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.

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/)

20th June 2019 / UIS Training

UIS: Research Computing Services

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.
Plan of the Course

Part 1: Basics
Part 2: Research Computing Services HPC
Part 3: Using HPC

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
  https://www.training.cam.ac.uk/ucs/Course/ucs-scriptsci

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).
- Please check your MCS workstation is booted into Ubuntu Linux, and logged in, ask if you need help with this.
- PDFs of the course notes and the exercises can be found in your MCS filespace.

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:
  https://help.uis.cam.ac.uk/service/security/stay-safe-online/malware
- Don’t share accounts (this is against the rules, and anyone can get their own).
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  
  - \( N \) is the number of CPUs.
Basics: Amdahl’s Law

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.

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.

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).

If you are using lots of R or python, you are probably high throughput, and possibly data intensive or compute intensive.
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.

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.

Larger computers have multiple sockets (each with their own local memory).

A supercomputer aggregates contemporary CPUs and memory to obtain increased computing power.

Usually today these are clusters.

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

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.

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.
  - Or simply use the memory accompanying the remaining CPUs.
  - Can replicate this across multiple nodes.

- 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.

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.
  - Parallel code may use pthreads/OpenMP/MPI within a node, or MPI across multiple nodes.
  - Serial code uses a single CPU and the memory of one node, but may be copied across many nodes.
Early History: EDSAC (1949–1958)

- **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.”

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.
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)


**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).

**Pascal**

- Each compute node:
  - 4x NVIDIA P100 GPUs
  - 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).

**KNL (Intel Phi)**

- Each compute node:
  - 64 cores, Intel Phi 7210256 CPUs
  - 96 GB RAM
  - 100 Gb/sec Omni-Path
  - 342 compute nodes.
  - Shared login nodes with Skylake.

**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.
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

Using HPC: Connecting to the RCS Clusters

- SSH secure protocol only.
  - Supports login, file transfer, remote desktop...
- SSH access is allowed from anywhere.
  - Fail2Ban will ban repeatedly failing clients for 20 minutes.
- Policies for other clusters may differ.
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 (provides an application environment similar to Linux)
  http://cygwin.com/install.html
  Includes X server for displaying graphical applications running remotely.
- MobaXterm
  http://mobaxterm.mobatek.net/

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: 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

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:HsiY1Oe0M8tS6JwR76PeQQA/VB7r8675BzG5OYQ4h34.
  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.
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.

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).

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.

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.

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

Filesystems: Quotas

- quota
  - 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   Used  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: 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.

### 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/lib/ibd/2017.4
  3) turbovnc/2.0.1 11) intel/lib/tbb/2017.4
  4) vgl/2.5.1/64 12) intel/lib/ipp/2017.4
  5) singularity/current 13) intel/lib/daal/2017.4
  6) rhel7/global 14) intel/lib/sif/2017.4
  7) intel/compilers/2017.4 15) rhel7/default-peta4
  8) intel/xk1/2017.4
  ```

- **Available:**
  ```
  module av
  ```

**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**

- **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 turbo vnc singularity
  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)

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

GCC: gcc, g++, gfortran

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

PGI: pgcc, pgCC, pgf90

```bash
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

- 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.
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:

  ```bash
  [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:

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

Job Submission: Monitor Job

- Examine a particular job:

  ```bash
  [abc123@login-e-1]$ scontrol show job=790290
  ```
Job Submission: Accounting Commands

▶ How many core hours available do I have?

```
mybalance
```

<table>
<thead>
<tr>
<th>User</th>
<th>Usage</th>
<th>Account</th>
<th>Usage</th>
<th>Account Limit Available (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sjr20</td>
<td>3</td>
<td>SUPPORT-CPU</td>
<td>2,929</td>
<td>22,425,600 22,422,671</td>
</tr>
<tr>
<td>sjr20</td>
<td>0</td>
<td>SUPPORT-CPU</td>
<td>0</td>
<td>87,600 87,600</td>
</tr>
</tbody>
</table>

▶ How many core hours does some other project or user have?

```
gbalance -p SUPPORT-CPU
```

<table>
<thead>
<tr>
<th>User</th>
<th>Usage</th>
<th>Account</th>
<th>Usage</th>
<th>Account Limit Available (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>pfb29</td>
<td>2,925</td>
<td>SUPPORT-CPU</td>
<td>2,929</td>
<td>22,425,600 22,422,671</td>
</tr>
<tr>
<td>sjr20</td>
<td>3</td>
<td>SUPPORT-CPU</td>
<td>2,929</td>
<td>22,425,600 22,422,671</td>
</tr>
</tbody>
</table>

(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"
```

<table>
<thead>
<tr>
<th>JobID</th>
<th>User</th>
<th>Account</th>
<th>JobName</th>
<th>Partition</th>
<th>End Time</th>
<th>Exit Code</th>
<th>State</th>
<th>CompHrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>263</td>
<td>xyz10</td>
<td>support-c+ _interact+</td>
<td>skylake</td>
<td>2018-04-18T19:44:40</td>
<td>0:0</td>
<td>TIMEOUT</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>264</td>
<td>xyz10</td>
<td>support-c+ _interact+</td>
<td>skylake</td>
<td>2018-04-18T19:48:07</td>
<td>0:0</td>
<td>CANCELLED</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>275</td>
<td>xyz10</td>
<td>support-c+ _interact+</td>
<td>skylake</td>
<td>Unknown</td>
<td>0:0</td>
<td>RUNNING</td>
<td>0.3</td>
<td></td>
</tr>
</tbody>
</table>

... (Output truncated for brevity)

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=116
#! 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 cpu16 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 --tasks=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=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: 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).

---

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).

---

Job Submission: High Throughput Jobs

- Multiple serial jobs across multiple nodes.
  
  ```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
  ```

- Use `srun` to launch tasks (job steps) within a job.

---

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:
  ```bash
  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.
  * SLURM-aware MPI will do this automatically.

Job Submission: Array Jobs

- http://slurm.schedmd.com/job_array.html
- Used for submitting and managing large sets of similar jobs.
- Each job in the array has the same initial options.
- SLURM

```bash
$[abc123@login-e-1]$ sbatch --array=1-7:21,3,5,7 -A TRAINING-CPU submit_script
```
Submitted batch job 791609

```bash
$[abc123@login-e-1]$ 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>791609_1</td>
<td>skylake</td>
<td>hpl</td>
<td>abc123</td>
<td>R</td>
<td>0:06</td>
<td>1</td>
<td>cpu-a-6</td>
</tr>
<tr>
<td>791609_3</td>
<td>skylake</td>
<td>hpl</td>
<td>abc123</td>
<td>R</td>
<td>0:06</td>
<td>1</td>
<td>cpu-a-16</td>
</tr>
<tr>
<td>791609_5</td>
<td>skylake</td>
<td>hpl</td>
<td>abc123</td>
<td>R</td>
<td>0:06</td>
<td>1</td>
<td>cpu-a-7</td>
</tr>
<tr>
<td>791609_7</td>
<td>skylake</td>
<td>hpl</td>
<td>abc123</td>
<td>R</td>
<td>0:06</td>
<td>1</td>
<td>cpu-a-7</td>
</tr>
</tbody>
</table>

i.e. ```

```bash
$ \{SLURM_ARRAY_JOB_ID\}.$\{SLURM_ARRAY_TASK_ID\}
```
SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

Job Submission: Array Jobs (ctd)

- Updates can be applied to specific array elements using
  ```bash
  $\{SLURM_ARRAY_JOB_ID\}.$\{SLURM_ARRAY_TASK_ID\}
  ```
- Alternatively operate on the entire array via
  ```bash
  $\{SLURM_ARRAY_JOB_ID\}.
  ```
- Some commands still require the SLURM_JOB_ID (sacct, sreport, sshare, sstat and a few others).
- Exercise 9 - Array Jobs.

Scheduling

- SLURM scheduling is multifactor:
  - QoS — payer or non-payer?
  - Age — how long has the job waited?
  - Fair Share — how much recent usage?
    
    | Don’t cancel jobs that seem to wait too long. | 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.
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.

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:
  
  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.