Your trainers for today will be:

- **Stuart Rankin**
  Research Computing User Services

- **Chris Hadjigeorgiou**
  Research Software Engineering
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.
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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Part 2: Research Computing Services HPC
Part 3: Using HPC
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Basics: Login nodes

- For our practical exercises we will use the login nodes `login.hpc.cam.ac.uk`.
- We will be using the skylake nodes which are part of the CPU cluster.
- We also have knl (specialised CPU) and pascal (GPU) nodes.
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Basics: Security

- **Boring but very, very important...**
- Cambridge IT is under constant attack by would-be intruders.
- Your data and research career are potentially threatened by intruders.
- Cambridge systems are high profile and popular targets (be paranoid, because they *are* out to get you).
- Don’t be the weakest link.
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- Always choose strong passwords.
- 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.
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▶ Basic Unix/Linux command line experience:
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*Compute Intensive:* A single problem requiring a large amount of computation.

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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.

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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):

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

- \(S(N)\) is the fraction by which the program has sped up relative to \(N = 1\)
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- Aim to make both $p$ and performance per CPU as large as possible.

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The Bottom Line

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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 -
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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 \textit{probably} high throughput, and \textit{possibly} data intensive or compute intensive.
Basics: Memory Intensive Problems

- Require aggregation of large memory, rather than many CPUs.
  
  NB Memory (fast, volatile) not disk (slow, non-volatile).

- Performance optimisation is harder (memory layout tends to be highly nonuniform).

- More technically difficult and expensive to scale beyond a single box.

- If you think you have a memory intensive problem, are you sure it needs to be?
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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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but users still see a single computer (single system image).
Basics: How to Build a Supercomputer

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   - Could be an off-the-shelf server, or something more special.
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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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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, transparently to the user.
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  - A single process can span the entire system.
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  - Private networks allow CPUs to see CPUs and memory in other nodes, transparently to the user.
    - These are shared memory machines, but very NUMA.
    - Logically a single system - 1 big node
    - A single process can span the entire system.
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.
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Basics: Programming a Multiprocessor Machine

- 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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Parallel code
- Shared memory methods within a node.
  E.g. pthreads, OpenMP. Intra-node only.
- Distributed memory methods spanning one or more nodes.
  Message Passing Interface (MPI). Both intra and inter-node.
- Some codes use both forms of parallel programming (hybrid).
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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.
- Parallel code uses shared memory (pthreads/OpenMP/MPI) within a node, distributed memory (MPI) across multiple nodes.
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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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TITAN (1964–1973) Multiuser system, designed with Ferranti.


Mainframe service morphs into distributed research computing support with central services.
Specialised research computing needs remain!
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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.

User base: Includes external STFC & EPSRC plus industrial users.

Plus: Dedicated group nodes and research projects.

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History of Performance

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
2017  1.697 CPU + 1.193 GPU Pflop/s
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)
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*
  - GPUs specialise in this type of work
  - Also competitor many-core architectures such as the Intel Phi
CPU coprocessors — GPUs etc.

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- Single Instruction, Multiple Data (SIMD)
- *Think pixels on a screen*
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- Also competitor many-core architectures such as the Intel Phi
Pascal

- Each compute node:
  - 4 × NVIDIA P100 GPU
  - 1×12 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
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](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

- SSH secure protocol only.
  - SSH access is allowed from anywhere.
  - Policies for other clusters may differ.
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- **putty, pscp, psftp**

- **WinSCP**
  [http://winscp.net/eng/download.php](http://winscp.net/eng/download.php)

- **TurboVNC (remote desktop, 3D optional)**

- **Cygwin**
  [http://cygwin.com/install.html](http://cygwin.com/install.html)

- **MobaXterm**
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- Cygwin (provides an application environment similar to Linux)  
  http://cygwin.com/install.html  
  Includes X server for displaying graphical applications running remotely.
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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 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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  i.e. one of `login-e-9, login-e-10, ..., login-e-16`
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:HsiY1Oe0M8tS6JwR76PeQQA/VC7r8675BzG50YQ4h34.

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.
Designed to detect fraudulent servers.
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Connecting: First time login

- Exercise 1 - Log into your RCS training account.
- Exercise 2 - Simple command line operations.
Connecting: First time login

- Exercise 1 - Log into your RCS training account.
- Exercise 2 - Simple command line operations.
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.
Connecting: File Transfer

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

  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`.

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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.
Connecting: Remote Desktop

First time starting a remote desktop:

```bash
[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.

The VNC password protects your desktop from other users.

Remember the unique host and display number (login-e-1 and 99 here) of your desktop.
Remote desktop already running:

$ vncserver -list

TigerVNC server sessions:

<table>
<thead>
<tr>
<th>X DISPLAY #</th>
<th>PROCESS ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>:99</td>
<td>130655</td>
</tr>
</tbody>
</table>

Kill it:

$ vncserver -kill :99
Killing Xvnc process ID 130655

Typically you only need one remote desktop.

Keeps running until killed, or the node reboots.
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.
Using HPC: User Environment

- **Scientific Linux 7.x** *(Red Hat Enterprise Linux 7.4 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.
Red Hat Enterprise Linux 7

- 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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Red Hat Enterprise Linux 7

- But you don't need to know that.
- NOT Ubuntu or Debian!
- CentOS 7 is OK.
Red Hat Enterprise Linux 7

- But you don't need to know that.
- NOT Ubuntu or Debian!
- CentOS 7 is OK.
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

- `/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`
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  - Intended for job inputs and outputs.
  - Not backed up.
  - Research Data Storage
  - [https://www.hpc.cam.ac.uk/research-data-storage-services](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.
### 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       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**

```
[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

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

<table>
<thead>
<tr>
<th>Filesystem</th>
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<th>quota</th>
<th>limit</th>
<th>grace</th>
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</tr>
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<td>No ZFS File Quotas</td>
<td>------</td>
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<td></td>
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<td>-</td>
<td>8</td>
<td>1048576</td>
<td>1048576</td>
<td>-</td>
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</tr>
</tbody>
</table>

- 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.
Directories under /rds/user and /rds/project are automounted.

- They only appear when explicitly referenced.
- Thus when browsing these directories may appear too empty — use `ls` or `cd` to reference /rds/user/abc123 explicitly.
- We create convenience symlinks (shortcuts) under ~/rds.
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.
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.
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.
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.
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.
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

▶ **Whatis:**

```
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
```
Matlab

\[ \text{module load matlab/r2017b} \]

- Invoking matlab in batch mode:
  \[ \text{matlab -nodisplay -nojvm -nosplash command} \]
  where the file command.m contains your matlab code.
- The University site license contains the Parallel Computing Toolbox.
- MATLAB Parallel Server coming soon!
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 coming soon!
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 coming soon!
Matlab

```bash
module load matlab/r2017b
```

Invoking matlab in batch mode:

```bash
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 coming soon!
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.
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
```
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 4: Modules and Compilers
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.
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.
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.
Jobs may use part or all of one or more nodes — the owner can specify \texttt{--exclusive} to force exclusive node access (automatic on KNL).

Template submission scripts are available under \\
\texttt{/usr/local/Cluster-Docs/SLURM}. 
Prepare a shell script and submit it to SLURM:

[abc123@login-e-1] $ sbatch slurm_submission_script
Submitted batch job 790299
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]
```
Submitted job scripts are copied and stored in a queue:

```
[abc123@login-e-1]$ squeue -u abc123

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>NODELIST(REASON)</th>
</tr>
</thead>
<tbody>
<tr>
<td>790299</td>
<td>skylake</td>
<td>Test3</td>
<td>abc123</td>
<td>PD</td>
<td>0:00</td>
<td>2</td>
<td>(Resources)</td>
</tr>
<tr>
<td>790290</td>
<td>skylake</td>
<td>Test2</td>
<td>abc123</td>
<td>R</td>
<td>27:56:10</td>
<td>2</td>
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</table>
```
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: 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`.

  ```bash
  #!/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`.

```bash
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#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=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`.

  ```bash
  #!/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: 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
...`
Serial jobs requiring large memory, or OpenMP codes.

```bash
#!/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
...
```
Serial jobs requiring large memory, or OpenMP codes.

```bash
#!/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.

```bash
#!/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
...
Serial jobs requiring large memory, or OpenMP codes.

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

```bash
#!/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

Outlet 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.

```bash
#!/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.

```bash
#!/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).
Parallel job across multiple nodes.

```bash
#!/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.

```bash
#!/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.

```bash
#!/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).
Parallel jobs using both MPI and OpenMP.

```bash
#!/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.

```bash
#!/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 5 - Submitting Jobs.
Job Submission: High Throughput Jobs

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

```bash
#!/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 5 - Submitting Jobs.
Job Submission: High Throughput Jobs

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

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

# Exercise 5 - 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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...
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srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 5 - 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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...
cd directory_for_job1
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...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 5 - Submitting Jobs.
Job Submission: High Throughput Jobs

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

```bash
#!/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 5 - Submitting Jobs.
Job Submission: Interactive

- Compute nodes are accessible via SSH while you have a job running on them.
- Alternatively, submit an interactive job:
  ```
  sinter -A TRAINING-CPU -N1 -n8 -t 2:0:0
  ```
- Within the window (screen session):
  - Launches a shell on the first node (when the job starts).
  - Graphical applications should display correctly (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.
  - SLURM-aware MPI will do this automatically.
Compute nodes are accessible via SSH while you have a job running on them.

Alternatively, submit an interactive job:
```
sintr -A TRAINING-CPU -N1 -n8 -t 2:0:0
```

Within the window (screen session):
* Launches a shell on the first node (when the job starts).
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Compute nodes are accessible via SSH while you have a job running on them.

Alternatively, submit an interactive job:

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- `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](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

<table>
<thead>
<tr>
<th>JOBID</th>
<th>PARTITION</th>
<th>NAME</th>
<th>USER</th>
<th>ST</th>
<th>TIME</th>
<th>NODES</th>
<th>Nodelist(Reason)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>hpl</td>
<td>abc123</td>
<td>R</td>
<td>0:06</td>
<td>1</td>
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</tr>
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<td>0:06</td>
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</tbody>
</table>

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

- [http://slurm.schedmd.com/job_array.html](http://slurm.schedmd.com/job_array.html)
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- Each job in the array has the same initial options.
- SLURM

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

```
[abc123@login-e-1]$ squeue -u abc123

<table>
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i.e. `{SLURM_ARRAY_JOB_ID}` _`{SLURM_ARRAY_TASK_ID}`

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.
Job Submission: Array Jobs

- [link](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=1,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

```
[abc123@login-e-1]$ squeue -u abc123

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791609_1, 791609_3, 791609_5, 791609_7
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i.e. `{$SLURM_ARRAY_JOB_ID}``${$SLURM_ARRAY_TASK_ID}`

$SLURM_ARRAY_JOB_ID = $SLURM_JOBID for the first element.
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[abc123@login-e-1]$ sbatch --array=1,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

```
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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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```
[abc123@login-e-1]$ sbatch --array=1,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609
```

```
[abc123@login-e-1]$ squeue -u abc123

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791609_1, 791609_3, 791609_5, 791609_7
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i.e. `{$SLURM_ARRAY_JOB_ID}_{$SLURM_ARRAY_TASK_ID}`

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[abc123@login-e-1]$ sbatch --array=1,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609
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[abc123@login-e-1]$ squeue -u abc123

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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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```bash
[abc123@login-e-1]$ sbatch --array=1,3,5,7 -A TRAINING-CPU submit_script
Submitted batch job 791609

[abc123@login-e-1]$ squeue -u abc123

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```

791609_1, 791609_3, 791609_5, 791609_7

i.e. `$$\{\text{SLURM ARRAY JOB ID}\}$$_{\{\text{SLURM ARRAY TASK ID}\}}$`

SLURM ARRAY JOB ID = SLURM JOBID for the first element.
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.
Updates can be applied to specific array elements using
${\text{SLURM ARRAY JOB ID}}_n{\text{SLURM ARRAY TASK ID}}$

Alternatively operate on the entire array via
${\text{SLURM ARRAY JOB ID}}$.

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.
  - `sprio -j jobid`

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

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Wait Times

- 36 hour job walltimes are permitted.
- This sets the timescale at busy times \((without\ backfilling)\).
- Use backfilling when possible.
- Short (1 hour or less) jobs have higher throughput.
Wait Times

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Wait Times

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- This sets the timescale at busy times (without backfilling).
- Use backfilling when possible.
- Short (1 hour or less) jobs have higher throughput.
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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Checkpointing

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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.