Introduction to High Performance Computing (HPC) – Session 2

using the "**C**omputational **S**hared **F**acility" (CSF)

Research Platforms, Research IT, IT Services

Course materials / Slides available from:
https://ri.itservices.manchester.ac.uk/course/rcsf/

CSF online documentation
https://ri.itservices.manchester.ac.uk/csf3/

Contact Research Platforms via the Connect Portal
https://ri.itservices.manchester.ac.uk/csf3/help/

Recap slide skipped in training room

https://ri.itservices.manchester.ac.uk/course/rcsf/

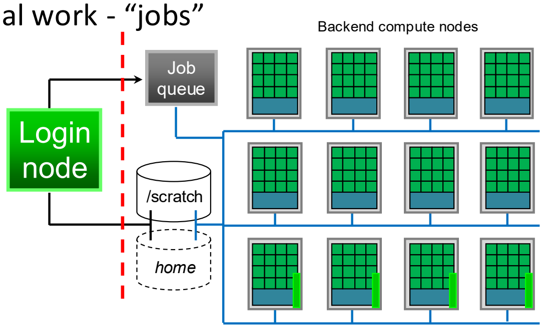
Housekeeping

- Please let me know if you're leaving
  - Morning: Session one: 10am – 12:30pm (practicals 1, 2, & 3)
  - Afternoon: Session two: 1:30pm - 4pm (practicals 4 & 5)
- 1-to-1 help is available if needed during exercises. We'll describe how this works before the first one.
- Please give feedback on this course
  - Quick form at https://goo.gl/forms/zfZyTLw4DDaySnCF3 (choose "*Introduction to HPC (Using CSF)*")
  - Feedback is important to help us improve our courses
  - Records your attendance on the course

Recap slide skipped in training room

Jobs, Jobscripts and the Batch System

- We want to do computational work - "jobs"



- You decide:
  - Which program(s) to run
  - Which resources it needs (#cores, CPU type, memory, GPU?)
  - How much time the job will need to complete its work
  - Which of your folders ("directory") to run the job in
- You'll put these requirements into a *jobscript* file
- Then submit your *jobscript* to the batch system ("Slurm")
- Slurm decides *when* the job runs and on which compute node(s). It ensures you get all of your requested resources.

Recap slide skipped in training room

A simple Jobscript – *Serial* (1 core)

`#!` on first line only (a special line)

First line indicates we use the *bash* scripting language to write our jobscript.

`#SBATCH` indicates a **batch system parameter** to specify our job requirements. We'll use various combinations of these.

myjob.txt

```
#!/bin/bash --login

#SBATCH -p serial
#SBATCH -n 1
#SBATCH -t 5

# Let's do some work
date
hostname
sleep 120
date
```

`-p` (`--partition=`) think of this as the queue, for serial (1-core) jobs in this case.

`-n` (`--ntasks=`) number of cores, which is 1 by default for serial jobs (**optional**).

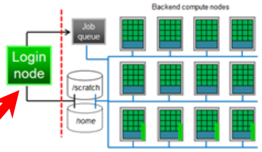
`#` lines are just comments - anything on the line after it will be ignored.

`-t` (`--time=`) maximum "wallclock" time the job is allowed to run for. Various formats. 5 is 5 minutes. 4-0 would be 4 days (0 hours).

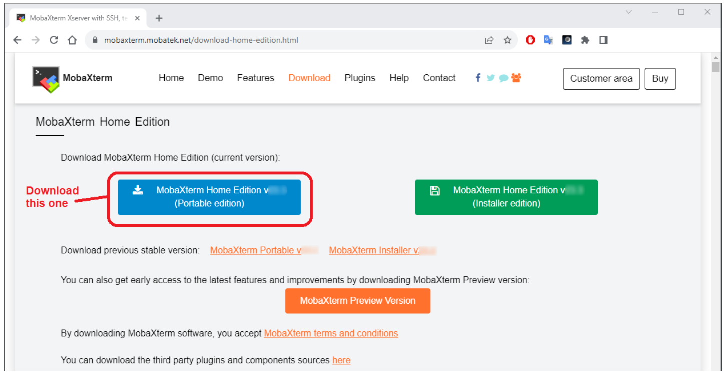
Actual Linux commands we run in our job. They will execute on a compute node.

Recap slide skipped in training room

Connect to CSF from Windows



- Access the CSF from a PC / laptop using an SSH (**S**ecure **Sh**ell) app
  - Sometimes called a "terminal".
  - There's no web-site or other fancy GUI on the CSF – use the "command-line".
- **Windows users** need to install a free *terminal* app called MobaXterm
- https://mobaxterm.mobatek.net/download-home-edition.html
  the Home edition (portable edition) does *not require* Administrator rights - just *extract* the small .zip file in your P-Drive or USB stick for example.



MobaXterm Home Edition

Download MobaXterm Home Edition (current version):

Download this one

MobaXterm Home Edition v[redacted] (Portable edition)

MobaXterm Home Edition v[redacted] (Installer edition)

Download previous stable version: MobaXterm Portable v[redacted] MobaXterm Installer v[redacted]

You can also get early access to the latest features and improvements by downloading MobaXterm Preview version:

MobaXterm Preview Version

By downloading MobaXterm software, you accept MobaXterm terms and conditions

You can download the third party plugins and components sources here

1. Download using the blue box.
2. Once downloaded, *right-click* on the .zip file and select:

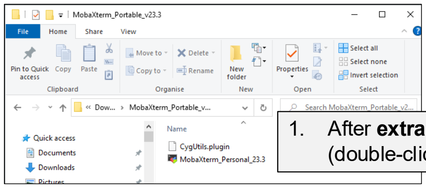
   "Extract all ..."

   This will *unpack* the .zip file to a folder.

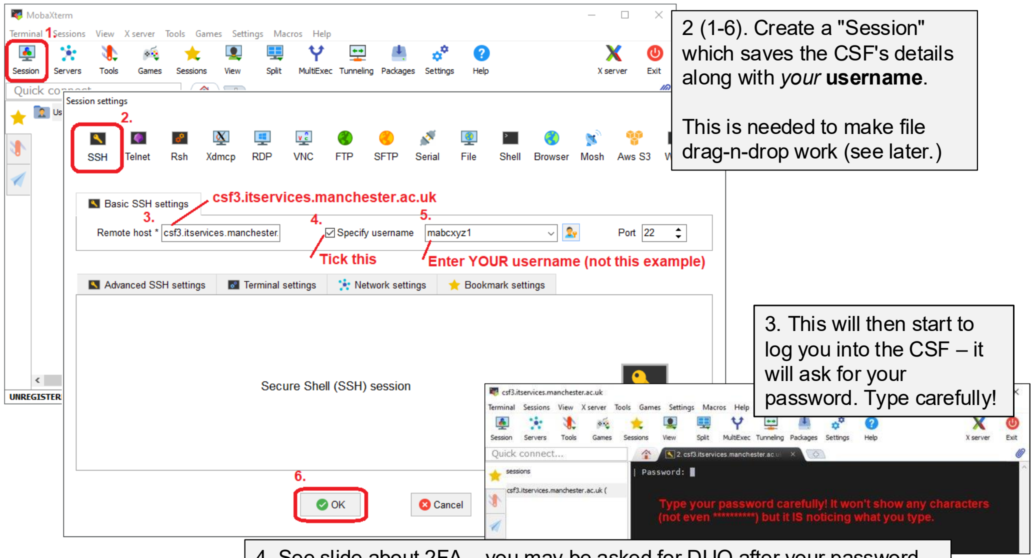
Recap slide skipped in training room

MobaXterm "Session"

(username saved in the session setup)



1. After **extracting** the .zip file, start MobaXterm_Personal_*xy.z* (double-click on the icon)



1. Session

2. SSH

3. csf3.itservices.manchester.ac.uk

Remote host * csf3.itservices.manchester

4. ☑ Specify username

Tick this

5. mabcxyz1

Enter YOUR username (not this example)

Port 22

6. OK

2 (1-6). Create a "Session" which saves the CSF's details along with *your* **username**.

This is needed to make file drag-n-drop work (see later.)

3. This will then start to log you into the CSF – it will ask for your password. Type carefully!

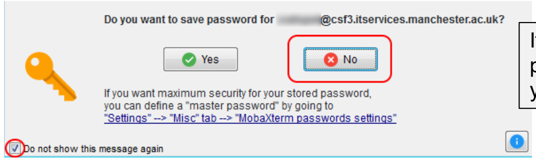
Password:

Type your password carefully! It won't show any characters (not even *********) but it IS noticing what you type.

4. See slide about 2FA – you may be asked for DUO after your password

---

Recap slide skipped in training room



Do you want to save password for [redacted]@csf3.itservices.manchester.ac.uk?

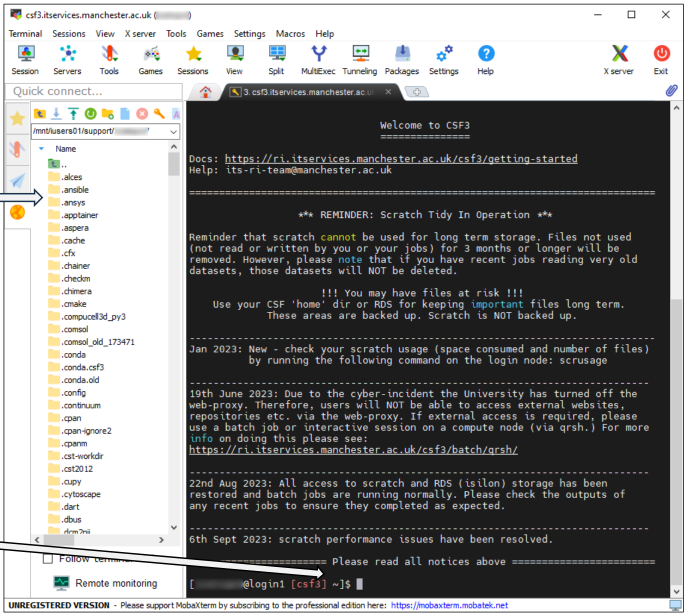
Yes

No

If you want maximum security for your stored password, you can define a "master password" by going to "Settings" --> "Misc" tab --> "MobaXterm passwords settings"

☑ Do not show this message again

If asked to save your password, we recommend you say "No", for security.



```
                    Welcome to CSF3
                    ===============

Docs: https://ri.itservices.manchester.ac.uk/csf3/getting-started
Help: its-ri-team@manchester.ac.uk

===============================================================================

            *** REMINDER: Scratch Tidy In Operation ***

Reminder that scratch cannot be used for long term storage. Files not used
(not read or written by you or your jobs) for 3 months or longer will be
removed. However, please note that if you have recent jobs reading very old
datasets, those datasets will NOT be deleted.

                 !!! You may have files at risk !!!
    Use your CSF 'home' dir or RDS for keeping important files long term.
         These areas are backed up. Scratch is NOT backed up.

------------------------------------------------------------------------------
Jan 2023: New - check your scratch usage (space consumed and number of files)
          by running the following command on the login node: scrusage

------------------------------------------------------------------------------
19th June 2023: Due to the cyber-incident the University has turned off the
web-proxy. Therefore, users will NOT be able to access external websites,
repositories etc. via the web-proxy. If external access is required, please
use a batch job or interactive session on a compute node (via qrsh.) For more
info on doing this please see:
https://ri.itservices.manchester.ac.uk/csf3/batch/qrsh/

------------------------------------------------------------------------------
22nd Aug 2023: All access to scratch and RDS (isilon) storage has been
restored and batch jobs are running normally. Please check the outputs of
any recent jobs to ensure they completed as expected.

------------------------------------------------------------------------------
6th Sept 2023: scratch performance issues have been resolved.

=================== Please read all notices above ===========================

[[redacted]@login1 [csf3] ~]$
```

Drag-n-drop file browser for upload / download

(new users won't have as many items in the list!)

We're on (one of) the CSF login nodes. Any commands you use will be typed "at the prompt", which shows your username and current directory (folder.)

Recap slide skipped in training room

Connecting from Linux / Mac

- From MacOS using a *Terminal* window (after installing Xquartz)

  ```
  ssh -Y username@csf3.itservices.manchester.ac.uk
  ```

  UPPERcase Y

  Central IT Services username.
  Answer 'Yes' to continue *if* asked.
  Enter central IT password when asked (same as for email)

- From Linux using a Terminal window

  ```
  ssh -X username@csf3.itservices.manchester.ac.uk
  ```

  UPPERcase X

  Central IT Services username.
  Answer 'Yes' to continue *if* asked.
  Enter central IT password when asked (same as for email)

- Finished using CSF? Log out with: `logout` or `exit`

Training room presentation begins here

https://ri.itservices.manchester.ac.uk/course/rcsf/

https://ri.itservices.manchester.ac.uk/csf3

ACCESSING APPLICATION S/W

Modules

Access to Application Software

- Lots of different pieces of software installed
  - Many different applications
  - Different *versions* of an application
  - Need to ensure job knows where an app is installed
    - Try `echo $PATH` to see all directories the CSF will look in
- Use "*modules*" to set up *environment* for software
  - In your jobscript, add some `module` commands
  - Sets up all necessary *environment variables*
  - Apps use these *env vars* to get various settings
  - Can also run `module` commands on the login node (e.g., to check what apps are available)

Module Commands

- `module avail` – lists all available modules
- `module search` *`keyword`* – lists all modules with *keyword* in their name
- `module list` – lists currently loaded modules
- `module load` *`modulename`* – loads module
- `module unload` *`modulename`* – unloads module
- `module purge` – **unload all modules**
- `man module` – man pages for the module command
- Examples:

```
module load apps/binapps/matlab/R2024b
module load apps/intel-19.1/amber/20-bf12-at21-bf12
module load apps/gcc/R/4.4.1
module unload apps/binapps/starccm/18.02-double
module help compilers/intel/19.1.2
module load tools/gcc/cmake/3.28.6
```

- See documentation for more info
  https://ri.itservices.manchester.ac.uk/csf3/software/modules/

Modulefile settings

- What "settings" do modulefiles actually make?
  - Depends on the application (eg the installation instructions)
- Try the following commands on the login node:

```
which matlab
/usr/bin/which: no matlab in(/opt/site/sge………

module load apps/binapps/matlab/R2024b

which matlab
/opt/apps/apps/binapps/matlab/R2024b/bin/matlab
```

- This shows that the modulefile made the matlab 2024b installation available.
- A job can do this to run that version of matlab.
- If interested, to see all of the settings that a modulefile will make:

```
module show apps/binapps/matlab/R2024b
```

But the idea is you don't need to know the settings - modulefiles take care of the details so you can concentrate on what your jobs actually *do* with the application.

- See documentation for more info
  https://ri.itservices.manchester.ac.uk/csf3/software/modules/

Loading modulefiles:
On login nodes OR in the jobscript

Inherit from the login node (not recommended)

Jobs in Slurm will inherit any modulefile settings (i.e. loaded modules) from the login node at the point when you *submit* (sbatch) the job.

```
# On the login node:
module load apps/R/4.4.1
sbatch myjob.txt
```

myjob.txt

```
#!/bin/bash --login
#SBATCH -p serial
#SBATCH -t 2-0



# We'll use whichever version
# of R was loaded on the login
# node. Which version of R did
# I use 6 months ago???
R CMD BATCH myscr.R
```

Only in the jobscript (recommended!)

```
# On the login node:
sbatch myjob.txt
```

myjob.txt

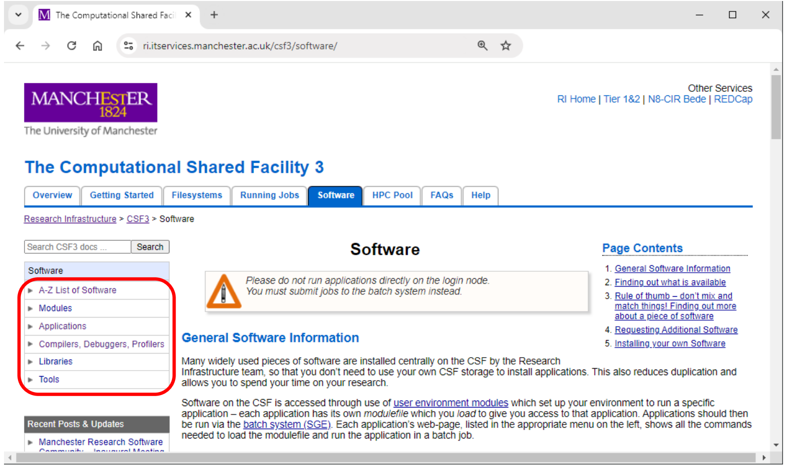
```
#!/bin/bash --login
#SBATCH -p serial
#SBATCH -t 2-0

# Start with a clean env then
# load module inside jobscript
module purge
module load apps/R/4.4.1

# We know the version of R!
R CMD BATCH myscr.R
```

Which Modulefiles to Load

- How do I know which modulefile to load for a particular app?
  - https://ri.itservices.manchester.ac.uk/csf3/software/



The Computational Shared Facility 3

Research Infrastructure > CSF3 > Software

Software

Please do not run applications directly on the login node.
You must submit jobs to the batch system instead.

Page Contents

1. General Software Information
2. Finding out what is available
3. Rule of thumb – don't mix and match things! Finding out more about a piece of software
4. Requesting Additional Software
5. Installing your own Software

General Software Information

Many widely used pieces of software are installed centrally on the CSF by the Research Infrastructure team, so that you don't need to use your own CSF storage to install applications. This also reduces duplication and allows you to spend your time on your research.

Software on the CSF is accessed through use of user environment modules which set up your environment to run a specific application – each application has its own *modulefile* which you *load* to give you access to that application. Applications should then be run via the batch system (SGE). Each application's web-page, listed in the appropriate menu on the left, shows all the commands needed to load the modulefile and run the application in a batch job.

A note about our documentation

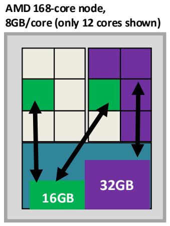
- Over the summer we change the batch system from SGE to Slurm
  - SGE uses #$ as the jobscript *sentinel*
  - Slurm uses #SBATCH (as we've seen earlier)
  - Our applications documentation is being updated to convert example jobscripts from SGE to Slurm
  - If you see #$ in our documentation, you'll need to write the equivalent Slurm jobscript (using #SBATCH).
  - See our SGE-to-Slurm guide, which shows how #$ flags map to #SBATCH flags https://ri.itservices.manchester.ac.uk/csf3/batch-slurm/sge-to-slurm/

PARALLEL COMPUTING

Background

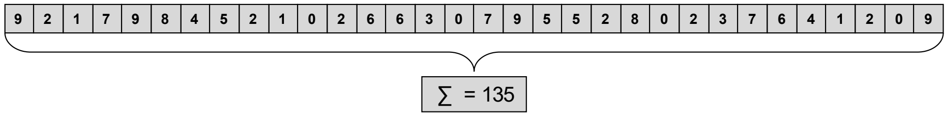
Motivations for Parallel Computing

- CSF compute nodes have multiple CPU cores (32, 168)
- Many apps can use multiple cores to speed up the computation
  - Split the "work" over multiple CPU cores
    - Each core does a small(er) part of the computation, all in parallel
    - "Data parallelism" (same instructions run on each portion of "data")
  - May need to *combine* partial results together at end
  - Should get the final result quicker
    - Ideally *N* cores giving results *N* times quicker
- Also provides access to more memory
  - Each core has access to 8GB RAM (AMD nodes)
    - Ideally *M* cores for *M* times larger problem
- Both of the above!
- Another "parallel" method: High *Throughput* Computing
  - Multiple instances of an app with different params or data

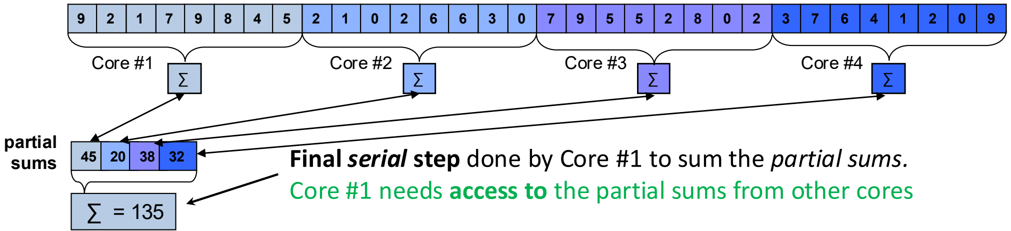


Simple example: sum a list of numbers

- Could do this example manually with 4 volunteers
- 1-core: sum = sum + number_i (for i = 1 to N)
  - Let's say it takes T_1 seconds to complete



- 4-cores: Each core sums a smaller list of numbers



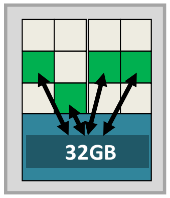
Final *serial* step done by Core #1 to sum the *partial sums.*

Core #1 needs **access to** the partial sums from other cores

  - Takes $T_4 \approx T_1/4 + T_{serial}$ seconds to complete ($< T_1$)

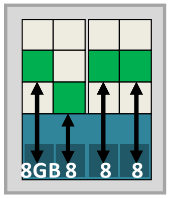
Parallel Job Type #1 - single node

- A program runs on *multiple CPU cores* of **one** compute node
- Two common techniques used by apps:
  - Typically, one copy of the program runs
    - *"Shared memory"* (all cores see same memory)
    - Cores synchronize access to shared memory (data)
    - Look for "OpenMP" / "multi-threaded" / "Java threads" … in an application's docs



Shared Memory

  - Or coordinated copies of the program run, each communicating with each other
    - *"Distributed memory"* (each core has its own mem)
    - They communicate to share data, results
    - Look for "MPI" or "message passing" in the application's docs

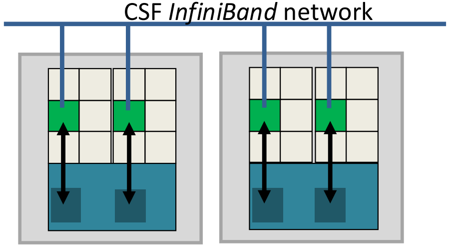


Distributed Memory

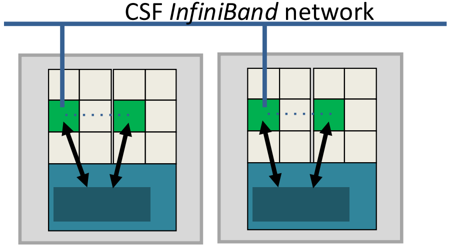
- **Your app must have been written to use one (or both) of the above parallel techniques!**
- We'll run this "single compute-node" type of job today

Parallel Job Type #2 - multi-node

- Running a program over *several* compute nodes (and the many cores on those nodes)
  - Must be the "MPI" / "message passing" style of app (see above)
  - Uses *more* cores than available in a *single* compute node
    - On CSF we require you to use *all* of the cores in *each* compute node!
  - They communicate to share data, results etc (as before)
    - Over the fast internal *InfiniBand* network
    - Possibly via shared memory as before, if on same compute node
- **Your app must have been written to support this!**
- We will *not* run this type of job today (see the HPC Pool.)



Distributed Memory



Hybrid Memory (often MPI+OpenMP)

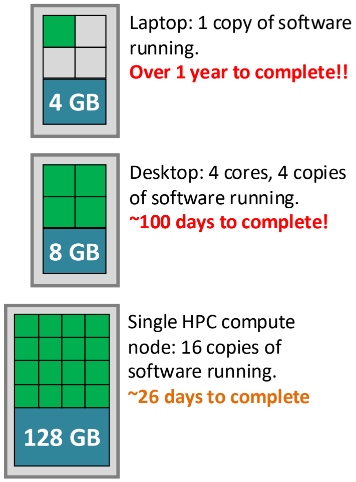
Note: the diagrams only show a few cores in use for simplicity. On the CSF you must use *all* cores in *each* node.

Parallel Job Type #3 - High Throughput Computing (HTC)

- Lots of *independent* computations. EG:
  - Processing lots of data files (e.g., image files)
  - Running the same simulation many times over with different parameters ("parameter sweeps")
- Run many copies of your program
  - Programs may be serial (single core) but running lots of them at once. They don't communicate.
- Easy to do on CSF. See also the UoM Condor Service (formerly the EPS Condor Pool)
  - Free resource, uses UoM idle desktops over night

Example: Image Analysis

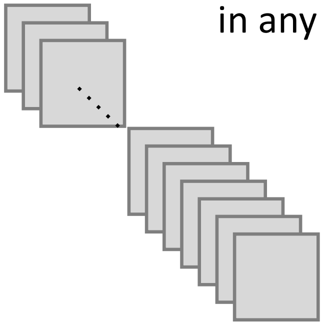
- High Throughput Computing
  - Not all s/w is "HPC" / parallel
  - But you might have *lots* of data
  - Each image takes 1hr to process (and are *independent* - process in any order)



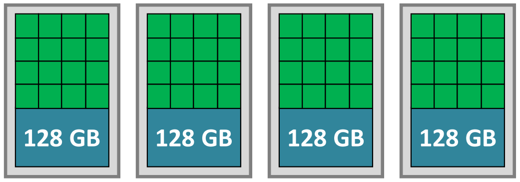
Laptop: 1 copy of software running.
Over 1 year to complete!!

Desktop: 4 cores, 4 copies of software running.
~100 days to complete!

Single HPC compute node: 16 copies of software running.
~26 days to complete



Example: 10,000 image scans to be analysed by an image processing application. Each image takes *1 hour* to process.



Multiple HPC compute nodes: 64 copies of software running.
~6 days to complete

Which style of parallel job to use

- Mostly determined by the capability of your app
  - Is it serial (1-core) only? Is it multi-core (single-node) only? Is it multi-node capable?
- A serial app will only ever use 1 core
  - But run as an HTC job, you can still process lots of data in parallel
    - Use many cores, running multiple *independent* jobs (see later)
- Parallel app using only *shared memory*
  - "OpenMP", "multithreaded", "Java threads", "shared memory"
  - Can only use 1 compute node (2--32 Intel or 2--168 AMD cores)
- Parallel app using *distributed memory*
  - "MPI" (message passing interface), "distributed memory"
  - Can use many cores across multiple compute nodes
  - But consider: the network
    - Communication faster *within* same compute node
    - Communication slower on network *between* nodes
    - Apps may not speed up, the more cores (and nodes) you use (see later)

Parallel Jobscript on CSF

- Use a jobscript to ask the batch system to find *N* free cores
  - While matching other requirements (memory, architecture, fast networking, GPU etc).

1. Add extra lines in jobscript to request:
   - *a parallel partition* (for multi-core or multi-node jobs)
   - *and number of cores* to reserve
2. Inform your app how many cores to use
   - Remember, the jobscript says how many cores your *job* requires (the batch system will allocate those cores to your job.)
   - **But** *you* must still ensure your app uses no more!!
     - This is not always automatic and how you do it varies from app to app

Parallel Jobscript – Multi-core (*single compute-node*)

#! - see serial jobscript earlier.

`myparajob.txt`

```
#!/bin/bash --login
#SBATCH -p multicore
#SBATCH -n 4
#SBATCH -t 3-0

# Set up to use a chemistry app
module purge
module load apps/gcc/gromacs/2023.3/double

# Inform app how many cores to use
export OMP_NUM_THREADS=4

# This job runs "gromacs"
mdrun_d
```

multicore is the partition name. This one means: app will multiple cores on a single compute node (2 to 168 AMD "Genoa" cores.)

-n (--ntasks=) **4** is the number of **cores** we want to *reserve* in the system. Each **partition** has a maximum number.

-t wallclock time limit for the job. This jobs is given 3 days (0 hours).

The commands we run in our job. They execute on a compute node that has the required number of cores free. `mdrun_d` is Gromacs.

Key concept!

Must *somehow* inform the app how many cores we *reserved*. Must use the number (**4**) given on the -n line. **Our app** wants `OMP_NUM_THREADS` environment variable setting. **Your app** may use a different method!

Avoid a common mistake

- Can use **`$SLURM_NTASKS`** to get the number of cores reserved by the job

`myparajob.txt`

```
#!/bin/bash --login
#SBATCH -p multicore    # Use the AMD "Genoa" nodes
#SBATCH -n 4            # Can be 2-168 in "multicore"
#SBATCH -t 3-0          # 3-day wallclock (max is 7-0)

# Set up to use a chemistry app
module purge
module load apps/gcc/gromacs/2023.3/double

# Inform app how many cores to use
export OMP_NUM_THREADS=$SLURM_NTASKS

# This job runs "gromacs"
mdrun_d
```

Our app wants `OMP_NUM_THREADS` environment variable to be set. **Your app** might use a different method!

`$SLURM_NTASKS` is automatically set to the number, **4** in this case, given on -n line. Will be **1** in "serial" partition.

Parallel jobscript - Multi-core (cont…)

- That was a multicore (*single* compute node) example
- Using an app named Gromacs as an example
  https://ri.itservices.manchester.ac.uk/csf3/software/applications/gromacs/
- Requested a partition (-p) and number of cores (-n)
  - Job will run the app on a single AMD "Genoa" node, allocating multiple cores on that node to the job.
- Then informed the app to use 4 cores via **`OMP_NUM_THREADS`** environment variable (very common).
  - Special **`$SLURM_NTASKS`** variable is always set to the number of cores requested on the -n (--ntasks=) line.

Parallel jobscript - Multi-core (cont…)

- As with the serial job, submit it to the system with
  `sbatch` *`jobscript`*
- Monitor with `squeue`
- It may take longer for *more* cores to become free in the system)
- You'll get the usual output file
  `slurm-`*`JOBID.out`*

Intel nodes

- If you need Intel CPUs (Haswell or Skylake architectures), use the "multcore_small" partition
    - Slurm will choose the architecture
    - Force it by adding "`#SBATCH -C skylake`", say.
    - These are older, but possibly less busy, nodes.

```
#!/bin/bash --login
#SBATCH -p multicore_small  # Use the Intel CPU nodes
#SBATCH -n 4                # Can be 2-32 in multicore_small
#SBATCH -t 3-0              # 3-day wallclock limit (max 7-0)

# Set up to use "gromacs"
module purge
module load apps/gcc/gromacs/2023.3/double

# Inform app how many cores to use
export OMP_NUM_THREADS=$SLURM_NTASKS

# This job runs "gromacs"
mdrun_d
```

Parallel Jobscript – multi-*node*

#! line from serial jobscript earlier.

hpcpool is the **partition** name. It means: app will use multiple compute nodes (Intel 32-core nodes, all 32 cores **must** be used on each) and has fast InfiniBand networking between the nodes.

-A gives an *account code*, needed for this restricted partition.

```
#!/bin/bash --login
#SBATCH -p hpcpool
#SBATCH -N 4  # Nodes: 4-32
#SBATCH -n 128  # Cores: 128-1024
#SBATCH -A hpc-projectcode
#SBATCH -t 4-0  # Max is 4-0 here
# Set up to use MrBayes
module purge
module load apps/gcc/mrbayes/3.2.6

# App uses MPI to run across nodes
mpirun -n $SLURM_NTASKS pmb in.nex
```

-N (--nodes=) 4 is the total number of **nodes** we want to *reserve* in the system.

-t wallclock time limit for the job. Max in hpcpool is 4 days.

-n (--ntasks=) 128 is the total number of **cores for MPI processes** we want to *reserve* in the system.

The commands we run in our job. They will execute on the compute nodes assigned to the job. `pmb` is the app name and is started via `mpirun` (very common for multi-node apps).

Must inform the app how many cores we *reserved*. `$SLURM_NTASKS` is automatically set to number (128) given on -n line. `mpirun` accepts a "`-n` ***numcores***" flag (which is optional – `mpirun` reads the `-n` number from Slurm if you don't supply it!!)

Parallel jobscript - Multi-node (cont…)

- A multi-*node* multi-core example
- Using an app named gulp as an example
  https://ri.itservices.manchester.ac.uk/csf3/software/applications/mrbayes/
- Requested a parallel environment (pe) & 128 cores

```
#SBATCH -p hpcpool
#SBATCH -N 4
#SBATCH -n 128
#SBATCH -A hpc-projectcode
```

  - Informed the app to use **4 nodes** (32-core Intel Skylake nodes) with **128 cores** used via "`mpirun -n $SLURM_NTASKS` ***appname***" (very common – lots of apps use this method.)
  - **`mpirun`** starts multiple copies of an MPI app on allocated nodes
  - Special **`$SLURM_NTASKS`** variable always set to number of cores on **`-n`** line
  - Can actually just use "**`mpirun`** ***appname***" and it will use the **`-n`** number.
- Access to the "HPC Pool" requires an application form, completed by PI/Supervisors on a per-project basis
  - https://ri.itservices.manchester.ac.uk/csf3/hpc-pool/application-questions/

Parallel Partitions

https://ri.itservices.manchester.ac.uk/csf3/batch/parallel-jobs/

Partition Name	Description
`multicore`	2-168 cores, single compute node. 8GB per core. Jobs will be placed on AMD EPYC "Genoa" (max 168 cores/job)
No optional flags	

Partition Name	Description
`multicore_small`	2-32 cores, single compute node. ~4-5GB per core. Jobs will be placed on Intel "haswell" (max 24 cores/job) or Skylake (max 32 cores/job)
`-C` *`architecture`*	**Not recommended!** (`haswell` or `skylake`)

Partition Name	Description
`hpcpool`	32 cores, multiple compute nodes. 5GB per core. Jobs will be placed on Intel Skylake (max 32 cores/job) CPUs. Jobs must use 4-32 compute nodes. 4-day runtime limit.
`-A` ***`hpc-projectcode`***	You must have an approved HPC Pool project code.

- **7-day runtime limit** on jobs unless otherwise indicated in table.
- Our simple jobscript did *not* use any of the above extra flags. Not needed in most cases.
- If you limit a job by *architecture* it may wait longer in the queue.

Choosing the partition

- Choosing the partition is fairly simple, but:
  - Check the app's webpage for advice and examples https://ri.itservices.manchester.ac.uk/csf3/software
  - Check the partition page for limits on number of cores https://ri.itservices.manchester.ac.uk/csf3/batch-slurm/partitions/
  - Avoid using `#SBATCH -C architecture`
- Use Intel (**multicore_small**) or AMD (**multicore**) nodes?
  - Most (all) apps will run on both, but AMD nodes are newer
  - The high memory nodes are all Intel CPUs (e.g., `-p himem`)
  - There are now *a lot* more AMD CPUs available than Intel CPUs
    - Submitting to **multicore** may result in shorter wait times
    - **multicore** nodes have 8GB/core (**multicore_small** nodes have ~5-6GB/core)

Parallel Software Performance

- You'll probably be running an app many times
- Worth small investigation to find optimal performance parameters (#cores & #nodes)
  - How many cores should I use?
- Do a few runs, change the number of cores
  - Plot time vs number of cores
  - Easy to do on CSF: remove "`-n numcores`" from jobscript, add it to `sbatch` command instead:

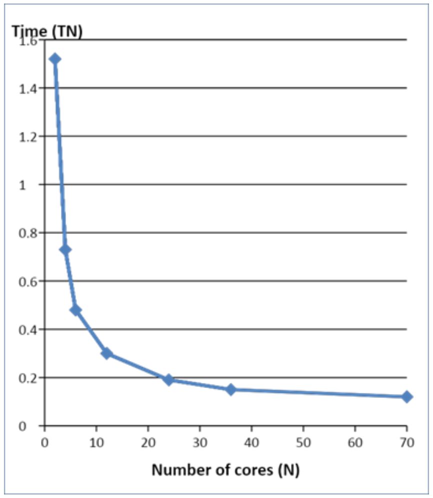
```
sbatch -n 2 myjobscript.txt
sbatch -n 4 myjobscript.txt
sbatch -n 8 myjobscript.txt
```

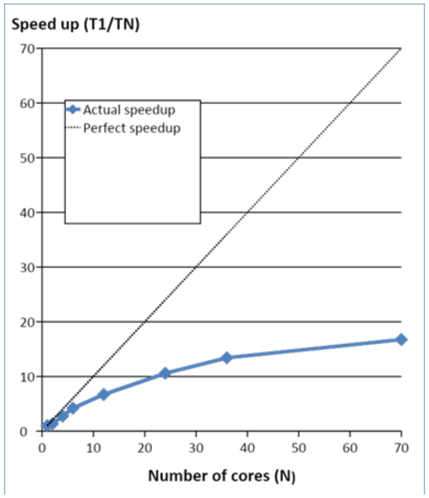
To Assess Parallelism

- Plot the following against "Number of Cores":
  - "Speed-up" or "Parallel Efficiency"
  - Total memory usage?
- Look for the sweet-spot
- Calculate: Speed-up = T_1 / T_N
  - Compare results against "ideal" scaling (where *N*-cores makes it go *N*-times faster)
- Calculate: Parallel Efficiency = $T_1 / (N \times T_N)$
  - N = number of cores, T_N = time take on N cores
- Pick a typical problem size for your work

Examples of Speed-up

- Data for popular Finite Element app on CSF
  - The 'Time' graphs shows it getting faster. But…





Examples of Speed-up & Efficiency

- Example showing Speed-up and Efficiency values
  - App multiplies two square matrices
    - Measured a single multiplication of two 2000x2000 matrices

No. cores	Time (Seconds)	Speed-up	Efficiency
1	45.0	1x	1.00
2	22.8	1.97x	0.99
4	11.7	3.84x	0.96
8	7.1	6.33x	0.80

- The speed-up is reasonably close to “perfect” & efficiency is reasonably close to 100% but…
  - How will this scale as we go multi-node?
  - How will this scale as the problem size increases?
  - How will this scale on other hardware?

PRACTICAL SESSION 4

Parallel job and scaling

Practical Session 4 - Parallel jobs

- Follow the handout ‘Practical Session 4’
  - Use **`sbatch`** to submit a simple parallel (2-core) job on the CSF
  - Modify the jobscript to use different numbers of cores
  - Determine whether the application "scales" with the number of cores.
- Exercise sheet (pdf) available at: https://ri.itservices.manchester.ac.uk/course/rcsf/

MULTIPLE SIMILAR JOBS

High Throughput Computing and "Job arrays"

Multiple Runs of an Application

- We want to run an application many times to process *many different* input files
  - For example, on a desktop PC you might run

```
myapp.exe -in mydata.1.tif -out myresult.1.tif
(wait for it to finish)
myapp.exe -in mydata.2.tif -out myresult.2.tif
(wait for it to finish)
myapp.exe -in mydata.3.tif -out myresult.3.tif
…
myapp.exe -in mydata.1000.tif -out myresult.1000.tif
```

  - If it takes 5 minutes to process one file, it will take 1000 x 5 minutes to process them all (~3.5 days)

How **Not** To Do It on the CSF (1)

- Inefficient method 1: one after another in *one* job? `sbatch jobscript-all.txt`

`jobscript-all.txt`

```
#!/bin/bash --login
#SBATCH -p serial
#SBATCH -t 4-0      # Wallclock is 4 days for all images

myapp.exe -in mydata.1.tif -out myresult.1.tif
(will wait for it to finish)
myapp.exe -in mydata.2.tif -out myresult.2.tif
(will wait for it to finish)
myapp.exe -in mydata.3.tif -out myresult.3.tif
…
myapp.exe -in mydata.1000.tif -out myresult.1000.tif
```

- This is *no better* than the desktop PC method

How **Not** To Do It on the CSF (2)

- Inefficient method 2: lots of individual jobscripts?

`jobscript1.txt`

```
#!/bin/bash --login
#SBATCH -p serial
#SBATCH -t 10    # Wallclock is 10 mins for one image

myapp.exe -in mydata.1.tif -out myresult.1.tif
```

Make 1000 copies of this jobscript, edit each one to process a different file (mydata.2.tif, …)

```
sbatch jobscript1.txt
sbatch jobscript2.txt
sbatch jobscript3.txt
…
sbatch jobscript1000.txt
```

Then **submit each job**

- Strains the batch system queue manager
- But, you will get many jobs running in parallel
  - EG: approx 100-200 jobs running at same time

How To Do It - a "Job Array" Jobscript

-t wallclock. Each individual array task has a wallclock of 10 minutes. There is no overall time limit for the job.

1-1000 (start-end) says how many tasks to run and how they should be numbered. Note: **Can** start at **0**. Can use start-end:increment to increase the ID by more than 1.

`arrayjob.txt`

```
#!/bin/bash --login
#SBATCH -p serial     # Each task gets 1 core
#SBATCH -t 10         # 10 minutes per task
#SBATCH -a 1-1000     # 1000 tasks

echo "I am task ${SLURM_ARRAY_TASK_ID}"
myapp.exe \
   -in mydata.${SLURM_ARRAY_TASK_ID}.tif \
   -out myresult.${SLURM_ARRAY_TASK_ID}.tif
```

-a an array job. Runs multiple copied of the job a specified number of times. These are called **array tasks**. Each is numbered uniquely 1, 2, 3 …, 1000.

The commands we run in our job. They will execute on backend nodes (different cores and nodes for different tasks).

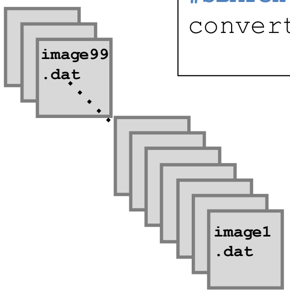
`${SLURM_ARRAY_TASK_ID}` is automatically set by the batch system and tells us which array task we are (1,2,…). We can use this to do something different in array task.

"Job Array" Jobscript

- Our app is a serial (1-core) app
  - But you *could* use the mutlicore partition if your app is multi-core capable.
- The total number of tasks can be 100s, 1000s, 10000s (max 25,000 on CSF)
- The system will run *many* of the tasks concurrently
  - Usually 100s - "High-throughput Computing"
  - You get lots of work done sooner
  - It will eventually churn through all of them
  - They are started in numerical order but no guarantee they'll finish in that order!
- The extra jobscript `#SBATCH -a` line is easy. Using the `$SLURM_ARRAY_TASK_ID` number *creatively* **is the key to job arrays**.
- **Note**: Do not confuse Slurm's `-n/--ntasks` (number of cores) flag with `-a/--array` (start-end for array tasks) flag. The names can be confusing :-(

The $SLURM_ARRAY_TASK_ID variable (1)

- Want to do something different in each task. EG:
  - Read a different data file to process
  - Pass a different parameter to an application
- You can get this different "thing" in many ways:
  - EG: Use the $SLURM_ARRAY_TASK_ID in filenames:



```
#SBATCH -a 1-1000
convert -i image_${SLURM_ARRAY_TASK_ID}.jpg \
        -o image_${SLURM_ARRAY_TASK_ID}.png
```

Task 1 reads `image_1.jpg` writes `image_1.png`
Task 2 reads `image_2.jpg` writes `image_2.png`
…
Task 1000 reads `image_1000.jpg` writes `image_1000.png`

The $SLURM_ARRAY_TASK_ID variable (2)

- Or have a "master" list (a text file) of names etc
- The Nth task reads the Nth line from that text file:

```
#SBATCH -a 1-4000
# Read the Nth line of filenamelist.txt and save in variable MYFILENAME
MYFILENAME=$(awk "NR==${SLURM_ARRAY_TASK_ID}" filenamelist.txt)

# Now use whatever the value of variable is in the next command
myapp.exe -input ${MYFILENAME} -output ${MYFILENAME}.out
```

```
filenamelist.txt
ptn1511.dat
ptn7235.dat
ptn7AFF.dat
ptn6E14.dat
ptn330D.dat
…
```

Task 1 reads `ptn1511.dat` writes `ptn1511.dat.out`
Task 2 reads `ptn7235.dat` writes `ptn7235.dat.out`
…

- Number of lines in master file **must** match number of tasks
- To get number of lines in master file use:
  `wc -l filenamelist.txt`
- bash: **`VAR=$(`*`command arg1 arg2`*`)`** captures output from *command* and assigns to variable VAR for use later.

https://ri.itservices.manchester.ac.uk/csf3/batch/job-arrays/

The $SLURM_ARRAY_TASK_ID variable (3)

- Another way to use the "master" list method
- The Nth task reads the Nth line from that text file:

```
#SBATCH -a 1-50
# Read the Nth line of foldernamelist.txt and save as $FOLDER
FOLDER=$(awk "NR==${SLURM_ARRAY_TASK_ID}" foldernamelist.txt)

# Now use whatever the value of variable is in the next command
cd ~/scratch/experiments/${FOLDER}
mdrun_d
```

```
foldernamelist.txt
znc24/100p/a1
znc24/200p/b2
ag80/100p/b1
ag81/100q/c1
ptn2/50a/a1
ptn3/50b/c1
…
```

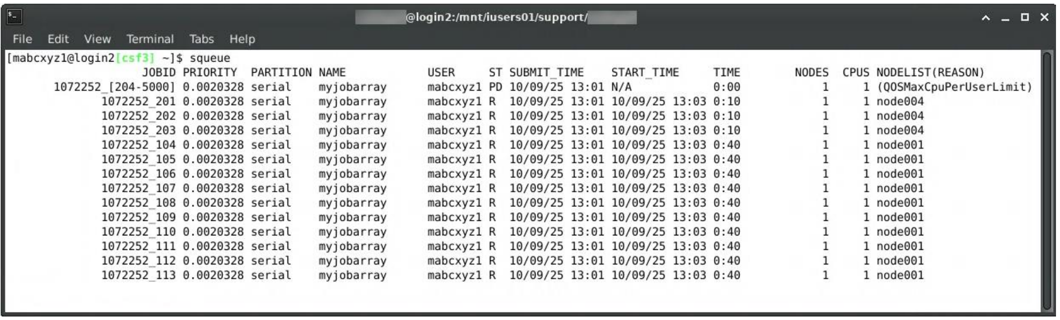
Task 1 reads `znc24/100p/a1` as folder name
Task 2 reads `znc24/200p/b2` as folder name
…

- Number of lines in master file **must** match number of tasks
- To get number of lines in master file use:
  `wc -l foldernamelist.txt`
- bash: **`VAR=$(`*`command arg1 arg2`*`)`** captures output from *command* and assigns to variable VAR for use later.

https://ri.itservices.manchester.ac.uk/csf3/batch/job-arrays/

Jobarrays – squeue and scancel

- `squeue` shows pending and running tasks
  - `QOSMaxCpuPerUserLimit` means the limit of number of CPUs in use at any one time (for this user) has been reached.
  - Hence some array tasks must wait until earlier ones have finished.



```
[mabcxyz1@login2[csf3] ~]$ squeue
             JOBID PRIORITY  PARTITION NAME           USER     ST SUBMIT_TIME    START_TIME     TIME         NODES  CPUS NODELIST(REASON)
      1072252_[204-5000] 0.0020328 serial    myjobarray      mabcxyz1 PD 10/09/25 13:01 N/A            0:00             1     1 (QOSMaxCpuPerUserLimit)
           1072252_201 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:10             1     1 node004
           1072252_202 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:10             1     1 node004
           1072252_203 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:10             1     1 node004
           1072252_104 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_105 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_106 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_107 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_108 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_109 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_110 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_111 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_112 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
           1072252_113 0.0020328 serial    myjobarray      mabcxyz1 R  10/09/25 13:01 10/09/25 13:03 0:40             1     1 node001
```

- scancel can remove all tasks or just some

`scancel 1072252`	Remove all running and waiting tasks
`scancel 1072252_300`	Remove task 300 (a bit strange)
`scancel 1072252_[4000-5000]`	Remove last 1000 tasks

Jobarray Output Files

- You'll get the usual Slurm output file but
  - One per task
  - Potentially a lot of files!
- Look for
  `slurm-JOBID_TASKID.out`

```
EG: slurm-1046732_1.out
    slurm-1046732_2.out
    ...
    slurm-1046732_1000.out
```

- You should delete empty / unwanted files soon and often

PRACTICAL SESSION 5

Job array examples

Practical Session 5 – Job arrays

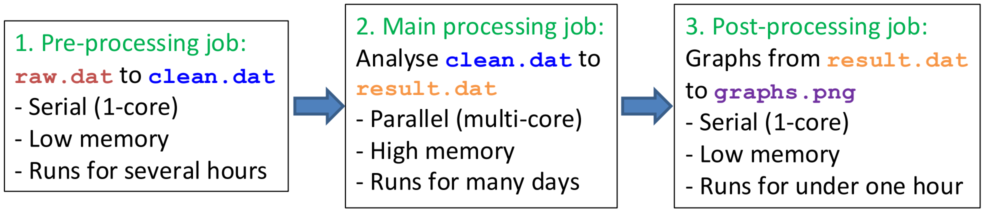
- Follow the handout 'Practical Session 5'
  - Modify, and run, a simple job-array jobscript to run an app with different input values.
  - Write a new job-array jobscript to do some python image processing on a set of Hubble Ultra Deep Field images.
- Exercise sheet (pdf) available at:
  https://ri.itservices.manchester.ac.uk/course/rcsf/

JOB PIPELINES

Ordering jobs

A Job Pipeline (aka workflow)

- Suppose you have several apps that:
  - Need to run in a specific order - a "pipeline"
    - There is a *dependency* between apps
  - Each might have different CPU-core and memory requirements
  - Each might take different amounts of time to run



1. Pre-processing job:
`raw.dat` to `clean.dat`
- Serial (1-core)
- Low memory
- Runs for several hours

2. Main processing job:
Analyse `clean.dat` to `result.dat`
- Parallel (multi-core)
- High memory
- Runs for many days

3. Post-processing job:
Graphs from `result.dat` to `graphs.png`
- Serial (1-core)
- Low memory
- Runs for under one hour

How **not** to do it on the CSF (1)

- Put all steps in one job?
  - Wastes resources (some cores and memory)
  - May go over 7-day runtime limit

mypipeline_bad.txt

```
#!/bin/bash --login
#SBATCH -p himem      # Uses a high-memory node
#SBATCH --mem 2000G   # … with 2TB of RAM
#SBATCH -n 16         # … and 16 cores
#SBATCH -t 7-0        # … for 7 days
module purge
module load apps/………

# First app (1-core, low memory usage)
preproc -in raw.dat -out clean.dat
# Second app (multiple cores, high memory usage)
mapper -p $SLURM_NTASKS -in clean.dat -out result.dat
# Third app (1-core, low memory usage)
drawGraphs -in result.dat -out graphs.png
```

Only one command uses all of the cores

Better but still not perfect

- Split into multiple jobs, notice when jobs finish, submit next…?
  - Log in to CSF, check if previous job has finished…. wastes time!

A serial job (no wasted cores)

firstjob.txt

```
#!/bin/bash --login
#SBATCH -p serial    # 1-core job
#SBATCH -t 0-2       # 2 hour wallclock
module load apps/………
# First 'job' (1-core, low memory usage)
preproc -i raw.dat -o clean.dat
```

A parallel, high-mem job

secondjob.txt

```
#!/bin/bash --login
#SBATCH -p himem     # Uses a high-memory node
#SBATCH --mem 2000G # … with 2TB RAM
#SBATCH -n 16        # … and 16 cores
#SBATCH -t 7-0       # … 7 day wallclock
module load apps/………
# Second 'job' (multiple cores, high memory usage)
mapper -p $SLURM_NTASKS -i clean.dat -o result.dat
```

A serial job (no wasted cores)

thirdjob.txt

```
#!/bin/bash --login
#SBATCH -p serial    # 1-core job
#SBATCH -t 30        # 30 minute wallclock
module load apps/………
# Third 'job' (1-core, low memory usage)
drawGraphs -i result.dat -o graphs.png
```

`sbatch firstjob.txt`
(now you need to wait until this job has finished before submitting the next one!)
`sbatch secondjob.txt`
(now you need to wait until this job has finished before submitting the next one!)
`sbatch thirdjob.txt`

How to do it - Job Dependencies

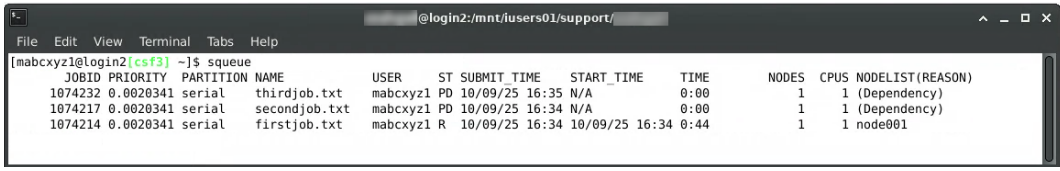
- Using the previous individual jobscripts
  - Add a `-d` / `--dependency=` flag when submitting them
  - Use the JOBID of the previous job to make the current job wait for it

```
sbatch firstjob.txt
Submitted batch job 1074214
                      ↓
sbatch -d afterok:1074214 secondjob.txt
Submitted batch job 1074217
                      ↓
sbatch -d afterok:1074217 thirdjob.txt
Submitted batch job 1074232
```

  - The `afterok` flag means do not run this job until the earlier dependency job has finished successfully.
  - Note, you cannot you use jobscript names. You must use the JOBID of an earlier job.
  - There are lots of dependency parameters (e.g, afterany, afternotok, and multiple dependencies can be setup.)

Job Dependencies

- You *must* submit the jobs in the correct order
  - EG: If `secondjob.txt` is submitted first, it runs immediately (no dependency job exists to wait for)
- `squeue` shows `(Dependency)` for jobs on hold



```
[mabcxyz1@login2[csf3] ~]$ squeue
       JOBID PRIORITY  PARTITION NAME            USER     ST SUBMIT_TIME    START_TIME     TIME         NODES  CPUS NODELIST(REASON)
     1074232 0.0020341 serial    thirdjob.txt    mabcxyz1 PD 10/09/25 16:35 N/A            0:00             1     1 (Dependency)
     1074217 0.0020341 serial    secondjob.txt   mabcxyz1 PD 10/09/25 16:34 N/A            0:00             1     1 (Dependency)
     1074214 0.0020341 serial    firstjob.txt    mabcxyz1 R  10/09/25 16:34 10/09/25 16:34 0:44             1     1 node001
```

- Later jobs may still *wait* to be scheduled
  - They don't always run *immediately* after earlier jobs finish

---

Job Dependencies

- Can submit the jobs in a more programmatic manner:
  - Use `--parsable` flag to get *just* the JOBID of the submitted job (instead of 'long' message):
    - `sbatch myjobscript`
      `Subimtted batch job 1074233`
    - `sbatch --parsable myjobscript`
      `1074233`
  - Capture output of command into shell variable

```
JOBID=$(sbatch --parsable firstjob.txt)
JOBID=$(sbatch --parsable -d afterok:$JOBID secondjob.txt)
JOBID=$(sbatch --parsable -d afterok:$JOBID thirdjob.txt)
```

Job-Array Dependencies (1)

- An ordinary job can wait for a *job array* to finish
  - All tasks in the job array must have finished

arrayjob.txt

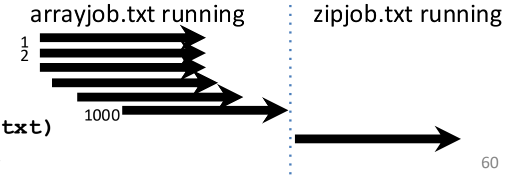
```
#!/bin/bash --login
#SBATCH -p serial      # 1-core job
#SBATCH -t 30          # 30 minute wallclock
#SBATCH -a 1-1000      # Job array with 1000 tasks
convert img.${SLURM_ARRAY_TASK_ID}.tif img.${SLURM_ARRAY_TASK_ID}.pdf
```

zipjob.txt

```
#!/bin/bash --login
#SBATCH -p serial      # 1-core job
#SBATCH -t 5           # 5 minute wallclock
zip conference.zip img.*.pdf
```

Add a job dependency so that second job waits until entire job-array has finished.

```
JID=$(sbatch --parsable arrayjob.txt)
sbatch -d afterok:$JID zipjob.txt
```

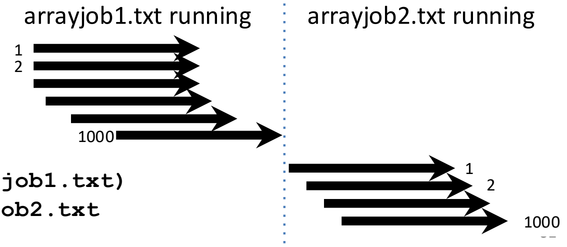


Job-Array Dependencies (2)

- A *job array* can wait for a *job array* to finish
  - – *All* tasks in the *first* job array must have finished

arrayjob1.txt
```
#!/bin/bash --login
#SBATCH -p serial        # 1-core job
#SBATCH -t 30            # 30 minute wallclock for each task
#SBATCH -a 1-1000        # Job array with 1000 tasks
someapp data.${SLURM_ARRAY_TASK_ID}.xyz  data.${SLURM_ARRAY_TASK_ID}.dat
```

arrayjob2.txt
```
#!/bin/bash --login
#SBATCH -p multicore     # Multicore job
#SBATCH -n 4             # Each task can use 4 cores.
#SBATCH -t 60            # 60 minute wallclock for each task
#SBATCH -a 1-1000        # Job array with 1000 tasks
otherapp data.${SLURM_ARRAY_TASK_ID}.dat result.${SLURM_ARRAY_TASK_ID}.dat
```



Add a job dependency so that second job array waits until entire first job-array has finished.

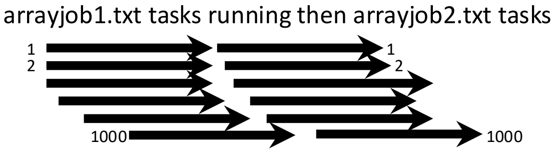
```
JID=$(sbatch --parsable arrayjob1.txt)
sbatch -d afterok:$JID arrayjob2.txt
```

Job-Array Dependencies (3)

- A *job array* can wait for a *job array* to finish
  - – Each task in *second* job array waits for *corresponding* task in *first* job array to finish

arrayjob1.txt
```
#!/bin/bash --login
#SBATCH -p serial        # 1-core job
#SBATCH -t 30            # 30 minute wallclock for each task
#SBATCH -a 1-1000        # Job array with 1000 tasks
someapp data.${SLURM_ARRAY_TASK_ID}.xyz  data.${SLURM_ARRAY_TASK_ID}.dat
```

arrayjob2.txt
```
#!/bin/bash --login
#SBATCH -p multicore     # Multicore job
#SBATCH -n 4             # Each task can use 4 cores.
#SBATCH -t 60            # 60 minute wallclock for each task
#SBATCH -a 1-1000        # Job array with 1000 tasks
otherapp data.${SLURM_ARRAY_TASK_ID}.dat result.${SLURM_ARRAY_TASK_ID}.dat
```



Add a job dependency so that second job array tasks wait for corresponding tasks in first job-array to finish.

```
JID=$(sbatch --parsable arrayjob1.txt)
sbatch -d aftercorr:$JID arrayjob2.txt
```

INTERACTIVE JOBS

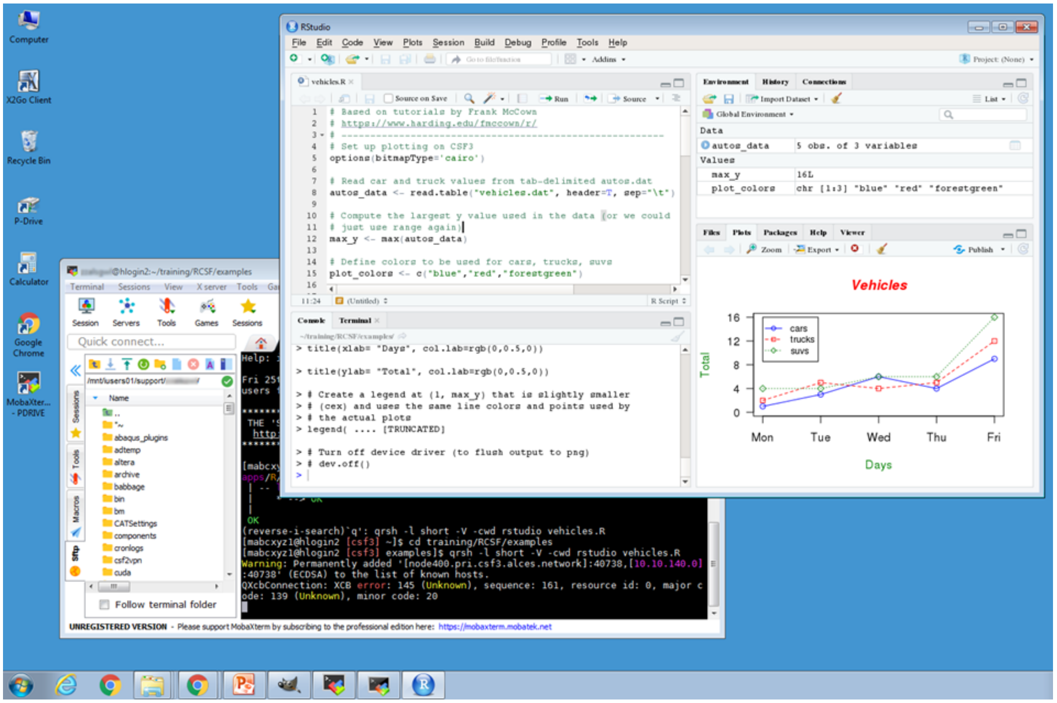
Compute apps with GUIs

Interactive work

- Some apps (eg Rstudio, VMD, molden, paraview) may have a GUI but should not be run on the login node.
  - The GUI itself might be quite a light-weight program, but if you then load a huge dataset in, or set off some long-running multi-process computation, via the GUI, you'll "hammer" the login node.
- Use the **srun** command to get an *interactive session* on a compute node

```
# We are on the login node here
module purge
module load apps/gcc/R/4.5.0
module load apps/binapps/rstudio/2025.05.0-any-r
srun -p interactive -t 60 -n 1 rstudio vehicles.R
```

- No dedicated resource, priority to batch jobs.
- Runs on an AMD 168-core node, hence 8GB per core.
- Max 60 minutes wallclock limit.
- Remember - a GUI app, as with `gedit`, needs an X-server running on your PC (as provided by MobaXTerm, or X-Quartz, or a Linux desktop)
- Remember to exit your GUI app when you have finished so the resource is made available for others.



```
# Based on tutorials by Frank McCown
# https://www.harding.edu/fmccown/r/
# ------------------------------------------------------------
# Set up plotting on CSF3
options(bitmapType='cairo')

# Read car and truck values from tab-delimited autos.dat
autos_data <- read.table("vehicles.dat", header=T, sep="\t")

# Compute the largest y value used in the data (or we could
# just use range again)
max_y <- max(autos_data)

# Define colors to be used for cars, trucks, suvs
plot_colors <- c("blue","red","forestgreen")
```

```
Data
autos_data    5 obs. of 3 variables
Values
max_y         16L
plot_colors   chr [1:3] "blue" "red" "forestgreen"
```

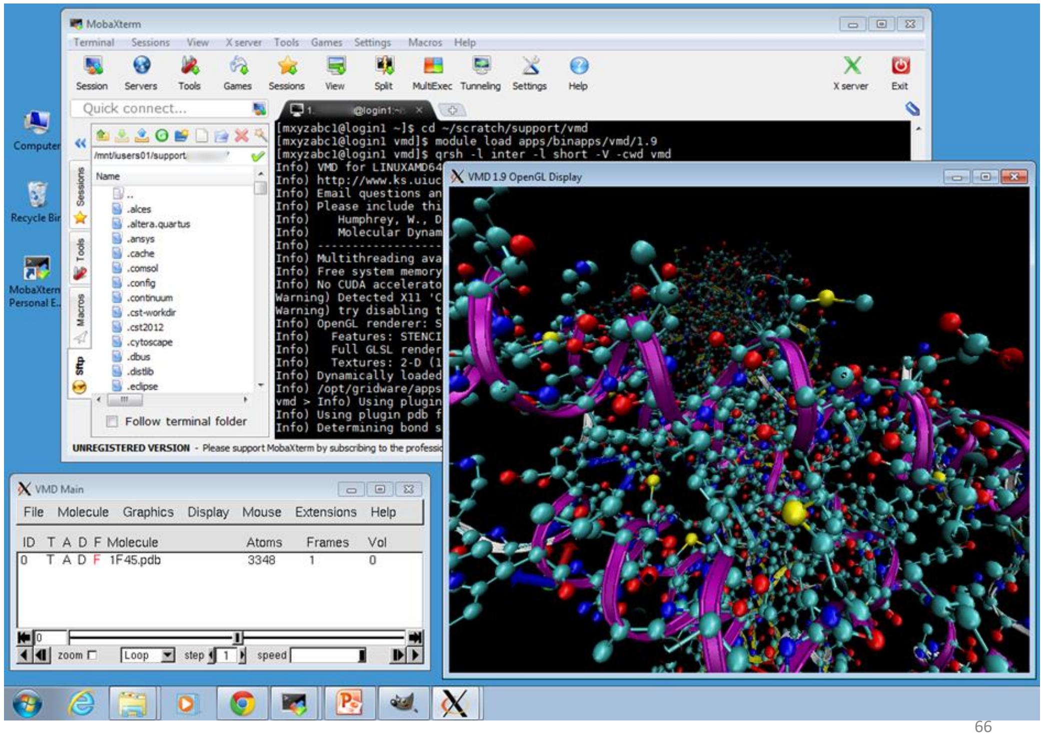
```
> title(xlab= "Days", col.lab=rgb(0,0.5,0))

> title(ylab= "Total", col.lab=rgb(0,0.5,0))

> # Create a legend at (1, max_y) that is slightly smaller
> # (cex) and uses the same line colors and points used by
> # the actual plots
> legend( .... [TRUNCATED]

> # Turn off device driver (to flush output to png)
> # dev.off()
>
```

```
 OK
(reverse-i-search)`q': qrsh -l short -V -cwd rstudio vehicles.R
[mabcxyz1@hlogin2 [csf3] ~]$ cd training/RCSF/examples
[mabcxyz1@hlogin2 [csf3] examples]$ qrsh -l short -V -cwd rstudio vehicles.R
Warning: Permanently added '[node400.pri.csf3.alces.network]:40738,[10.10.140.0]
:40738' (ECDSA) to the list of known hosts.
QXcbConnection: XCB error: 145 (Unknown), sequence: 161, resource id: 0, major c
ode: 139 (Unknown), minor code: 20
```



```
[mxyzabc1@login1 ~]$ cd ~/scratch/support/vmd
[mxyzabc1@login1 vmd]$ module load apps/binapps/vmd/1.9
[mxyzabc1@login1 vmd]$ qrsh -l inter -l short -V -cwd vmd
Info) VMD for LINUXAMD64
Info) http://www.ks.uiuc
Info) Email questions an
Info) Please include thi
Info)    Humphrey, W., D
Info)    Molecular Dynam
Info) ------------------
Info) Multithreading ava
Info) Free system memory
Info) No CUDA accelerato
Warning) Detected X11 'C
Warning) try disabling t
Info) OpenGL renderer: S
Info)   Features: STENCI
Info)   Full GLSL render
Info)   Textures: 2-D (1
Info) Dynamically loaded
Info) /opt/gridware/apps
vmd > Info) Using plugin
Info) Using plugin pdb f
Info) Determining bond s
```

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	1F45.pdb	3348	1	0

GPU Jobs

Accessing the GPUs

Nvidia GPUs

- CSF3 has 164 x Nvidia GPUs
  - v100, A100(80GB), L40S (and some A100(40GB) for a specific research group) are available to all users.

24 x Volta v100 GPUs in total – 4 GPUs/node
16GB GPU memory, Mem bandwidth 900GB/s
5120 CUDA cores (80 Multiprocessors, 64 cores/MP)
640 Tensor cores
Peak FP64 7.5 TFLOPS
32-core Intel Xeon Gold "Cascade Lake"
192GB RAM host node

84 x Ampere A100 GPUs in total – 4 GPUs/node
80GB(**76x**) or 40GB(**8x**) GPU mem, Mem b/w 2TB/s
6912 CUDA cores (108 Multiprocessors, 64 cores/MP)
432 Tensor cores
Peak FP64 9.7 TFLOPS
48-core AMD Epyc "Milan"
512GB RAM host node
40GB A100 nodes restricted to one research group

56 x Ada Lovelace L40S GPUs in total – 4 GPUs/node
48GB GPU memory, Mem bandwidth 864GB/s
18176 CUDA cores (142 Multiprocessors, 128 cores/MP)
142 RT cores
568 Tensor cores
Peak SP 91.6 TFLOPS
48-core Intel Xeon Gold "Sapphire Rapids"
512GB RAM host node

Parallel Jobscript – multi-*node*

`gpuV, gpuA, gpuL,` or `gpuA40GB` is the **partition** name. It means: app will use a GPU compute node containing the indicated type of GPU - v100, A100, L40S or gpuA40GB (this one has restricted access.)

`-t` wallclock time limit for the job. Max in `gpuX` is 4 days.

```
#!/bin/bash --login
#SBATCH -p gpuX     # Partition (V,A,L)
#SBATCH -G 2        # GPUs: 1-4
#SBATCH -n 8        # Cores: 1-8,12
#SBATCH -t 4-0      # Max is 4-0 here
# Set up to use the CUDA toolkit
module purge
module load libs/cuda/12.4.1

# Run a GPU app. Slurm will ensure no
# other jobs can use your GPUs.
deviceQuery
```

-G (--gpus=) 2 is the total number of **GPUs** we want to *reserve* in the system.

-n (--ntasks=) 8 is the total number of **host CPU cores** we want to *reserve* in the system.

Slurm will set some environment variables for use in your jobscript:
`$CUDA_VISIBLE_DEVICES` gives the device IDs (`0` or `0,1` or `0,1,2` or `0,1,2,3`) depending number of GPUs.
`$SLURM_GPUS` gives the number of GPUs you request on the -G line.
`$SLURM_NTASKS` as previous jobs, the number on the –n (host CPU cores).

GPU Limits

- Most users get access to **up to two GPUs** from the gpuV, gpuA or gpuL partitions, in use at any one time with a max of 2 overall (e.g., 1xv100 + 1xA100. Or 2xL40S.)
  - This is "free at point of use access", funded by the Research Lifecycle Programme, managed by Research IT.
  - Users from some contributing groups who have funded GPUs may get access to more GPUs.
  - All GPU nodes contain 4 GPUs. Multi-node (>4 GPU jobs) are NOT possible.
- CPU host cores are limited by number of GPUs in job and by node-type
  - Note that unless the jobscript contains the `-n` flag, jobs will only have one host CPU core.
  - Many GPU apps can still make use of multiple host CPU cores for some of their processing.

GPU Partition (GPU type)	Host CPU type	Max host CPU cores per GPU	Host RAM per CPU core (GB)	Max host RAM per GPU (GB)
`gpuV` (v100)	23-core Intel Xeon "Cascade Lake"	8	5.8	46
`gpuA` (A100 80GB)	48-core AMD EPYC "Milan"	12	10.4	125
`gpuL` (L40s)	48-core Intel Xeon "Sapphire Rapids"	12	10.4	125
`gpuA40GB` (A100 40GB)	48-core AMD EPYC "Milan"	12	10.4	125

Other GPU Notes

- GPUs are run in **`DEFAULT`** compute mode (not **`EXCLUSIVE_PROCESS`**.)
  - You can run multiple processes / apps on the same GPU – e.g., several small chemistry simulations.
- You can monitor your GPU jobs by accessing the compute node and GPU once your job as started.
  - Use the `srun` command on the login node to "login" to the compute node and resource container where your job is running:
    `srun --jobid=`*`JOBID`*` --pty bash`
    (wait until you are logged into the compute node where you job is running. You'll see the same GPUs.)
    `nvidia-smi`
    or, for example:
    `module load libs/cuda/12.4.1`
    `ncu-ui` or **`nvvp`** (or other Nvidia tool)
- A quick exercise 6:
  - If you are logged-in to the CSF, try editing the `~/training/RCSF/examples/dq_gpu.sbatch` jobscript (change the `-p` line to request one of the `gpuV`, `gpuA` or `gpuL` partitions.) Then *submit* the job.
  - It runs the Nvidia `deviceQuery` utility to return some stats about the GPU assigned to your job.

High Memory Jobs

Accessing the high memory nodes

High Memory Jobs

- So far, our serial and parallel jobs have access to a fixed amount of memory
  - The partitions provide a specific amount of memory per core.
    - e.g. the multicore partition provides 8GB/core
  - If you want more memory, you need to request more cores.
  - Max in **`multicore`** is ~ 1.5 TB if all 168 cores used.
  - Can be very wasteful of CPU resources
- The **`himem`** and **`vhimem`** partitions provide access to more memory (up to 2TB and 4TB.)
  - Memory is a "consumable" - the amount of memory can be requested independently of the number of cores.

Do you need more memory?

- If a job fails and reports an "OOM" error in the **`slurm-`*`JOBID`*`.out`** file, you should request more memory.
- You can also check a previous job to see how much memory it used with "**`seff`**"

```
[mabcxyz1@login1[csf3] ~]$ seff 12345
Job ID: 12345
Cluster: csf3.man.alces.network
User/Group: username/xy01
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 2
CPU Utilized: 00:04:13
CPU Efficiency: 49.41% of 00:08:32 core-walltime
Job Wall-clock time: 00:04:16
Memory Utilized: 21.45 GB             # Peak memory usage
Memory Efficiency:33.5% of 64.00 GB   # A low memory efficiency means this job did NOT need
                                      # to use the himem partition. You should check this.
```

High-memory Compute Nodes

- The 2TB (**`himem`**) partition contains various Intel compute nodes.
  - Slurm will place your job on any of the node-types that have enough resources (memory, cores) as requested by your job.
- The 4TB (**`vhimem`**) partition is restricted
  - Please request access via the Connect Portal
  - We will need evidence from previous jobs that you need >2TB of RAM.

Partition (required)	Default job mem-per-core if memory not requested (GB)	Max job size (cores)	Max job memory (GB)	Arch Flag (optional, but will activate specific limits shown in the next columns)	Max job size (cores)	Max job memory (GB)	Has SSD storage	Old SGE flag (DO NOT USE)
`himem`	31	32	2000	`-C haswell`	16	496	No	mem512
				`-C cascadelake`	32	1472	No	mem1500
				`-C icelake` (also `ssd`)	32	2000	Yes	mem2000
`vhimem`	125	32	4000	`-C icelake` (also `ssd`)	32	4000	Yes	mem4000

High Memory Jobscripts

```
#!/bin/bash --login
#SBATCH -p himem                 # Partition
#SBATCH -n 2                     # Cores: Can be 1-32
#SBATCH --mem=1200G              # Total memory for the job
#SBATCH -t 4-0                   # Wallclock (max is 7-0 here)

# Set up to use your app
module purge
module load apps/gcc/something/1.2.3

# Run a GPU app. Slurm will ensure no
someApp -in hugh_dataset.dat -out results.dat
```

```
#!/bin/bash --login
#SBATCH -p himem                 # Partition
#SBATCH -n 2                     # Cores: Can be 1-32
#SBATCH --mem-per-cpu=600G       # OR specify the Memory per Core
                                 # (note: name of flag uses 'cpu')
#SBATCH -t 4-0                   # Wallclock (max is 7-0 here)
```

OTHER PARALLEL HARDWARE

What else is available?

HPC Pool

- Dedicated pool for HPC jobs
  - 4096 cores of Infiniband connected Skylake
  - Minimum 128-core job size, maximum 1024
  - Frontend shared with CSF3
    - You just submit HPC jobs like any other CSF job (with a different "partition" name and an account code.)
  - Lightweight application process – must be made by PI
  - Currently free

  https://ri.itservices.manchester.ac.uk/csf3/hpc-pool

N8 Bede (NICE)

- 32 IBM Power 9 dual-CPU nodes
  - ○ Each node comprises 4 NVIDIA V100 GPUs and high performance interconnect.
- 5 Nvidia GH200 Grace Hopper nodes
  - ○ Each node comprises 1x NVIDIA H100 96GB with 900 GB/s NVLink-C2C and 1x NVIDIA Grace aarch64 CPU @ 3.483 GHz (72 Arm Neoverse V2 cores)
- Same architecture as the US government’s SUMMIT and SIERRA supercomputers which occupied the top two places in a recently published list of the world’s fastest supercomputers.
- Contact Research IT for advice
- https://n8cir.org.uk/supporting-research/facilities/bede/docs/

ARCHER2

- National supercomputer funded by UK Research Councils
  - Archer2 has replaced Archer which was 118,080 cores
  - Now 5,848 compute nodes, each with dual AMD EPYC Zen2 (Rome) 64 core CPUs at 2.2GHz, giving 748,544 cores in total.
  - Estimated peak performance of 28 PFLOP/s
- Mostly open source / free HPC software
- See https://www.archer2.ac.uk/
  - Info for how to apply for access
    - Applications assessed for suitability
- IT Services can help you apply for access

FINAL POINTS

Further info

News

- MOTD when you log into the CSF - please read it
- Problems e.g. system down, can’t log in, minor changes to the service (and other services - e.g storage):
  https://ri.itservices.manchester.ac.uk/services-news/
- Prolonged problems or major changes emailed to all users

https://ri.itservices.manchester.ac.uk/csf3/help/

- CSF Slurm documentation
  https://ri.itservices.manchester.ac.uk/csf3/batch-slurm/
- Job Arrays - multiple similar jobs from a single submission script
  https://ri.itservices.manchester.ac.uk/csf3/batch-slurm/job-arrays-slurm/
- SSHFS - another means of file transfer
  https://ri.itservices.manchester.ac.uk/userdocs/file-transfer/
  Virtual Desktop Service – another means of connecting and running GUIs and logging in from off campus
  https://ri.itservices.manchester.ac.uk/virtual-desktop-service/
- Please give feedback: Quick form at https://goo.gl/forms/zfZyTLw4DDaySnCF3 (choose "*Introduction to HPC (Using CSF)*")

Thank you!