

Batch Systems

Running your jobs on an HPC machine



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Outline

- What is a batch system and why do we need them?
- How do I use a batch system to run my jobs?
 - 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

Using batch systems

How can I use them to run and manage my jobs?

How to use a batch system

1. Set up a job, consisting of:

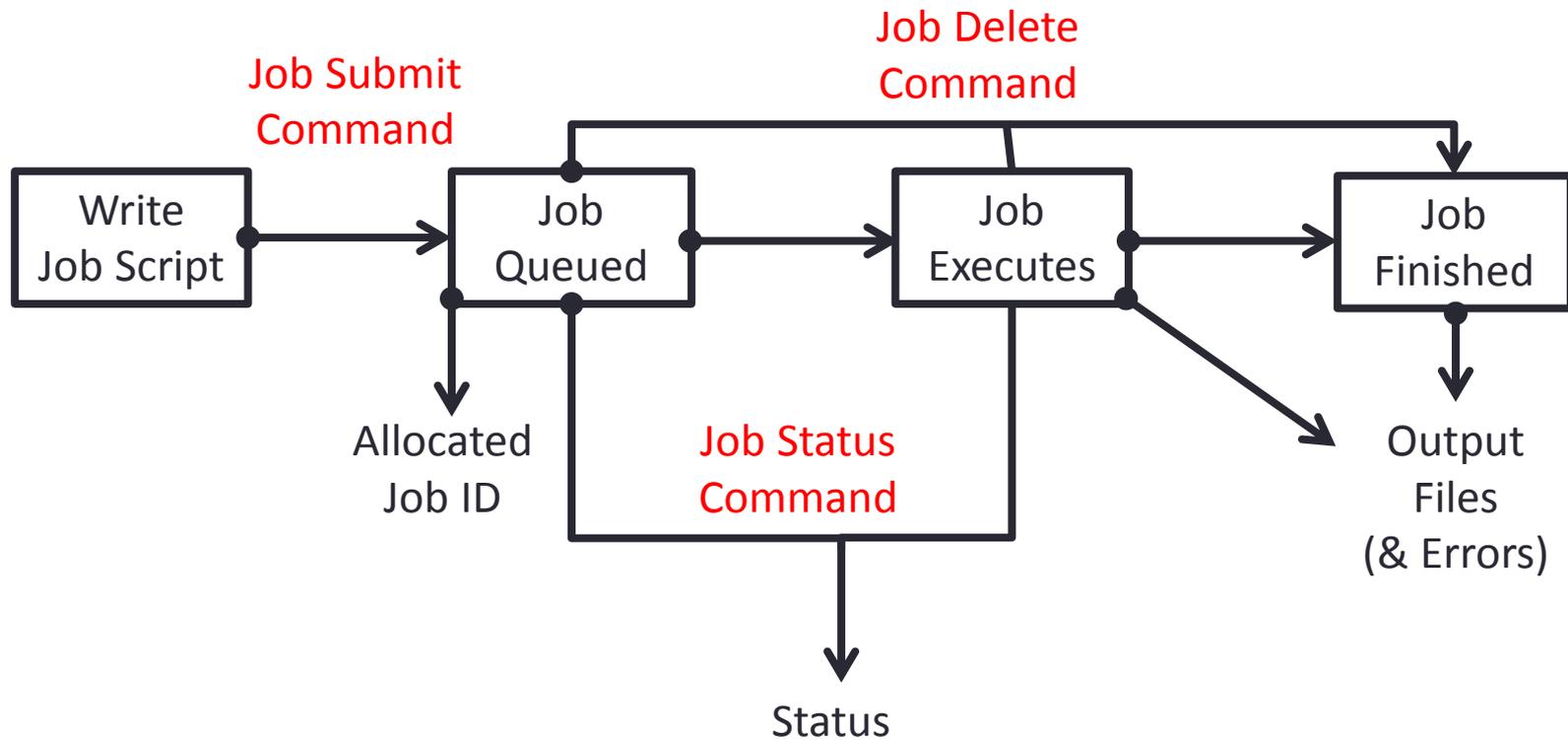
- Commands that run one or more calculations / simulations
- Specification of compute resources needed to do this

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

E.g. on ARCHER:

- “standard” queue (24 hour limit, no limit on number of nodes)
- “short” queue (max 20 minutes & 8 nodes, weekdays 08:00-22:00 only)

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)

Batch system commands & job states

	PBS (ARCHER & Cirrus)	SLURM
Job submit command	<code>qsub myjob.pbs</code>	<code>sbatch myjob_sbatch</code>
Job status command	<code>qstat -u \$USER</code>	<code>squeue -u \$USER</code>
Job delete command	<code>qdel #####</code>	<code>scancel #####</code>

PBS job state (ARCHER & Cirrus)	Meaning
Q	The job is <i>queued</i> and waiting to start
R	The job is currently <i>running</i>
E	The job is currently <i>exiting</i>
H	The job is <i>held</i> 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	
<code>aprun -n 48 -N 12 -d 2 my_program</code>	(ARCHER)
<code>mpiexec_mpt -n 48 -ppn 24 my_program</code>	(Cirrus)
<code>mpirun -ppn 12 -np 48 my_program</code>	
<code>mpiexec -n 48 my_program</code>	

Job submission scripts

PBS example:

```
#!/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 -n 4800 weathersim
```

Parallel job launcher

Number of parallel
instances of program
to launch

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
```

← Linux shell to run job script in

← Job name

← Number of nodes requested

← Requested job duration

← Number of parallel tasks

← Queue to submit job to (GPU queue)

Parallel job launcher

Number of parallel instances of program to launch

Program name

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 interactive jobs from the batch scheduler
 - Use same resource request variables as batch jobs (duration, size)
 - Wait until job runs to get an interactive session
 - Within interactive session run serial code or parallel programs using parallel launcher as for batch 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
 - May be limited in performance, available libraries, parallelism, etc.

Scheduling of jobs

A brief look under the hood at when jobs are run

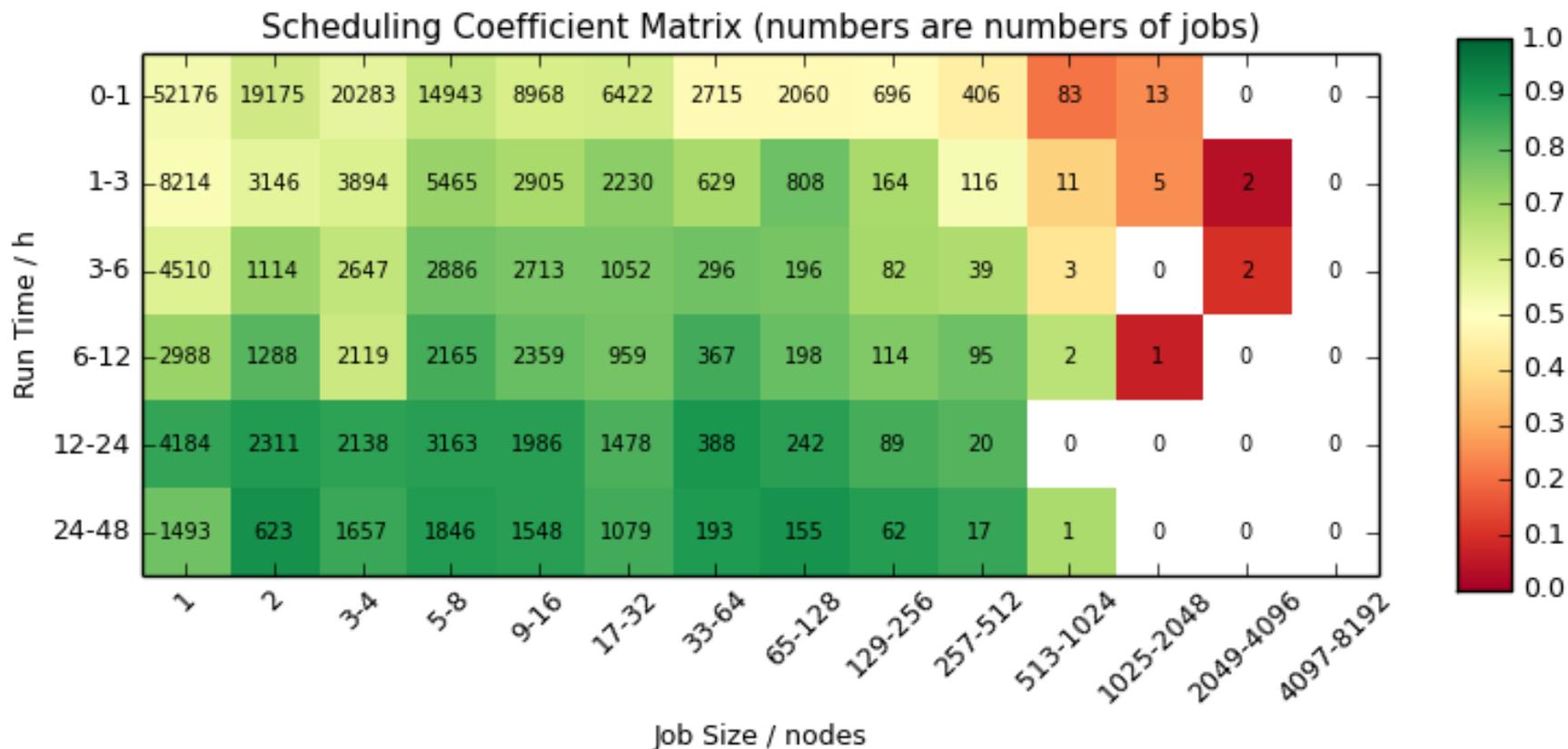
Scheduling

- Complex scheduling algorithms try to run many jobs of different sizes on system to ensure maximum utilisation and minimum wait time
- Batch schedulers can implement scheduling policy that varies from machine to machine by allowing control over the relative importance to job prioritisation of:
 - Waiting times
 - Large vs small jobs
 - Long vs short jobs
 - Power consumption

Scheduling

- Backfilling:
 - Assign all jobs priority according to policy & scheduling algorithm
 - Starting with highest priority job, run each lesser priority job that can run with current free resources
 - For highest priority job *A* that can't currently run, calculate when required resources will become available and schedule job *A* to run at this 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
- Active area of research
- For example on ARCHER you can view detailed statistics on this
 - <http://archer.ac.uk/status/>
- How long until my job executes?
 - Not always an easy question to answer!

Scheduling



Best practice

Tips for making the most effective use of batch systems

Best practice

- Run short tests using interactive jobs if possible
- Once you are happy the setup works write a short test job script and submit it to the batch system
- 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 and Cirrus), Torque
- Grid Engine
- SLURM
- LSF – IBM Systems
- LoadLeveller – IBM Systems

- It is not unusual for applications to run over many different HPC machines using different queue systems
 - You often see sets of submission scripts for different systems
 - From a user's perspective different commands are used to submit and manage jobs

Submission script 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
- Tends to be a fairly mechanical - some utilities can help
 - Bolt – from EPCC, generates job submission scripts for a variety of batch systems/HPC resources: <https://github.com/aturner-epcc/bolt>
- HPC machine documentation often provides significant reference material
 - Especially true for ARCHER and Cirrus

Summary

Summary

- Submitting jobs through a batch system represents a different way of interacting with a computer than you might be used to
 - But this has a crucial role in enabling potentially thousands of users to easily run jobs on the same machine concurrently
- A number of different batch system technologies
 - Fundamentally the same concepts, but different options and commands
 - These are all well documented
 - Many applications are shipped with submission scripts for multiple systems