

# 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

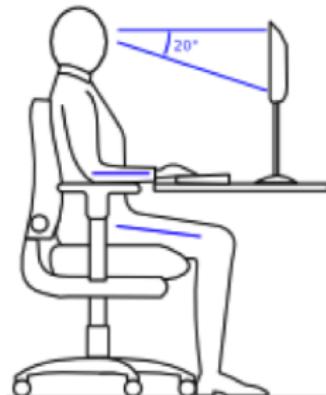
- ▶ Please sign in on the **attendance sheet**.
- ▶ Please fill in the **online feedback** at the end of the course: There is a link to this on your desktop.
- ▶ Keep your belongings with you.
- ▶ Course files can be downloaded from: [www.cs3.cam.ac.uk](http://www.cs3.cam.ac.uk)

# 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 trainers for today will be:

- ▶ Paul Sumption — Research Computing Technical Liaison
- ▶ Simon Flood — Research Computing System Administrator
- ▶ Matthew Archer — Research Software Engineering Team
- ▶ 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 two pieces of paper on your desk.
- ▶ 1: A terms and conditions form for you to sign.
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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>
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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.

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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.
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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  $N = 1$

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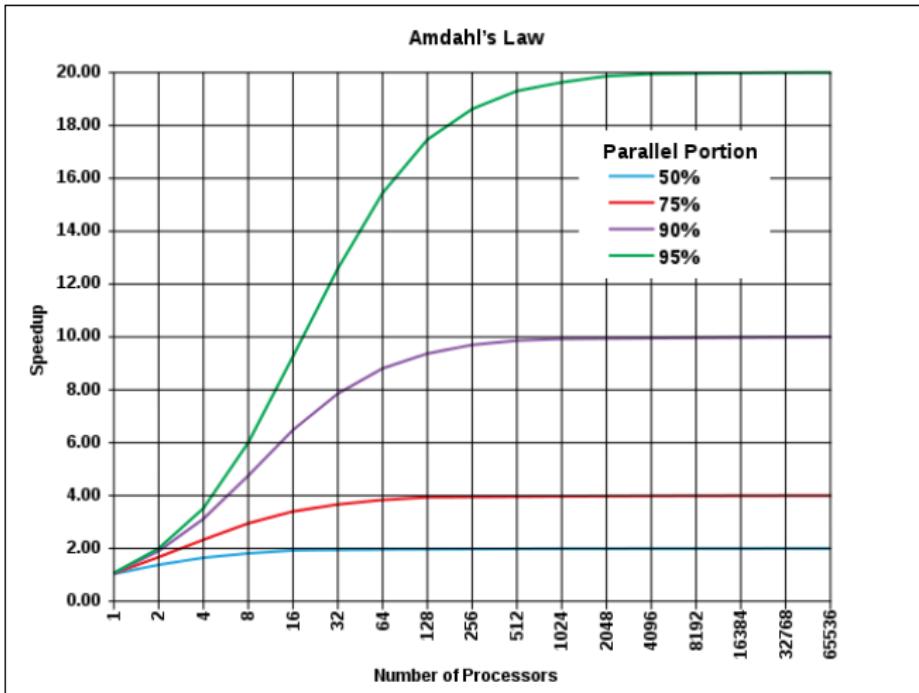
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<http://en.wikipedia.org/wiki/File:AmdahlsLaw.svg>

# 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.
- ▶ Rapid movement of data to and from disk is more important than inter-CPU communication.
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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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# Basics: Memory Intensive Problems

- ▶ 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).
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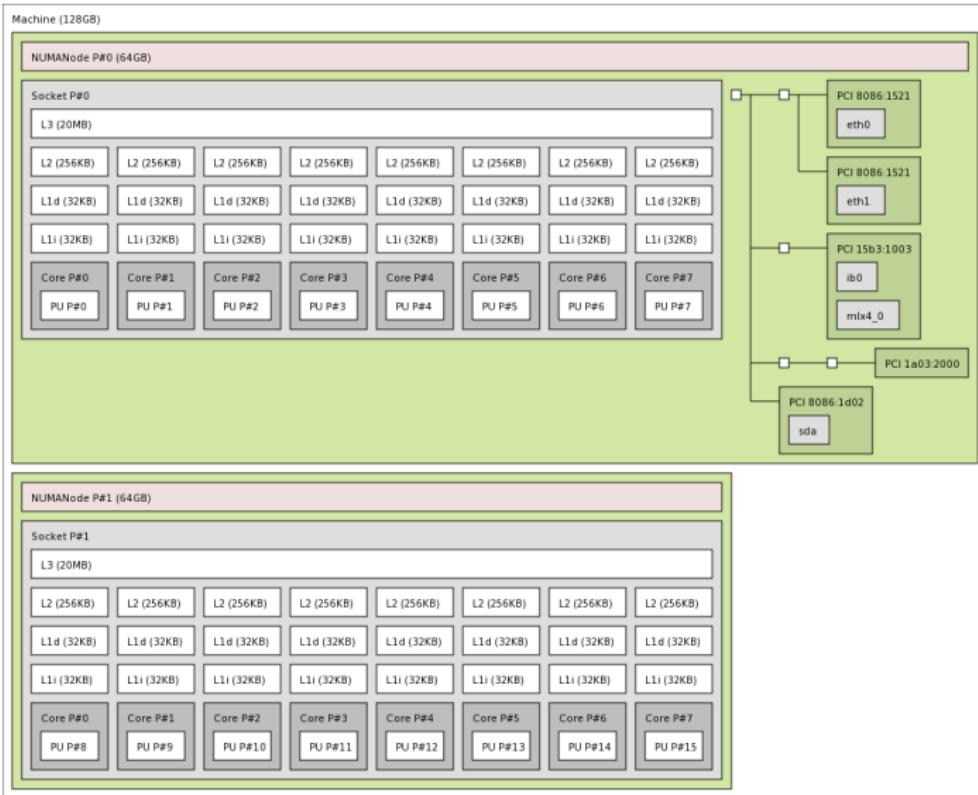
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    but users still see a single computer (**single system image**).

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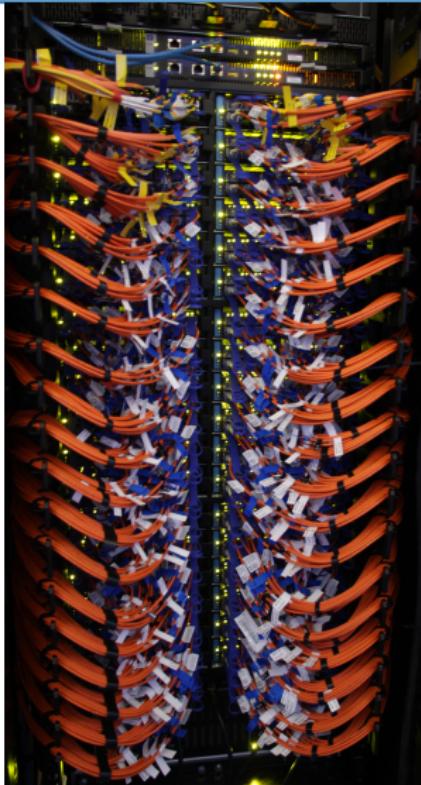
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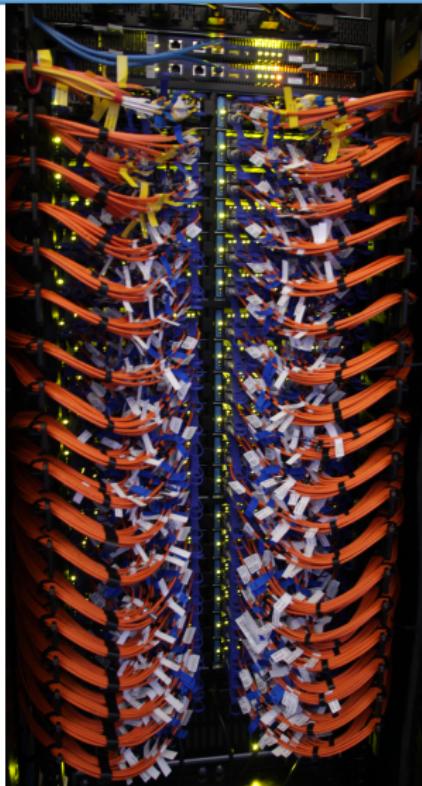
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Slower network for **management** and **provisioning**.  
**Storage** may use either.



# 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).
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## 3. Logically bind the nodes

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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
  - ▶ Burst buffer
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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
- ▶ 8 login nodes ([login-cpu.hpc.cam.ac.uk](http://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
- ▶ 8 login nodes ([login-cpu.hpc.cam.ac.uk](http://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](http://login-gpu.hpc.cam.ac.uk)).

- ▶ 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](http://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

- ▶ 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:
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## 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.

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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:  
ssh <username>@login-gpu.hpc.cam.ac.uk

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

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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.hpc.cam.ac.uk:scratch/new_directory`  
copies contents of old\_directory to `~/scratch/new_directory`.

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- ▶ When using your own computer you may need to install some software in order to connect.
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- ▶ ssh, scp, sftp, rsync

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

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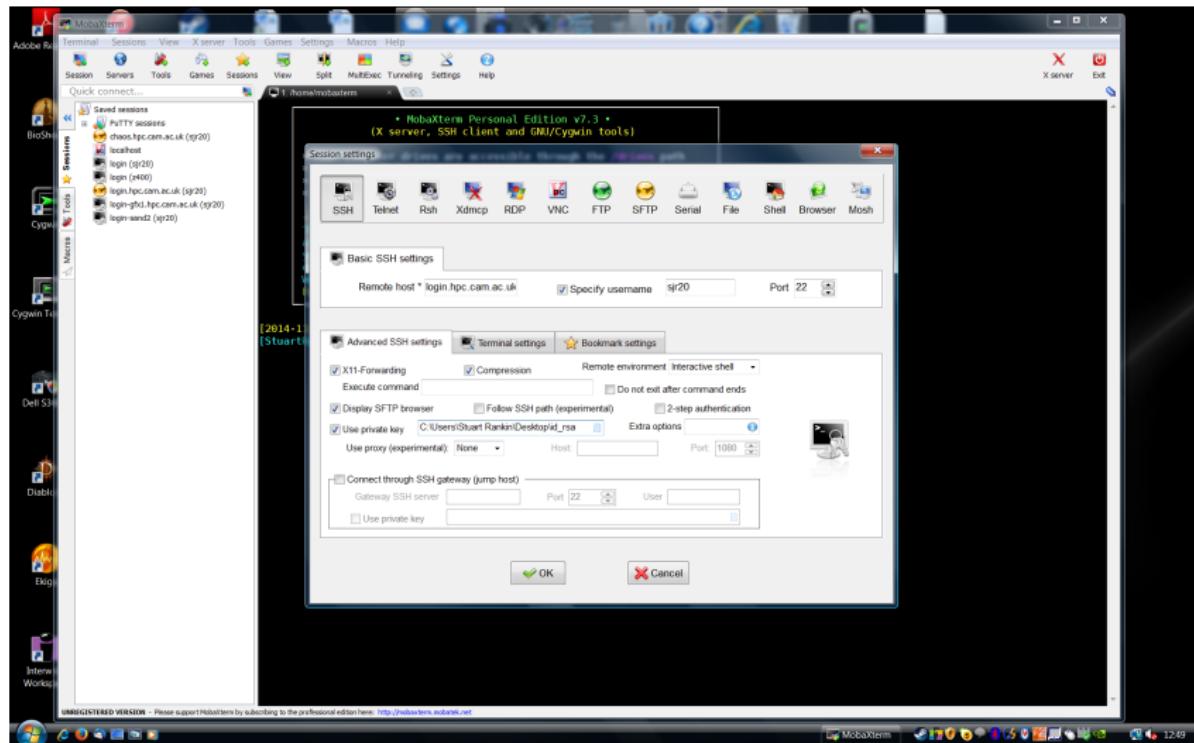
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- ▶ Cygwin (provides an application environment similar to Linux)  
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Includes X server for displaying graphical applications running remotely.
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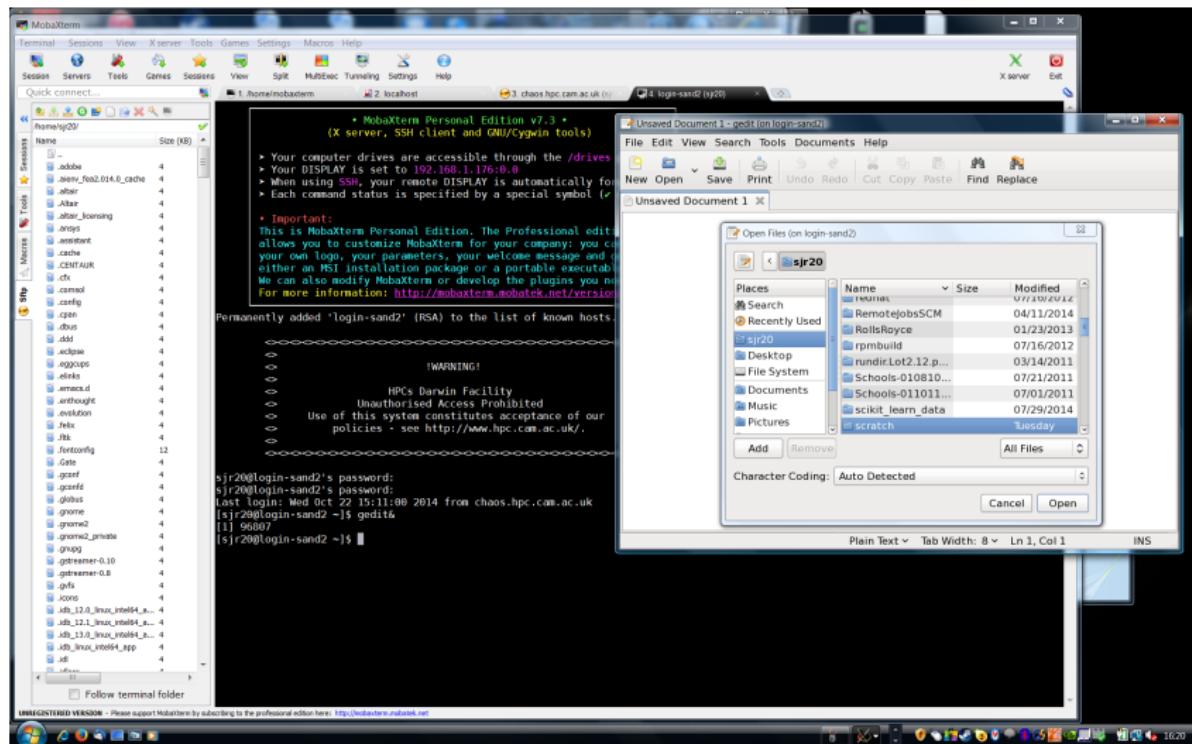
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# MobaXterm SSH (Windows)



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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: Learn more about a command
- ▶ Exercise 4: Unzip the exercises.tar file
- ▶ Exercise 5: Navigating the command line

## 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 2!

## Exercise 2: Transfer some files

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

- ▶ Open a second 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 3: Transfer some files

Transfer the exercises.tar to your HPC home folder.

- ▶ `sftp abc123@login.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

## Exercise 3: Learn more about a command

- (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) Copy `exercises.tar` to the `~/hpc-work` directory. Note that `~` is just a convenient shorthand for your home directory. Omitting the `~/` will look for a `hpc-work` in the current directory.

## Exercise 3: Learn more about a command

- (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) Copy `exercises.tar` to the `~/hpc-work` directory. Note that `~` is just a convenient shorthand for your home directory. Omitting the `~/` will look for a `hpc-work` in the current directory.

*Hints:* Do `cp exercises.tar ~/hpc-work/`. Note that you can often reduce typing by pressing **TAB**.

## Exercise 4: Unzip the excercises.tar file

- (a) Use the `cd` command to enter the `~/hpc-work` directory and then list the contents — you should see the copy of `exercises.tgz`.
- (b) Unpack the tar archive to create an exercise subdirectory.

## Exercise 4: Unzip the excercises.tar file

- (a) Use the `cd` command to enter the `~/hpc-work` directory and then list the contents — you should see the copy of `exercises.tgz`.
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## Exercise 4: Unzip the excercises.tar file

- (a) Use the `cd` command to enter the `~/hpc-work` directory and then list the contents — you should see the copy of `exercises.tgz`.

*Hints:* Do `cd ~/hpc-work/` then `ls -al`. Note that `cd ..` will take you back up one step to the home directory.

- (b) Unpack the tar archive to create an exercise subdirectory.

## Exercise 4: Unzip the excercises.tar file

- (a) Use the `cd` command to enter the `~/hpc-work` directory and then list the contents — you should see the copy of `exercises.tgz`.

*Hints:* Do `cd ~/hpc-work/` then `ls -al`. Note that `cd ..` will take you back up one step to the home directory.

- (b) Unpack the tar archive to create an exercise subdirectory.

*Hints:* Do `tar -zxvf exercises.tar`

## Exercise 5: File listings

- (a) In a terminal logged into the cluster 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 “exercise”**.
- (c) Print a long listing of the subdirectory `hpc-work`.

## Exercise 5: File listings

- (a) In a terminal logged into the cluster 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 "exercise"`.  
*Hints:* Do `ls -al exercise*`
- (c) Print a long listing of the subdirectory `hpc-work`.

## Exercise 5: File listings

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

*Hints:* Do `ls -al exercise*`

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

*Hints:* Do `ls -al hpc-work/`. Note that omitting the `/` reveals that the item `hpc-work` is actually a shortcut (technically a symbolic link) to `/hpc-work/username`.

## Part V: Using HPC

# Using HPC: User Environment

- ▶ CentOS 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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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](#)

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- ▶ **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.
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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.
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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.
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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.

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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
```

# 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

```
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
```

## 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` note the lower case 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 there is a file called test.r
- ▶ Run this script using: Rscript hello.r
- ▶ Load the module for: R/3.3.2

*Hints:* [module load R/3.3.2](#)

- ▶ Run the script again: Rscript hello.r

## 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

- ▶ Our R modules: `module load r/(version)`. We have two sets of R modules, those with an upper case R where compiled for an older version of Linux and should be ignored (Darwin legacy)
- ▶ `echo " " outputs the text between the quotes, >redirects the text into the .Renviron file.`
- ▶ When we start R the `.Renviron` 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 `exercises` directory that you unzipped in hpcwork.  
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

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*Hints:* `gcc hello.c -o hello`

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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`

- ▶ 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 9: 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  
[~/job\\_templates](#).

# 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]
```

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 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 TRAININGCPU
#! 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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# 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 TRAININGCPU
#! 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
...
```

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#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
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$application $options
...
```

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- ▶ 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
...
```

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- ▶ The template script uses \$SLURM\_TASKS\_PER\_NODE to set PPN.

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...
```

- ▶ 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).

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```
#!/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.

```
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...
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...
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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
```

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...
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...
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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
```

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```
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...
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cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
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...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

## Exercise 10: 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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- Hints:*
1. Load the matlab module using the `job_script` in your exercises directory.
  2. Set the value of application to  
`"matlab -nodesktop -nosplash -nojvm"`
  3. Set the value of options to `"-r file"`
  4. Submit the job with `sbatch job_script`. The jobid is then printed.
  5. Watch the job in the queue with `squeue`.
  6. After it has disappeared, open the output file `slurm-jobid.out` in your editor. It should contain a list of licensed Matlab features.
  7. For more demanding work you can increase the available memory by increasing the number of cpus.

## Exercise 11: 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 -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](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 TRAININGCPU 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 TRAININGCPU submit_script
Submitted batch job 791609
```

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

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- ▶ Exercise 7 - Array Jobs.

## Exercise 11: 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 11: 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 11: 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 ${SLURM_ARRAY_JOB_ID}`  
i.e. use the array id to release the entire array.
4. When all the jobs complete you should have 64 `slurm-${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?
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    - 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.
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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.