Batch Systems

Running your jobs on an HPC machine

Outline

- What are batch systems?
- Why are they needed?
- How to run jobs on an HPC machine via a batch system:
  - Concepts
  - Resource scheduling and job execution
  - Job submission scripts
  - Interactive jobs
- Scheduling
- Best practice
- Common batch systems
  - Converting between different batch systems

Batch Systems

What are they and why do we need them?

What is a batch system?

- Mechanism to control access by many users to shared computing resources
- Queuing / scheduling system for users' jobs
- Manages the reservation of resources and job execution
- Allows users to "fire and forget" large, long calculations or many jobs ("production runs")

Why do we need a batch system?

- Ensure all users get a fair share of compute resources (demand usually exceeds supply)
- To ensure the machine is utilised as efficiently as possible
- To track usage - for accounting and budget control
- To mediate access to other resources e.g. software licences

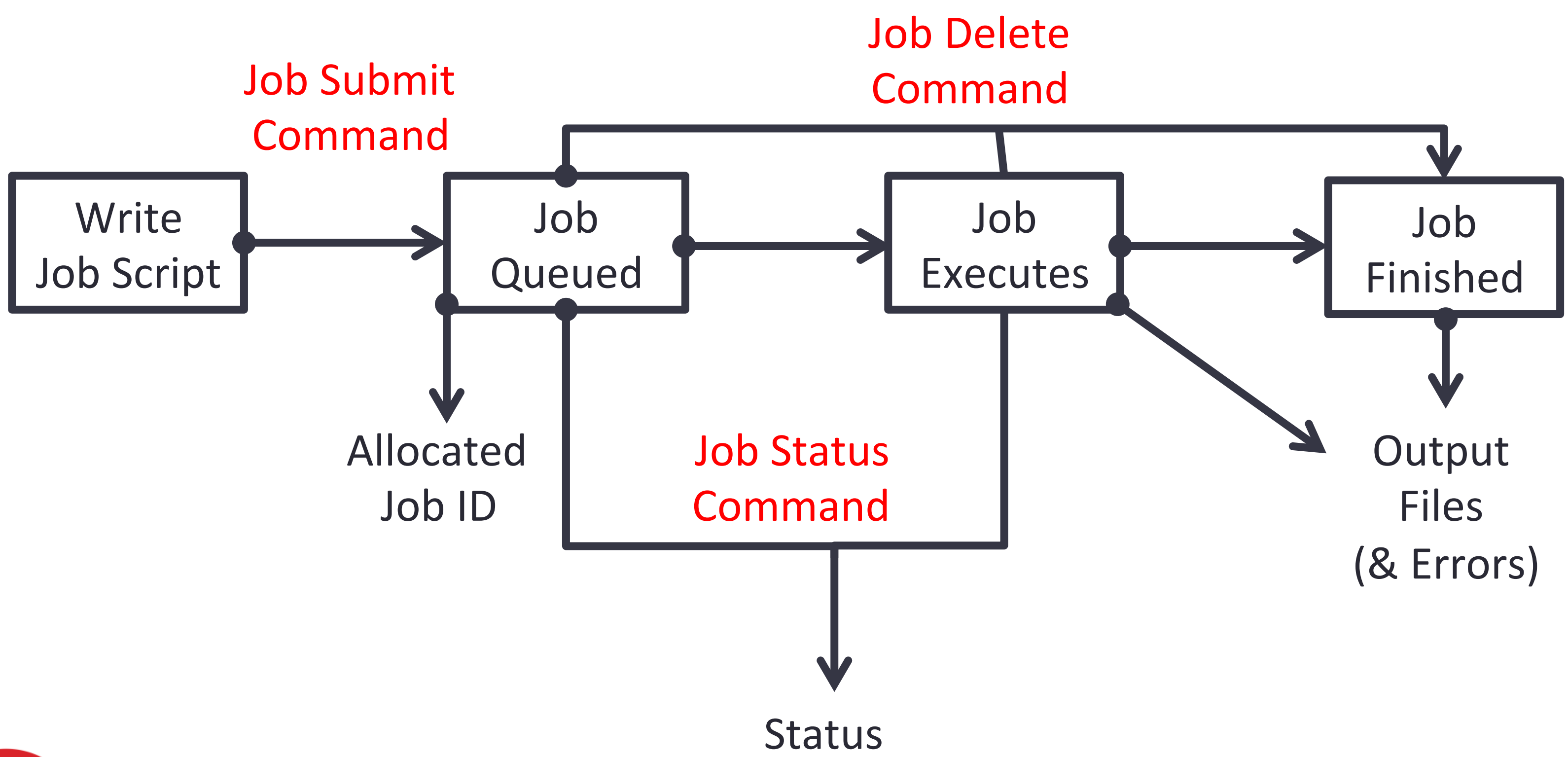
How to use a batch system

1. Set up a job, consisting of:
   - Commands that run one or more calculations / simulations
   - Specification of compute resources needed to do this

2. Submit your job to the batch system
   - Job is placed in a queue by the scheduler
   - Will be executed when there is space and time on the machine
   - Job runs until it finishes successfully, is terminated due to errors, or exceeds a time limit

3. Examine outputs and any error messages

Batch system flow



Resource scheduling & job execution

- When you submit a job to a batch system you specify the resources it requires (number of nodes / cores, job time, etc.)
- The batch system schedules a block of resources that meet these requirements to become available for your job to use
- When it runs, your job can use these resources however it likes (specified in advance in your job script):
  - Run a single calculation / simulation that spans all cores and full time
  - Run multiple shorter calculations / simulations in sequence
  - Run multiple smaller calculations / simulations running in parallel for the full time

Batch system concepts

- Queue – a logical scheduling category that may correspond to a portion of the machine:
  - Different time constraints
  - Nodes with special features such as large memory, different processor architecture or accelerators such as GPUs, etc.
  - Nodes reserved for access by a subset of users (e.g. for training)
  - Generally have a small number of defined queues
  - Jobs contend for resources within the queue in which they sit

Queues on ARCHER

- “standard” queue: 24 hour limit, up to ~4000 nodes
- “short” queue: max 20 minutes, up to 8 nodes, available weekdays 09:00-20:00 only
- “long” queue: 48 hour limit, up to ~900 nodes
- “largemem” queue: 48 hour limit, up to ~ 400 nodes, 128GB RAM
- “serial” queue

Batch system concepts

- Priority – numerical ranking of a job by the scheduler that influences how soon it will start (higher priority more likely to start sooner)
- Account name / budget code – identifier used to charge (£) time used
  - Jobs may be rejected when you submit with insufficient budget
- Walltime – the time a job takes (or is expected to take)

Using Batch Systems

Command and examples

Batch system commands & job states

	PBS (ARCHER)	SLURM
Job submit command	qsub myjob.pbs	sbatch myjob_sbatch
Job status command	qstat –u $USER	squeue –u $USER
Job delete command	qdel #########	scancel #########

PBS job state (ARCHER)	Meaning
Q	The job is *queued* and waiting to start
R	The job is currently *running*
E	The job is currently *exiting*
H	The job is *held* and not eligible to run

Parallel application launcher commands

Use these commands inside a job script to launch a parallel executable

Parallel application launcher commands	
aprun –n 48 –N 12 –d 2 my_program	(ARCHER)
mpirun –ppn 12 –np 48 my_program	
mpiexec –n 48 my_program	

Job submission scripts

PBS example:

```
#!/bin/bash --login
#PBS -N Weather1
#PBS -l select=200
#PBS -l walltime=1:00:00
#PBS -q short
cd $PBS_O_WORKDIR
aprun -n 4800 weathersim
```

- `#!/bin/bash --login` ← Linux shell to run job script in
- `#PBS -N Weather1` ← Job name
- `#PBS -l select=200` ← Number of nodes requested
- `#PBS -l walltime=1:00:00` ← Requested job duration
- `#PBS -q short` ← Queue to submit job to
- `cd $PBS_O_WORKDIR` ← Changing to directory to run in
- `aprun` ← Parallel job launcher
- `4800` ← Number of parallel instances of program to launch
- `weathersim` ← Program name

Job submission scripts

SLURM example:

```
#!/bin/bash
#SBATCH -J Weather1
#SBATCH --nodes=2
#SBATCH --time=12:00:00
#SBATCH --ntasks=24
#SBATCH -p tesla
mpirun -np 24 weathersim
```

- `#!/bin/bash` — Linux shell to run job script in
- `#SBATCH -J Weather1` — Job name
- `#SBATCH --nodes=2` — Number of nodes requested
- `#SBATCH --time=12:00:00` — Requested job duration
- `#SBATCH --ntasks=24` — Number of parallel tasks
- `#SBATCH -p tesla` — Queue to submit job to (GPU queue)
- `mpirun` — Parallel job launcher
- `-np 24` — Number of parallel instances of program to launch
- `weathersim` — Program name

archer

epcc

Interactive jobs

Testing, development and visualisation

Interactive jobs

- Most HPC machines allow both batch and interactive jobs

- **Batch jobs** are non-interactive.
  - You write a *job submission script* to run your job
  - Jobs run without user intervention and you collect results at the end
- **Interactive jobs** allow you to use compute resources interactively
  - For testing, debugging/profiling, software development work
  - For visualisation and data analysis
- How these are set up and charged varies from machine to machine

Interactive jobs

- If using the same compute resource as batch jobs then need to request an interactive job from the batch scheduler
  - Use same resource request variables as for batch jobs (duration, size, queue, etc.):

```
qsub -I -l select=1,walltime=0:10:0 -A y14 -q short
```

  - Wait until job runs to get an interactive terminal session
  - Within interactive session run serial code or parallel programs using parallel launcher (aprun, mpirun, etc.) as for batch jobs

Interactive jobs

- May have a small part of the HPC machine dedicated to interactive jobs
  - Typically for visualisation & postprocessing / data analysis
  - May bypass the batch scheduler for instant access (serial nodes on ARCHER)
  - May be limited in performance, available libraries, parallelism, etc.

Scheduling

How does the scheduler decide which job to run when?

Scheduling

- Complex scheduling algorithms try to run many jobs of different sizes on system to ensure
  - maximum utilisation
  - minimum wait time

- Batch schedulers can be configured to implement scheduling policy that varies from machine to machine, allowing control over the relative importance to job prioritisation of:
  - Waiting times
  - Large vs small jobs
  - Long vs short jobs
  - Power consumption
  - Some other metric ….

Scheduling

- Backfilling strategy in scheduling algorithms:
  - Assign all jobs priority according to policy
  - If you have a high priority job *A* that can not currently run given available resources, calculate when the required resources will become available and schedule *A* to run at that future time.
  - Until such time, run any less high priority jobs that will complete before job *A* starts and for which sufficient resources are currently available
  - This "fills gaps" and improves resource utilisation

- Scheduling algorithms are an active area of research

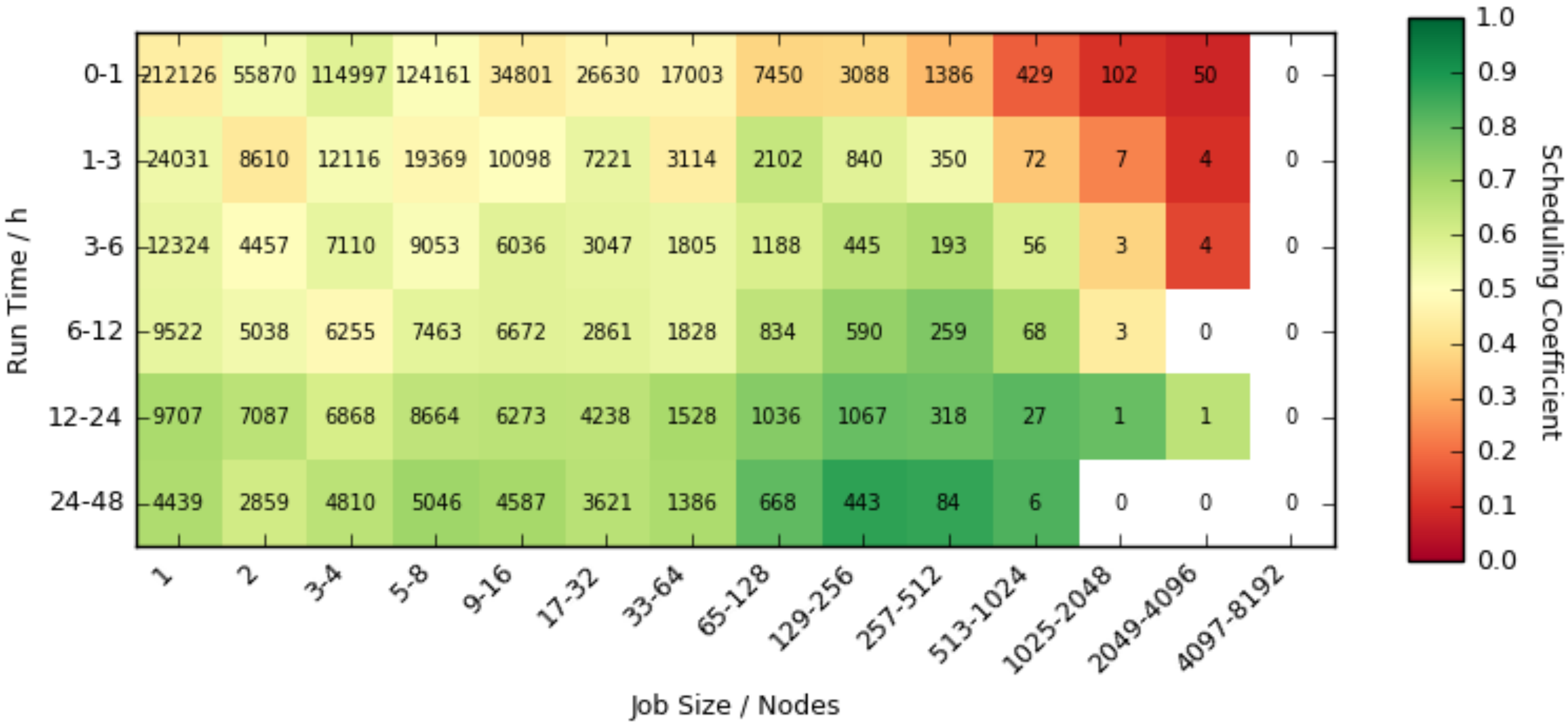
http://archer.ac.uk/status/

- How long until my job executes?

Scheduling Coefficient

Scheduling coefficient = runtime / (runtime + queuedtime)

Statistics over last year:



Best Practice

Tips for using HPC batch systems

Best practice

- Run short tests using interactive jobs if possible (firing off large jobs without first testing may burn resources without producing good results)
- Once you are happy the setup works write a short test job script and submit it to the batch system (e.g. to short queue)
- Finally, produce scripts for full production runs
- Remember you have the full functionality of the Linux command line (bash or other) available in scripts
  - This allows for sophisticated scripts if you need them
  - Can automate a lot of tedious data analysis and transformation
  - …be careful to test when moving, copying deleting important data – it is very easy to lose the results of a large simulation due to a typo (or unforeseen error) in a script

Migrating

Changing your scripts from one batch system to another

Batch systems

- PBS (on ARCHER), Torque
- Grid Engine
- SLURM
- LSF – IBM Systems
- LoadLeveller – IBM Systems

Conversion

- Usually need to change the batch system options
- Sometimes need to change the commands in the script
  - Particularly to different paths
  - Usually the order (logic) of the commands remains the same
- There are some utilities that can help
  - Bolt – from EPCC, generates job submission scripts for a variety of batch systems/HPC resources: https://github.com/aturner-epcc/bolt

Summary

Summary

- Batch systems exist to manage access to shared resources on HPC systems and maximise utilisation
- Allow users to submit jobs and go and do other things while they queue and run
  - No need to stay logged in or monitor your jobs
- There are a number of different batch systems
  - But they all work in broadly the same way
  - Usually *request* resources using batch syntax…
  - … then specify how to *use* resources using parallel job launcher
- Complex scheduling algorithms maximise resource utilisation according to policy