

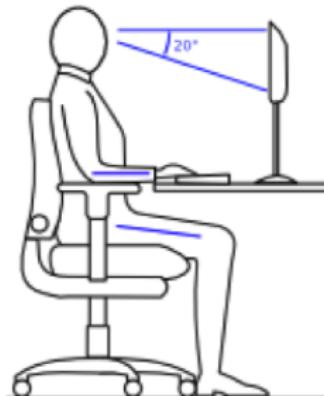
# An Introduction to High Performance Computing

Stuart Rankin

[sjr20@cam.ac.uk](mailto: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
- ▶ **Mark Sharpley**  
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

16:30 CLOSE

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- ▶ 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.
- ▶ Your UIS password is used for multiple systems so keep it secure!
- ▶ Keep the software on your laptops/tablets/PCs up to date — this includes home computers.
- ▶ Check out and install free anti-malware software available for work and home:  
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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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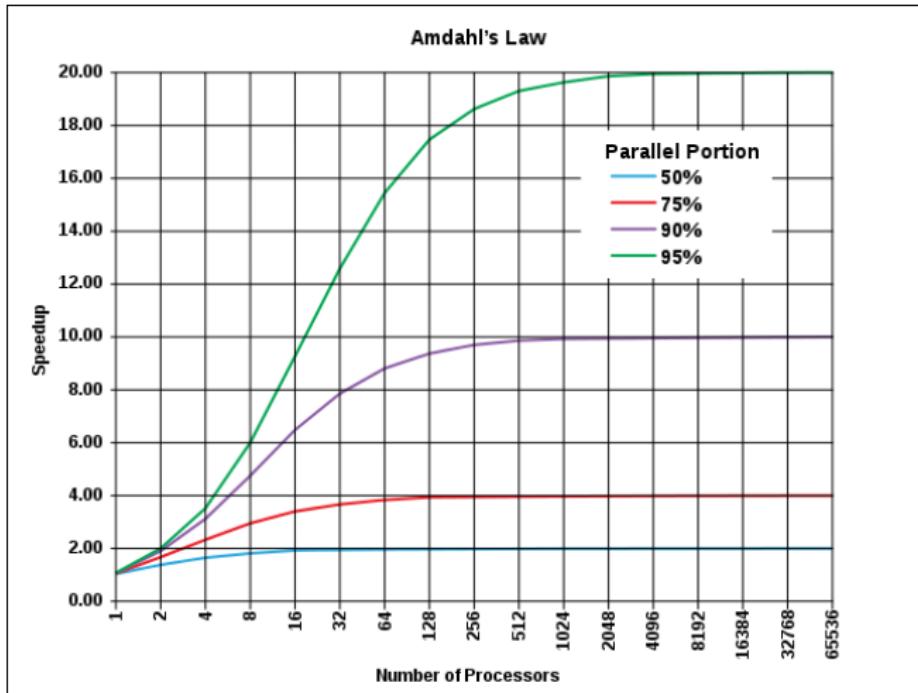
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<http://en.wikipedia.org/wiki/File:AmdahlsLaw.svg>

# 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.
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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
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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.
- ▶ Compute intensive capable  $\Rightarrow$  high throughput capable (not conversely).

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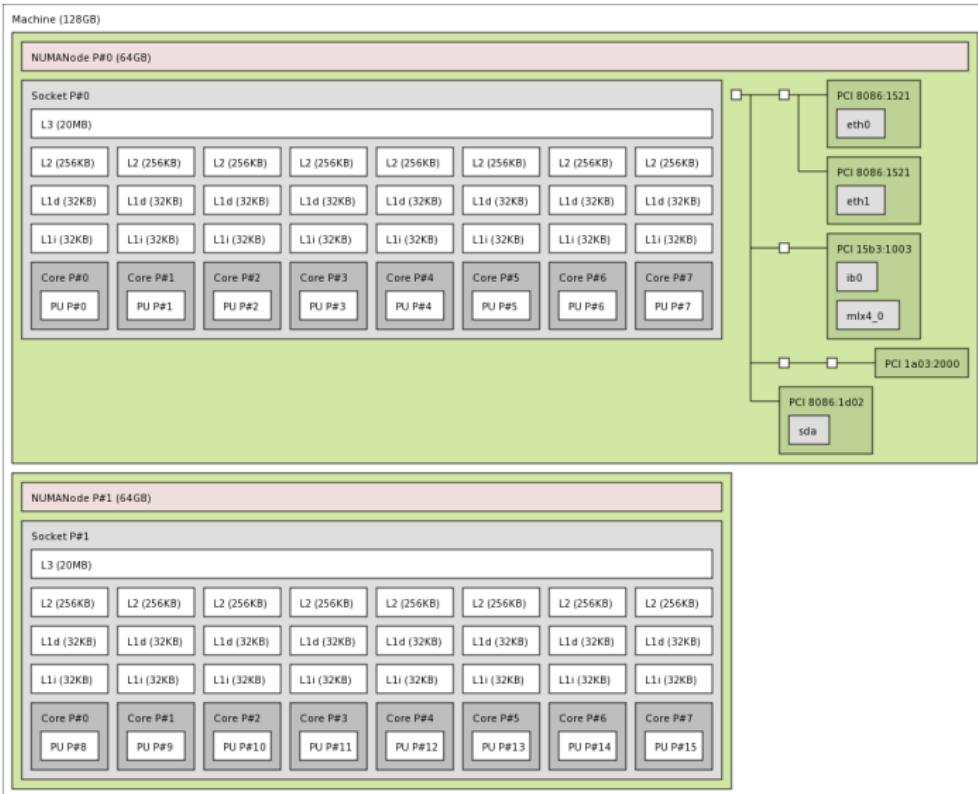
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1. Take some (multicore) processors plus some memory to make a node.
  - ▶ Could be an off-the-shelf server, or something more special.

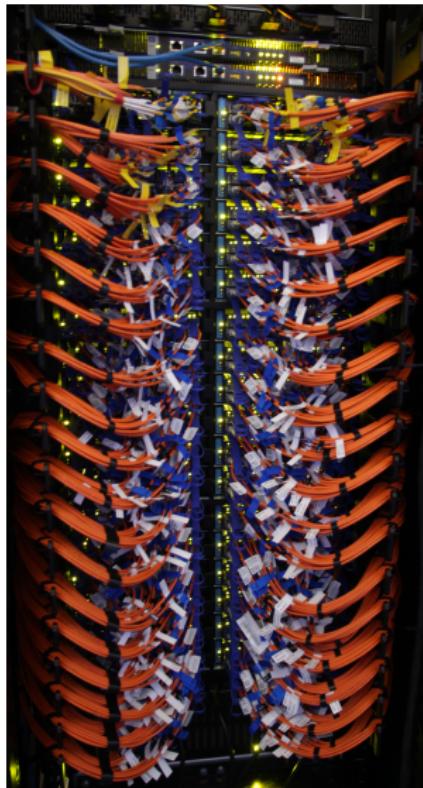
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2. Connect similar nodes with one or more **networks**. E.g.  
Gbit Ethernet: 100 MB/sec  
Omni-Path: 10 GB/sec

Faster network is for inter-CPU communication across nodes.  
Slower network is for management and provisioning.  
Storage may use either.

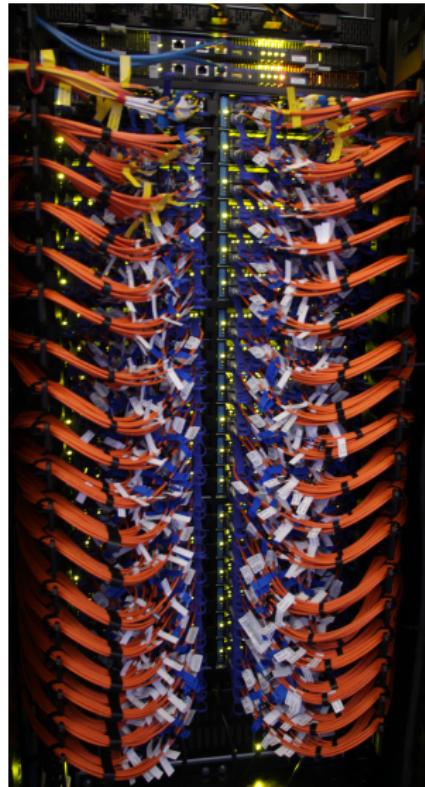


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# Basics: How to Build a Supercomputer

## 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: How to Build a Supercomputer

## 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.
  - \* E.g. SGI UV.

# Basics: Running Applications on a Cluster

- ▶ Non-parallel (serial) code
  - \* For a single node as for a workstation.
  - \* Typically run as many copies per node as CPUs, assuming node memory is sufficient.
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E.g. pthreads, OpenMP.
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# Basics: Summary

- ▶ Why have a supercomputer?
  - ▶ Single problems requiring great time or big data; many problems.
  - ▶ Most current supercomputers are clusters of separate nodes.
  - ▶ Each node has multiple CPUs and (non-uniform, shared) memory.
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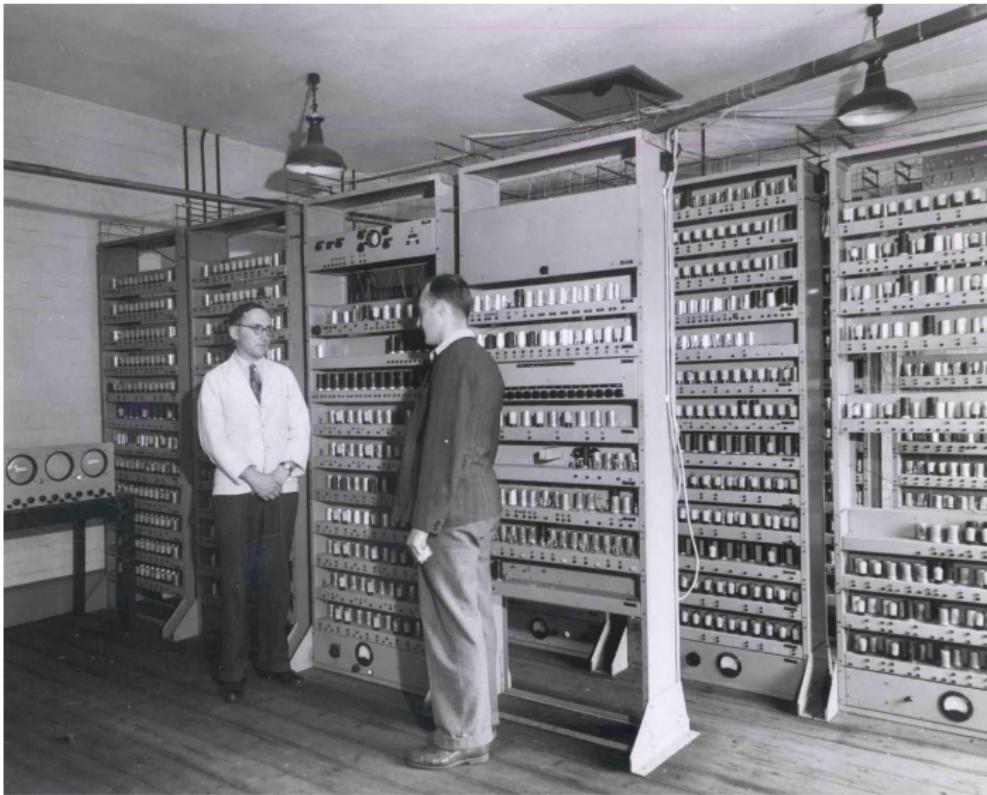
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## Part II: Research Computing Services HPC

# 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.

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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](http://login-cpu.hpc.cam.ac.uk)).

# Skylake

- ▶ Each compute node:
  - \* 32 CPUs
  - \* 6 GB or 12 GB per CPU
  - \* 10 GB/sec (for MPI and storage)
- ▶ 1152 compute nodes.
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# 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](http://login-gpu.hpc.cam.ac.uk)).

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

# 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](mailto:support@hpc.cam.ac.uk)

## Part III: Using HPC

# Using HPC: Connecting to the RCS Clusters

- ▶ SSH secure protocol only.
- ▶ SSH access is allowed from anywhere.
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- ▶ 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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- ▶ 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.  
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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.
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ECDSA key fingerprint is SHA256:HsiY1Oe0M8tS6JwR76PeQQA/VB7r8675BzG50YQ4h34.
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ECDSA key fingerprint is MD5:34:9b:f2:d2:c6:b3:5c:63:99:b7:27:da:5b:c8:16:fe.
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```
Are you sure you want to continue connecting (yes/no)? yes
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Warning: Permanently added 'login-cpu,128.232.224.50' (ECDSA) to the list of known hosts.
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- ▶ One should always check the fingerprint before typing “yes”.
- ▶ Graphical SSH clients *should* ask a similar question.
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- ▶ Exercise 2 - Simple command line operations.

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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/`

`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`

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copies old\_directory (and contents) to

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- \* 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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# 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.

# Connecting: Remote Desktop

- ▶ To connect to the desktop from Linux:

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- ▶ Press F8 to bring up the control panel.
- ▶ 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

- ▶ But you don't need to know that.
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# Using HPC: User Environment

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# 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>

# User Environment: Filesystems

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# 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

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

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- ▶ Aim to stay below the soft limit (*quota*).
- ▶ Once over the soft limit, you have 7 days grace to return below.
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- ▶ 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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## 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                               9) intel/impi/2017.4/intel
 2) slurm                            10) intel/libs/idb/2017.4
 3) turbovnc/2.0.1                   11) intel/libs/tbb/2017.4
 4) vgl/2.5.1/64                     12) intel/libs/ipp/2017.4
 5) singularity/current              13) intel/libs/daal/2017.4
 6) rhel7/global                      14) intel/bundles/complib/2017.4
 7) intel/compilers/2017.4            15) rhel7/default-peta4
 8) intel/mkl/2017.4
```

- ▶ 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/r2017b
```

- ▶ 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/r2017b
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module load matlab/r2017b
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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**
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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 (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:  
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#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

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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`.

```
#!/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
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```

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

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...
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$application $options
...
```

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

# Job Submission: Single Node Jobs

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

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

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

# Job Submission: Single Node Jobs

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

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

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

# Job Submission: Single Node Jobs

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

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

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

# Job Submission: MPI Jobs

- ▶ Parallel job across multiple nodes.

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

- ▶ SLURM-aware MPI launches remote tasks via SLURM (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).

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# 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.

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- ▶ Exercise 6–8 - 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 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`.
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# Job Submission: Array Jobs

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

```
[abc123@login-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
    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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791609\_1, 791609\_3, 791609\_5, 791609\_7

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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}`
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- ▶ Some commands still require the SLURM\_JOB\_ID (sacct, sreport, sshare, sstat and a few others).
- ▶ Exercise 9 - 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.
  - ▶ `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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<http://dmtcp.sourceforge.net/index.html>

# 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.