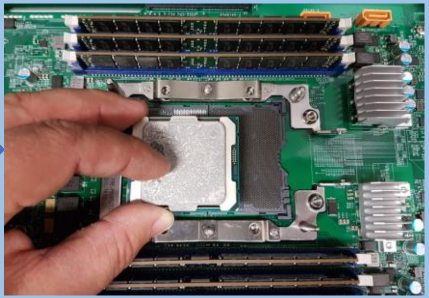
## Some definitions

- A **processor** is a small chip that responds to and processes the basic instructions that drive a computer. The term *processor* is used interchangeably with the term **central processing unit** (CPU)
- **Core**: The smallest compute unit that can run a program
- **Socket:** A compute unit, packaged as one and usually made of a single chip often called processor. Modern sockets carry many cores (10, 14, or 20, 24, 28, etc. on most servers)
- **Node:** A stand-alone computer system that contains one or more sockets, memory, storage, etc. connected to other nodes via a fast network interconnect.

## From a CPU to a Cluster

CPU

(Has Multiple cores)



Socket

(Can have Multiple CPUs)

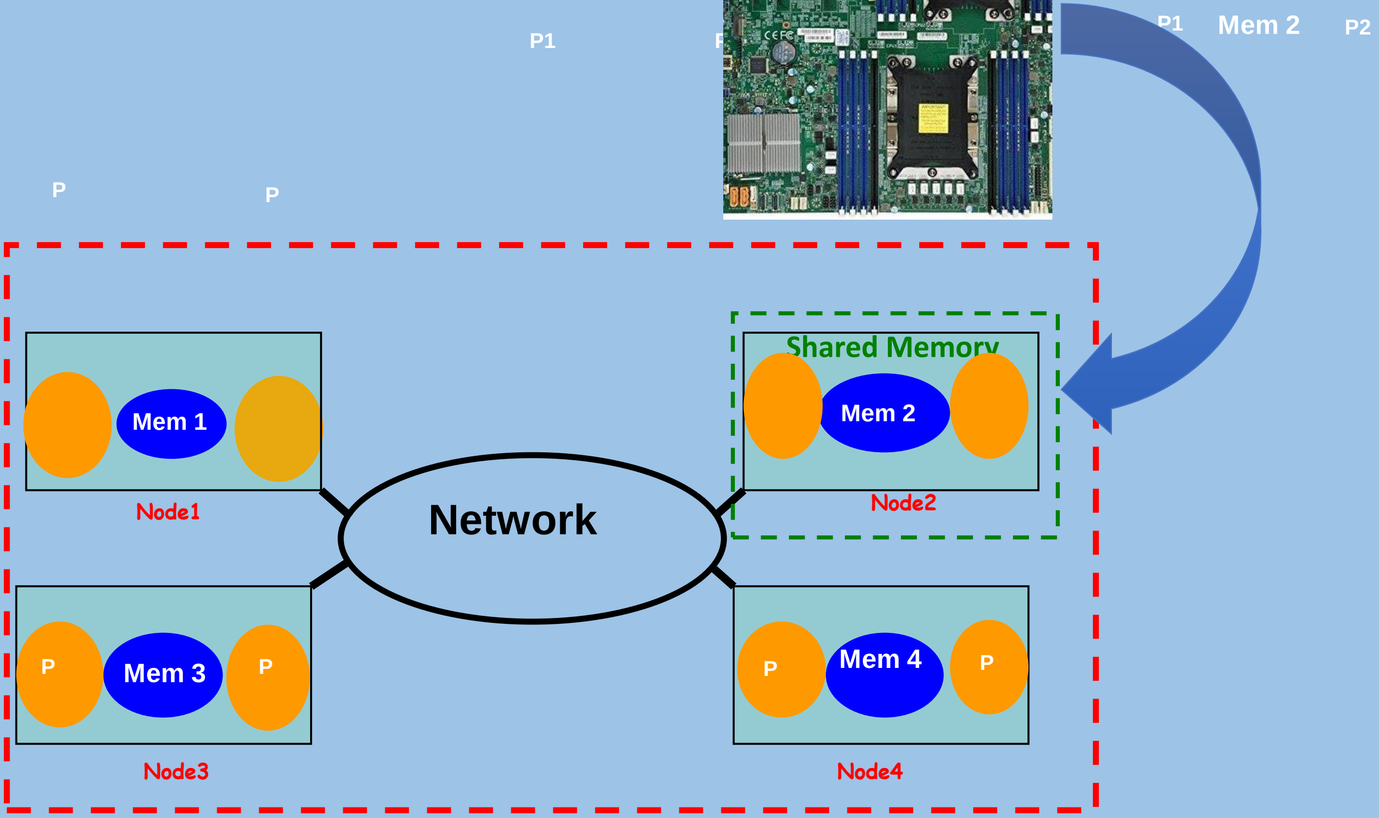
Motherboard

Compute Node

Rack

Cluster

# Distributed vs Shared Memory Systems



Distributed Shared Memory

## How to
## Run jobs

**Either Interactively or submitting jobs to a queue using Slurm**

## Slurm: Some key terms to remember

A **job** is the resources you are using and the code you are running

The **queue** in Slurm is all RUNNING and all PENDING jobs
To see every job in the queue on Oscar, use the command

```
squeue
```

To see your jobs in the queue

```
squeue -u <cnetid>
```

```
or
```

```
myq
```

## What goes into a batch script?

A batch script is list of instructions for slurm.

```
#!/bin/bash

# Here is a comment
#SBATCH --time=1:00:00

#SBATCH –nodes=1
#SBATCH –ntasks-per-node=1
#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

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#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

This #! is a shebang

It tells operating system to use
/bin/bash
with this script

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#SBATCH –nodes=1
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#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

# is a comment

everything after # is ignored by bash

## What goes into a batch script?

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#Run your code
```

#SBATCH is a directive

It is a comment in Bash

#SBATCH is only relevant to slurm:
sbatch my_script.sh

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#Run your code
```

#SBATCH is a directive

It is a comment in Bash

#SBATCH is only relevant to slurm:
sbatch my_script.sh

To comment out directives, break the pattern, e.g.
##SBATCH
# SBATCH

# What goes into a batch script?

A batch script is list of instructions for slurm.

```
#!/bin/bash

# Here is a comment
#SBATCH --time=1:00:00

#SBATCH –nodes=1
#SBATCH –ntasks-per-node=1
#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

Instructions for Slurm must go at the top of the script

Any #SBATCH lines you put after your program will be ignored

## What goes into a batch script?

A batch script is list of instructions for slurm.

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#!/bin/bash

# Here is a comment
#SBATCH --time=1:00:00

#SBATCH –nodes=1
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#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

Slurm has some variables you can use. %j is the job number. When the job runs %j will be expanded to the job number. In this example %j is used in the output file and error file names:

MyJob-13571056.out
MyJob-13571056.err

%j is unique. By using %j in your filenames you guarantee a unique file name, which means you won't accidentally overwrite previous output.

# What goes into a batch script?

A batch script is list of instructions for slurm.

```
#!/bin/bash

# Here is a comment
#SBATCH --time=1:00:00

#SBATCH –nodes=1
#SBATCH –ntasks-per-node=1
#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.ou
#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
```

=> Time your job is allowed to run

=> Number of nodes to run on
=> Number of cores on each node to use
=> Memory per cpu => 2000Mb or 2Gb
=> Name of the job.
=> Job output file behaves as stdout for the code.
=> Error file. behaves as stderr for the code.

=> Load any modules you need for your application
=> run the code you want

## Running batch jobs using a Submission Script

- A simple job submission script (saved as python.sbatch):

Slurm

Your Job

```
#!/bin/bash
#SBATCH --job-name=first_python_job
#SBATCH --output=first_python_job_%j.out
#SBATCH --error=first_python_job_%j.err
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --mem-per-cpu=2000M
#SBATCH --partition=broadwl
#SBATCH --reservation=kicpworkshop-cpu
#SBATCH --time=00:30:00
module load python
python hello_world.py
echo “job finished at `date`”
```

- • To submit the above script:
  - sbatch python.sbatch

## Exercise;
## Ex-1 in Repo

# How to submit OpenMP jobs?

```
#!/bin/bash

#Here is a comment
#SBATCH --time=1:00:00
#SBATCH –partition=broadwl
#SBATCH –nodes=1
#SBATCH –ntasks-per-node=8
#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err

module load <module name>
export OMP_NUM_THREADS=8
#Run your code
./my_executable
```

Specify number of cores > 1.

OMP_NUM_THREADS is an environment variable.

## Exercise;
## Ex-2 in Repo

# How to submit Parallel MPI jobs?

```
#!/bin/bash

#Here is a comment
#SBATCH --time=1:00:00
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err
#SBATCH –partition=broadwl
#SBATCH –nodes=4
#SBATCH –ntasks-per-node=8
#SBATCH --mem-per-cpu=2000
module load openmpi
module load <module name>
#Run your code
mpirun  ./my_executable
```

Specify number of nodes > 1.

Specify number of cores >= 1.

Load OPENMPI MPI library or IntelMPI

## Exercise;
## Ex-3 in Repo

## How to submit GPU jobs?

```
#!/bin/bash

#Here is a comment
#SBATCH --time=1:00:00
#SBATCH –partition=gpu2
#SBATCH –gres=gpu:1
#SBATCH –nodes=1
#SBATCH –ntasks-per-node=8
#SBATCH --mem-per-cpu=2000
#SBATCH –job-name=MyJob
#SBATCH –output= MyJob-%j.out
#SBATCH –error=MyJob-%j.err

module load <module name>
#Run your code
./my_executable
```

Specify partition gpu2

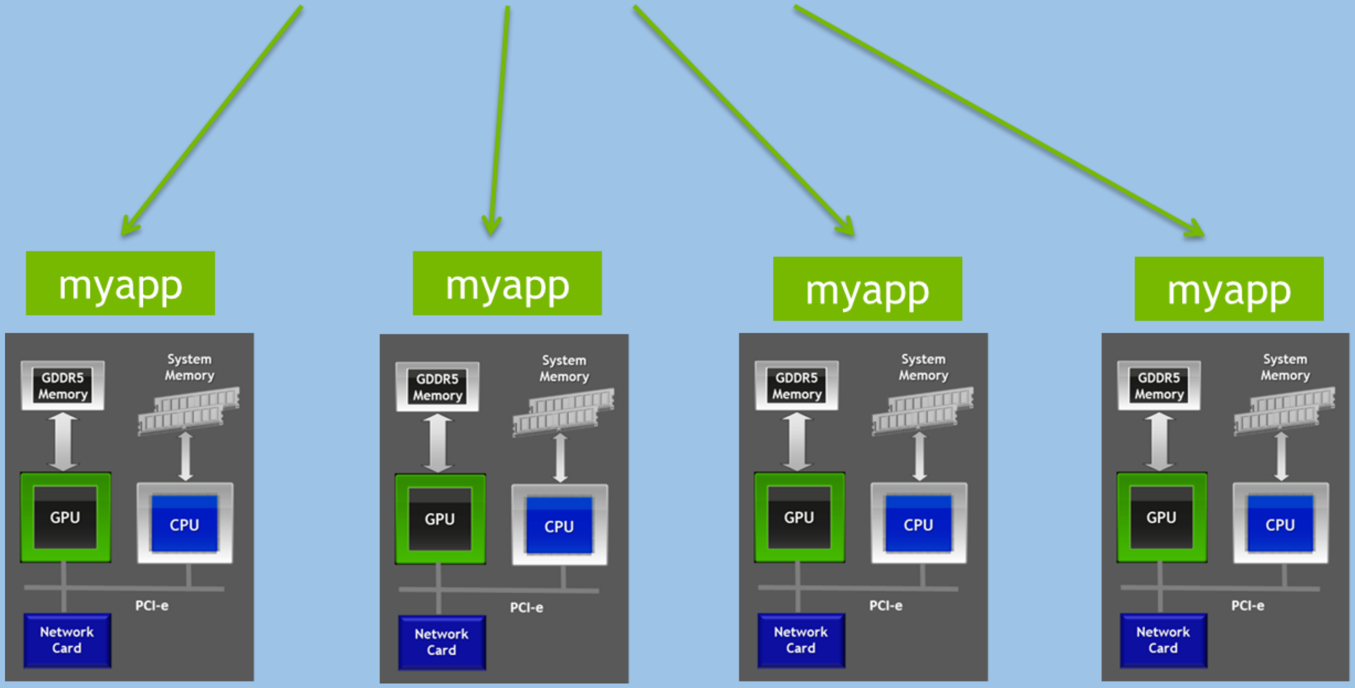
Specify number of gpus, like *gpu*:1

## Exercise;
## Ex-4 in Repo

## How to submit MPI + GPU jobs?

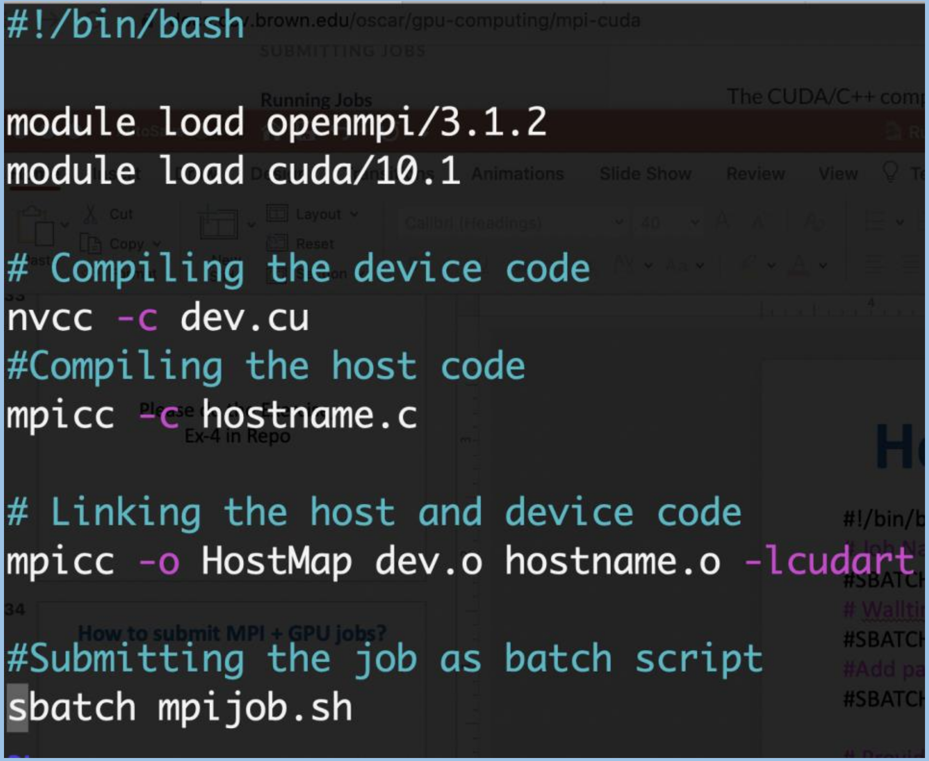
CUDA Aware MPI

```
mpirun -np 4 ./myapp <args>
```



# How to submit MPI + GPU jobs?

Compilation



```
#!/bin/bash

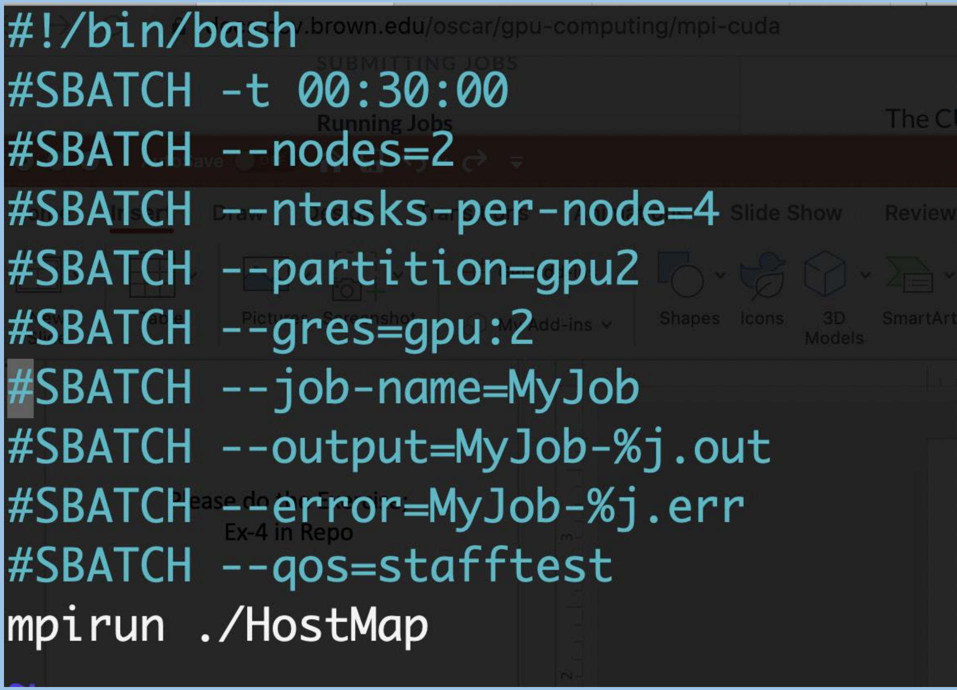
module load openmpi/3.1.2
module load cuda/10.1

# Compiling the device code
nvcc -c dev.cu
#Compiling the host code
mpicc -c hostname.c

# Linking the host and device code
mpicc -o HostMap dev.o hostname.o -lcudart

#Submitting the job as batch script
sbatch mpijob.sh
```

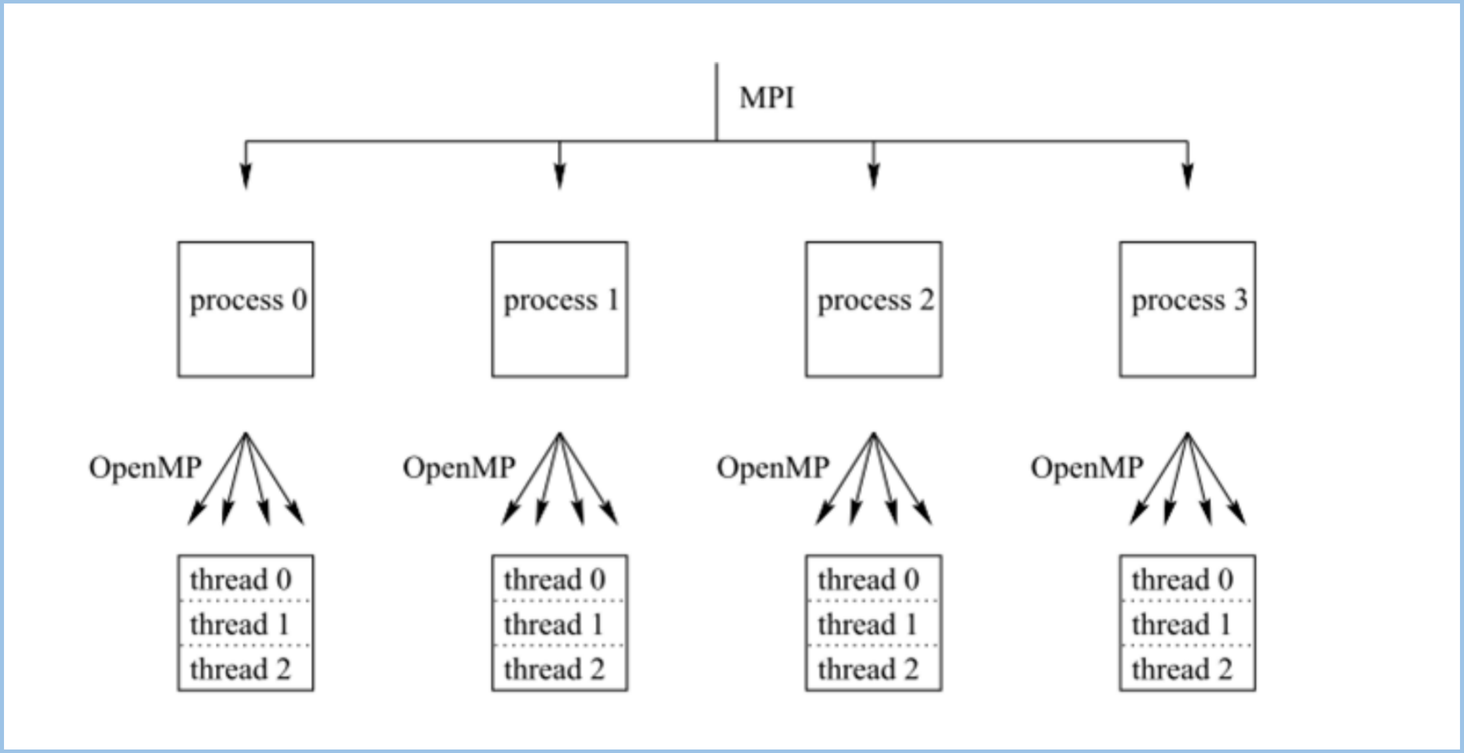
Job Submission

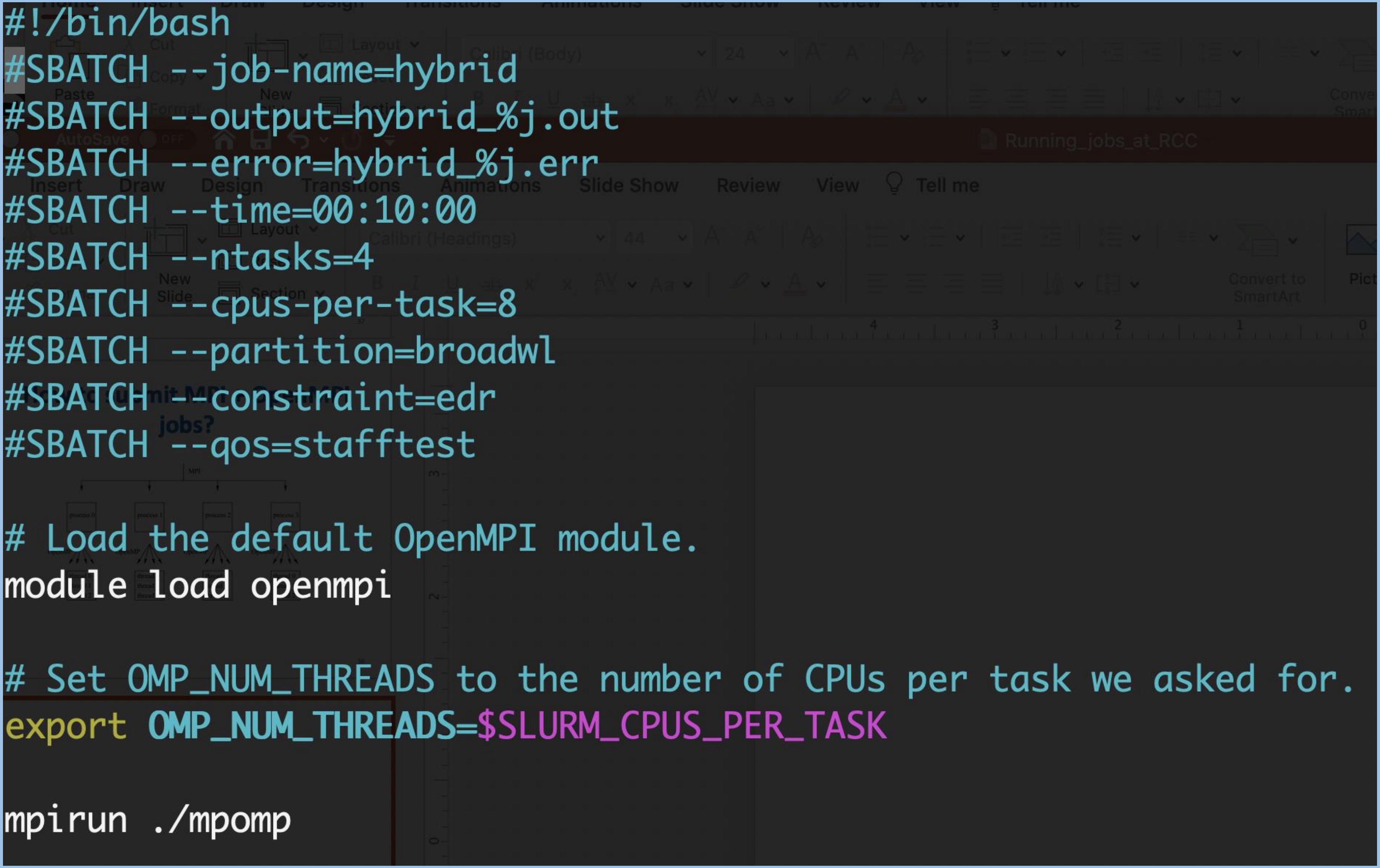


```
#!/bin/bash
#SBATCH -t 00:30:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --partition=gpu2
#SBATCH --gres=gpu:2
#SBATCH --job-name=MyJob
#SBATCH --output=MyJob-%j.out
#SBATCH --error=MyJob-%j.err
#SBATCH --qos=stafftest
mpirun ./HostMap
```

## Exercise;
## Ex-5 in Repo

## How to submit MPI + OpenMPI jobs?





```
#!/bin/bash
#SBATCH --job-name=hybrid
#SBATCH --output=hybrid_%j.out
#SBATCH --error=hybrid_%j.err
#SBATCH --time=00:10:00
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=8
#SBATCH --partition=broadwl
#SBATCH --constraint=edr
#SBATCH --qos=stafftest

# Load the default OpenMPI module.
module load openmpi

# Set OMP_NUM_THREADS to the number of CPUs per task we asked for.
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

mpirun ./mpomp
```

Exercise;
Ex-5a in Repo

# How to submit array based jobs

```
#!/bin/bash
# Job Name
#SBATCH --job-name=arrayjob
# Walltime requested
#SBATCH --time=0:10:00
#Add partition
#SBATCH --partition=broadwl-lc

# Provide index values (TASK IDs)
#SBATCH --array=1-16

# Use '%A' for array-job ID, '%J' for job ID and '%a' for task ID
#SBATCH --error=maths%A-%a.err
#SBATCH --output=maths%A-%a.out

# single core
#SBATCH --ntasks-per-node=1
#SBATCH --mem-per-cpu=2000

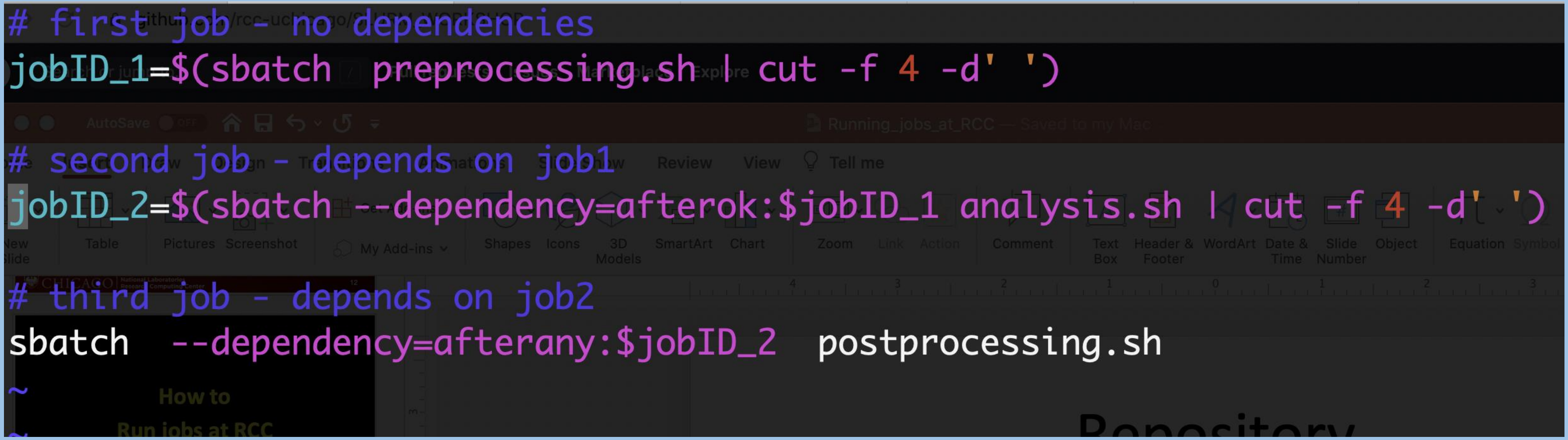
# Use the $SLURM_ARRAY_TASK_ID variable to provide different inputs for each job
input=$((SLURM_ARRAY_TASK_ID*1000+2))
```

## Exercise;
## Ex-6 in Repo

# How to submit dependent jobs

SLURM Rule:

*sbatch --dependency=type:job_id jobfile*



```
# first job - no dependencies
jobID_1=$(sbatch  preprocessing.sh | cut -f 4 -d' ')

# second job - depends on job1
jobID_2=$(sbatch  --dependency=afterok:$jobID_1 analysis.sh | cut -f 4 -d' ')

# third job - depends on job2
sbatch  --dependency=afterany:$jobID_2  postprocessing.sh
~
~
```

# How to submit dependent jobs

| | |
|---|---|
| after | This job can begin execution after the specified jobs have begun execution |
| afterany | This job can begin execution after the specified jobs have terminated. |
| aftercorr | A task of this job array can begin execution after the corresponding task ID in the specified job has completed successfully |
| afternotok | This job can begin execution after the specified jobs have terminated in some failed state |
| afterok | This job can begin execution after the specified jobs have successfully executed |
| singleton | This job can begin execution after any previously launched jobs sharing the same job name and user have terminated |

Exercise;
Ex-7 in Repo

# How to submit Parallel batch jobs

```
#!/bin/sh
#SBATCH --time=01:00:00
#SBATCH --partition=broadwl
#SBATCH --ntasks=28
#SBATCH --mem-per-cpu=2G # NOTE DO NOT USE THE --mem= OPTION
# Load the default version of GNU parallel. module load parallel
# set the max number of processes (which determine the max per processor)
ulimit -u 10000
# This specifies the options used to run srun. The "-N1 -n1" options are
# used to allocates a single core to each task.
srun="srun --exclusive -N1 -n1”
#Run GNU parallel
parallel="parallel --delay 0.2 -j $SLURM_NTASKS --joblog runtask.log --resume"
# Run a script, runtask.sh, using GNU parallel and srun.
$parallel "$srun ./runtask.sh arg1:{1} > runtask.sh.{1}" ::: {1..128}
# Note that if your program does not take any input, use the -n0 option to call the
parallel command: # # $parallel -n0
"$srun ./run_noinput_task.sh > output.{1}" ::: {1..128}
```

## How to submit Parallel batch jobs

Exercise;
Ex-8 in Repo

## What resources should I ask for?

This depends on the code you are running

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This depends on the code you are running

**Nodes/Cores**

- Question: is your code parallel? You will need to find out if your code can
    - Run on multiple cores? Run across multiple nodes?
    - Check if your code is threaded, multiprocessor, MPI
- Question: Is your code serial?
    - This means it can only make use of one core

## What resources should I ask for?

This depends on the code you are running

**Wall Time**

Make an estimate of your job run and add a bit.

e.g. if think your code will take an hour, give it 1 hour and 30 min

- If your job runs out of time, your job will be killed, so
- be accurate with your estimate without going below.

## What resources should I ask for?

This depends on the code you are running

**Memory**

For memory, this can take some trial and error.  You can ask for a lot, then measure your usage.  If you have asked for more memory and then  reduce your memory with the next job.

- To ask for all the memory available on a node, use #SBATCH --mem=0

## What if I need an entire node or specific features?

Add this in your batch script

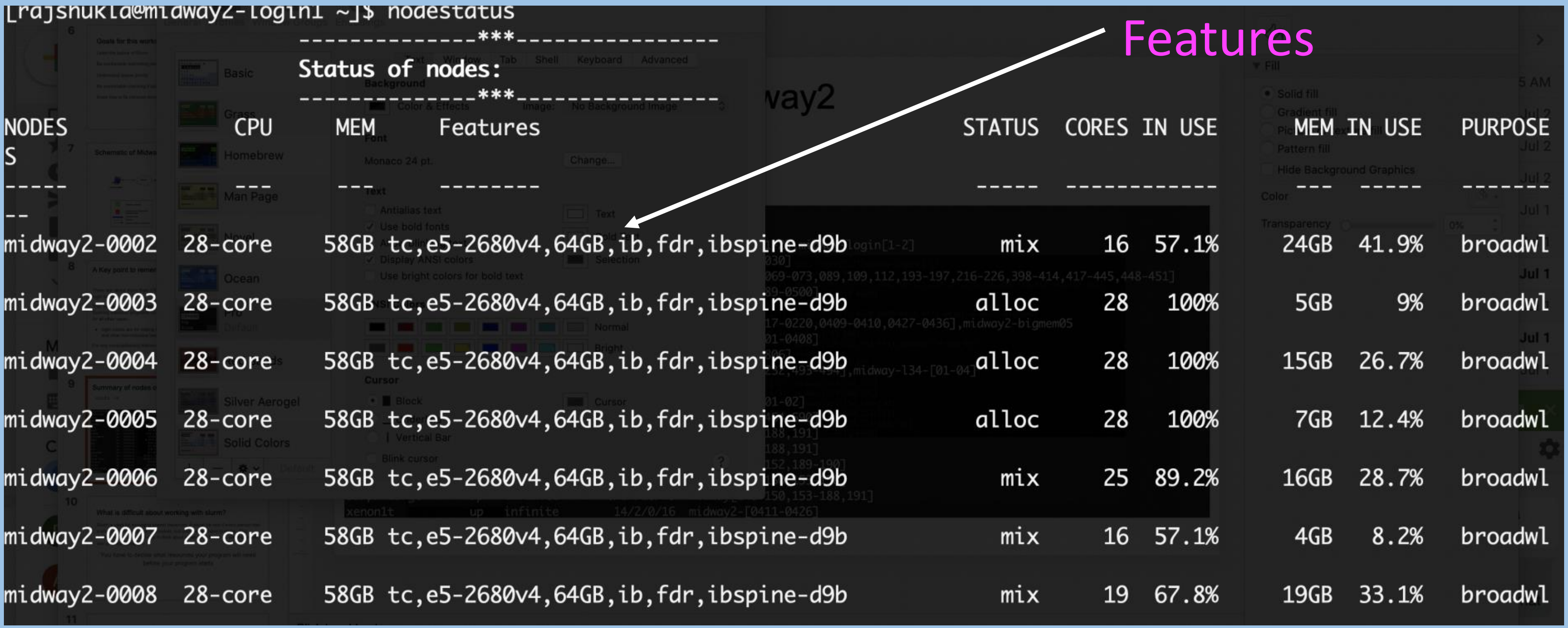
*#SBATCH –exclusive*

Add this in your batch script

*#SBATCH –constraint=v100*

## How do I know the features of the node to use with #SBATCH -constraint?

**nodestatus**



```
[rajshukla@midway2-login1 ~]$ nodestatus
                   --------------***----------------
                   Status of nodes:
                   --------------***----------------
NODES          CPU      MEM     Features                                       STATUS  CORES IN USE      MEM IN USE     PURPOSE
S
-----          ---      ---     --------                                       -----   ------------      ---  -----     -------
--
midway2-0002  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b              mix       16   57.1%     24GB  41.9%    broadwl
midway2-0003  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b            alloc       28    100%      5GB     9%    broadwl
midway2-0004  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b            alloc       28    100%     15GB  26.7%    broadwl
midway2-0005  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b            alloc       28    100%      7GB  12.4%    broadwl
midway2-0006  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b              mix       25   89.2%     16GB  28.7%    broadwl
midway2-0007  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b              mix       16   57.1%      4GB   8.2%    broadwl
midway2-0008  28-core   58GB tc,e5-2680v4,64GB,ib,fdr,ibspine-d9b              mix       19   67.8%     19GB  33.1%    broadwl
```

## What resources should I ask for?

This depends on the code you are running

**GPUs** If you code is build to use gpus you can submit to the gpu partition.  To request 1 gpu:

```
#SBATCH -p gpu2 --gres=gpu:1
```

## What resources did my job actually use?

It is good practice to occasionally check what resources your job is using.  For example if you are going to be submitting hundreds of similar jobs, you may save yourself a lot of waiting time in the queue by checking that you are not over requesting resources.

# Why did my job fail?

- Ran out of Memory
- Ran out of Time
- Problem in your submit script
- Problem with your code
- Node failure

## Why did my job fail?

- Ran out of Memory
- Ran out of Time
- Problem in your submit script
- Problem with your code
- Node failure

**You can fix these**

## Why did my job fail?

- Ran out of Memory
- Ran out of Time
- Problem in your submit script
- Problem with your code
- Node failure

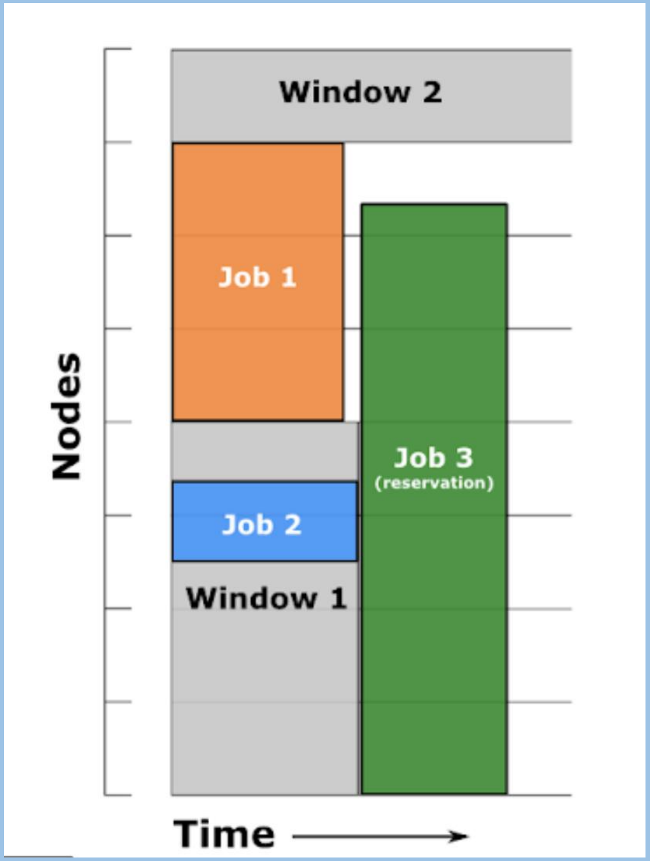
**You can fix these**

# Job Priority

- Priority is calculates using a **Fairshare** algorithm
- Fairshare is function of
  - Requested wall clock, memory, nodes/cores, etc.
  - Length of time in queue
  - Number of jobs in a time window and per PI group
  - Backfill
  - Etc.

# Job Priority

**Backfill**



the x axis is time

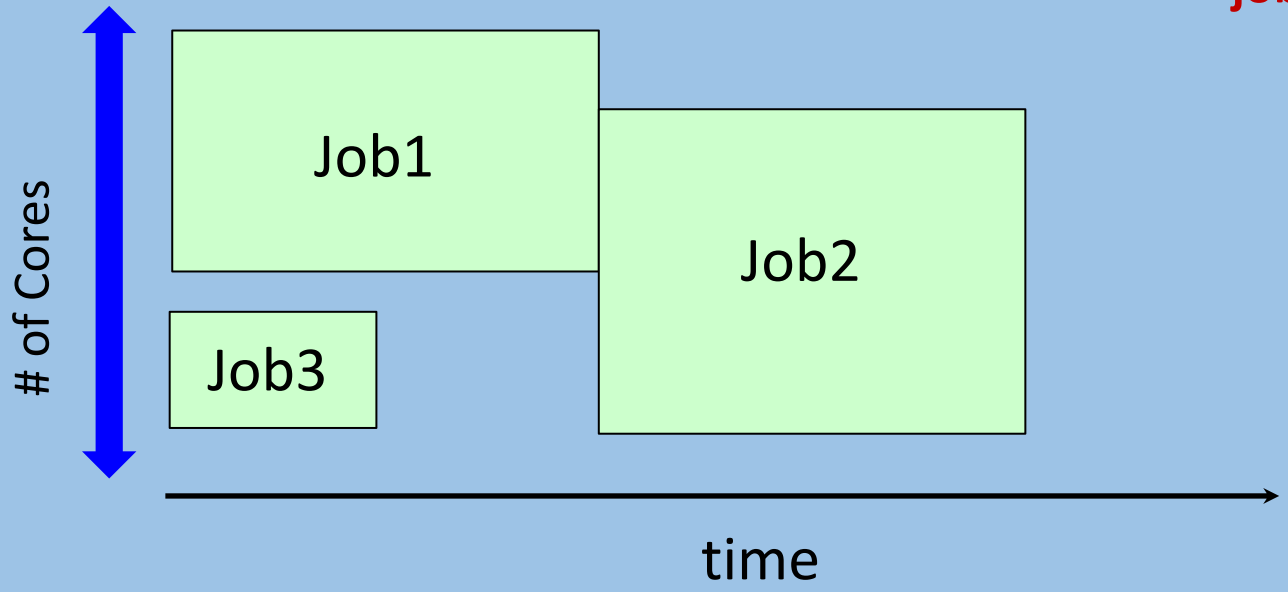
time

# Job Priority

## Backfill

Why has someone else's job started before mine?

**The scheduler can fit smaller jobs in before big jobs are due to start**

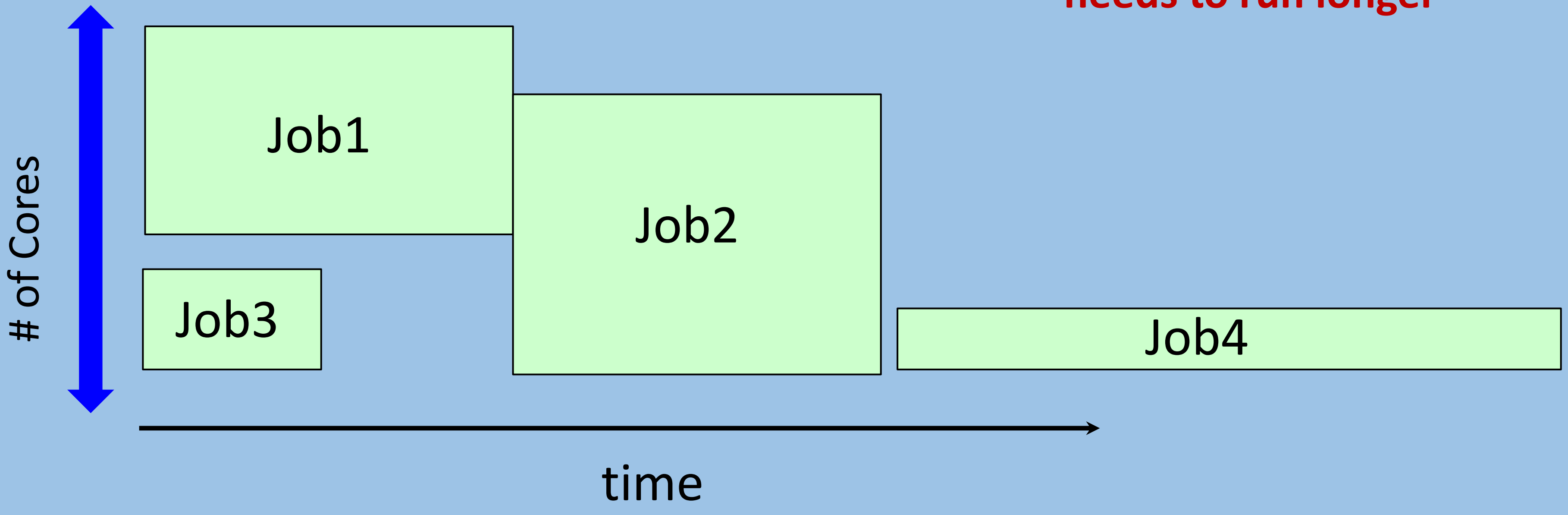


# Job Priority

## Backfill

Why has someone else's job started before mine?

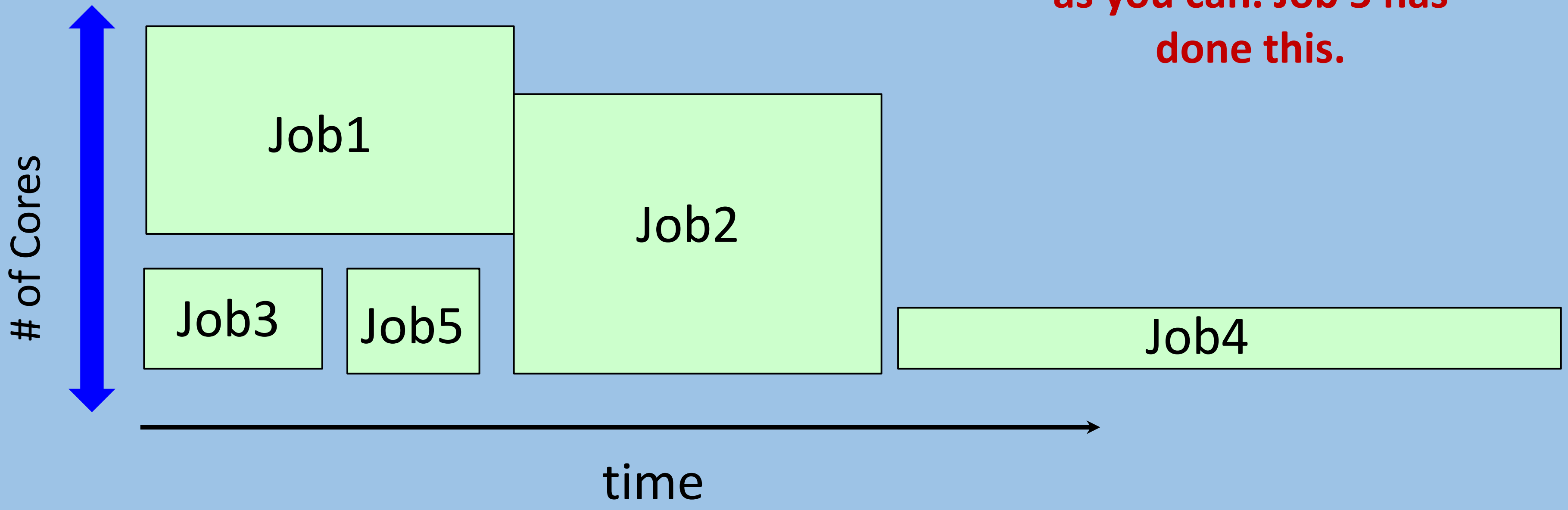
**Job4 while requesting less nodes, it can not be backfilled because it needs to run longer**



# Job Priority

## Backfill

Why has someone else's job started before mine?

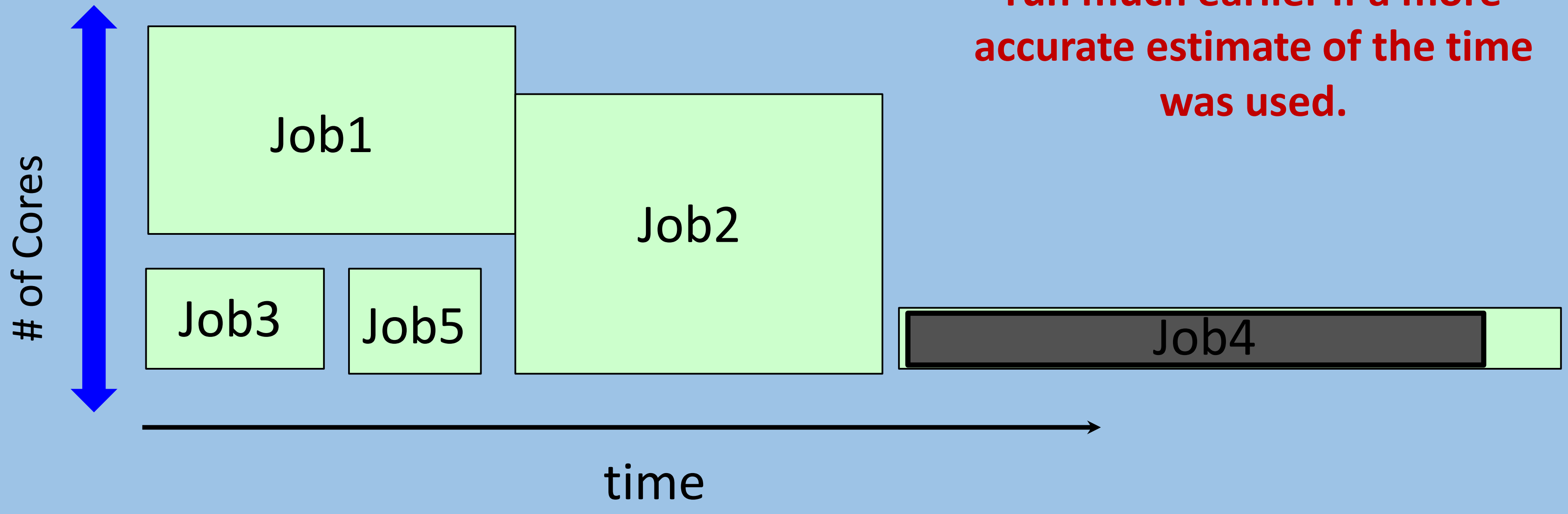


**You can take advantage of backfill by specifying wall time as accurately as you can. Job 5 has done this.**

# Job Priority

## Backfill

Why has someone else's job started before mine?



**You can take advantage of backfill by specifying wall time as accurately as you can. In this example job 4 could have run much earlier if a more accurate estimate of the time was used.**

# Job submission and monitoring
## SLURM Commands

| Command | Description |
|---|---|
| `sbatch script.sbatch` | Submits `script.sbatch` job script |
| `squeue –u $USER or myq` | Reports the status of your jobs |
| `sacct –u $USER` | Displays accounting data for your job(s) |
| `scancel jobid` | Cancels a running job or removes it from the queue |
| `scontrol show job jobid or jobinfo` | Displays details of a running job |