uc-cmyk

An Introduction to High Performance Computing on the CSD3 Cluster

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

Welcome

- Paul Sumption — Research Computing Technical Liaison
- Jeffrey Salmond — Research Software Engineering Team
- Course files can be downloaded from: `www.csd3.cam.ac.uk`
- Please ask questions and let us know if you need assistance.

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Plan of the Course

Part 1: Basics

Part 2: HPC Facilities

Part 2: Using HPC

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11:30-11:45	Break
13:00-14:00	LUNCH
15:30-15:45	Break
16:30	CLOSE

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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):

$$S(N) = \frac{1}{\left(1 - p + \frac{p}{N}\right)}$$

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.

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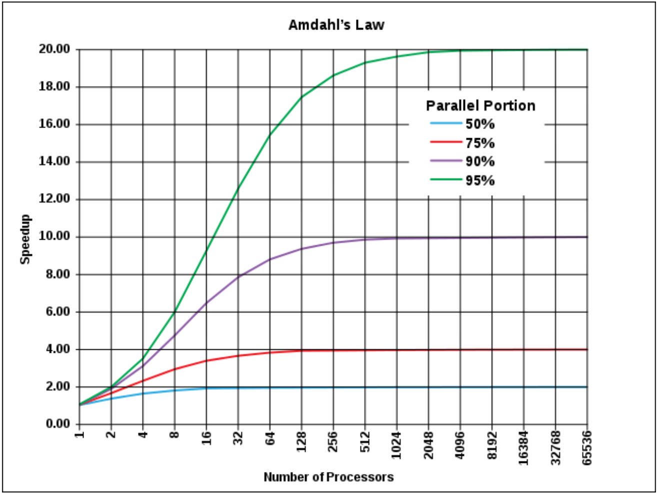

http://en.wikipedia.org/wiki/File:AmdahlsLaw.svg

The Bottom Line

- Parallelisation requires effort:
  - There are libraries to help (e.g. OpenMP, MPI).
  - First optimise performance on one CPU, then make p as large as possible.
- The scaling limit: eventually using more CPUs becomes detrimental instead of helpful.

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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 -
- Hadoop/MapReduce
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Basics: High Throughput

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- 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
- Compute intensive capable $\not\Leftarrow$ high throughput capable

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Basics: Memory Intensive Problems

- Require aggregation of large memory into a single system image (i.e. a single computer running Linux).
- Technically more challenging to build machines (very fast, low latency interconnection between all CPUs and all memory).
- Coding/porting easier (memory appears seamless).
- Optimisation harder (memory is actually highly nonuniform).
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- Nowadays, similar complexity inside single commodity servers.

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Basics: Inside a Modern Computer

- Today's commodity servers already aggregate both CPUs and memory to make a single system image in a single box.
- Even small computers now have multiple CPU cores per socket
- Larger computers have multiple sockets (each with local memory): all CPU cores (unequally) share the node memory

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  with Non-Uniform Memory Architecture (NUMA)
  but users still see a single computer (single system image).

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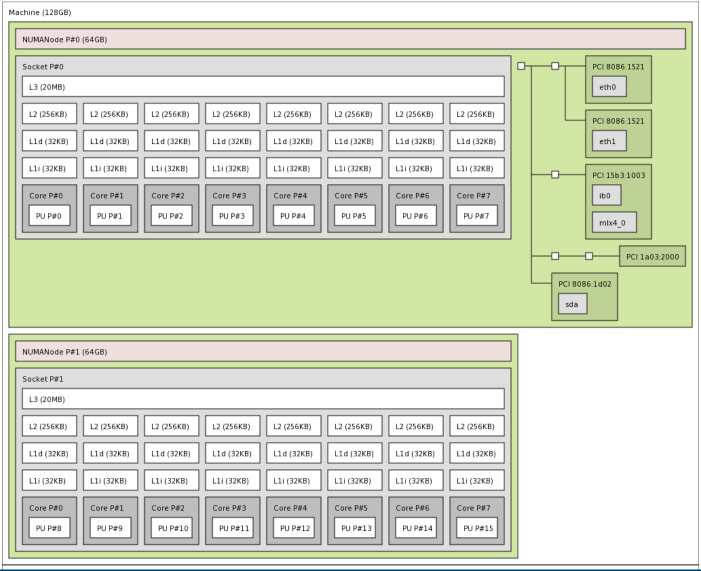

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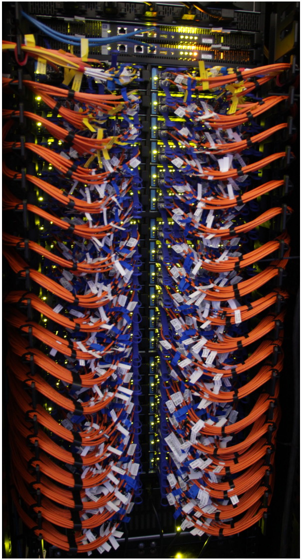
2. Connect the nodes with one or more networks. E.g.

   Gbit Ethernet: 100 MB/sec

   Omni-Path: 10 GB/sec

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



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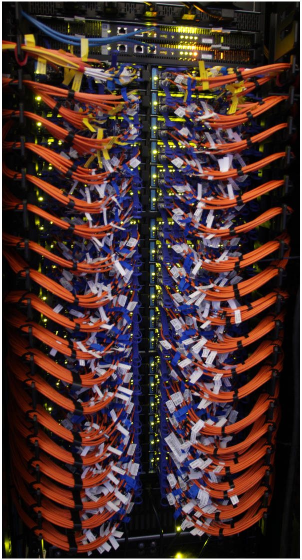

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3. Logically bind the nodes
   - Clusters consist of distinct nodes (i.e. separate Linux computers) on common private network(s) and controlled centrally.
     - Private networks allow CPUs in different nodes to communicate.
     - Clusters are distributed 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.
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Part II: **HPC Facilities**

Minerva

- Each compute node:
  - 2x16 cores, Intel Skylake 2.6 GHz
  - 192 GB RAM
  - 100 Gb/sec Omni-Path
- 16 compute nodes
- 1 high-memory login/head node (minerva-login1.npl.co.uk), 768 GB RAM.
- 1 GPU node, 2 $\times$ NVIDIA P100 GPU, 192 GB RAM.

Minerva

- Each compute node:
  - 32 CPUs
  - 6 GB per CPU
  - 10 GB/sec (for MPI and storage)
- 16 compute nodes
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CSD3 - University of Cambridge

- Cambridge Service for Data Driven Discovery
- Peta4 — Intel CPU cluster
- Wilkes2 — NVIDIA GPU cluster
- Hadoop-based data analytic platform
- Burst buffer
- Some NPL users through CORE.

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CSD3 - University of Cambridge

- Cambridge Service for Data Driven Discovery
- Peta4 — Intel CPU cluster
- Wilkes2 — NVIDIA GPU cluster
- Hadoop-based data analytic platform
- Burst buffer
- Some NPL users through CORE.

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Peta4-Skylake

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

Peta4-Skylake

- Each compute node:
  - 32 CPUs
  - 6 GB or 12 GB per CPU
  - 10 GB/sec (for MPI and storage)
- 768 compute nodes
- 8 login nodes (login-cpu.hpc.cam.ac.uk)

Coprocessors — GPUs etc

- CPUs are general purpose
- Some types of parallel workload fit vector processing well:
  - Single Instruction, Multiple Data (SIMD)
  - *Think pixels on a screen*
  - GPUs specialise in this type of work
  - Also competitor many-core architectures such as the Intel Phi

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Wilkes2-GPU

- Each compute node:
  - $4 \times$ 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).

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Wilkes2-GPU

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

Peta4-KNL (Intel Phi)

- Each compute node:
  - 64 cores, Intel Phi 7210
  - 96 GB RAM
  - 100 Gb/sec Omni-Path
- 342 compute nodes
- Shared login nodes with Peta4-Skylake

Peta4-KNL (Intel Phi)

- Each compute node:
  - 256 CPUs
  - 96 GB RAM
  - 10 GB/sec (for MPI and storage)
- 342 compute nodes
- Shared login nodes with Peta4-Skylake

Cluster Storage

- Minerva uses NFS to share user directories between all cluster nodes (150 TB).
- CSD3 uses the 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.

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Obtaining an Account and Support

- Please contact the NPL IT Service Desk:
  - itservicedesk@npl.co.uk
  - Room F12-CS1
  - Tel. 6000
- Second line support is provided by the Cambridge RCS.

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Part III: **Using HPC**

Using HPC: Connecting

- SSH secure protocol only.

Using HPC: Connecting

- SSH secure protocol only.
  Supports login, file transfer, remote desktop. . .

Connecting: Windows Clients

- putty, pscp, psftp
  http://www.chiark.greenend.org.uk/ sgtatham/putty/download.html
- WinSCP
  http://winscp.net/eng/download.php
- TurboVNC (remote desktop, 3D optional)
  http://sourceforge.net/projects/turbovnc/files/
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  http://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.
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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.
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Connecting: Login

- From graphical clients:
  Host: minerva-login1.npl.co.uk
  Username: **npl\abc123** (your NPL AD account name)
- From Linux/MacOSX/UNIX (or Cygwin):

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

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

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Connecting: First time login

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

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

ECDSA key fingerprint is SHA256:k/eB+LjcAfQW56XCzK9QptT0wVWF7j3a/CPxPRd7+lE.
ECDSA key fingerprint is MD5:18:9a:97:e2:87:4c:07:60:cb:43:46:f2:bb:d8:3d:01.

Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'minerva-login1.npl.co.uk (139.143.201.10)' (ECDSA) to the list of known
hosts.
```

- One should always check the fingerprint before typing "yes".
- Graphical SSH clients *should* ask a similar question.
- Designed to detect fraudulent servers.

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- Exercise 1 - Log into your Minerva account.
- 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/**

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

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

  rsync -av **old_directory**

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

  copies old_directory (and contents) to ~/hpc-work/new_directory/old_directory.

  - Rerun to update or resume after interruption.
  - All transfers are checksummed.
  - For transfers in the opposite direction, place the remote machine as the first argument.
- Exercise 3 - File transfer.

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Connecting: Remote Desktop

- First time starting a remote desktop:

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

You will require a password to access your desktops.

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

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

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

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

Connecting: Remote Desktop

- Remote desktop already running:

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

TigerVNC server sessions:

X DISPLAY #     PROCESS ID
:99             130655
```

- Kill it:

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

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

Connecting: Remote Desktop

- To connect to the desktop from Linux:

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

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

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Connecting: Remote Desktop

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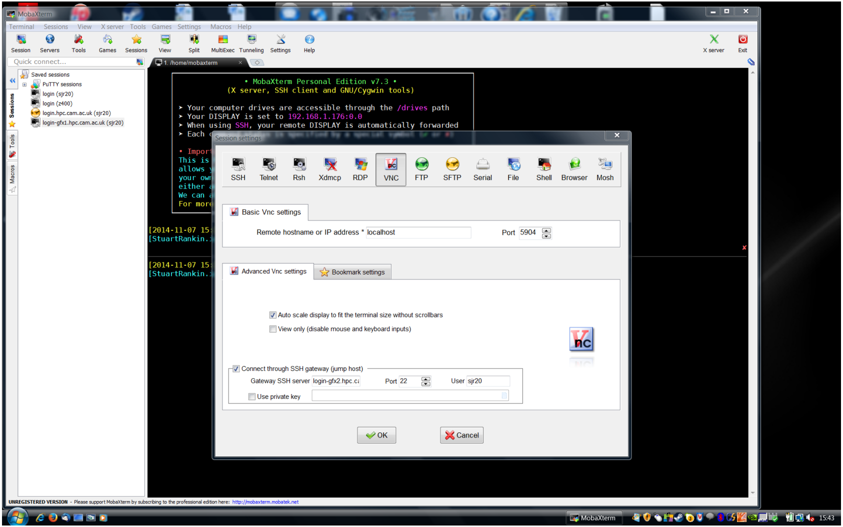
- Exercise 4 - Remote desktop (from Windows)

Connecting: Remote Desktop (MobaXterm)



Using HPC: User Environment

- CentOS Linux 7.4 (Red Hat Enterprise Linux 7.4 rebuild)
  - bash shell
  - Gnome or XFCE4 desktop (if you want)
  - GCC compilers and other development software.
- But you don't need to know that.

Using HPC: User Environment

Red Hat Enterprise Linux 7

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User Environment: Filesystems

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

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Filesystems: Quotas

- quota

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

- Aim to stay below the soft limit (*quota*).
- Once over the soft limit, you have 7 days grace to return below.
- When the grace period expires, or you reach the hard limit (*limit*), no more data can be written.
- It is important to rectify an out of quota condition ASAP.

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Filesystems: Permissions

- Be careful and if unsure, please ask support.
  - Can lead to accidental destruction of your data or account compromise.
- Avoid changing the permissions on your home directory.
  - Files under /home are particularly security sensitive.
  - Easy to break passwordless communication between nodes.

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User Environment: Software

- Free software accompanying Red Hat Enterprise Linux is (or can be) provided.
- Other software (free and non-free) is available via modules.
- Proprietary software currently available includes Matlab and COMSOL.
- New software may be possible to provide on request.
- Self-installed software should be properly licensed.
- *sudo will not work.* (You should be worried if it did.)

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User Environment: Environment Modules

- Modules load or unload additional software packages.
- Some are required and automatically loaded on login.
- Others are optional extras, or possible replacements for other modules.
- Beware unloading default modules in ~/.bashrc.
- Beware overwriting environment variables such as PATH and LD_LIBRARY_PATH in ~/.bashrc. If necessary append or prepend.

User Environment: Environment Modules

- Currently loaded:

```
module list
Currently Loaded Modulefiles:
  1) dot                          3) centos7/global
  2) slurm                        4) centos7/default-basic
```

- Available:

```
module av
```

User Environment: Environment Modules

- Whatis:

```
module whatis openmpi-3.0.0-gcc-4.8.5-n2hvjgm
openmpi-3.0.0-gcc-4.8.5-n2hvjgm: The Open MPI Project is an open source...
```

- Load:

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

- Unload:

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

- Matlab

```
module load matlab/r2018a
```

- Invoking matlab in batch mode:
  matlab -nodisplay -nojvm -nosplash command
  where the file command.m contains your matlab code.
- The current site license contains the Parallel Computing Toolbox.

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User Environment: Environment Modules

- Purge:

```
module purge
```

- Defaults:

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

- Run time environment must match compile time environment.

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User Environment: Compilers

- GCC

```
gcc -O3 -mtune=native code.c -o prog
gfortran -O3 -mtune=native code.f90 -o prog
```

```
module load openmpi-3.0.0-gcc-4.8.5-n2hvjgm
mpicc -O3 -mtune=native mpi_code.c -o mpi_prog
mpif90 -O3 -mtune=native mpi_code.f90 -o mpi_prog
```

- Exercise 5: Modules and Compilers

User Environment: Compilers

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```

- 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.

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Using HPC: Job Submission

- Jobs are submitted from the login node
  — not itself managed by the scheduler.
- Jobs may be either non-interactive (batch) or interactive.
- Batch jobs run a shell script on the first of a list of allocated nodes.
- Interactive jobs provide a command line on the first of a list of allocated nodes.

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Using HPC: Job Submission

- Jobs 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 `--exclusive` to force exclusive node access.
- Template submission scripts are available under ~/job_templates.

Job Submission: Using SLURM

- Prepare a shell script and submit it to SLURM:

```
[abc123@login-a-1]$ sbatch slurm_submission_script
Submitted batch job 790299
```

Job Submission: Show Queue

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

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

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Job Submission: Show Queue

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

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

Job Submission: Show Queue

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

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

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Job Submission: Monitor Job

- Examine a particular job:

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

Job Submission: Cancel Job

- Cancel a particular job:

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

Job Submission: Scripts

- SLURM
  In ~/job_templates, see examples: slurm_submit.skylake.generic, slurm_submit.skylake.matlab.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A NPL-GENERAL-CPU
#! How many whole nodes should be allocated?
#SBATCH --nodes=1
#! How many tasks will there be in total? (<= nodes*32)
#SBATCH --ntasks=1
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

- #SBATCH lines are *structured comments*
  — correspond to sbatch command line options.
- The above job will be given 1 cpu on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

Job Submission: Scripts

- SLURM
  In ~/job_templates, see examples: slurm_submit.skylake.generic, slurm_submit.skylake.matlab.

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#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).

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#SBATCH --ntasks=1
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

- #SBATCH lines are *structured comments*
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Job Submission: Scripts

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  In ~/job_templates, see examples: slurm_submit.skylake.generic, slurm_submit.skylake.matlab.

```
#!/bin/bash
#! Name of the job:
#SBATCH -J myjob
#! Which project should be charged:
#SBATCH -A NPL-GENERAL-CPU
#! How many whole nodes should be allocated?
#SBATCH --nodes=1
#! How many tasks will there be in total? (<= nodes*32)
#SBATCH --ntasks=16
#! How much wallclock time will be required?
#SBATCH --time=02:00:00
#! Select partition:
#SBATCH -p skylake
...
```

- #SBATCH lines are *structured comments*
  — correspond to sbatch command line options.
- The above job will be given 16 cpus on 1 node for 2 hours (by default there is 1 task per node, and 1 cpu per task).

Job Submission: Accounting Commands

- How many core hours available do I have?

```
mybalance

User          Usage |        Account     Usage | Account Limit Available (hours)
---------- --------- + -------------- --------- + ------------- ---------
sjr20             3 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
sjr20             0 |    SUPPORT-GPU         0 |        87,600    87,600
```

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

```
gbalance -p SUPPORT-CPU

User          Usage |        Account     Usage | Account Limit Available (hours)
---------- --------- + -------------- --------- + ------------- ---------

pfb29         2,925 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
sjr20 *           3 |    SUPPORT-CPU     2,929 |    22,425,600 22,422,671
...
(Use -u for user.)
```

- List all jobs charged to a project/user between certain times:

```
gstatement -p NPL-GENERAL-CPU  -u xyz10 -s "2018-04-01-00:00:00" -e "2018-04-30-00:00:00"
       JobID      User    Account    JobName  Partition                 End ExitCode      State  CompHrs
------------ --------- ---------- ---------- ---------- ------------------- -------- ---------- --------
263              xyz10 support-c+ _interact+    skylake 2018-04-18T19:44:40      0:0    TIMEOUT      1.0
264              xyz10 support-c+ _interact+    skylake 2018-04-18T19:48:07      0:0 CANCELLED+      0.1
275              xyz10 support-c+ _interact+    skylake             Unknown      0:0    RUNNING      0.3
...
```

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

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

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

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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
...
```

uc-rev-cmyk

Job Submission: Single Node Jobs

- Serial jobs requiring large memory, or OpenMP codes.

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

uc-rev-cmyk

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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
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export OMP_NUM_THREADS=  # For OpenMP across  cores
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```

uc-rev-cmyk

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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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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
...
```

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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
...
```

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Job Submission: MPI Jobs

- Parallel job across multiple nodes.

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

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64     # i.e.  16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 16 -np 64 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: MPI Jobs

- Parallel job across multiple nodes.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64      # i.e.  16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
mpirun -ppn 16 -np 64 $application $options
...
```

- SLURM-aware MPI launches remote tasks via SLURM.
- The template script uses $SLURM_TASKS_PER_NODE to set PPN.

Job Submission: Hybrid Jobs

- Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64     # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2   # i.e. 2 threads per MPI task.
mpirun -ppn 16 -np 64 $application $options
...
```

- This job uses 128 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: Hybrid Jobs

- Parallel jobs using both MPI and OpenMP.

```
#!/bin/bash
...
#SBATCH --nodes=4
#SBATCH --ntasks=64     # i.e. 16x4 MPI tasks in total.
#SBATCH --cpus-per-task=2
...
export OMP_NUM_THREADS=2   # i.e. 2 threads per MPI task.
mpirun -ppn 16 -np 64 $application $options
...
```

- This job uses 128 CPUs (each MPI task splits into 2 OpenMP threads).

Job Submission: High Throughput Jobs

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

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

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

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 6 - Submitting Jobs.

Job Submission: High Throughput Jobs

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

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 6 - Submitting Jobs.

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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 - Submitting Jobs.

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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 - Submitting Jobs.

Job Submission: High Throughput Jobs

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

```
#!/bin/bash
...
#SBATCH --nodes=2
...
cd directory_for_job1
srun --exclusive -N 1 -n 1 $application $options_for_job1 > output 2> err &
cd directory_for_job2
srun --exclusive -N 1 -n 1 $application $options_for_job2 > output 2> err &
...
cd directory_for_job64
srun --exclusive -N 1 -n 1 $application $options_for_job64 > output 2> err &
wait
```

- Exercise 6 - Submitting Jobs.

Job Submission: Interactive

- Compute nodes are accessible via SSH while you have a job running on them.
- Alternatively, submit an interactive job:

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

- Within the window (screen session):
  - Launches a shell on the first node (when the job starts).
  - Graphical applications should display correctly.
  - Create new shells with ctrl-a c, navigate with ctrl-a n and ctrl-a p.
  - ssh or srun can be used to start processes on any nodes in the job.
  - SLURM-aware MPI will do this automatically.

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  - Launches a shell on the first node (when the job starts).
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  - 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*
- Used for submitting and managing large sets of similar jobs.
- Each job in the array has the same initial options.
- SLURM

```
[abc123@login-a-1]$ sbatch --array=1-7 -A NPL-GENERAL-CPU submit_script
Submitted batch job 791609
```

```
[abc123@login-a-1]$ squeue -u abc123
            JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         791609_1 skylake      hpl    abc123  R       0:06      1 cpu-a-6
         791609_3 skylake      hpl    abc123  R       0:06      1 cpu-a-16
         791609_5 skylake      hpl    abc123  R       0:06      1 cpu-a-7
         791609_7 skylake      hpl    abc123  R       0:06      1 cpu-a-7
```

791609_1, 791609_3, 791609_5, 791609_7

i.e. ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

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

```
[abc123@login-a-1]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         791609_1 skylake      hpl    abc123  R       0:06      1 cpu-a-6
         791609_3 skylake      hpl    abc123  R       0:06      1 cpu-a-16
         791609_5 skylake      hpl    abc123  R       0:06      1 cpu-a-7
         791609_7 skylake      hpl    abc123  R       0:06      1 cpu-a-7
```

791609_1, 791609_3, 791609_5, 791609_7

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```
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Submitted batch job 791609
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          791609_3 skylake      hpl    abc123  R        0:06      1 cpu-a-16
          791609_5 skylake      hpl    abc123  R        0:06      1 cpu-a-7
          791609_7 skylake      hpl    abc123  R        0:06      1 cpu-a-7
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         791609_7 skylake      hpl    abc123  R       0:06      1 cpu-a-7
```

791609_1, 791609_3, 791609_5, 791609_7

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[abc123@login-a-1]$ squeue -u abc123
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
         791609_1 skylake      hpl    abc123  R       0:06      1 cpu-a-6
         791609_3 skylake      hpl    abc123  R       0:06      1 cpu-a-16
         791609_5 skylake      hpl    abc123  R       0:06      1 cpu-a-7
         791609_7 skylake      hpl    abc123  R       0:06      1 cpu-a-7
```

791609_1, 791609_3, 791609_5, 791609_7

i.e. ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}

SLURM_ARRAY_JOB_ID = SLURM_JOBID for the first element.

Job Submission: Array Jobs

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

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

```
[abc123@login-a-1]$ squeue -u abc123
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Job Submission: Array Jobs (ctd)

- Updates can be applied to specific array elements using ${SLURM_ARRAY_JOB_ID}_${SLURM_ARRAY_TASK_ID}
- Alternatively operate on the entire array via ${SLURM_ARRAY_JOB_ID}.
- Some commands still require the SLURM_JOB_ID (sacct, sreport, sshare, sstat and a few others).
- Exercise 7 - Array Jobs.

uc-rev-cmyk

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Scheduling

- SLURM scheduling is multifactor:
  - QoS — payer or non-payer?
  - Age — how long has the job waited?
    Don't cancel jobs that seem to wait too long.
  - Fair Share — how much recent usage?
    Payers with little recent usage receive boost (not implemented yet).
  - sprio -j jobid
- Backfilling
  - Promote lower priority jobs into gaps left by higher priority jobs.
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- 36 hour job walltimes are permitted.
- This sets the timescale at busy times (*without* backfilling).
- Use backfilling when possible.
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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.