

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

Part 1: Course Introduction

Part 2: HPC - Basic Concepts

Part 3: HPC - Facilities

Part 4: HPC - Connecting

10:00 WELCOME

11:30-11:45 Break

13:00-14:00 LUNCH

15:30-15:45 Break

16:30 CLOSE

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Part I: Introduction

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.

Basics: 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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- ▶ 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

- ▶ A pre-requisite of this course:
- ▶ Basic Unix/Linux command line experience
- ▶ <https://www.training.cam.ac.uk/ucs/Course/ucs-unixintro1>
Unix: Introduction to the Command Line Interface (Self-paced)
- ▶ 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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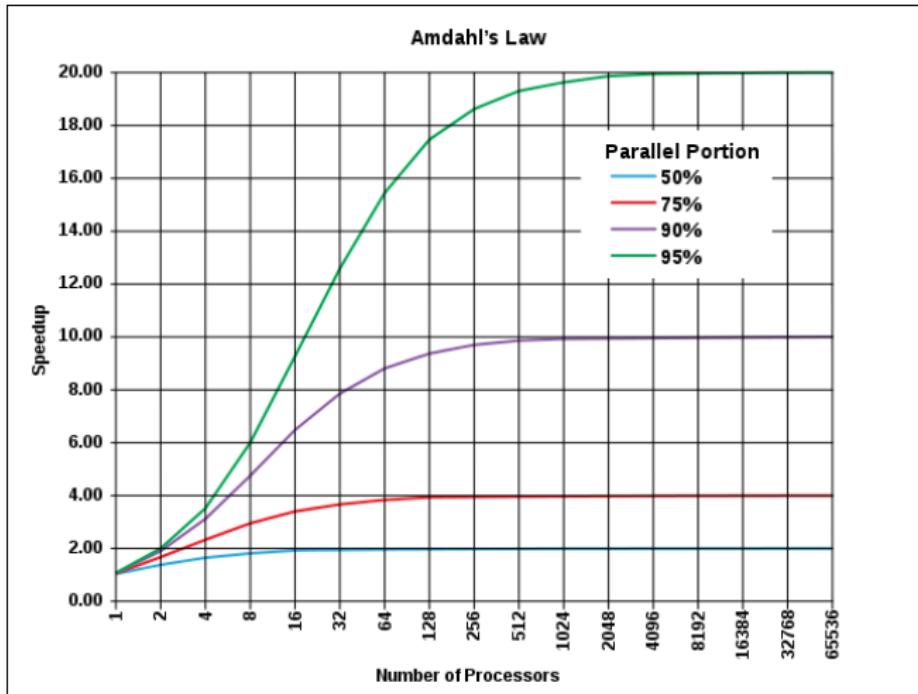
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The Bottom Line

- ▶ Parallelisation requires effort:
 - ▶ There are libraries to help (e.g. [OpenMP](#), [MPI](#)).
 - ▶ First optimise performance on one CPU, then make p as large as possible.
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Basics: Data Intensive Problems

- ▶ Distribute the **data** for a **single problem** across multiple CPUs to reduce the overall execution time.
- ▶ 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.
- ▶ **Big Data** problems of great current interest -
- ▶ Hadoop/MapReduce
- ▶ Life Sciences (genomics) and elsewhere.

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- ▶ Distribute **independent, multiple problems** across multiple CPUs to reduce the overall execution time.
- ▶ 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).
 - * Little or no inter-CPU communication.
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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).
- ▶ Coding/porting easier (memory appears seamless).
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- ▶ Historically, the arena of large **SGI** systems.
- ▶ Nowadays, similar complexity inside single commodity servers.

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Basics: Inside a Modern Computer

- ▶ Today's commodity servers already aggregate both CPUs and memory to make a single system image in a single box.
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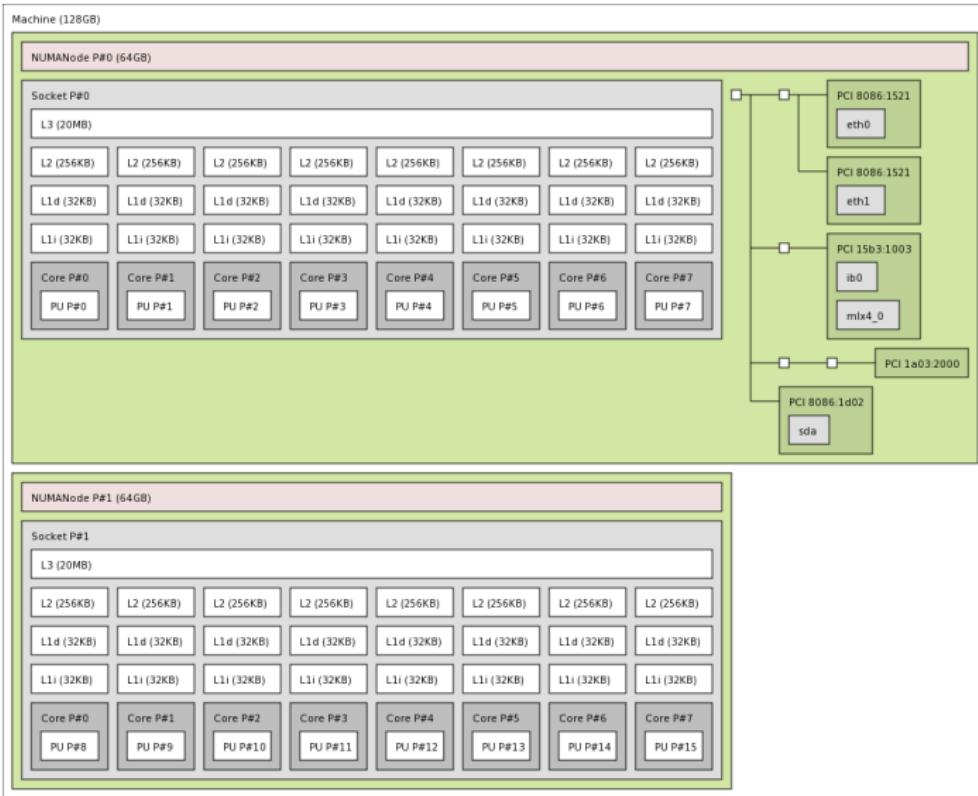
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 with Non-Uniform Memory Architecture (**NUMA**)
 but users still see a single computer (**single system image**).

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

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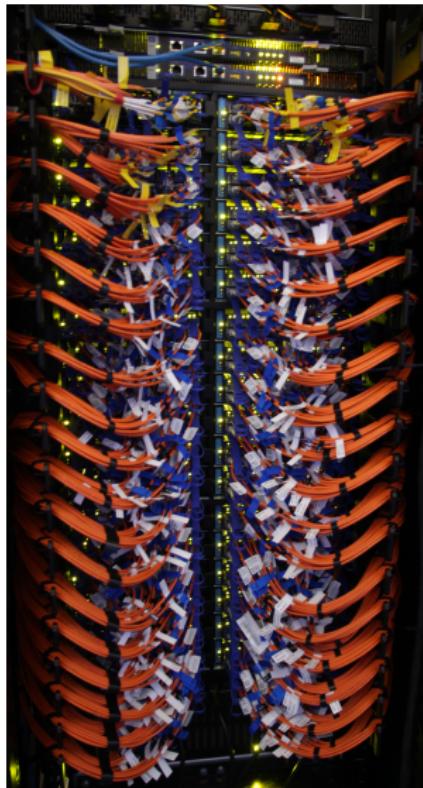
2. Connect the nodes with one or more **networks**. E.g.

Gbit Ethernet: 100 MB/sec

Omni-Path: 10 GB/sec

Faster network is for inter-CPU communication across nodes.

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



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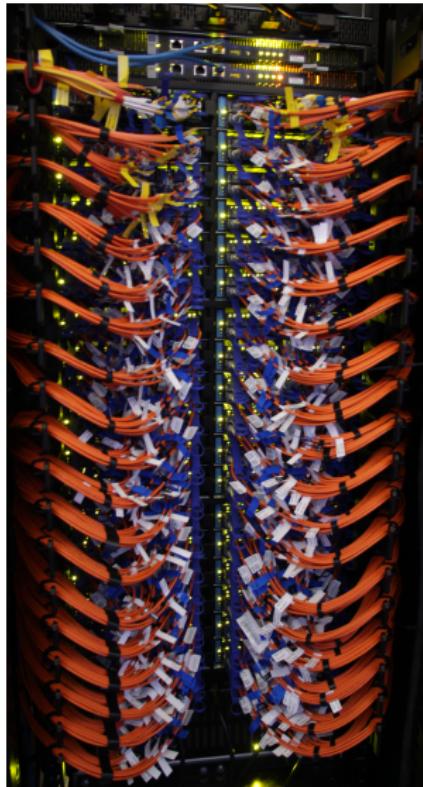
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Basics: How to Build a Supercomputer

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.
- ▶ More expensive machines logically bind nodes into a single system i.e. CPUs and memory.
 - * E.g. SGI UV.
 - * Private networks allow CPUs to see CPUs and memory in other nodes.
 - * These are shared memory machines.
 - * Logically a single system - 1 big node - but very non-uniform.
 - * A single process can span the entire system.

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 - * Private networks allow CPUs to see CPUs and memory in other nodes.
 - * These are **shared memory** machines.
 - * Logically a single system - 1 big node - but very non-uniform.
 - * A single process can span the entire system.

Basics: How to Build a Supercomputer

3. Logically bind the nodes

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- ▶ Non-parallel (serial) code
 - * For a single node as for a workstation.
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Basics: Summary

- ▶ Why have a supercomputer?
 - ▶ Big single problems, many problems, Big Data.
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- ▶ Each node has multiple CPUs and non-uniform shared memory.
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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)

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)

Coprocessors — GPUs etc

- ▶ CPUs are **general purpose**
- ▶ Some types of parallel workload fit **vector processing** well:
 - ▶ Single Instruction, Multiple Data (SIMD)
 - ▶ *Think pixels on a screen*
 - ▶ GPUs specialise in this type of work
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- ▶ 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
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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:
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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.

Basics: Connecting

- ▶ SSH secure protocol only.
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or SSH tunnel through a departmental gateway.

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.hpc.cam.ac.uk`
- ▶ From graphical clients:
Host: `login.hpc.cam.ac.uk`
Username: `abc123` (your UCAM account name)
- ▶ `login.hpc` will map to a random login node
i.e. one of `login-sand1`, `login-sand2`, ..., `login-sand8`
NB Not `darwin.hpc` (the head node).
- ▶ Non-registered addresses will fail with “Connection refused”.
- ▶ Similarly for other systems (e.g. `cardio-login.hpc`,
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Connecting: First time login

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

```
The authenticity of host 'login-sand2.hpc.cam.ac.uk (131.111.1.214)'  
can't be established.
```

RSA key fingerprint is

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0b:ef:59:90:fb:13:4a:c9:56:82:7b:cd:4b:2b:e1:3b.
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Are you sure you want to continue connecting (yes/no)? yes

Warning: Permanently added 'login-sand2.hpc.cam.ac.uk' (RSA) to the
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- ▶ One should always check the fingerprint before typing “yes”.
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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`.

`rsync -av old_directory abc123@login.hpc.cam.ac.uk:scratch/new_directory`
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- ▶ 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)

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

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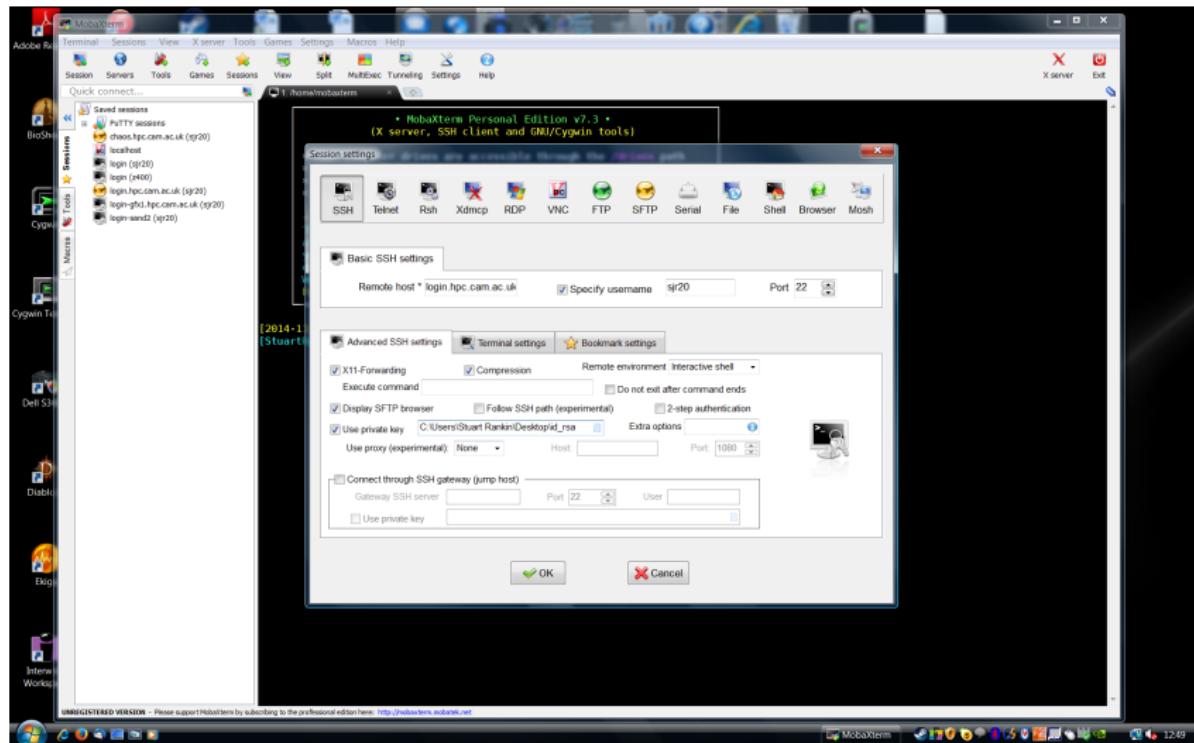
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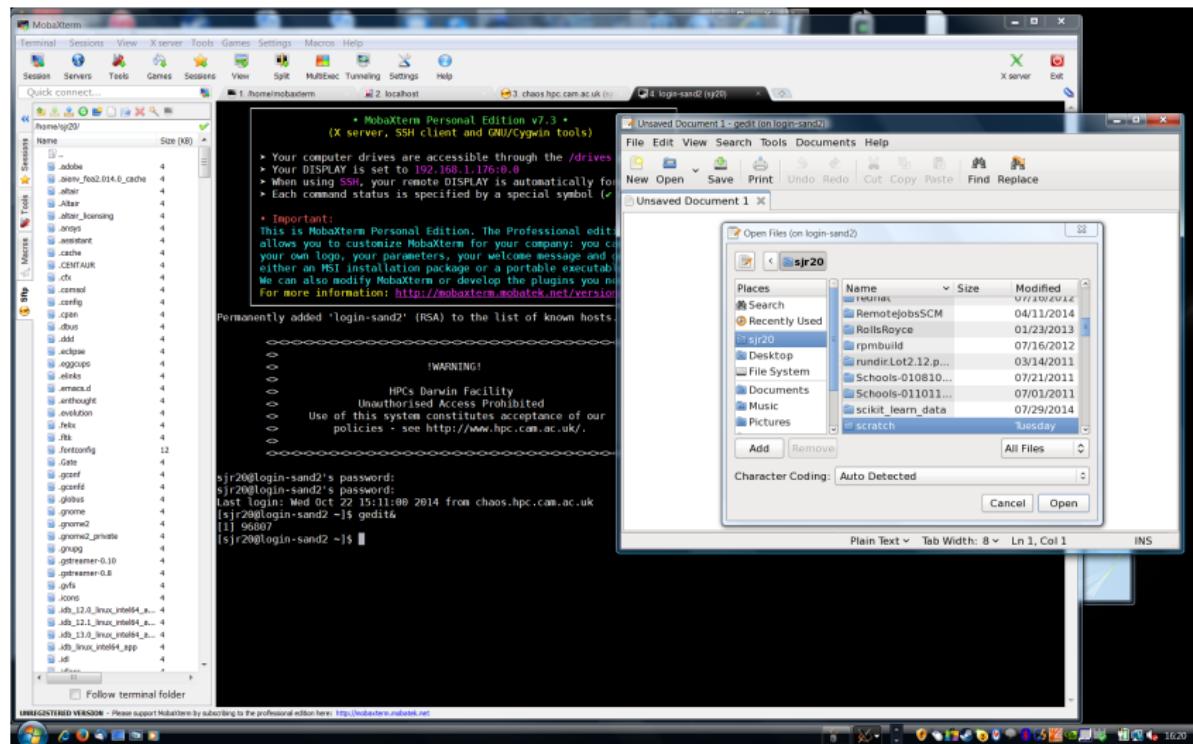
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Basics: A practical example before some theory

- ▶ Some simple exercises will help us gauge your experience.
- ▶ Exercise 1: Login with SSH.
- ▶ Exercise 2: Navigating the command line.
- ▶ Exercise 3: SFTP file transfer.

Exercise 1: Navigating your terminal

- ▶ Start a terminal by double clicking on the terminal icon
- ▶ Try the `ls` and `cd` commands in a terminal.
- ▶ Look at the man page for the `ls` command
- ▶ Close the terminal

Exercise 2: 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.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!

Exercise 3: 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.gz' is in your directory listing
- ▶ Hint: `ls`

Exercise 3: Transfer some files

Transfer the exercises.tar.gz to your HPC home folder.

- ▶ `sftp abc123@login.hpc.cam.ac.uk`
Change abc123 to your training account username
- ▶ The command: `put exercises.tar.gz` will transfer the file from your local computer to the remote one
- ▶ In terminal logged into the cluster type: `ls`
- ▶ Use: `tar -xvf exercise.tar -` to unzip the file

Connecting: File Transfer

In exercise 3 we used sftp. Another tool to be familiar with is rsync especially when you want to transfer lots of directories and files.

- ▶ rsync is a powerful tool and has many features.
 - * You can rerun it to update or resume after interruption.
 - * All transfers are checksummed.

Using HPC: Connecting

- ▶ SSH secure protocol only.

Using HPC: Connecting

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Supports login, file transfer, remote desktop...

Connecting: Windows Clients

- ▶ putty, pscp, psftp

<http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html>

- ▶ WinSCP

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

- ▶ TurboVNC (remote desktop, 3D optional)

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

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<http://winscp.net/eng/download.php>
- ▶ TurboVNC (remote desktop, 3D optional)
<http://sourceforge.net/projects/turbovnc/files/>
- ▶ Cygwin (provides an application environment similar to Linux)
<http://cygwin.com/install.html>
Includes X server for displaying graphical applications running remotely.
- ▶ MobaXterm
<http://mobaxterm.mobatek.net/>

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Connecting: Linux/MacOSX/UNIX Clients

- ▶ ssh, scp, sftp, rsync
[Installed \(or installable\).](#)
- ▶ TurboVNC (remote desktop, 3D optional)
<http://sourceforge.net/projects/turbovnc/files/>
- ▶ On MacOSX, install XQuartz to display remote graphical applications.
<http://xquartz.macosforge.org/landing/>

Connecting: Linux/MacOSX/UNIX Clients

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Connecting: Login

- ▶ From graphical clients:

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

Username: `npl\abc123` (your NPL AD account name)

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

`ssh -Y npl\\abc12@minerva-login1.npl.co.uk`

Note the double backslash — this is because UNIX command interpreters treat `\` as special.

Connecting: Login

- ▶ From graphical clients:

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

Username: `npl\abc123` (your NPL AD account name)

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`ssh -Y npl\\abc12@minerva-login1.npl.co.uk`

Note the double backslash — this is because UNIX command interpreters treat `\` as special.

Connecting: First time login

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

```
The authenticity of host 'minerva-login1.npl.co.uk (139.143.201.10)' can't be established.
```

```
ECDSA key fingerprint is SHA256:k/eB+LjcAfQW56XCzK9QptT0wVWF7j3a/CPxPRd7+1E.
```

```
ECDSA key fingerprint is MD5:18:9a:97:e2:87:4c:07:60:cb:43:46:f2:bb:d8:3d:01.
```

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

```
Warning: Permanently added 'minerva-login1.npl.co.uk (139.143.201.10)' (ECDSA) 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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Connecting: First time login

- ▶ Exercise 1 - Log into your Minerva account.
- ▶ Exercise 2 - Simple command line operations.

Connecting: First time login

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Connecting: File Transfer

- ▶ With graphical clients, connect as before and drag and drop.

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

`rsync -av old_directory/`

`npl\\abc12@minerva-login1.npl.co.uk:hpc-work/new_directory`

copies contents of `old_directory` to `~/hpc-work/new_directory`.

`rsync -av old_directory`

`npl\\abc12@minerva-login1.npl.co.uk:hpc-work/new_directory`

copies `old_directory` (and contents) to

`~/hpc-work/new_directory/old_directory`.

- * Rerun to update or resume after interruption.
- * All transfers are checksummed.
- * For transfers in the opposite direction, place the remote machine as the first argument.

- ▶ Exercise 3 - File transfer.

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- ▶ Exercise 3 - File transfer.

Connecting: Remote Desktop

- ▶ First time starting a remote desktop:

```
[sjr20@login-a-1 ~]$ vncserver
```

You will require a password to access your desktops.

Password:

Verify:

Would you like to enter a view-only password (y/n)? n

New 'login-a-1:99 (sjr20)' desktop is login-a-1:**99**

Starting applications specified in /home/sjr20/.vnc/xstartup
Log file is /home/sjr20/.vnc/login-a-1:99.log

- ▶ NB Choose a **different** password for VNC.
- ▶ The VNC password protects your desktop from other users.
- ▶ Remember the unique display number (**99** here) of your desktop.

Connecting: Remote Desktop

- ▶ Remote desktop already running:

```
[sjr20@login-a-1 ~]$ vncserver -list
```

TigerVNC server sessions:

X DISPLAY #	PROCESS ID
:99	130655

- ▶ Kill it:

```
[sjr20@login-a-1 ~]$ vncserver -kill :99  
Killing Xvnc process ID 130655
```

- ▶ Typically you only need **one** remote desktop.
- ▶ Keeps running until killed, or the node reboots.

Connecting: Remote Desktop

- ▶ To connect to the desktop from Linux:

```
vncviewer -via npl\\abc12@minerva-login1.npl.ad.local localhost:99
```

- ▶ The display number **99** will be different in general and unique to each desktop.
- ▶ You will be asked firstly for your AD login password, and secondly for your VNC password.
- ▶ Press F8 to bring up the control panel.
- ▶ Exercise 4 - Remote desktop (from Windows)

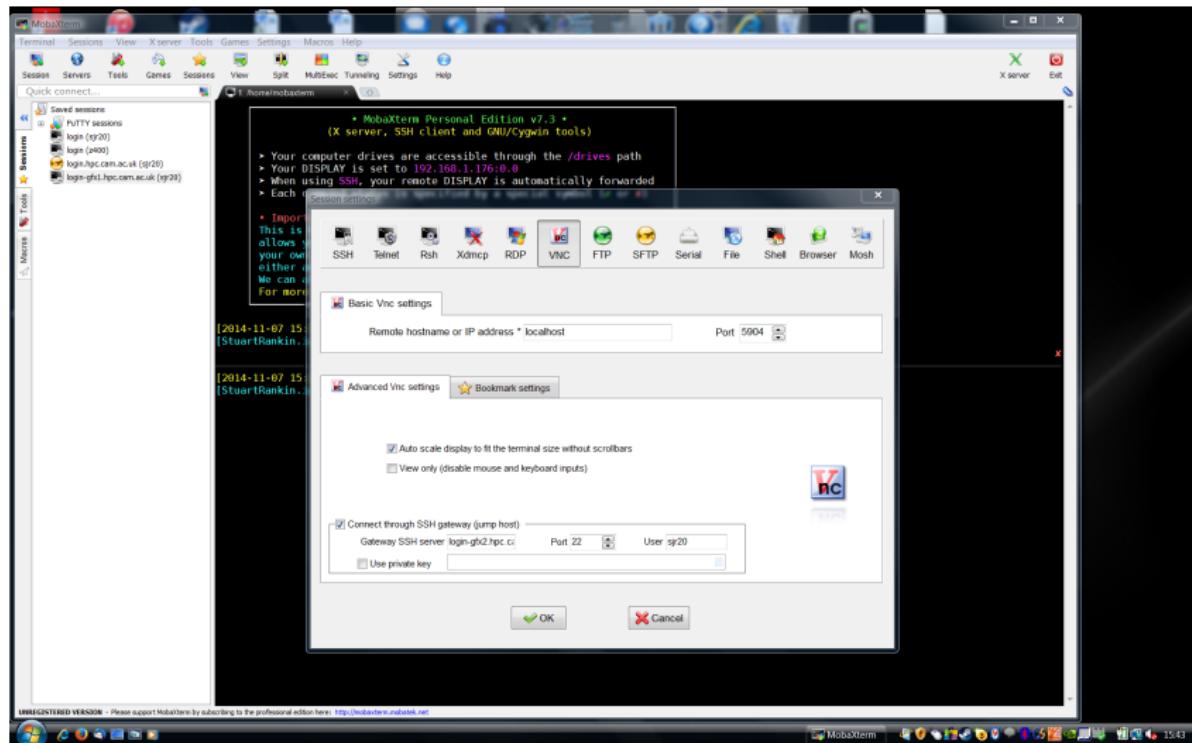
Connecting: Remote Desktop

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- ▶ Press **F8** to bring up the control panel.
- ▶ Exercise 4 - Remote desktop (from Windows)

Connecting: Remote Desktop (MobaXterm)



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

- ▶ [/home/abc12@npl.ad.local](#)
 - ▶ 50GB quota.
 - ▶ Visible equally from all nodes.
 - ▶ Single storage server.
 - ▶ Regular backups.
 - ▶ Not intended for job outputs or large/many input files.
- ▶ [~/hpc-work](#)
 - ▶ Visible equally from all nodes.
 - ▶ Larger (1TB initial quota).
 - ▶ Intended for job inputs and outputs.
 - ▶ **Not backed up by default.**

Filesystems: Quotas

► quota

```
[sjr20@login-a-1 ~]$ quota -s
Disk quotas for user sjr20 (uid 1004):
  Filesystem   space   quota   limit   grace   files   quota   limit   grace
10.44.82.252:/hpc-work
                      OK    1024G   1126G
10.44.82.252:/home
                13272K  51200M  56320M
                                         345      0      0
```

- 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.
- It is important to rectify an out of quota condition ASAP.

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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.

User Environment: Software

- ▶ Free software accompanying Red Hat Enterprise Linux is (or can be) provided.
- ▶ Other software (free and non-free) is available via modules.
- ▶ Proprietary software currently available includes Matlab and COMSOL.
- ▶ New software may be possible to provide on request.
- ▶ **Self-installed software should 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                      3) centos7/global
 2) slurm                    4) centos7/default-basic
```

- ▶ 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-4.8.5-n2hvjgm
```

- ▶ Unload:

```
module unload openmpi-3.0.0-gcc-4.8.5-n2hvjgm
```

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2018a
```

- ▶ 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

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```
module load matlab/r2018a
```

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

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

User Environment: Environment Modules

- ▶ Purge:

```
module purge
```

- ▶ Defaults:

```
module show centos7/default-basic  
module load centos7/default-basic
```

- ▶ Run time environment must match compile time environment.

User Environment: Compilers

► GCC

```
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
```

► Exercise 5: Modules and Compilers

User Environment: Compilers

- ▶ **GCC**

```
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
```

- ▶ **Exercise 5: Modules and Compilers**

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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 - not itself managed by the scheduler.
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- ▶ **Batch** jobs run a shell script 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]
```

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:

```
[abc123@login-a-1]$ squeue -u abc123
      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 NPL-GENERAL-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).

Job Submission: Scripts

► SLURM

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

```
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#! Name of the job:
#SBATCH -J myjob
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#SBATCH -A NPL-GENERAL-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*

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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 NPL-GENERAL-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).

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 NPL-GENERAL-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:

```
gstatement -p NPL-GENERAL-CPU -u xyz10 -s "2018-04-01-00:00:00" -e "2018-04-30-00:00:00"
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
# 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=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=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=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
```

- ▶ Exercise 6 - Submitting Jobs.

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
```

- ▶ Exercise 6 - Submitting Jobs.

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
```

- ▶ Exercise 6 - Submitting Jobs.

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
```

- ▶ Exercise 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
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```
#!/bin/bash
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#SBATCH --nodes=2
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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
```

- ▶ Exercise 6 - Submitting Jobs.

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
```

- ▶ Exercise 6 - Submitting Jobs.

Job Submission: Interactive

- ▶ Compute nodes are accessible via SSH while you have a job running on them.
- ▶ Alternatively, submit an interactive job:
`sintr -A NPL-GENERAL-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.

Job Submission: Interactive

- ▶ Compute nodes are accessible via SSH while you have a job running on them.

- ▶ Alternatively, submit an interactive job:

```
sintr -A NPL-GENERAL-CPU -N1 -n8 -t 2:0:0
```

- ▶ Within the window (screen session):

- * Launches a shell on the first node (when the job starts).
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Job Submission: Interactive

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 - * `ssh` or `srun` can be used to start processes on any nodes in the job.
 - * SLURM-aware MPI will do this automatically.

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 NPL-GENERAL-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.

Job Submission: Array Jobs

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```
[abc123@login-a-1]$ sbatch --array=1-7:2 -A NPL-GENERAL-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
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```
[abc123@login-a-1]$ sbatch --array=1,3,5,7 -A NPL-GENERAL-CPU submit_script
Submitted batch job 791609
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```
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    791609_5 skylake     hpl    abc123 R   0:06      1 cpu-a-7
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```

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      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
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    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.

Job Submission: Array Jobs

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[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}

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Job Submission: Array Jobs

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```
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      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.

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

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.
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Wait Times

- ▶ 36 hour job walltimes are permitted.
- ▶ This sets the timescale at busy times (*without* backfilling).
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- ▶ Insurance against failures during long jobs.
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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.

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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Using HPC: User Environment

Red Hat Enterprise Linux 7

- ▶ But you don't need to know that.

User Environment: Filesystems

- ▶ [/home/abc12@npl.ad.local](#)
 - ▶ 50GB quota.
 - ▶ Visible equally from all nodes.
 - ▶ Single storage server.
 - ▶ Regular backups.
 - ▶ Not intended for job outputs or large/many input files.
- ▶ [~/hpc-work](#)
 - ▶ Visible equally from all nodes.
 - ▶ Larger (1TB initial quota).
 - ▶ Intended for job inputs and outputs.
 - ▶ **Not backed up by default.**

Filesystems: Quotas

► quota

```
[sjr20@login-a-1 ~]$ quota -s
Disk quotas for user sjr20 (uid 1004):
  Filesystem   space   quota   limit   grace   files   quota   limit   grace
10.44.82.252:/hpc-work
                      OK     1024G   1126G
10.44.82.252:/home
                 13272K  51200M  56320M
                                         345      0      0
```

- 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.
- It is important to rectify an out of quota condition ASAP.

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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.

User Environment: Software

- ▶ Free software accompanying Red Hat Enterprise Linux is (or can be) provided.
- ▶ Other software (free and non-free) is available via modules.
- ▶ Proprietary software currently available includes Matlab and COMSOL.
- ▶ New software may be possible to provide on request.
- ▶ **Self-installed software should 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                      3) centos7/global
 2) slurm                    4) centos7/default-basic
```

- ▶ 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-4.8.5-n2hvjgm
```

- ▶ Unload:

```
module unload openmpi-3.0.0-gcc-4.8.5-n2hvjgm
```

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2018a
```

- ▶ 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.

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

User Environment: Environment Modules

- ▶ Purge:

```
module purge
```

- ▶ Defaults:

```
module show centos7/default-basic  
module load centos7/default-basic
```

- ▶ Run time environment must match compile time environment.

User Environment: Compilers

► GCC

```
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
```

► Exercise 5: Modules and Compilers

User Environment: Compilers

- ▶ **GCC**

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

- ▶ **Exercise 5: Modules and Compilers**

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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- 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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[abc123@login-a-1]$ squeue -u abc123
      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 NPL-GENERAL-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).

Job Submission: Scripts

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

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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 NPL-GENERAL-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:

```
gstatement -p NPL-GENERAL-CPU -u xyz10 -s "2018-04-01-00:00:00" -e "2018-04-30-00:00:00"
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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```
#!/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
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...
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).

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- ▶ 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
```

- ▶ Exercise 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

- ▶ Multiple serial jobs across multiple nodes.
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...
cd directory_for_job64
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wait
```

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wait
```

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wait
```

- ▶ Exercise 6 - Submitting Jobs.

Job Submission: Interactive

- ▶ Compute nodes are accessible via SSH while you have a job running on them.

- ▶ Alternatively, submit an interactive job:

```
sintr -A NPL-GENERAL-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.
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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 NPL-GENERAL-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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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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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.
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- ▶ 36 hour job walltimes are permitted.
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- ▶ Insurance against failures during long jobs.
- ▶ Restart from checkpoints to work around finite job length.
- ▶ Application native methods are best. Failing that ...

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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.