks=1
# Default is 1 task per node
#SBATCH --cpus-per-task=32 # Whole node

#SBATCH --mem=5990
# Memory per node in MB - default is pro rata by cpu number
# Increasing --mem or --cpus-per-task implicitly increases the other
...
export OMP_NUM_THREADS=16 # For OpenMP across 16 cores (using all memory)
$application $options
...
```

Job Submission: MPI Jobs

- ▶ Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=128      # i.e. 32x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -np 128 $application $options
...
```

- ▶ SLURM-aware MPI launches remote tasks via SLURM.
- ▶ The template script uses \$SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- ▶ Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 16 -np 64 $application $options
...
```

- ▶ SLURM-aware MPI launches remote tasks via SLURM.
- ▶ The template script uses \$SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- ▶ Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 16 -np 64 $application $options
...
```

- ▶ SLURM-aware MPI launches remote tasks via SLURM.
- ▶ The template script uses \$SLURM_TASKS_PER_NODE to set PPN.

Job Submission: Hybrid Jobs

- ▶ Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2  # i.e. 2 threads per MPI task.
mpirun -ppn 16 -np 64 $application $options
...
```

- ▶ This job uses 128 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: Hybrid Jobs

- ▶ Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2  # i.e. 2 threads per MPI task.
mpirun -ppn 16 -np 64 $application $options
...
```

- ▶ This job uses 128 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
- ▶ Use `srun` to launch tasks (**job steps**) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
- ▶ Use `srun` to launch tasks (**job steps**) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
- ▶ Use `srun` to launch tasks (**job steps**) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
- ▶ Use `srun` to launch tasks (**job steps**) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
- ▶ Use `srun` to launch tasks (**job steps**) within a job.

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

If you are attending the HPC Course:

README: Job Scripts!

If you are attending the HPC Course:

- ▶ Use job_script for the exercises when running the exercises during the course
- ▶ Use slurm_submit.peta4-skylake if running the exercises outside of the course
- ▶ I recommend you make a copy of the job script for each exercise

Exercise 11: Submitting a Matlab job

- ▶ Submit a job which will run `matlab` on the `file.m` command file (which contains just the `ver` command).

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- ▶ Submit a job which will run `matlab` on the `file.m` command file (which contains just the `ver` command).

Hints: 1. Edit the `job_script` in your exercises directory.

2. In the module load section: `module load matlab/r2017b`
3. Set the value of application to
`"matlab -nodesktop -nosplash -nojvm"`
4. Set the value of options to `"-r file"`
5. Submit the job with `sbatch job_script`. The jobid is then printed.
6. Watch the job in the queue with `squeue`.
7. After it has disappeared, open the output file `slurm-jobid.out` in your editor. It should contain a list of licensed Matlab features.
8. For more demanding work you can increase the available memory by increasing the number of cpus.

Exercise 12: Submitting compiled code

- ▶ Submit a job which will run a copy of your hello program on 1 cpu.

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- ▶ Submit a job which will run a copy of your hello program on 1 cpu.

Hints: 1. Edit the script `job_script` in your exercises directory.

Set:

```
#SBATCH --nodes=1  
#SBATCH --ntasks=1  
application=". ./hello"
```

2. Submit the job with `sbatch job_script`. The jobid is then printed.
3. Watch the job in the queue with `squeue`.
4. After it has disappeared, open the output file `slurm-jobid.out` in your editor. There should be exactly one “Hello, World!” message.

Job Submission: Interactive

- ▶ Compute nodes are accessible via SSH while you have a job running on them.
- ▶ Alternatively, submit an interactive job:
`sintr -A TRAINING-CPU -N1 -n8 -t 2:0:0`
- ▶ Within the window (screen session):
 - * Launches a shell on the first node (when the job starts).
 - * Graphical applications should display correctly.
 - * Create new shells with `ctrl-a c`, navigate with `ctrl-a n` and `ctrl-a p`.
 - * `ssh` or `srun` can be used to start processes on any nodes in the job.
 - * SLURM-aware MPI will do this automatically.

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Job Submission: Array Jobs

- ▶ http://slurm.schedmd.com/job_array.html
- ▶ Used for submitting and managing large sets of similar jobs.
- ▶ Each job in the array has the same **initial** options.
- ▶ SLURM

```
[abc123@login-a-1]$ sbatch --array=1-7 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

```
[abc123@login-a-1]$ squeue -u abc123
      JOBID PARTITION     NAME     USER ST      TIME  NODES NODELIST(REASON)
    791609_1 skylake     hpl    abc123 R   0:06      1 cpu-a-6
    791609_3 skylake     hpl    abc123 R   0:06      1 cpu-a-16
    791609_5 skylake     hpl    abc123 R   0:06      1 cpu-a-7
    791609_7 skylake     hpl    abc123 R   0:06      1 cpu-a-7
```

791609_1, 791609_3, 791609_5, 791609_7

i.e. \${SLURM_ARRAY_JOB_ID} - \${SLURM_ARRAY_TASK_ID}

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

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```
[abc123@login-a-1]$ sbatch --array=1-7:2 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

```
[abc123@login-a-1]$ squeue -u abc123
      JOBID PARTITION     NAME     USER ST      TIME  NODES NODELIST(REASON)
    791609_1 skylake     hpl    abc123 R   0:06      1 cpu-a-6
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Job Submission: Array Jobs (ctd)

- ▶ Updates can be applied to specific array elements using `${SLURM_ARRAY_JOB_ID} . ${SLURM_ARRAY_TASK_ID}`
- ▶ Alternatively operate on the entire array via `${SLURM_ARRAY_JOB_ID}`.
- ▶ Some commands still require the SLURM_JOB_ID (sacct, sreport, sshare, sstat and a few others).
- ▶ Exercise 7 - Array Jobs.

Job Submission: Array Jobs (ctd)

- ▶ Updates can be applied to specific array elements using
 `${SLURM_ARRAY_JOB_ID} . ${SLURM_ARRAY_TASK_ID}`
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Exercise 13: Array Jobs

- ▶ Submit your last job in the form of an array with indices 1-32. Use -H with sbatch to mark the array as held (so that it won't run immediately).
- ▶ Release array element 1 and allow it to run. Then release the others.

Exercise 13: Array Jobs

- ▶ Submit your last job in the form of an array with indices 1-32. Use -H with sbatch to mark the array as held (so that it won't run immediately).
Hints:
 1. Use `sbatch -H --array=1-32 job_script`
 2. Use `squeue -u userid` to see your array job. Note that `-r` reports each array element individually.
- ▶ Release array element 1 and allow it to run. Then release the others.

Exercise 13: Array Jobs

- ▶ Submit your last job in the form of an array with indices 1-32. Use -H with sbatch to mark the array as held (so that it won't run immediately).

Hints:

1. Use `sbatch -H --array=1-32 job_script`
2. Use `squeue -u userid` to see your array job. Note that `-r` reports each array element individually.

- ▶ Release array element 1 and allow it to run. Then release the others.

Hints:

1. Use `scontrol release ${SLURM_ARRAY_JOB_ID}_1`
2. Use `squeue -u userid` again to watch what happens.
3. Release the others with
`scontrol release ${SLURM_ARRAY_JOB_ID}`
i.e. use the array id to release the entire array.
4. When all the jobs complete you should have 32 `slurm-${SLURM_ARRAY_JOB_ID}_N.out` files saying hello from various cpus on possibly multiple nodes.

Scheduling

- ▶ SLURM scheduling is multifactor:
 - ▶ QoS — payer or non-payer?
 - ▶ Age — how long has the job waited?
 - Don't cancel jobs that seem to wait too long.
 - ▶ Fair Share — how much recent usage?
 - Payers with little recent usage receive boost (not implemented yet).
 - ▶ `sprio -j jobid`
- ▶ Backfilling
 - ▶ Promote lower priority jobs into gaps left by higher priority jobs.
 - ▶ Demands that the higher priority jobs not be delayed.
 - ▶ Relies on reasonably accurate wall time requests for this to work.
 - ▶ Jobs of default length will not backfill readily.

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 - ▶ `sprio -j jobid`
- ▶ Backfilling
 - ▶ Promote lower priority jobs into gaps left by higher priority jobs.
 - ▶ Demands that the higher priority jobs not be delayed.
 - ▶ Relies on reasonably accurate wall time requests for this to work.
 - ▶ Jobs of default length will not backfill readily.

Scheduling

- ▶ SLURM scheduling is multifactor:
 - ▶ **QoS** — payer or non-payer?
 - ▶ **Age** — how long has the job waited?
Don't cancel jobs that seem to wait too long.
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- ▶ 12 or 36 hour job walltimes are permitted.
- ▶ SL3 jobs, 12hrs (non payers), SL2 and 1, 36hrs (payers)
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Job Submission: Scheduling Top Dos & Don'ts

► Do ...

- ▶ Give reasonably accurate wall times (allows [backfilling](#)).
- ▶ Check your balance occasionally ([mybalance](#)).
- ▶ Test on a small scale first.
- ▶ Implement [checkpointing](#) if possible (reduces resource wastage).

► Don't ...

- ▶ Request more than you need
 - you will wait longer and use more credits.
- ▶ Cancel jobs unnecessarily
 - priority increases over time.