Introduction to High Performance Computing (HPC) – Session 2

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

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

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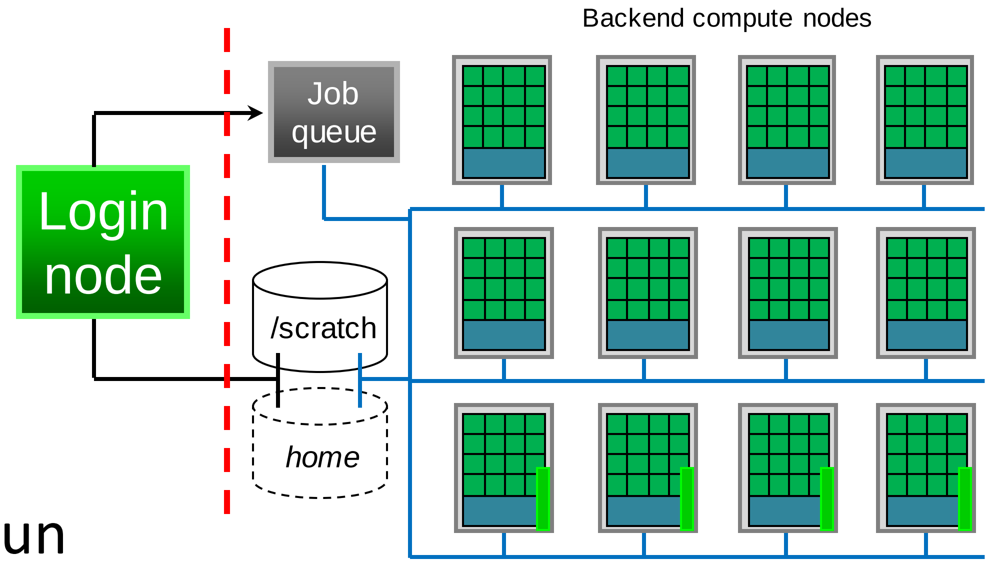
https://ri.itservices.manchester.ac.uk/csf3/

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

Jobs, Jobscripts and the Batch System

- We want to do computational work - "jobs"



- You decide:
  - What program(s) to run
  - Which directory to run from (within *scratch* :-))
  - What resources it needs (#cores, CPU type, memory)
- Write these requirements in a *jobscript*
- Submit your jobscript to the batch system (SGE)
- SGE decides exactly *when* and *where* the job runs

A simple Jobscript – *Serial* (1 core)

#! on first line only (a special line)

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

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

myjob.txt

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

#$ -cwd
#$ -N myjob
#$ -l resource

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

-cwd indicates we'll run from our current (working) directory. Input / output files will usually be found here.

-N (optional). Set the *jobname*. Otherwise will use name of your jobscript as the name.

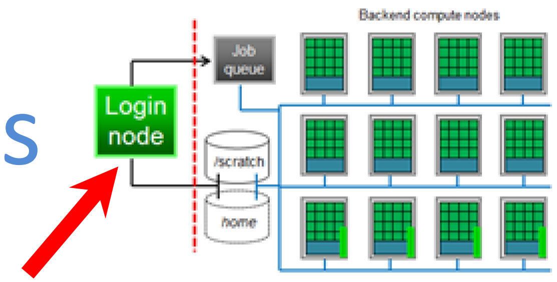
# lines are just comments - anything on the line after it will be ignored.

-l (optional) used to add extra resource requirements e.g. memory, time limits

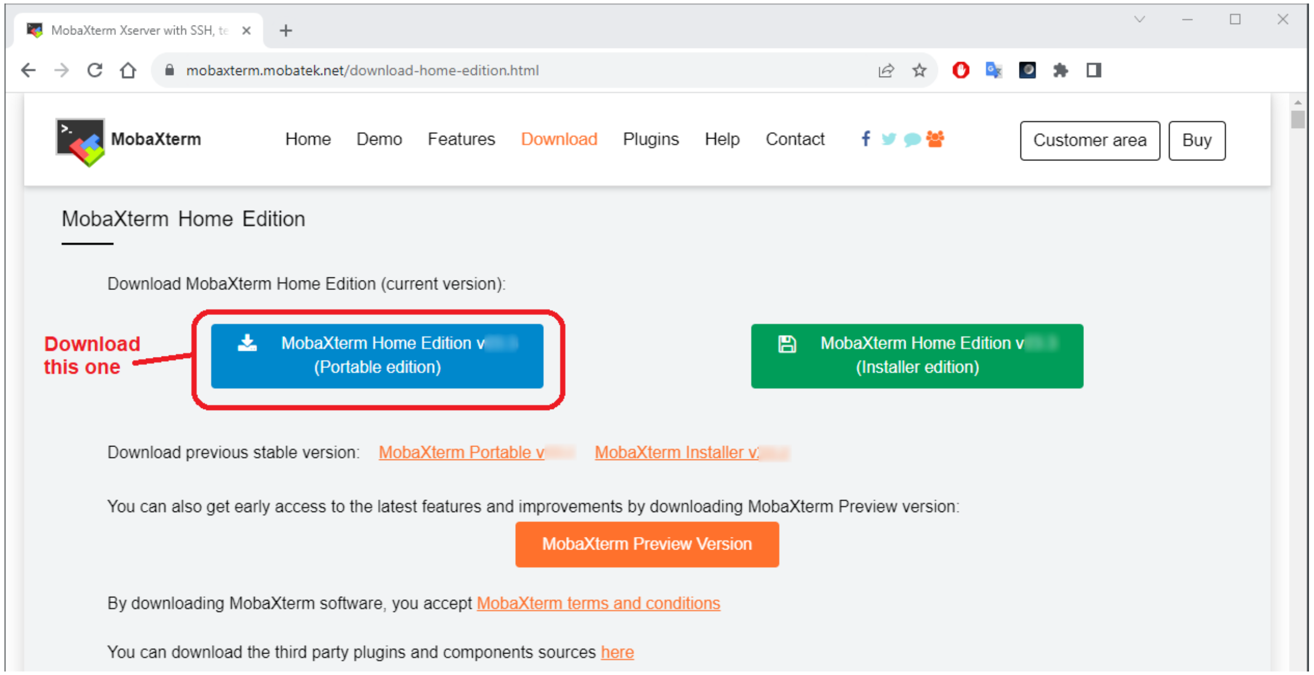
#$ -l course only works on the day of a course.

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

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 Xserver with SSH, te
mobaxterm.mobatek.net/download-home-edition.html
MobaXterm
Home
Demo
Features
Download
Plugins
Help
Contact
Customer area
Buy
Download this one
MobaXterm Home Edition v[redacted] (Portable edition)
MobaXterm Home Edition v[redacted] (Installer edition)
MobaXterm Preview Version

MobaXterm Home Edition

Download MobaXterm Home Edition (current version):

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:

By downloading MobaXterm software, you accept MobaXterm terms and conditions

You can download the third party plugins and components sources here

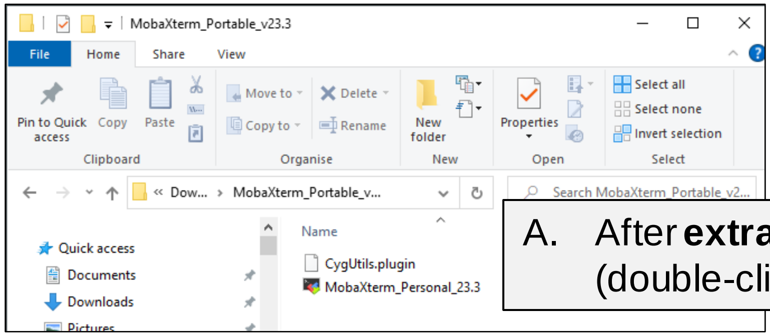
1. Download using the blue box.

2. Once downloaded, *right-click* on the .zip file and select:

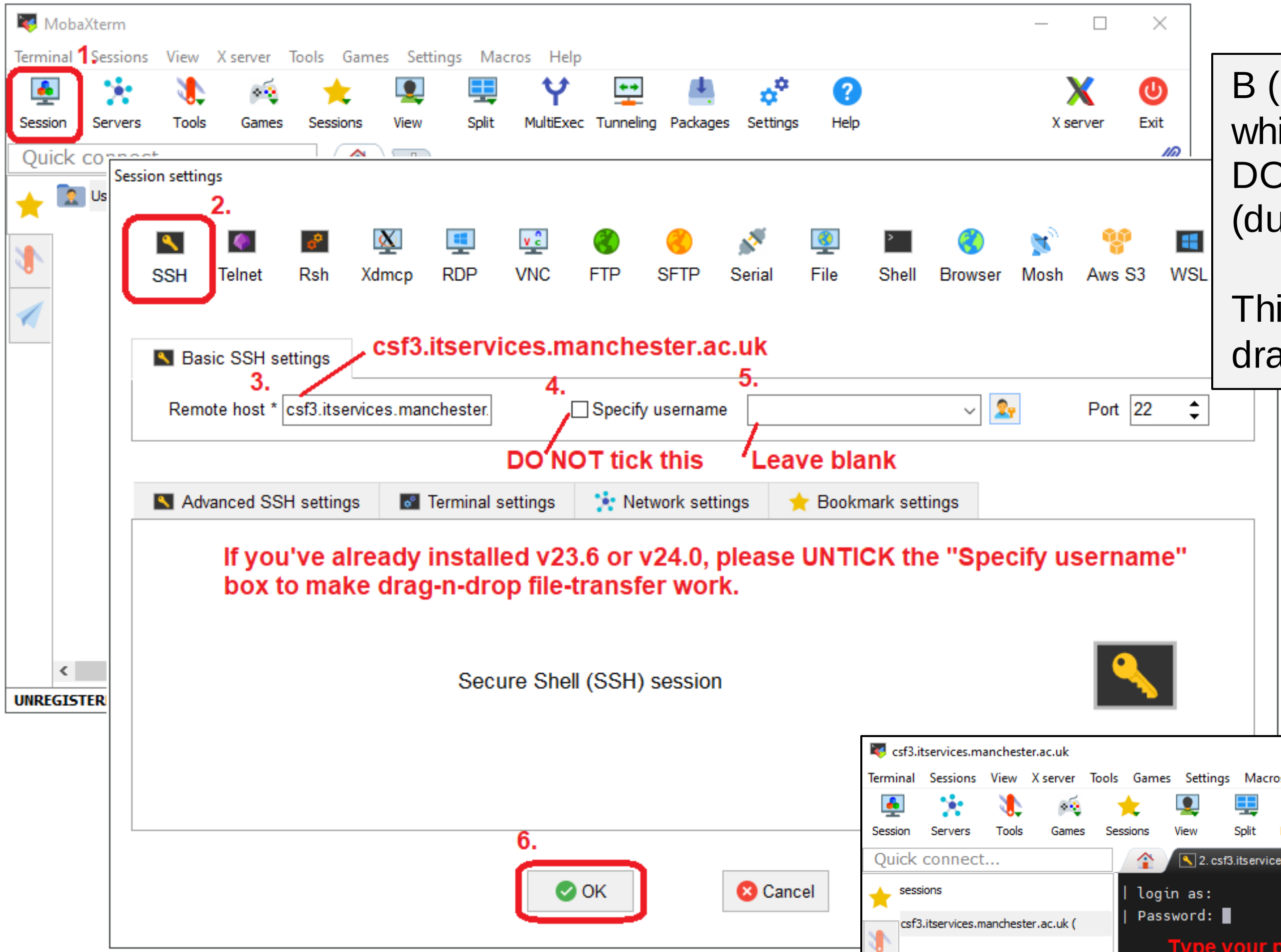
   "Extract all …"

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

MobaXterm



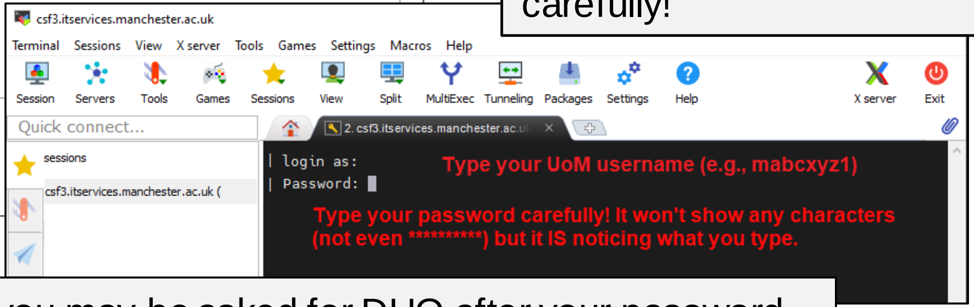
A. After **extracting** the .zip file, start MobaXterm_Personal_*xy.z* (double-click on the icon)



B (1-6). Create a "Session" which saves the CSF's details. DO NOT save your username (due to a bug in MobaXterm.)

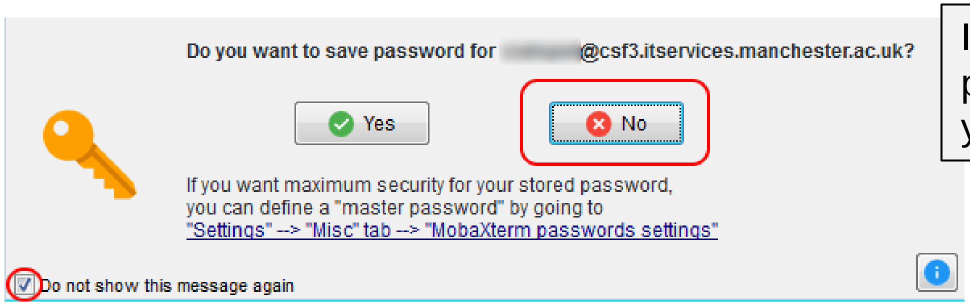
This is needed to make file drag-n-drop work (see later.)

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


csf3.itservices.manchester.ac.uk
Terminal
Sessions
View
X server
Tools
Games
Settings
Macros
Help
Session
Servers
Tools
Games
Sessions
View
Split
MultiExec
Tunneling
Packages
Settings
Help
X server
Exit
Quick connect...
2. csf3.itservices.manchester.ac.u
sessions
csf3.itservices.manchester.ac.uk (
Type your UoM username (e.g., mabcxyz1)
Type your password carefully! It won't show any characters (not even **********) but it IS noticing what you type.

```
login as:
Password:
```

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



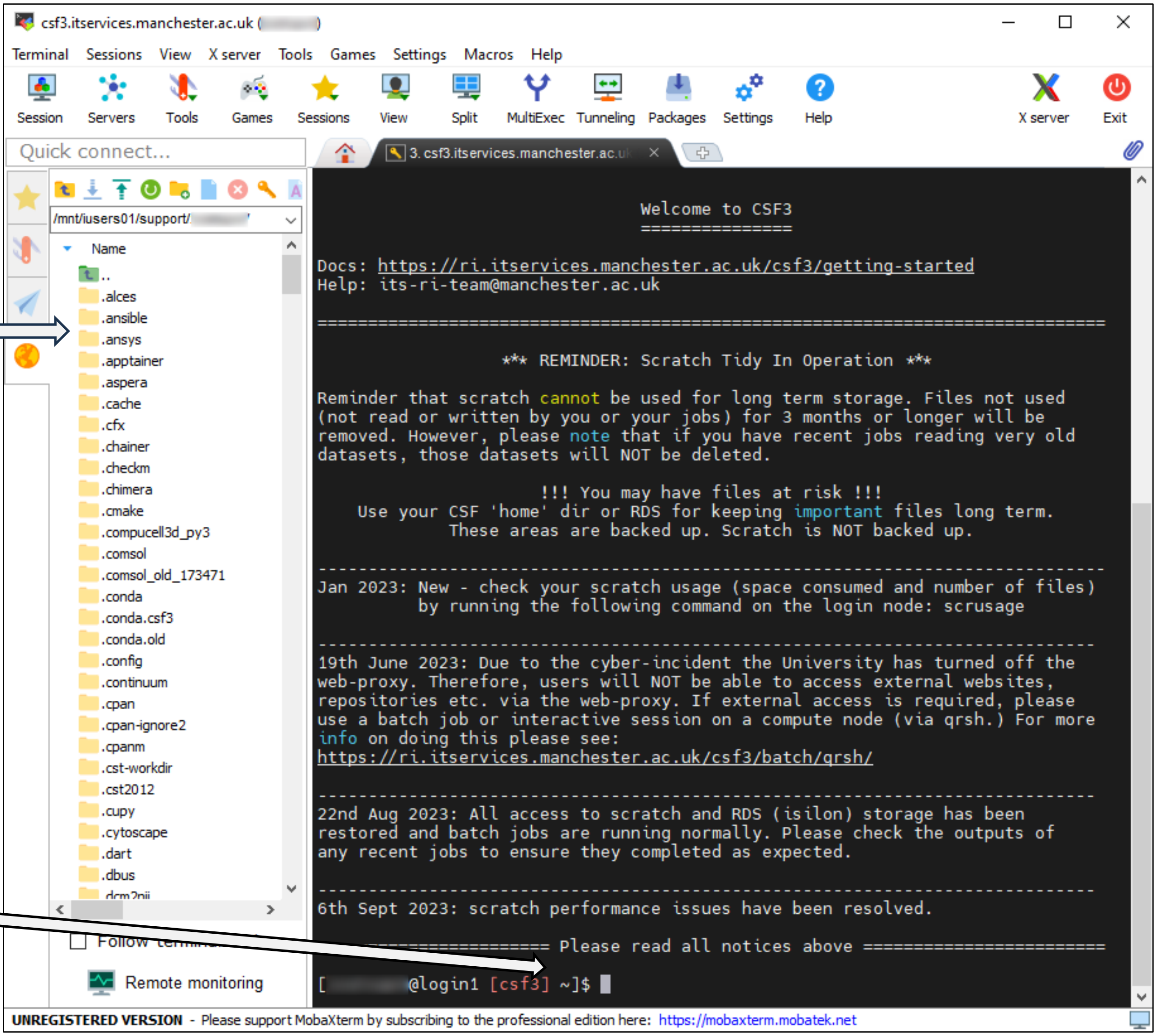
Do you want to save password for [redacted]@csf3.itservices.manchester.ac.uk?

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] ~]$
```

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net

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.)

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` 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 it 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 (hopefully)
- `man module` – man pages for the module command
- Examples:

```
module load apps/binapps/matlab/R2018a
module load apps/intel-17.0/amber/16
module load apps/gcc/R/3.4.2
module unload apps/binapps/starccm/12.04-double
module load compilers/intel/17.0.7
module load tools/gcc/cmake/3.13.2
```

- 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/R2022a

which matlab
/opt/apps/apps/binapps/matlab/R2022a/bin/matlab
```

- This shows that the modulefile made the matlab installation available.
- Hence your job will be able to run that version of matlab.
- If interested, to see all of the settings that a modulefile will make:

```
module show apps/binapps/matlab/R2022a
```

  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)

Extra flag needed to *inherit* all settings from login node (done when job *submitted*)

myjob.txt

```
#!/bin/bash
#$ -cwd
#$ -l resource
#$ -V   # Inherit login node env
        # (note: UPPERcase V)
        # Settings copied when
        # job is submitted

# Let's do some work
R CMD BATCH myscr.R
```

In the jobscript (recommended!)

Extra flag needed to load modulefiles in the jobscript

myjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -l resource


# Load module inside jobscript
module load apps/R/3.4.2

# Let's do some work
R CMD BATCH myscr.R
```

On the CSF login node run the following commands

```
module load apps/R/3.4.2
qsub myjob.txt
```

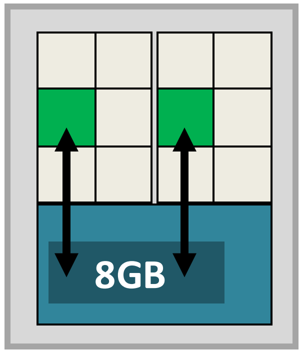
```
qsub myjob.txt
```

PARALLEL COMPUTING

Background

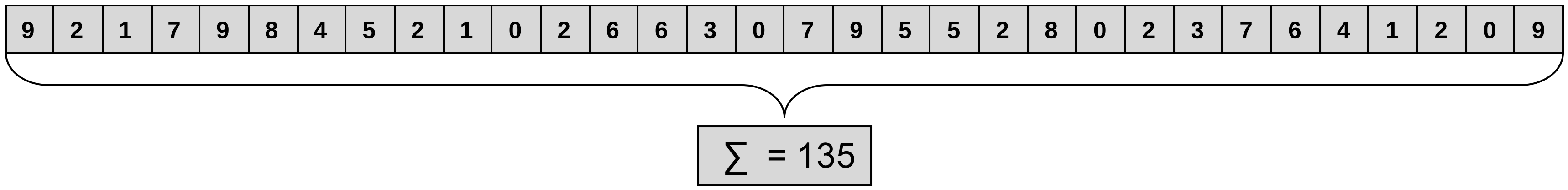
Motivations for Parallel Computing

- CSF compute nodes have multiple CPU cores (up to 32)
- Many apps can use several cores to speed up computation
  - Split the computation over multiple CPU cores?
    - Each core does a small(er) part of the computation
    - "Data parallelism"
  - May need to *combine* partial results together at end
  - Should get overall result quicker
    - Ideally *N* cores giving results *N* times quicker
- Also provides access to more memory
  - Each core has access to ~4GB RAM (std nodes)
    - Ideally *M* cores for *M* times larger problem
- Both of the above!
- Another way: High Throughput Computing
  - Repeated runs of an app with different params or data

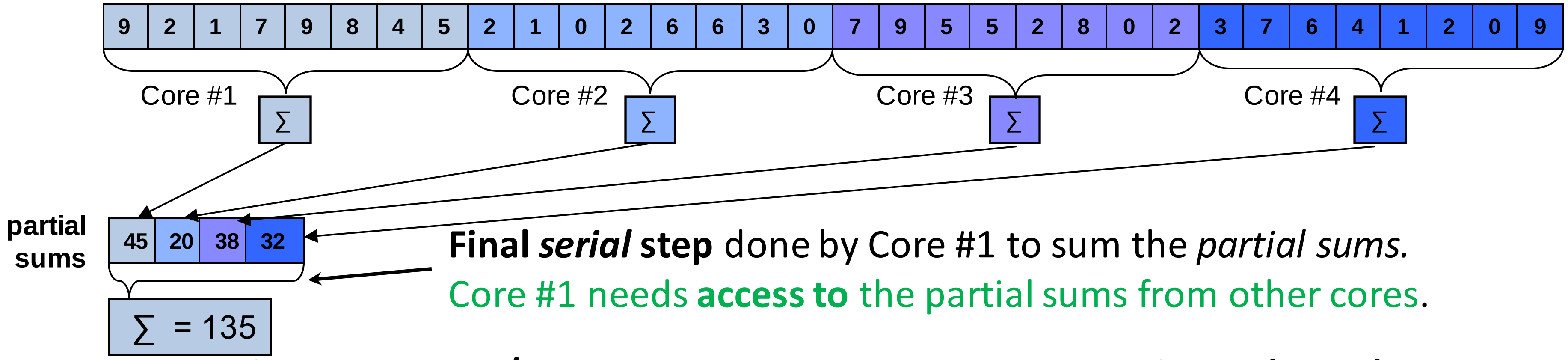


Simple example: sum a list of numbers

- Could do this example manually with 3 friends
- 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

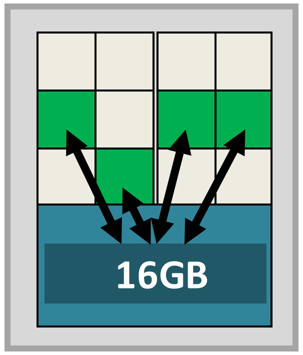


Final *serial* step done by Core #1 to sum the *partial sums.*
Core #1 needs **access to** the partial sums from other cores.

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

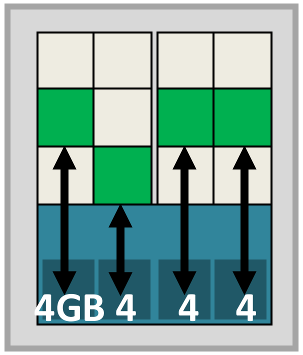
Parallel Job Type #1 - single node

- Running a program on multiple cores of **one** node
  - Typically, one copy of the program runs
    - *"Shared memory"* (all cores see same memory)
    - Cores synchronize access to shared data, results
    - 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

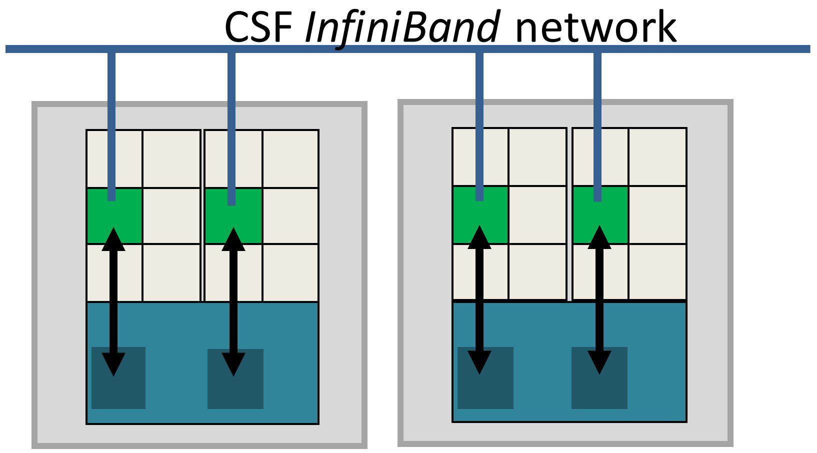


Distributed Memory

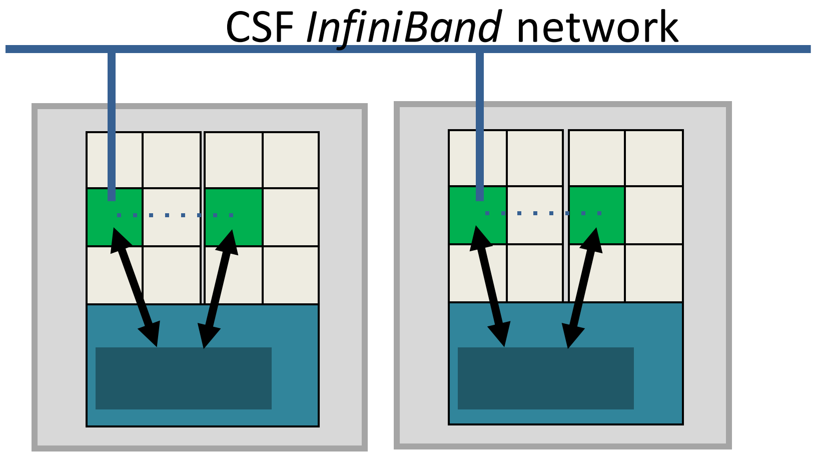
- Your app must have been written to use one (or both) of the above parallel techniques!

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 (as before)
  - Uses more cores than 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!



Distributed Memory



Hybrid Memory (only a few apps)

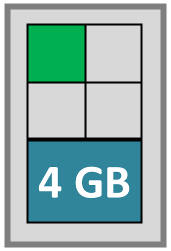
Note: the diagrams only show a few cores in use for simplicity. On the CSF you must use *all* cores in *each* node.

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

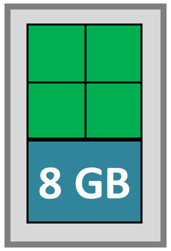
- Lots of *independent* computations. EG:
  - Processing lots of data files (e.g., image files)
  - Running the same simulation many times over with different parameters ("parameter sweeps")
- Run many copies of your program
  - Programs may be serial (single core) but running lots of them at once. They 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

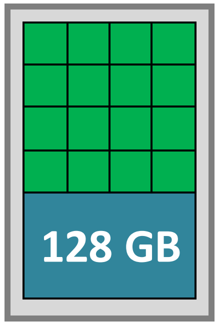
- High Throughput Computing
  - Not all apps do "HPC" / parallel
  - But you have *lots* of data
  - Each image takes 1hr to process (and are *independent* - process in any order)



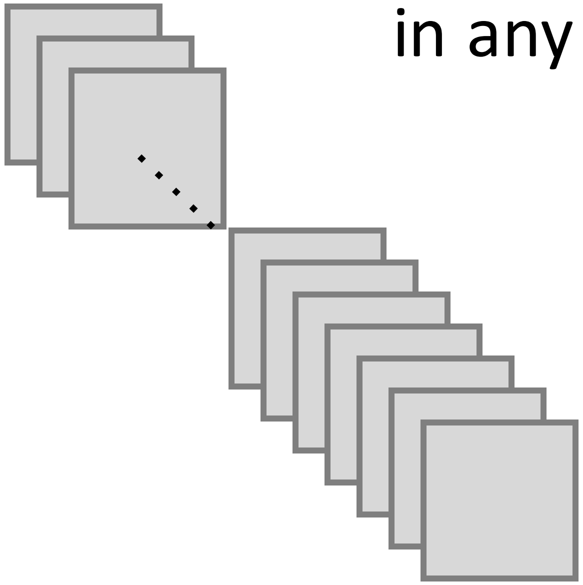
Laptop: 1 copy of software running.
Over 1 year to complete!!

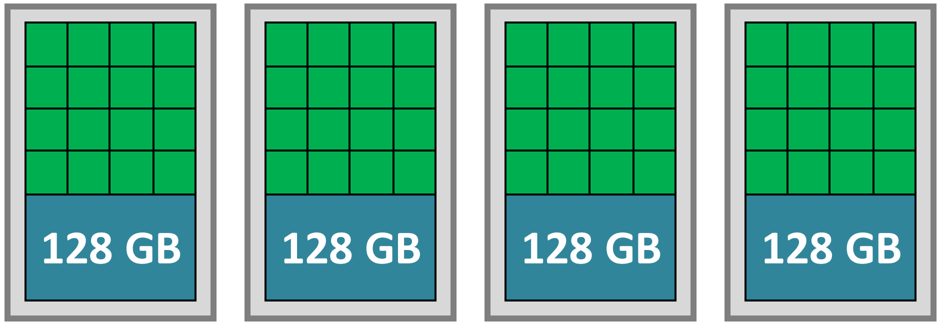


Desktop: 4 cores, 4 copies of software running.
~100 days to complete!



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





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

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

Which style of parallel job to use

- Mostly determined by the capability of your app
  - Is it serial only? Is it multi-core only? Is it MPI / multi-node?

- A serial app will only ever use 1 core
  - But run as HTC jobs they can still process lots of data in parallel
  - Use many cores, running *independent* jobs
- Parallel app using only *shared memory*
  - "OpenMP", "multithreaded", "Java threads", "shared memory"
  - Can only use 1 compute node (2 to 32 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

- Ask batch system to find *N* free cores
  - While matching other requirements (memory, architecture, fast networking etc).

1. Add one extra line in jobscript to request:
   - *parallel environment* (multi-core or multi-node)
   - *and number of cores* to reserve
2. Inform your app how many cores to use
   - The jobscript ensures your job has the correct number of cores available (and other resources)
   - You must ensure your app uses no more!!
     - This is not automatic and varies from app to app

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

#! and #$ see serial jobscript earlier.

-pe indicates we'll run a parallel job in a particular **p**arallel **e**nvironment.

# indicates line is a comment so does nothing.

myparajob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -pe smp.pe 4

# Set up to use a chemistry app
module load apps/intel-17.0/gromacs/2018.4/double

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

# This job runs "gromacs"
mdrun_d
```

smp.pe is the **p**arallel **e**nvironment name. This one means: app will use a single compute node (up to 32 cores.)

4 is the number of **cores** we want to *reserve* in the system. Each **PE** has a maximum allowed.

Any commands we run in our job. They will execute on a backend node that has 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 -pe line. **Our app** wants `OMP_NUM_THREADS` environment variable setting.
Your app might use a different method!

Avoid a common mistake

- Can use **$NSLOTS** for correct number of cores

(Check: *your* app might not use `OMP_NUM_THREADS`)

```
#!/bin/bash --login
#$ -cwd
#$ -pe smp.pe 4

# Set up to use "gromacs"
module load apps/intel-17.0/gromacs/2018.4/double

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

# This job runs "gromacs"
mdrun_d
```

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

`$NSLOTS` is automatically set to number **(4)** given on **-pe** line.
Will be unset in a serial job (no **-pe** line).

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 parallel environment (-pe) & 4 cores

  ```
  $# -pe smp.pe 4
  ```

  CSF-speak for "multiple cores in a single node" **p**arallel **e**nvironment

  - smp=symmetric multi-processor
- Informed the app to use 4 cores via `OMP_NUM_THREADS` environment variable (very common).
  - Special `$NSLOTS` variable always set to number of cores on PE line

Parallel jobscript - Multi-core (cont…)

- As with the serial job submit it to the system with `qsub` and monitor with `qstat`
- It may take longer for *N* cores to become free in the system
- You'll get the usual output files
  - *`jobname.oJobID`* and *`jobname.eJobID`*

Parallel Jobscript – multi-*node*

#! and #$ lines from serial jobscript earlier.

mpi-24-ib.pe is the **p**arallel **e**nvironment name. This one means: app will use multiple compute nodes (all 24 cores **must** be used on each) and has fast **I**nfini**B**and networking between the nodes.

```
#!/bin/bash --login
#$ -cwd
#$ -pe mpi-24-ib.pe 48

# Set up to use MrBayes
module load apps/gcc/mrbayes/3.2.6

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

-pe indicates we'll run a parallel job in a particular **p**arallel **e**nvironment.

48 is the number of **cores** we want to *reserve* in the system. Each PE has a maximum allowed.

# indicates line is a comment so does nothing.

The commands we run in our job. They will execute on a backend node that has required number of cores free. `pmb` is the app name.

Must somehow inform the app how many cores we *reserved*. `$NSLOTS` is automatically set to number(48) given on -pe line. Our app is started via `mpirun` which has a `-n` *`numcores`* flag

Parallel jobscript - Multi-node (cont…)

- A multi-node (but also 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) & 48 cores

  ```
  $# -pe mpi-24-ib.pe 48
  ```

  CSF-speak for "multiple cores in multiple nodes" **p**arallel **e**nvironment (where all 24 cores per node will be used)

  - mpi=message passing interface, ib=InfiniBand (fast network)
- Informed the app to use 48 cores via `mpirun -n $NSLOTS` (very common).
  - `mpirun` starts multiple copies of an MPI app on allocated nodes
  - Special `$NSLOTS` variable always set to number of cores on PE line

Parallel Environments

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

PE Name	Description
`smp.pe` *N*	2-32 cores, single compute node. ~4-5GB per core. Jobs will be placed on Ivybridge (max 16 cores), Haswell / Broadwell (max 24 cores), Skylake (max 32 cores).
`-l` *architecture*	**Ignore** (`ivybridge` or `haswell` or `broadwell` or `skylake`)
`-l short`	4GB/core Ivybridge(**1 hour runtime limit**). For test work. Max job size of 12 cores.
`-l mem256`	16GB/core Haswell. Max job size of 16 cores.
`-l mem512`	32GB/core Haswell or Ivybridge. Max job size of 16 cores.

PE Name	Description
`mpi-24-ib.pe` *N*	Multi-node jobs only, 48 cores *or more*, multiple of 24 cores. Intel Haswell cores. ~5GB per core, 7 day runtime limit. Fast InfiniBand networking between the nodes.

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

Choosing your Parallel Environment (PE)

- Choosing the PE is fairly simple, but:
  - Check the app's webpage for advice and examples
    https://ri.itservices.manchester.ac.uk/csf3/software
  - Check the PE page for limits on number of cores
    https://ri.itservices.manchester.ac.uk/csf3/batch/parallel-jobs
  - Only use **`#$ -l`** ***`resource`*** if necessary
- If writing/compiling your own apps, multi-node (MPI) jobs require an MPI modulefile
  - EG:

```
module load mpi/intel-19.1/openmpi/4.1.1
```

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, vary the number of cores
  - Plot time versus num cores
  - Easy to do on CSF: remove PE setting from jobscript (and -N *name* if used), add PE to qsub command:

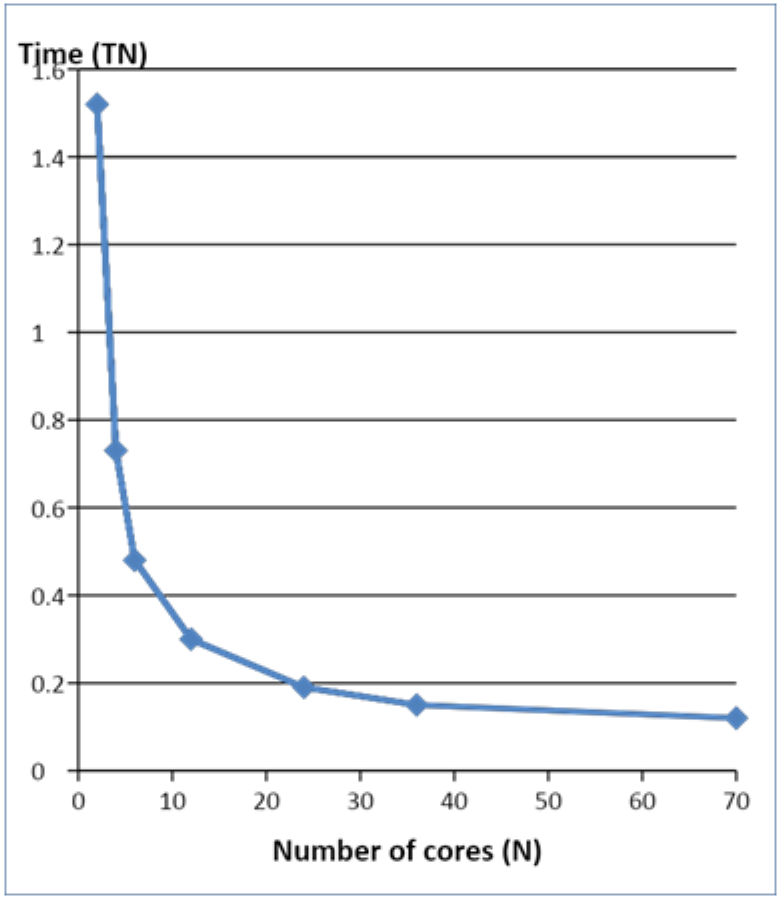
```
qsub -pe smp.pe 2 myjobscript.txt
qsub -pe smp.pe 4 myjobscript.txt
qsub -pe smp.pe 8 myjobscript.txt
```

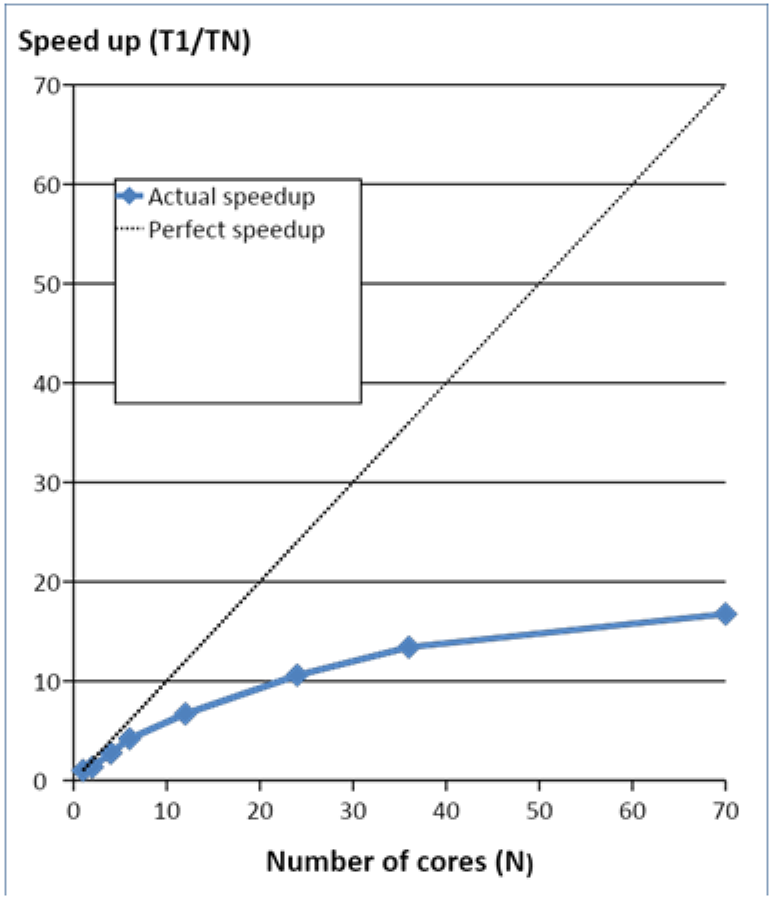
To Assess Parallelism

- 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 (no handout)

Practical Session 4 (Intro)

- We will measure parallel efficiency for a similar matrix multiplication program
- But this time
  - Same problem size: 2000 x 2000 matrices
  - Repeats 5 times with additional maths ops on elements
  - (*sort of simulates an app solving equations*)
- Hardware reserved today
  - Two compute nodes
  - 24 cores per node (for today's course)
    - Shared memory jobs: up to 24 cores
    - Distributed memory jobs: 48 cores
  - Faster InfiniBand networking used between nodes

Practical Session 4 (Intro)

- This is a distributed memory MPI program written in C
  - Already compiled: executable named `pmm.exe`
- Jobscript for a parallel job must specify:
  - Parallel environment (where job runs on CSF)
  - Number of cores (2 or more)
- For one compute node (2-24 cores) can use
  - Shared memory parallel env: **`smp.pe`**
- For two compute nodes (48 cores) can use
  - Distributed memory parallel env: **`mpi-24-ib.pe`**

Practical Session 4 - Part 1

- To set up the environment for the job, do the following:
  - `module load mpi/intel-19.1/openmpi/4.1.1`
- Submit the job to the batch system
  - `qsub pmm_jobscript`
- Immediately edit `pmm_jobscript` to change number of cores then resubmit (don't need to wait for previous job to run)
  - Use 1, 2, 4, 8, 12, 16, 24 cores.
  - Can also change the job name (`-N run_pmm_np2`) to make output filenames different (change the number of cores in the name - can't use `$NSLOTS` here sadly).
- Look at the output from SGE to find runtimes
  - Look in the `run_pmm_np2.o`*`JobID`* file (use `cat`, `less`, or `gedit`)
  - Check the `ru_wallclock` (seconds) using `qacct -j` *`JobID`*
- Calculate the speed-up or efficiency for your runs

Practical Session 4 - Part 2

- Try 48 core job using `mpi-24-ib.pe`
  - Does is go twice as fast as the 24-core job?
- View the CSF documentation that lists the different parallel options

  https://ri.itservices.manchester.ac.uk/csf3/batch/parallel-jobs/
- No pdf exercise sheet - see previous few slides - you should be more familiar with all of the tasks needed to complete this exercise now.

MULTIPLE SIMILAR JOBS

High Throughput Computing and "Job arrays"

Multiple Runs of Same App

- We want to make many runs of an application 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? `qsub jobscript-all.txt`

jobscript-all.txt
```
#!/bin/bash --login
#$ -cwd

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
#$ -cwd
myapp.exe -in mydata.1.tif -out myresult.1.tif
```

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

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

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 - "Job Array" Jobscript

-t makes the jobscript automatically run a specified number of times. These are called **tasks**. Each is numbered uniquely 1,2,3….1000.

1-1000 (start-end) says how many tasks to run and how they should be numbered. Note: **Cannot** start at **0**. Can use start-end:increment to increase the ID by more than 1.

arrayjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000

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

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

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

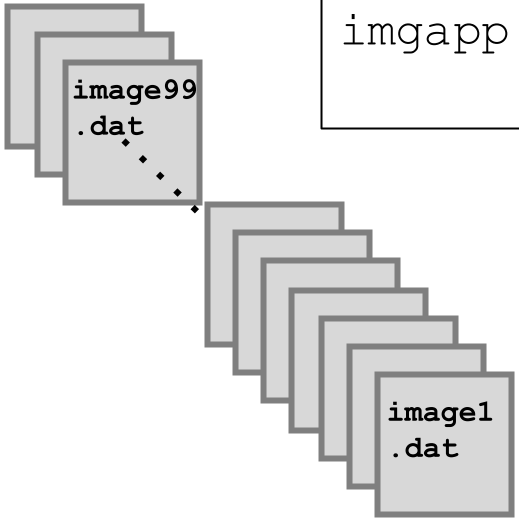
"Job Array" Jobscript

- Our app is serial (1-core) so no `#$ -pe` line
  - But you *could* add one if your app is multi-core
- The total number of tasks can be 100s, 1,000s, 10,000s (seen over 50,000 on CSF)
- The system will run many of the tasks in parallel
  - 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 `#$ -t` line is easy. Using the *task id* number *creatively* is the key to job arrays.

The `$SGE_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 $SGE_TASK_ID in filenames:

```
#$ -t 1-1000
imgapp -i image_${SGE_TASK_ID}.dat \
       -o image_${SGE_TASK_ID}.png
```



Task 1 reads `image_1.dat` writes `image_1.png`

Task 2 reads `image_2.dat` writes `image_2.png`

…

Task 1000 reads `image_1000.dat` writes `image_1000.png`

The `$SGE_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:

```
#$ -t 1-4000
# Read the Nth line of filenamelist.txt and save in variable MYFILE
MYFILE=$(awk "NR==${SGE_TASK_ID} {print}" filenamelist.txt)
# Now use whatever the value of variable is in the next command
myapp.exe -input ${MYFILE} -output ${MYFILE}.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 file **must** match number of tasks
- To get number of lines in master file use:
  `wc -l filenamelist.txt`
- NB: VAR=$(*command arg1 arg2…*) captures output from *command* and assigned to variable VAR

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

The `$SGE_TASK_ID` variable (3)

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

```
#$ -t 1-50
# Read the Nth line of dirnamelist.txt and save in variable SUBDIR
SUBDIR=$(awk "NR==${SGE_TASK_ID} {print}" dirnamelist.txt)
# Now use whatever the value of variable is in the next command
cd ~/scratch/experiments/${SUBDIR}
mdrun_d
```

`dirnamelist.txt`

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

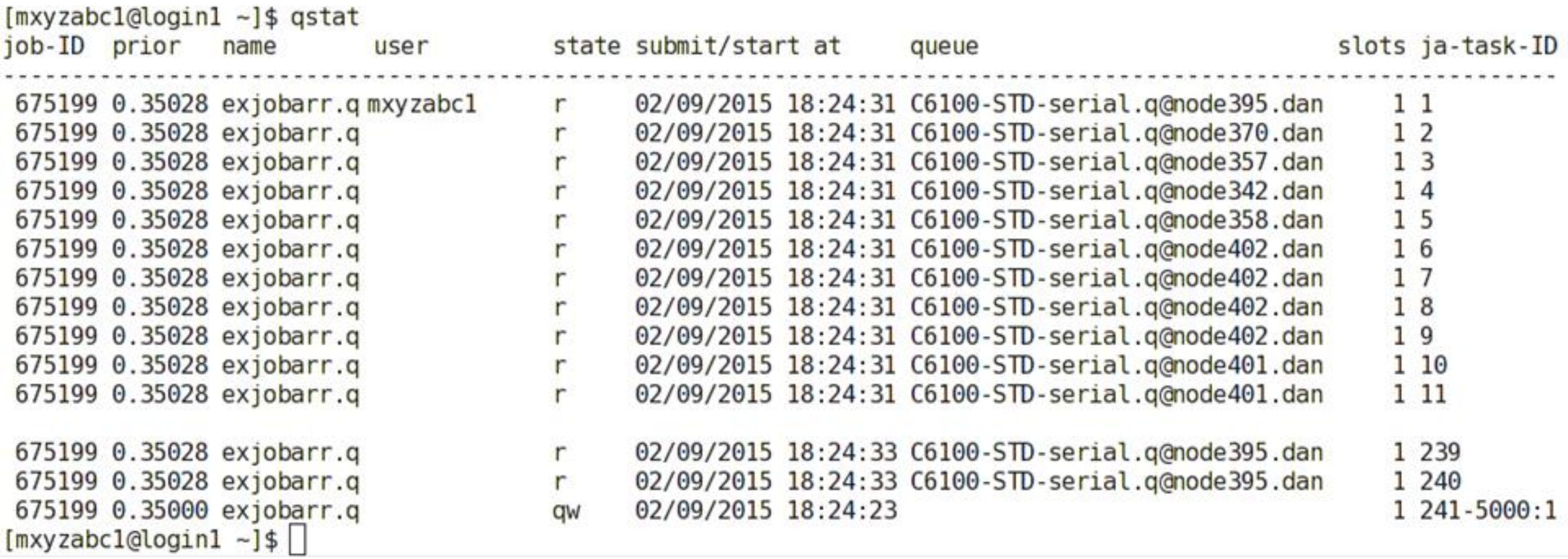
Task 1 reads `znc24/100p/a1` as subdir name
Task 2 reads `znc24/200p/b2` as subdir name
…

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

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

Jobarrays and qstat, qdel

- qstat shows running tasks and tasks still waiting



```
[mxyzabc1@login1 ~]$ qstat
job-ID  prior   name       user         state submit/start at     queue                          slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------
 675199 0.35028 exjobarr.q mxyzabc1     r     02/09/2015 18:24:31 C6100-STD-serial.q@node395.dan     1 1
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node370.dan     1 2
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node357.dan     1 3
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node342.dan     1 4
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node358.dan     1 5
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node402.dan     1 6
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node402.dan     1 7
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node402.dan     1 8
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node402.dan     1 9
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node401.dan     1 10
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:31 C6100-STD-serial.q@node401.dan     1 11

 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:33 C6100-STD-serial.q@node395.dan     1 239
 675199 0.35028 exjobarr.q              r     02/09/2015 18:24:33 C6100-STD-serial.q@node395.dan     1 240
 675199 0.35000 exjobarr.q              qw    02/09/2015 18:24:23                                    1 241-5000:1
[mxyzabc1@login1 ~]$ 
```

- qdel can remove all tasks or just some

`qdel 675199`	Remove all running and waiting
`qdel 675199 -t 300`	Remove task 300 (a bit strange)
`qdel 657199 -t 4000-5000`	Remove last 1000 tasks

Jobarray Output Files

- You'll get the usual output .o file and error .e file (hopefully empty) but
  - One per task
  - Potentially a lot of files!
- Look for

  `jobname.oJobID.TaskID` and

  `jobname.eJobID.TaskID`
- You should delete empty / unwanted files soon and often

PRACTICAL SESSION 5

Job array examples

Practical Session 5 (job array)

- Write a small job array to process some images
- Go to `~/training/RCSF/examples/hudf_images/`
  - Has some images from Hubble Ultra Deep Field
    https://esahubble.org/images/heic0611b/
    Credit: NASA, ESA, and S. Beckwith (STScI) and the HUDF Team
  - To list them: `ls -l`   To view one: `eog hudf_1.png`
  - Write a serial jobscript to process an image using:

    ```
    module load apps/binapps/anaconda3/2021.11
    python process.py filename.png
    ```
  - Add the jobarray **`#$ -t`** line to it (with *start* and *end*) and use **`$SGE_TASK_ID`** in the image filename
- Check the results in `xxxxx.oJobID.TaskID`
- **Q**: Which image has most objects detected?
- On login node run: `eog filename.png` to see images
- No exercise sheet again ;-)

Practical Session 5 (advanced job array)

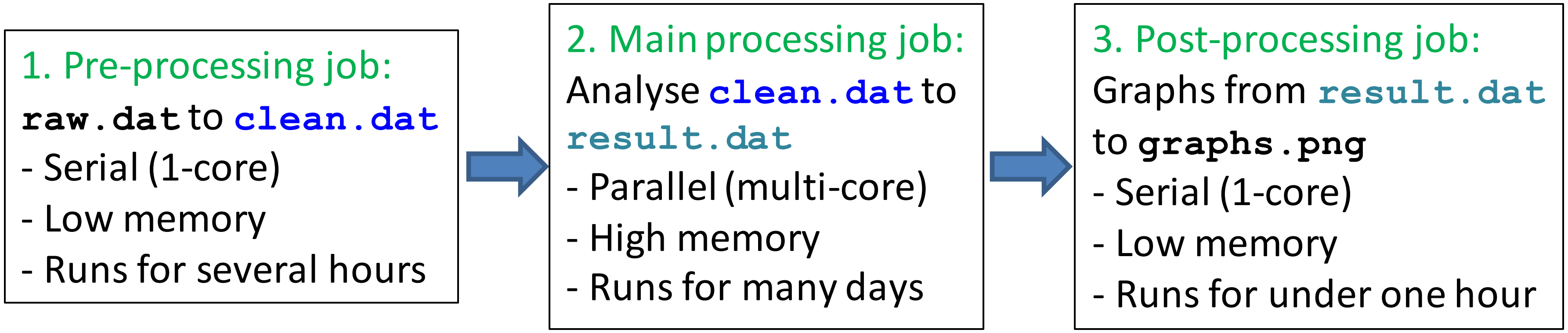
- Write a small job array to run an app with different input parameters (taken from a list of input params)
- Go to `~/training/RCSF/examples/`
- You should now be able to
  - Get number-of-lines in the **`numberlist.txt`** file (the list of inputs)
  - Begin writing a serial jobscript
  - Add the jobarray **`#$ -t`** line to it (with *start* and *end*)
  - Optional: Use CSF3 website to find the **`#$`** flag to "join" .o and .e outputs into only the .o file (for each task) to reduce number of files.
- Each task should read a line from **`numberlist.txt`** (each line in the file contains an integer)
  - Use that integer as a command-line param to a prime-factor program:
    `./prime_factor.exe`
- Check the results in `xxxxx.o`*`JobID`*`.`*`TaskID`*
- No exercise sheet again ;-)

JOB PIPELINES

Ordering jobs

A Job Pipeline (aka workflow)

- Suppose you have several jobs that:
  - Need to run in a specific order - a job "pipeline"
    - There is a *dependency* between jobs
  - Each might have different CPU-core or 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 mem)
  - May go over 7-day runtime limit

mypipeline_bad.txt

```
#!/bin/bash --login
#$ -cwd
#$ -l mem256              # Uses a high-memory node and
#$ -pe smp.pe 16          # … reserves 16 cores
                          # … for duration of job
module load apps/………

# First 'job' (serial)
preproc -in raw.dat -out clean.dat
# Second 'job' (parallel, needs lots of memory)
mapper -p $NSLOTS -in clean.dat -out result.dat
# Third 'job' (serial)
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
#$ -cwd
module load apps/………
# First 'job' (serial)
preproc -i raw.dat -o clean.dat
```

A parallel, high-mem job

secondjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -l mem256             # Uses a high-memory node and
#$ -pe smp.pe 16         # … reserves 16 cores
module load apps/………
# Second 'job' (parallel)
mapper -p $NSLOTS -i clean.dat -o result.dat
```

A serial job (no wasted cores)

thirdjob.txt

```
#!/bin/bash --login
#$ -cwd
module load apps/………
# Third 'job' (serial)
drawGraphs -i result.dat -o graphs.png
```

`qsub firstjob.txt`

(now wait until this job has finished before submitting the next one!)

`qsub secondjob.txt`

(now wait until this job has finished before submitting the next one!)

`qsub thirdjob.txt`

(now wait until this job has finished before submitting the next one!)

How to do it - Job Dependencies

- Split in to multiple jobs, submit all jobs, let SGE manage it!

The jobscripts are as before, but …

firstjob.txt

```
#!/bin/bash --login
#$ -cwd
module load apps/………
# First 'job' (serial)
preproc -i raw.dat -o clean.dat
```

The jobscript filename is used for the name of the job (if no **#$ -N *name***) flag supplied.

… added a job dependency

secondjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -l mem256              # Uses a high-memory node and
#$ -pe smp.pe 16          # … reserves 16 cores
#$ -hold_jid firstjob.txt
module load apps/………
# Second 'job' (parallel)
mapper -p $NSLOTS -i clean.dat -o result.dat
```

… added a job dependency

thirdjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -hold_jid secondjob.txt
module load apps/………
# Third 'job' (serial)
drawGraphs -i result.dat -o graphs.png
```

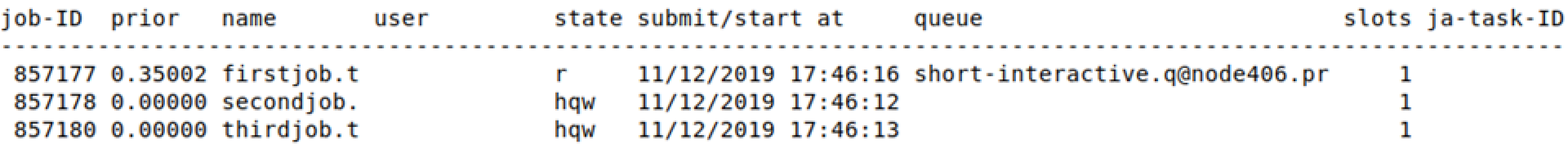
-hold_jid *name* (or *jobid*) makes the job automatically wait for the named (earlier) job **to finish**. The name can be a **job name** or a **job ID** number.

- Submit all of your jobs in one go

```
qsub firstjob.txt
qsub secondjob.txt
qsub thirdjob.txt
```

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)
- `qstat` shows `hqw` for jobs on hold



```
job-ID  prior   name       user         state submit/start at     queue                          slots ja-task-ID
-----------------------------------------------------------------------------------------------------------------
 857177 0.35002 firstjob.t              r     11/12/2019 17:46:16 short-interactive.q@node406.pr     1
 857178 0.00000 secondjob.              hqw   11/12/2019 17:46:12                                    1
 857180 0.00000 thirdjob.t              hqw   11/12/2019 17:46:13                                    1
```

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

Job Dependencies

- Using job names can become messy
  - Generalise using the job ID and `qsub` command-line
  - Firstly, remove all **`#$ -hold_jid`** ***`name`*** lines from the jobscripts!
  - Then add `-hold_jid` *`name`* to `qsub` command-line
  - Use `-terse` flag to get *just* the job ID of the submitted job (instead of 'long' message):
    - **`qsub myjobscript`**
      `Your job 19886 ("myjobscript") has been submitted`
    - **`qsub -terse myjobscript`**
      `19886`
  - Capture output of command into shell variable

```
JOBID=$(qsub -terse firstjob.txt)
JOBID=$(qsub -terse -hold_jid $JOBID secondjob.txt)
JOBID=$(qsub -terse -hold_jid $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

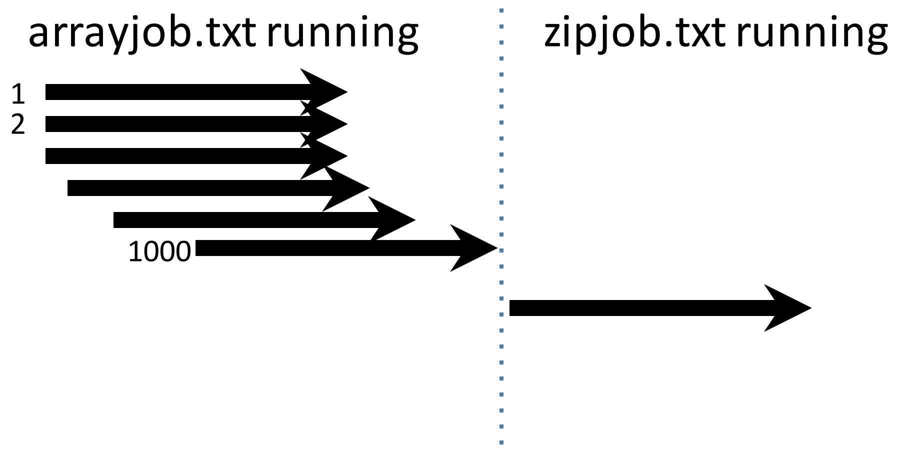
```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000           # Job array with 1000 tasks
convert img.${SGE_TASK_ID}.tif img.${SGE_TASK_ID}.pdf
```

zipjob.txt

```
#!/bin/bash --login
#$ -cwd
#$ -hold_jid arrayjob.txt
zip conference.zip img.*.pdf
```

Add a job dependency

```
qsub arrayjob.txt
qsub 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

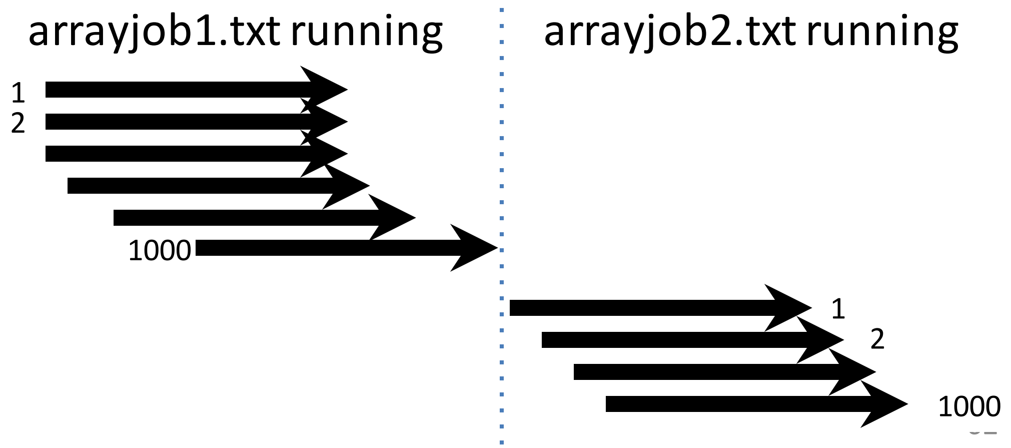
```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000           # Job array with 1000 tasks
someapp data.${SGE_TASK_ID}.xyz data.${SGE_TASK_ID}.dat
```

arrayjob2.txt

```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000           # Job array with 1000 tasks
#$ -hold_jid arrayjob1.txt
someotherapp data.${SGE_TASK_ID}.dat res.${SGE_TASK_ID}.dat
```

Add a job dependency

```
qsub arrayjob1.txt
qsub arrayjob2.txt
```



Job-Array Dependencies (3)

- Job array *tasks* can wait for other *tasks* to finish
  - A task in *second* job array waits for same task in first

arrayjob1.txt

```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000                # Job array with 1000 tasks
someapp data.${SGE_TASK_ID}.xyz data.${SGE_TASK_ID}.dat
```

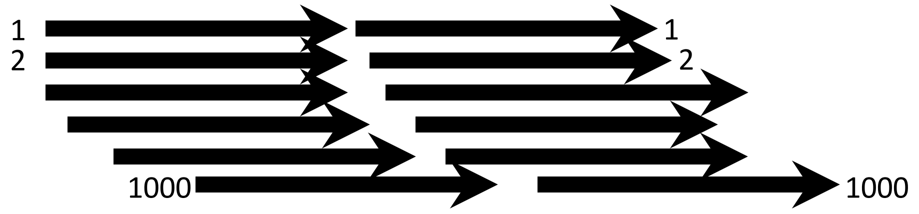
arrayjob2.txt

```
#!/bin/bash --login
#$ -cwd
#$ -t 1-1000                # Job array with 1000 tasks
#$ -hold_jid_ad arrayjob1.txt
someotherapp data.${SGE_TASK_ID}.dat res.${SGE_TASK_ID}.dat
```

Add a job *array* (_ad) dependency

```
qsub arrayjob1.txt
qsub arrayjob2.txt
```

arrayjob1.txt tasks running then arrayjob2.txt tasks



INTERACTIVE AND GPU COMPUTING

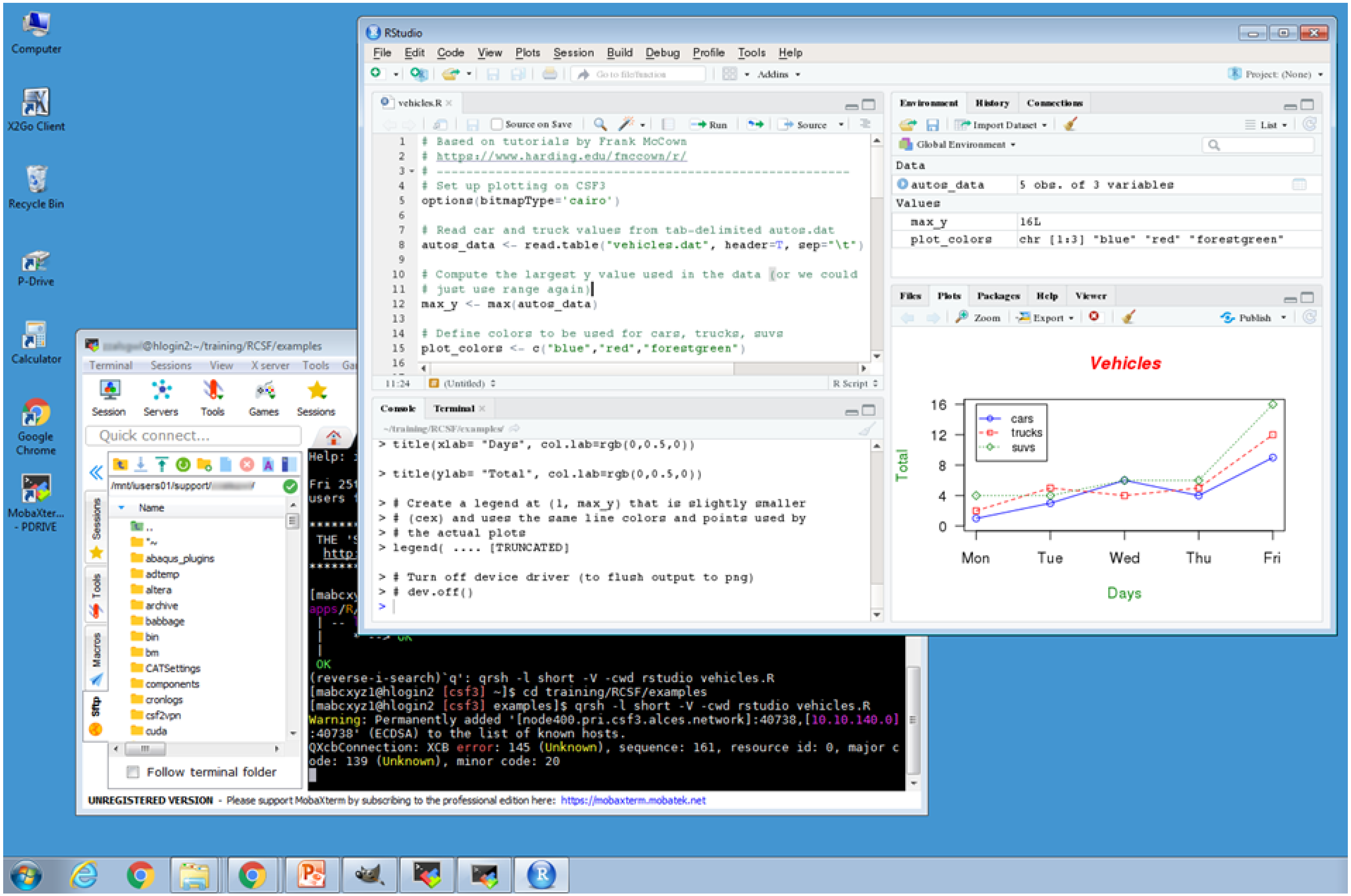
Compute apps with GUIs

Interactive work

- Some apps (eg Rstudio, VMD, molden, paraview) may have a GUI but should not be run on the login node!!
- Use the `qrsh` command to get an *interactive session* on a compute node

```
    module load apps/binapps/rstudio/1.1.463
    qrsh -l short -V -cwd rstudio vehicles.R
```

- No dedicated resource, priority to batch jobs
- Only 4GB per core (contact its-ri-team@manchester.ac.uk if you need more)
- Remember - it is a GUI app, as with `gedit` you need Xwindows running on your PC (MobaXTerm, X-Quartz, Linux)
- Remember to exit your GUI app when you have finished so the resource is made available for others
- Better options: Virtual Desktop Service and InCLine (Interactive Computational LInux Environment) also known as iCSF.



```
# 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()
> 
```

```
Help: i
Fri 25t
users t
*******
 THE 'S
  http:
*******

[mabcxy
apps/R/
 | -- 
 |
 |
 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
```

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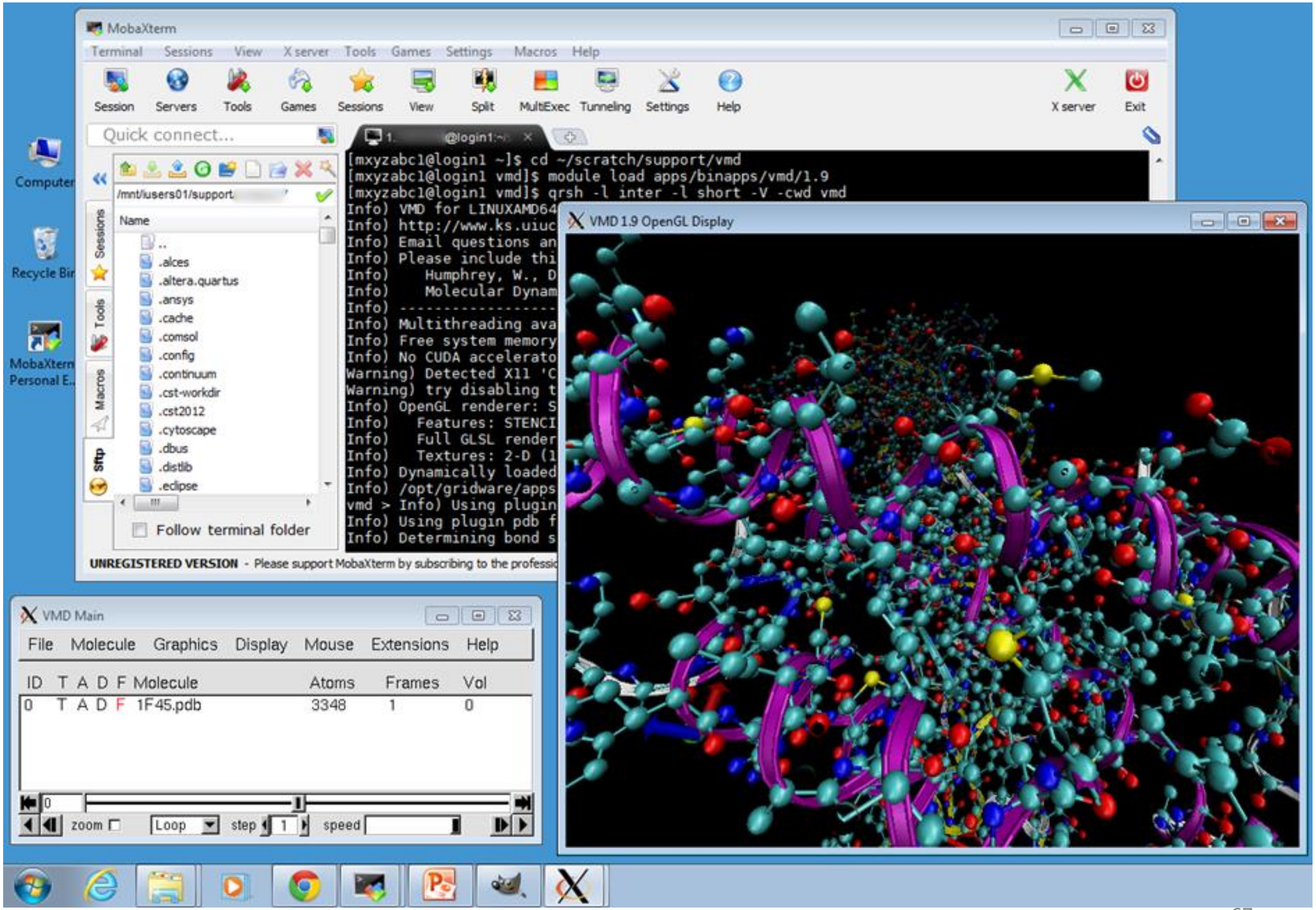
MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Settings Help X server Exit
Quick connect...
1. @login1:~
Sessions Tools Macros Sftp
Computer
Recycle Bin
MobaXterm Personal E...
VMD 1.9 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
zoom Loop step 1 speed

/mnt/iusers01/support

Name
..
.alces
.altera.quartus
.ansys
.cache
.comsol
.config
.continuum
.cst-workdir
.cst2012
.cytoscape
.dbus
.distlib
.eclipse

Follow terminal folder

```
[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
```

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

Nvidia GPUs

- CSF3 has 132 x Nvidia GPUs

68 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 "Skylake"
192GB RAM host node + InfiniBand

64 x Ampere A100 GPUs in total – 4 GPUs/node
80GB GPU memory, Mem bandwidth 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 + InfiniBand

- Faster for certain tasks
  - All cores perform same instruction
  - Operating on different items of data
- Code can be difficult to write (CUDA, OpenCL)
- Several CSF apps already support GPUs

OTHER PARALLEL HARDWARE

What else is available?

HPC Pool

- Dedicated pool for “true” 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 "PE" name and an account code.)
  - Lightweight application process – must be made by PI
  - Currently free

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

ITS Condor Service

- Formerly EPS Condor Pool
  - Condor manager HTC workflow
  - Condor pool is a group of cores available for use
  - Condor sends out jobs to the pool (similar to SGE)
  - Often cores become available when PCs are idle
    - UoM public clusters over night
    - Dedicated pool always available
- Condor pool available to all researchers for free
  - More than 2000 cores (if all configured PCs available)
  - Suitable for short lightweight computations
  - Can now burst to the cloud (AWS)!!!
  - See https://ri.itservices.manchester.ac.uk/htccondor/

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

Scafell Pike

- Hartree Centre
  - 25,728 Intel Skylake + ~55,680 Xeon Phi cores
- Common open source HPC software installed
- Focus on industry / academia collab. projects
- Contact Research IT for advice

N8 Bede (NICE)

- 32 IBM Power 9 dual-CPU nodes
- Each node comprises 4 NVIDIA V100 GPUs and high performance interconnect.
- 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/

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

its-ri-team@manchester.ac.uk

- More SGE options/parameters
  https://ri.itservices.manchester.ac.uk/csf3/batch/qsub-options/
- Job Arrays - multiple similar jobs from a single submission script
  https://ri.itservices.manchester.ac.uk/csf3/batch/job-arrays/
- 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!