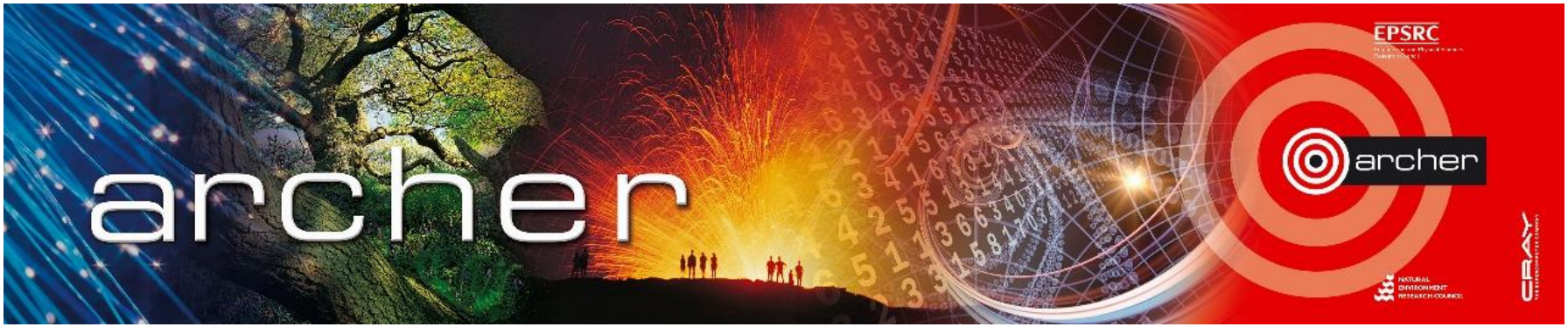

Welcome!

Virtual tutorial starts at 15:00 GMT

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PBS Job Submission

ARCHER Virtual Tutorial, Wed 11th February 2015

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Reusing this material

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A day in the life of a PBS job

Submitted to the PBS batch system using qsub

Held in a queue until able to run

Executed

Parallel jobs launched from script

Completed and job output written

Batch script written with a text editor

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Conception: batch script written …

- What is a batch script?
  - a list of commands that are executed in order exactly as if you typed them into the shell on the command line
  - recommended to use bash
- Lines starting "#" are comments
- Except …
  - **`#!`** is special to operating system
  - **`#!/bin/bash --login`** # Run script as if a bash login session
- and
  - **`#PBS`** is special to batch system
  - **`#PBS -N myjob`** # Pass on as arguments to qsub

Great! So I can run the batch script in advance to check it works since it's just a bunch of commands

I'm afraid it's not that simple

Why?

Your batch script runs on a different computer in a different environment

So some commands that work on the login nodes won't work under PBS?

Actually, some commands that *don't* work on the login nodes *will* work under PBS

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Birth: submitted to batch system

```
user@archer> qsub -l select=6 myjob.pbs
123456.sdb
```

- PBS takes a *copy* of your batch script and stores it
  - ascertains resource requirements (e.g. no. of nodes)
    - from command line arguments or from **`#PBS`** lines
  - other resources: **`-l walltime=03:00:00`**
- Job is queued until resources are available
  - query status with **`qstat -u <myusername>`**
  - job status set to “Q”

Great! So I can edit the same job script and resubmit straight away?

I'm afraid it's not that simple

Why?

You're probably running an executable from the script and it will see the version that's there at run time - OK for a package but not if you're recompiling

How does it decide when to run my job?

It's a balance of your requested number of nodes and the runtime compared to all the other jobs in the system

So I should take care when specifiying these?

Yes – don't ask for huge amounts of runtime if you don't need it!

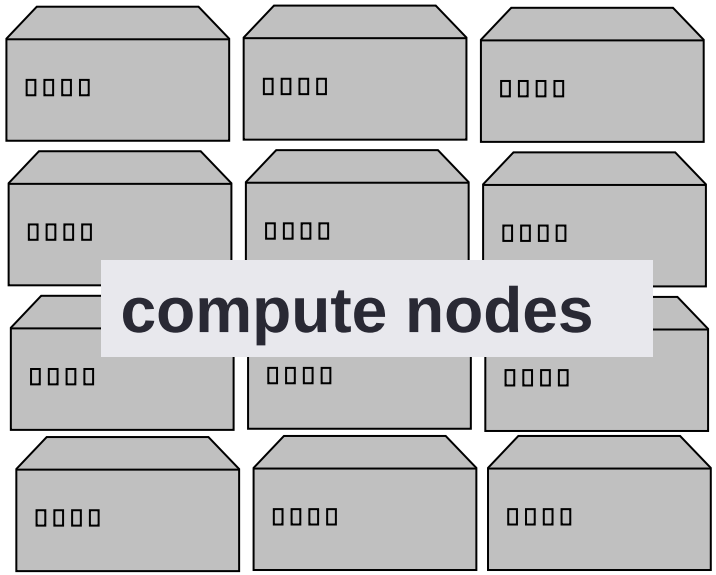
Childhood: job script runs

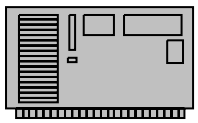
- A set of compute nodes is reserved for your job
  - but your batch script is actually executed on the **MOM nodes**
  - backronym for “Machine Oriented Mini-server”
  - **qstat** job status set to “R”

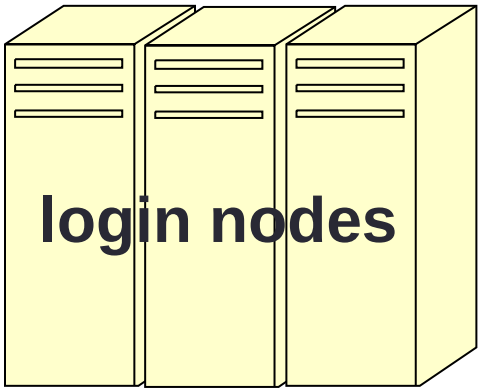
- The **only way** to access the compute nodes is with aprun

```
#PBS -N myjob
...
# Now run the job (assume I used select=6)
aprun -n 144 mympiprogram
```

Operating Systems







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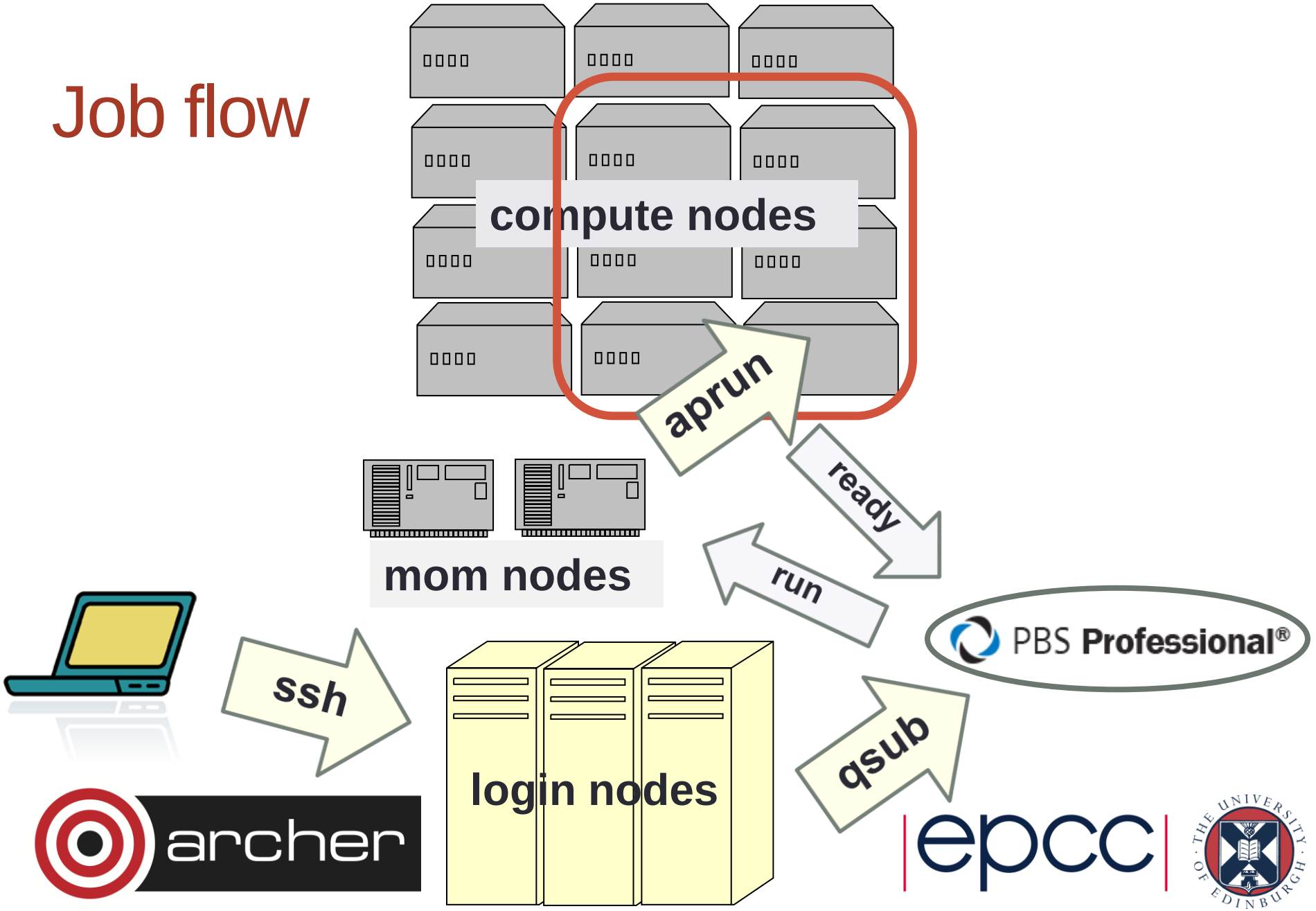
Job flow


compute nodes
aprun
ready
mom nodes
run
PBS Professional®
ssh
login nodes
qsub
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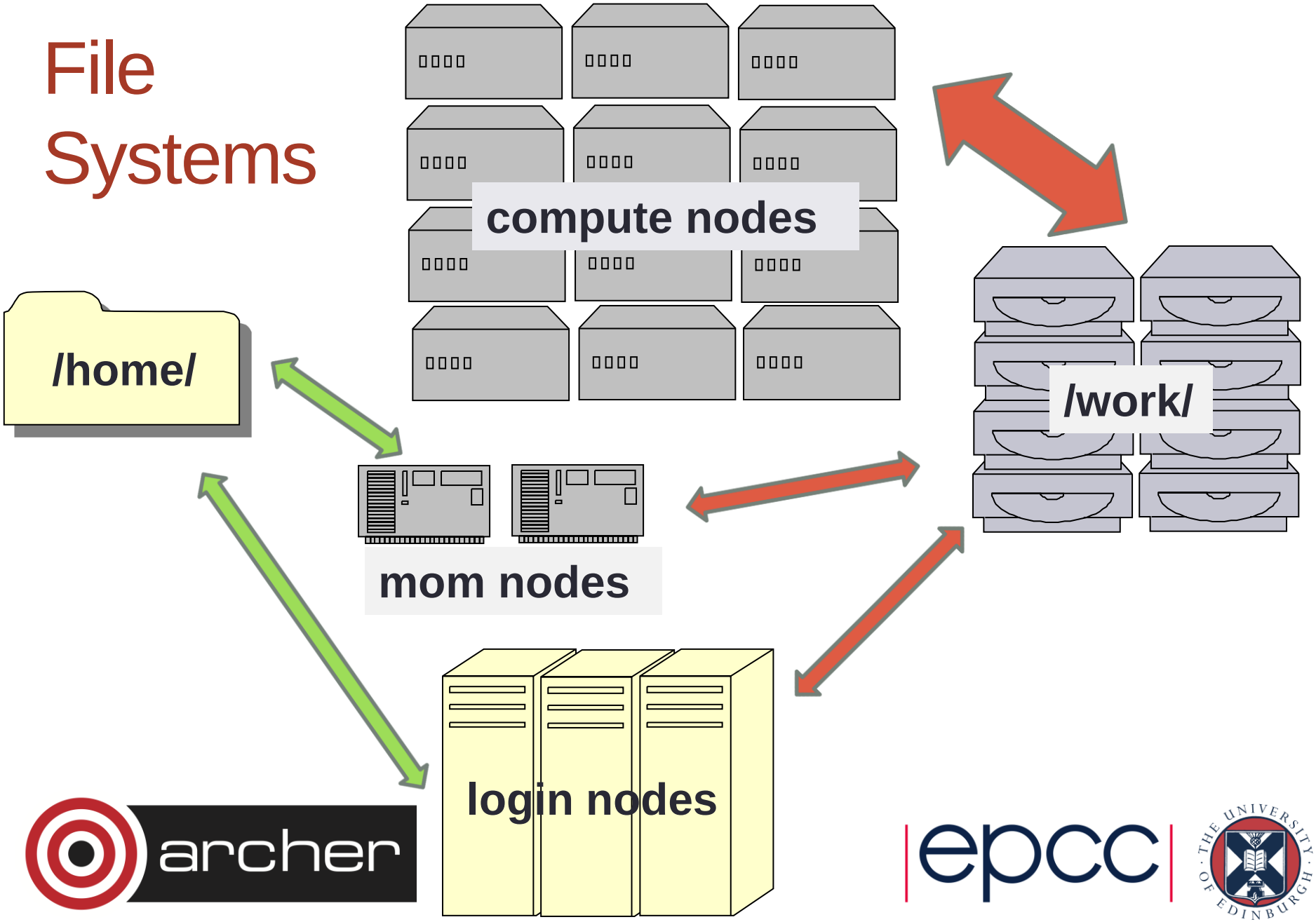
Adulthood: parallel jobs

- Compute nodes reserved for duration of job
  - PBS doesn't care if/how you use them!
  - all commands from batch script executed on MOM node
  - aprun on MOM node causes parallel jobs to run on compute nodes
- Do production runs in **`/work/`** filesystem, not **`/home/`**.
  - **`$PBS_O_WORKDIR`** is where the job was submitted from
- **`aprun`** does the following
  - **broadcasts the executable** to all the compute nodes
  - **gathers** the standard outputs / errors from all the PEs

File Systems



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Retirement: the end of your job

- Job finishes
  - after the all the commands in script have been executed …
  - … or the wallclock limit is exceeded
- All running parallel jobs are killed
  - e.g. wallclock exceeded or aprun running in background (see later)
- Standard outputs collated
  - written to **`myjob.o123456`**
- **qstat** job status may be set to “E” for a few minutes
  - job is “**E**xiting” (not “**E**xited”) but script has finished

aprun

- Can issue multiple aprun's in a single job
  - single job + many aprun's may be better than many jobs

```
#PBS -l select=6          # 6*24 = 144 cores
...
aprun -n 144 mympiprogram dataset1
aprun -n 144 mympiprogram dataset2
aprun -n 144 mympiprogram dataset3
...
```

aprun is quite clever

- Can manage multiple parallel jobs simultaneously
  - e.g. imagine we had 4 runs each using 72 cores

```
#PBS -l select=6          # 6*24 = 144 cores
...
aprun -n 72 mympiprogram dataset1
aprun -n 72 mympiprogram dataset2
aprun -n 72 mympiprogram dataset3
aprun -n 72 mympiprogram dataset4
# Incorrect! - all these run sequentially
```

Multiple aprun's in the background (i)

```
aprun -n 72 mympiprogram dataset1 &
aprun -n 72 mympiprogram dataset2 &
aprun -n 72 mympiprogram dataset3 &
aprun -n 72 mympiprogram dataset4 &

# Incorrect: "Job finishes after the all the
# commands in script have been executed".
# Final aprun returns immediately, script
# reaches end and finishes, aprun's killed.
```

Multiple aprun's in the background (ii)

```
aprun -n 72 mympiprogram dataset1 &
aprun -n 72 mympiprogram dataset2 &
aprun -n 72 mympiprogram dataset3 &
aprun -n 72 mympiprogram dataset4

# Incorrect: script finishes when dataset4
# finishes, but other datasets may still be
# running at that time.
```

Multiple aprun's in the background (iii)

```
aprun -n 72 mympiprogram dataset1 &
aprun -n 72 mympiprogram dataset2 &
aprun -n 72 mympiprogram dataset3 &
aprun -n 72 mympiprogram dataset4 &

wait

# Correct! "wait" blocks until all spawned
# processes are complete
```

Task farms with aprun

```
aprun -n 72 mympiprogram dataset1 &
aprun -n 36 mympiprogram dataset2 &
aprun -n 72 mympiprogram dataset3 &
aprun -n 36 mympiprogram dataset4 &
aprun -n 36 mympiprogram dataset5 &

wait

# ordering might be: 1, 2, 4, 3, 5
```

why can my job script see my home files but my MPI program can only see my work files?

Because the script runs on the MOM nodes which see /home but MPI runs on the compute nodes which only see /work

why can I store my MPI executable in /home but not its input files?

aprun broadcasts the executable from /home to the compute nodes, but not any dependent files

how do "interactive" batch jobs work?

You are effectively submitting a job which runs a bash shell on the MOM nodes

Special queues

- Regular jobs
  - up to 24 hours; 1-4,920 nodes (24-118,080 cores)
- Long jobs (qsub -q long)
  - up to 48 hours; 1-256 nodes (24-6,144 cores)
- Short (debug) jobs (qsub -q short)
  - up to 20 minutes; 1-8 nodes (24-192 cores)
  - only available 0900-1700 UK time Mon-Fri.
- Low priority jobs (qsub -q low)
  - up to 3 hours; 1-512 nodes (24-12288 cores)
  - uncharged, but only enabled when machine is lightly used
- Serial jobs (qsub -q serial)
  - run on separate postprocessing nodes – see documentation for details

THE END

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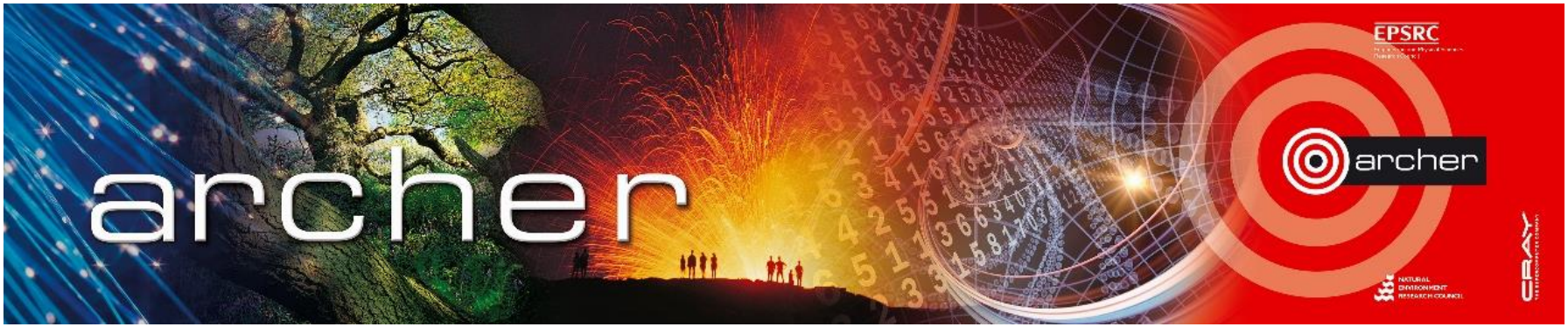

Goodbye!

Virtual tutorial has finished

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