

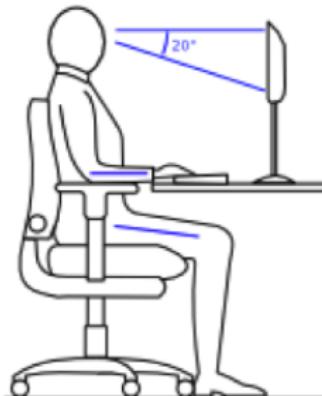
An Introduction to High Performance Computing

Stuart Rankin

sjr20@cam.ac.uk

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

Health and Safety



Welcome

- ▶ Please sign in on the **attendance sheet**.
- ▶ Please give your **online feedback** at the end of the course:
<http://feedback.training.cam.ac.uk/ucs/form.php>
- ▶ Keep your belongings with you.
- ▶ Please ask questions and let us know if you need assistance.

Your trainers for today will be:

- ▶ **Stuart Rankin**
Research Computing User Services
- ▶ **Joe Stankiewicz**
Research Computing Platforms
- ▶ We are generalists, but there is also the **Research Software Engineering** team.

You may be ...

- ▶ Programmers (or not).
- ▶ UNIX power users (or not).
- ▶ Researchers wishing to run large, parallel code.
- ▶ Researchers wishing to run many, non-parallel cases.
- ▶ Researchers interested in big data, machine learning, AI.
- ▶ Researchers requiring slightly more than an ordinary workstation.
- ▶ Many different disciplines and requirements.

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Plan of the Course

Part 1: Basics

Part 2: Research Computing Services HPC

Part 3: Using HPC

09:30 WELCOME

11:00-11:15 Break

12:30-13:30 LUNCH

15:30-15:45 Break

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Prerequisites

- ▶ Basic Unix/Linux command line experience:
Unix: Introduction to the Command Line Interface (self-paced)
<https://www.training.cam.ac.uk/ucs/Course/ucs-unixintro1>
- ▶ Shell scripting experience is desirable:
Unix: Simple Shell Scripting for Scientists
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Training accounts

- ▶ For our practical exercises we will use HPC training accounts. These are distinct from the MCS desktop training accounts.
- ▶ You will find HPC training account details on your desk.
- ▶ Your HPC training account is valid only for today.
- ▶ The name of the HPC account will be the same as your MCS desktop account: z4XY (where XY is the station number).
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Security

- ▶ Cambridge IT is under constant attack by would-be intruders.
- ▶ Choose strong passwords and keep it (or private key passphrase) safe.
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- ▶ Keep the software on your laptops/tablets/PCs up to date — this includes home computers.
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Part I: 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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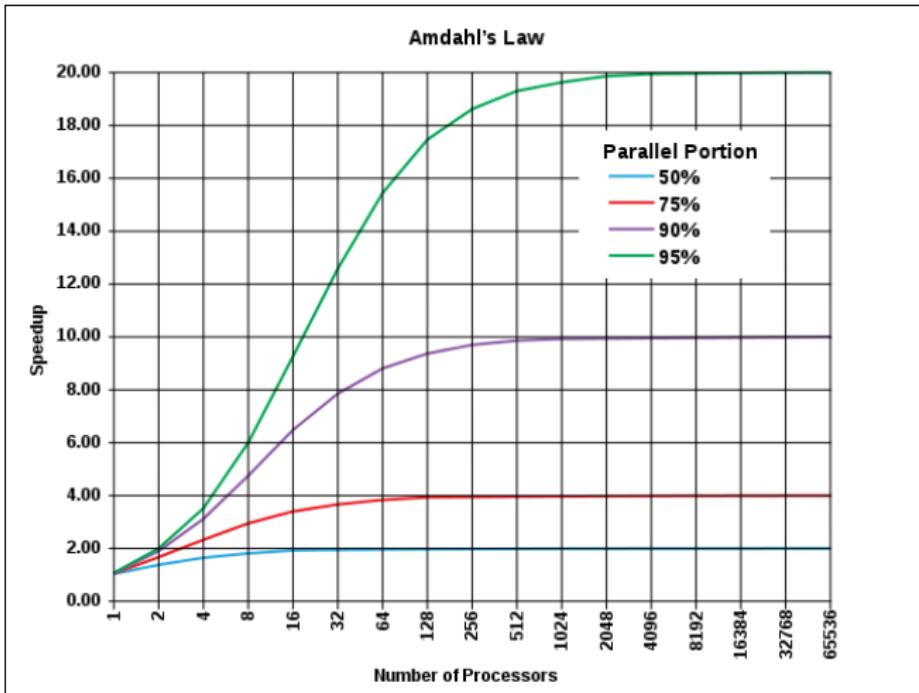
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<http://en.wikipedia.org/wiki/File:AmdahlsLaw.svg>

The Bottom Line

- ▶ Parallelisation requires effort:
 - ▶ There are libraries to help (e.g. OpenMP, MPI).
 - ▶ Aim to make both p and performance per CPU as large as possible.
- ▶ The scaling limit: eventually using more CPUs becomes detrimental instead of helpful.

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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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Basics: High Throughput

- ▶ 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.
- ▶ Emphasis is on throughput over a period, rather than on performance on a single problem.
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If you are using lots of R or python, you are probably high throughput, and possibly data intensive or compute intensive.

Basics: Putting it All Together

- ▶ Each of these types of problem requires combining many CPUs and memory modules.
- ▶ Nowadays, there can be many CPUs and memory modules inside a single commodity PC or server.
- ▶ HPC involves combining many times more than this.

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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.
- ▶ Even small computers now have multiple cores (fully functional CPUs) per socket
 - ⇒ each socket (plus its local memory) is a Symmetric Multi-Processor (SMP).
- ▶ Larger computers have multiple sockets (each with their own local memory):
 - all CPUs (unequally) share the node memory
 - ⇒ the node is a NUMA, shared memory multiprocessor (NUMA = Non-Uniform Memory Architecture).

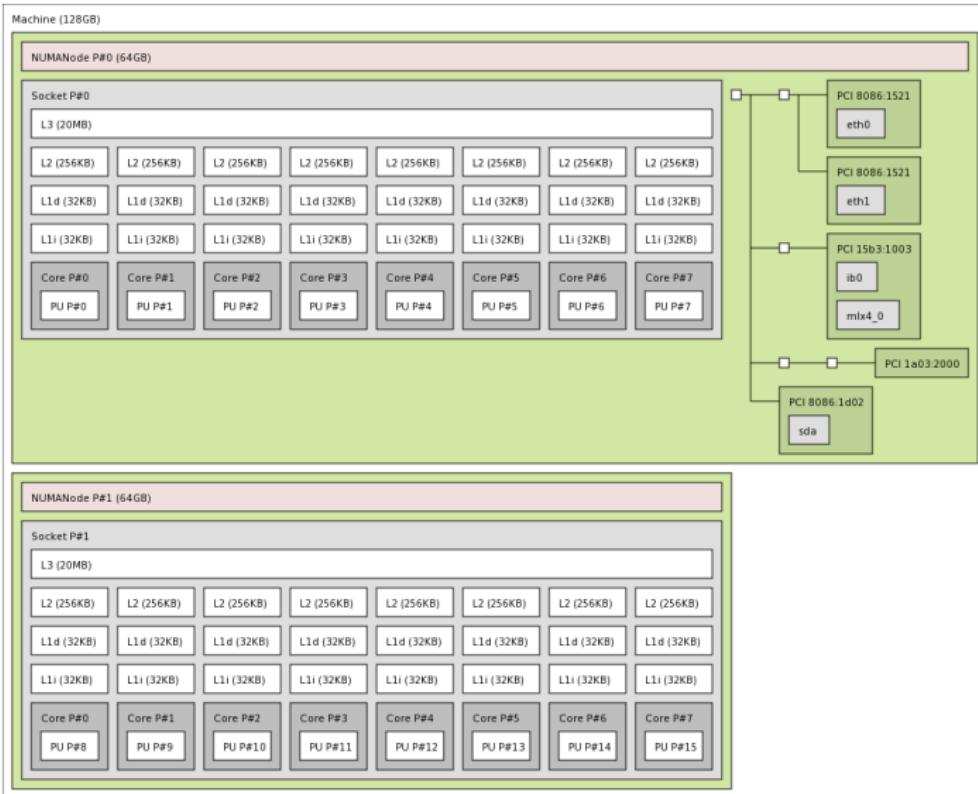
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1. Take some (multicore) processors plus some memory to make a node.
 - ▶ Could be an off-the-shelf server, or something more special.

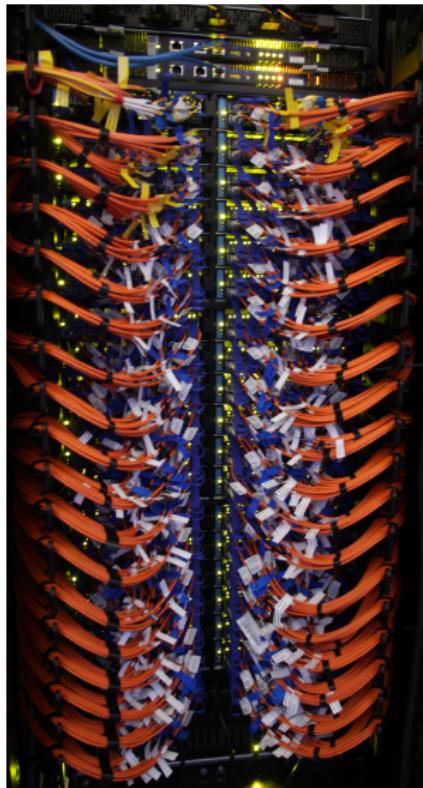
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2. Connect similar nodes with one or more networks. E.g.
Gbit Ethernet: 100 MB/sec
Omni-Path: 10 GB/sec

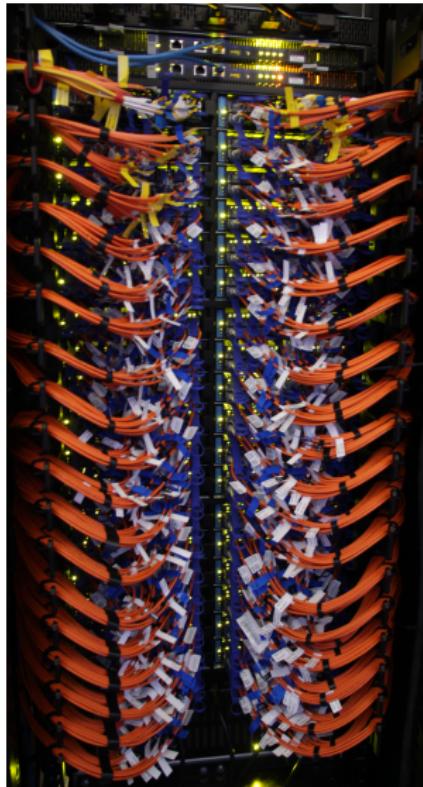
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Storage may use either.



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3. Allocate CPUs & memory to workload

- ▶ Clusters consist of distinct nodes (i.e. separate Linux computers), networked together and controlled centrally by a scheduler.
 - * Each process/thread can see only its local node's CPUs and memory (without help from e.g. MPI).
 - * Each process/thread must fit within a single node's memory.
- ▶ More expensive machines logically bind nodes into a single system.
 - * Logically one big node.
 - * A single process can see the entire system.
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Basics: Running Applications on a Cluster

- ▶ Non-parallel (serial) code
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Basics: Running Applications on a Cluster

- ▶ Parallel code
 - * Thread parallelism works **only** within a node.
E.g. pthreads, OpenMP.
 - * MPI parallelism works both intra- and inter-node.
 - * Some hybrid codes use both forms of parallel programming.

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- ▶ Why have a supercomputer?
 - ▶ Single problems requiring great time or big data; many problems.
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Login to the CSD3 Cluster

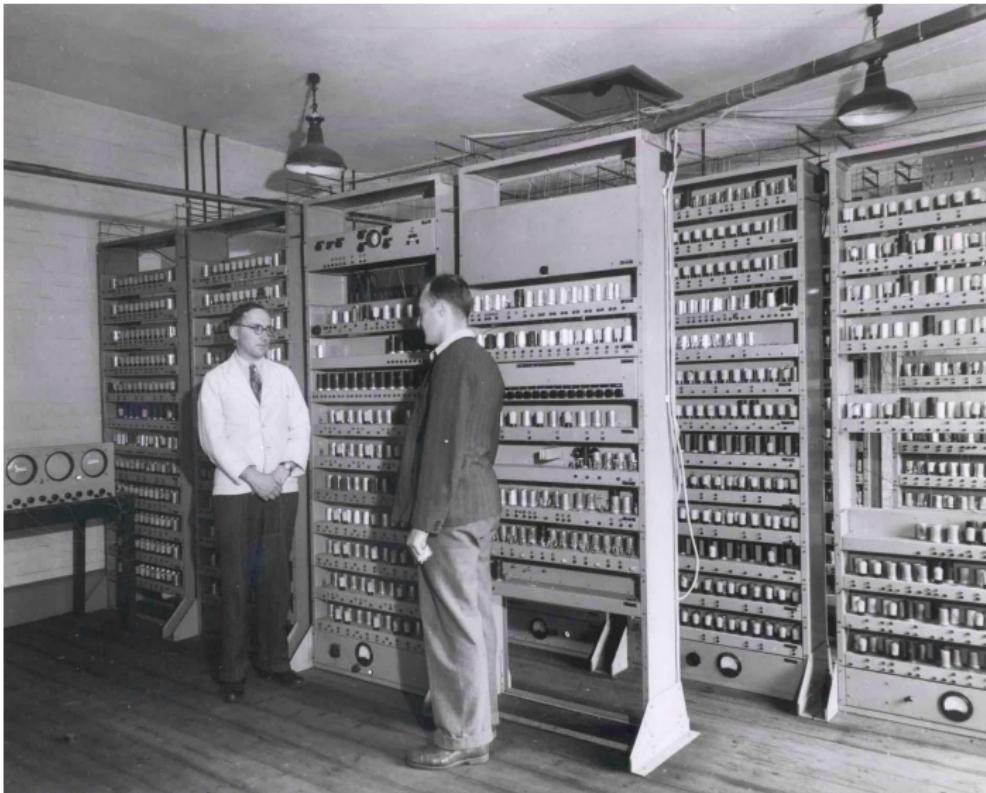
- ▶ Exercise 1 - Log into your RCS training account.
- ▶ Exercise 2 - Simple command line operations.

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Part II: Research Computing Services HPC

Early History: EDSAC (1949–1958)



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- ▶ **Electronic Delay Storage Automatic Calculator**
- ▶ The second general use, electronic digital (Turing complete) stored program computer
- ▶ 3,000 valves
- ▶ 650 instructions per second
- ▶ 2KB memory in mercury ultrasonic delay lines
- ▶ One program at a time!
- ▶ Used in meteorology, genetics, theoretical chemistry, numerical analysis, radioastronomy.
- ▶ *“On a few occasions it worked for more than 24 hours.”*

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Central HPC in Cambridge

Created: 1996 (as the HPCF).

Mission: Delivery and support of a large HPC resource for use by the University of Cambridge research community.

Self-funding: Paying and non-paying service levels.

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History of Performance

<http://www.top500.org>

1997 76.8 Gflop/s

2002 1.4 Tflop/s

2006 18.27 Tflop/s

2010 30 Tflop/s

2012 183.38 Tflop/s

2013 183.38 CPU + 239.90 GPU Tflop/s

2018 2.271 CPU + 1.193 GPU Pflop/s

Darwin1 (2006–2012)



Darwin3 (2012–2018)(b) & Wilkes (2013–2018)(f)



Peta4 (2017) Cumulus (2018)



Skylake

- ▶ Each compute node:
 - * 2x16 cores, Intel Skylake 2.6 GHz
 - * 192 GB or 384 GB RAM
 - * 100 Gb/sec Omni-Path
- ▶ 1152 compute nodes.
- ▶ 8 login nodes (login-cpu.hpc.cam.ac.uk).

- ▶ Each compute node:
 - * 32 CPUs
 - * 6 GB or 12 GB per CPU
 - * 10 GB/sec (for MPI and storage)
- ▶ 1152 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*
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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).

- ▶ 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).

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 Skylake

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 Skylake

Cluster Storage

- ▶ Lustre cluster filesystem:
 - * Very scalable, high bandwidth.
 - * Multiple RAID6 back-end disk volumes.
 - * Multiple object storage servers.
 - * Single metadata server.
 - * Tape-backed HSM on newest filesystems.
 - * 12 GB/sec overall read or write.
 - * Prefers big read/writes over small.

Obtaining an Account and Support

- ▶ <https://www.hpc.cam.ac.uk/applications-access-research-computing-services>
- ▶ Email support@hpc.cam.ac.uk

Part III: Using HPC

Using HPC: Connecting to the RCS Clusters

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- ▶ SSH access is allowed from anywhere.
- ▶ Policies for other clusters may differ.

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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/>

- ▶ Cygwin

<http://cygwin.com/install.html>

- ▶ MobaXterm

<http://mobaxterm.mobatek.net/>

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Includes X server for displaying graphical applications running remotely.
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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/>

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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-10, ..., login-e-16

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Connecting: First time login

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

```
The authenticity of host 'login-cpu (128.232.224.50)' can't be established.
```

```
ECDSA key fingerprint is SHA256:HsiY10e0M8tS6JwR76PeQQA/VB7r8675BzG50YQ4h34.
```

```
ECDSA key fingerprint is MD5:34:9b:f2:d2:c6:b3:5c:63:99:b7:27:da:5b:c8:16:fe.
```

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

```
Warning: Permanently added 'login-cpu,128.232.224.50' (ECDSA) to the list of known hosts.
```

- ▶ One should always check the fingerprint before typing “yes”.
- ▶ Graphical SSH clients *should* ask a similar question.
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File Transfer

- ▶ With graphical clients, connect as before and drag and drop.
- ▶ From Linux/MacOSX/UNIX (or Cygwin):

```
rsync -av old_directory/  
abc12@login-cpu.hpc.cam.ac.uk:rds/hpc-work/new_directory
```

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


```
rsync -av old_directory  
abc12@login-cpu.hpc.cam.ac.uk:rds/hpc-work/new_directory
```

copies old_directory (and contents) to
~/rds/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.

File Transfer

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- ▶ Exercise 3 - File transfer.

Connecting: Remote Desktop

- ▶ First time use of TurboVNC (recommended):

```
[sjr20@login-e-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-e-1:99 (sjr20)' desktop is **login-e-1:99**

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

- ▶ NB Choose a **different** password for VNC to protect your desktop from other users.
- ▶ Note the unique host and display number (**login-e-1** and **:99** here).

Connecting: Remote Desktop

- ▶ Remote desktop already running:

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

TigerVNC server sessions:

X DISPLAY #	PROCESS ID
:99	130655

- ▶ Kill it:

```
[sjr20@login-e-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 abc12@login-e-1.hpc.cam.ac.uk localhost:99
```

- ▶ The display number :99 will be different in general and unique to each desktop.
- ▶ You will be asked firstly for your cluster login password, and secondly for your VNC password.
- ▶ Press F8 to bring up the control panel.
- ▶ Exercise 4 - Connecting to a remote desktop running on the HPC cluster.

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- ▶ Exercise 4 - Connecting to a remote desktop running on the HPC cluster.

Using HPC: User Environment

- ▶ Scientific Linux 7.x (Red Hat Enterprise Linux 7.x rebuild)
 - ▶ bash shell
 - ▶ Gnome or XFCE4 desktop (if you want)
 - ▶ GCC, Intel, PGI compilers and other development software.
- ▶ But you don't need to know that.
- ▶ NOT Ubuntu or Debian!
- ▶ CentOS 7 is OK.

Using HPC: User Environment

Red Hat Enterprise Linux 7

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User Environment: Filesystems

- ▶ [/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](#) a.k.a. [/home/abc123/rds/hpc-work](#)
 - ▶ Visible equally from all nodes.
 - ▶ Larger and faster (1TB initial quota).
 - ▶ Intended for job inputs and outputs.
 - ▶ **Not backed up.**
 - ▶ [Research Data Storage](#)
 - ▶ <https://www.hpc.cam.ac.uk/research-data-storage-services>

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 - ▶ 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](#) a.k.a. [/home/abc123/rds/hpc-work](#)
 - ▶ Visible equally from all nodes.
 - ▶ Larger and faster (1TB initial quota).
 - ▶ Intended for job inputs and outputs.
 - ▶ **Not backed up.**
 - ▶ **Research Data Storage**
 - ▶ <https://www.hpc.cam.ac.uk/research-data-storage-services>

Filesystems: Quotas

- ▶ quota

```
[abc123@login-e-1 ~]$ quota
```

Filesystem	GiBytes	quota	limit	grace	files	quota	limit	grace	User/group
/home	10.6	40.0	40.0	0	-----	No ZFS File Quotas	-----	-----	U:abc123
/rds-d2	1.0	1024.0	1126.4	-	8	1048576	1048576	-	G:abc123

- ▶ 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.

Filesystems: Quotas

- ▶ quota

```
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```

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Filesystems: Quotas

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Filesystems: Quotas

- ▶ quota

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/rds-d2	1.0	1024.0	1126.4	-	8	1048576	1048576	-	G:abc123

- ▶ 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.

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.
- ▶ Some proprietary software may not be generally accessible.
- ▶ 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.)*
- ▶ Docker-compatible containers can now be downloaded and used via singularity.

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- ▶ Self-installed software should be properly licensed.
- ▶ *sudo will not work. (You should be worried if it did.)*
- ▶ Docker-compatible containers can now be downloaded and used via singularity.

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) slurm
 3) turbovnc/2.0.1
 4) vgl/2.5.1/64
 5) singularity/current
 6) rhel7/global
 7) intel/compilers/2017.4
 8) intel/mkl/2017.4
 9) intel/impi/2017.4/intel
10) intel/libs/idb/2017.4
11) intel/libs/tbb/2017.4
12) intel/libs/ipp/2017.4
13) intel/libs/daal/2017.4
14) intel/bundles/complib/2017.4
15) rhel7/default-peta4
```

► Available:

```
module av
```

User Environment: Environment Modules

- ▶ What is:

```
module whatis openmpi-1.10.7-gcc-5.4.0-jdc7f4f
openmpi-1.10.7-gcc-5.4.0-jdc7f4f: The Open MPI Project is an open source...
```

- ▶ Load:

```
module load openmpi-1.10.7-gcc-5.4.0-jdc7f4f
```

- ▶ Unload:

```
module unload openmpi-1.10.7-gcc-5.4.0-jdc7f4f
```

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2019b
```

- ▶ Invoking matlab in batch mode:

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

where the file command.m contains your matlab code.

- ▶ The University site license contains the Parallel Computing Toolbox.
- ▶ MATLAB Parallel Server is also available.

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2019b
```

- ▶ Invoking matlab in batch mode:

`matlab -nodisplay -nojvm -nosplash command`

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

- ▶ The University site license contains the Parallel Computing Toolbox.
- ▶ MATLAB Parallel Server is also available.

User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2019b
```

- ▶ Invoking matlab in batch mode:

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matlab -nodisplay -nojvm -nosplash command
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where the file `command.m` contains your matlab code.

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User Environment: Environment Modules

- ▶ Matlab

```
module load matlab/r2019b
```

- ▶ Invoking matlab in batch mode:

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

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

- ▶ The University site license contains the Parallel Computing Toolbox.
- ▶ MATLAB Parallel Server is also available.

User Environment: Environment Modules

- ▶ Purge:

```
module purge
```

- ▶ Defaults loaded on login (vary by cluster):

```
module show rhel7/default-peta4
```

```
/usr/local/Cluster-Config/modulefiles/rhel7/default-peta4:
```

```
module-whatis      default user environment for Peta4 nodes with Intel MPI
setenv            OMP_NUM_THREADS 1
module            add dot slurm turbovnc vgl singularity
module            add rhel7/global
module            add intel/bundles/complib/2017.4


---


```

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

- ▶ Run time environment must match compile time environment.

User Environment: Compilers

Intel: `icc`, `icpc`, `ifort` (recommended)

```
icc -O3 -xHOST -ip code.c -o prog  
mpicc -O3 -xHOST -ip mpi_code.c -o mpi_prog
```

GCC: `gcc`, `g++`, `gfortran`

```
gcc -O3 -mtune=native code.c -o prog  
mpicc -cc=gcc -O3 -mtune=native mpi_code.c -o mpi_prog
```

PGI: `pgcc`, `pgCC`, `pgf90`

```
pgcc -O3 -tp=skylake code.c -o prog  
mpicc -cc=pgcc -O3 -tp=skylake mpi_code.c -o mpi_prog
```

Exercise 5: Modules and Compilers

User Environment: Compilers

Intel: `icc`, `icpc`, `ifort` (recommended)

```
icc -O3 -xHOST -ip code.c -o prog  
mpicc -O3 -xHOST -ip mpi_code.c -o mpi_prog
```

GCC: `gcc`, `g++`, `gfortran`

```
gcc -O3 -mtune=native code.c -o prog  
mpicc -cc=gcc -O3 -mtune=native mpi_code.c -o mpi_prog
```

PGI: `pgcc`, `pgCC`, `pgf90`

```
pgcc -O3 -tp=skylake code.c -o prog  
mpicc -cc=pgcc -O3 -tp=skylake mpi_code.c -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.

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.

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 (automatic on KNL).
- ▶ Template submission scripts are available under
`/usr/local/Cluster-Docs/SLURM.`

Job Submission: Using SLURM

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

```
[abc123@login-e-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-e-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-e-[1,10]
```

Job Submission: Show Queue

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

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

Job Submission: Show Queue

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

```
[abc123@login-e-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-e-[1,10]
```

Job Submission: Monitor Job

- ▶ Examine a particular job:

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

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 SUPPORT-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: Cancel Job

- ▶ Cancel a particular job:

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

Job Submission: Scripts

► SLURM

In `/usr/local/Cluster-Docs/SLURM`, see examples:
`slurm_submit.peta4-skylake`, `slurm_submit.wilkes2`.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A CHANGEME
#! 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 `/usr/local/Cluster-Docs/SLURM`, see examples:
`slurm_submit.peta4-skylake`, `slurm_submit.wilkes2`.

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#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

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

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Job Submission: Scripts

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In `/usr/local/Cluster-Docs/SLURM`, see examples:
`slurm_submit.peta4-skylake`, `slurm_submit.wilkes2`.

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#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A CHANGEME
#! 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 `/usr/local/Cluster-Docs/SLURM`, see examples:
`slurm_submit.peta4-skylake`, `slurm_submit.wilkes2`.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A CHANGEME
#! 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: 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=
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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=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 (doesn't need a list of nodes).

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 (doesn't need a list of nodes).

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 (doesn't need a list of nodes).

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 6–8 – 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 6–8 – 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 &
...
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```

- ▶ Exercise 6–8 – Submitting Jobs.

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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#!/bin/bash
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#SBATCH --nodes=2
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Job Submission: Interactive

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

- ▶ Alternatively, submit an interactive job:

```
sintr -A TRAINING-CPU -N1 -n8 -t 1:0:0
```

- ▶ Within the window (screen session):

- * Launches a shell on the first node (when the job starts).
- * Graphical applications should display correctly (if they did from the login node).
- * 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-e-1]$ sbatch --array=1-7 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

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

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

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- ▶ Updates can be applied to specific array elements using
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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.
 - ▶ `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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- ▶ 36 hour job walltimes are permitted.
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Checkpointing

- ▶ Insurance against failures during long jobs.
- ▶ Restart from checkpoints to work around finite job length.
- ▶ Application native methods are best. Failing that, one can try DMTCP:
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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.