

# Running Jobs on RCC Systems Using the SLURM Scheduler

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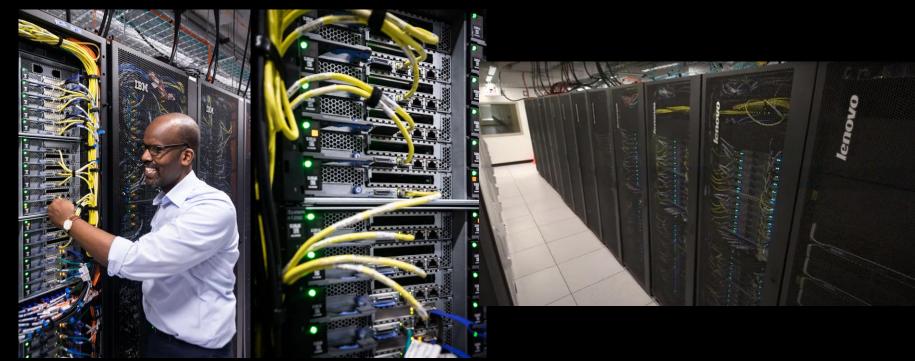
October 15th, 2020

#### Agenda

- The RCC Midway compute systems
- Using SLURM (Simple Linux Utility for Resource Management) to submit jobs to the RCC Midway systems
- => Goals of this workshop
  - Learn the basics of SLURM
  - Submit jobs on Midway HPC systems
  - Understand priority queue
  - Check if your jobs succeeded/failed
  - Know how to fix common errors

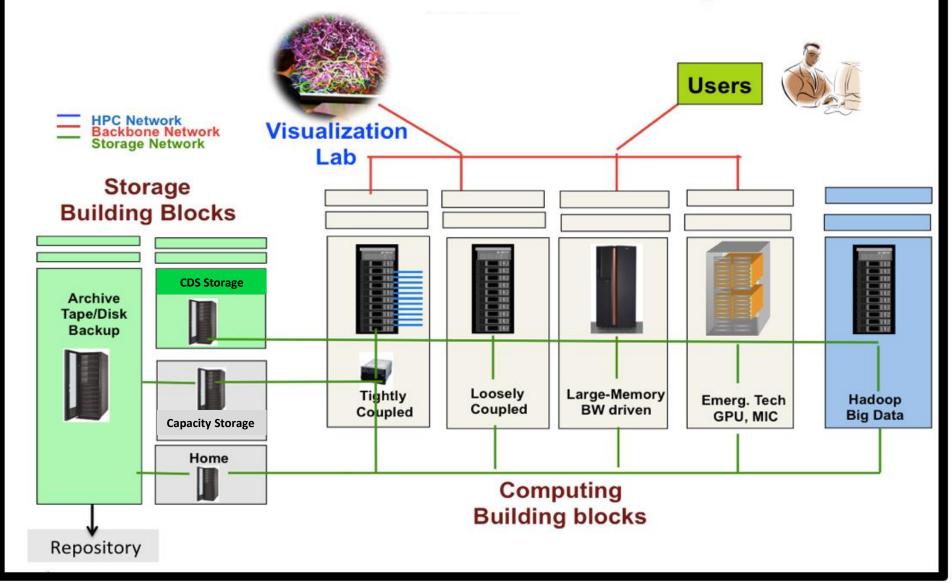
#### **Understanding the RCC Compute Ecosystem**

Midway is a constellation a of many compute systems and storage with various architectures coupled together in one system.



SLURM is the software used to manage the workload on Midway

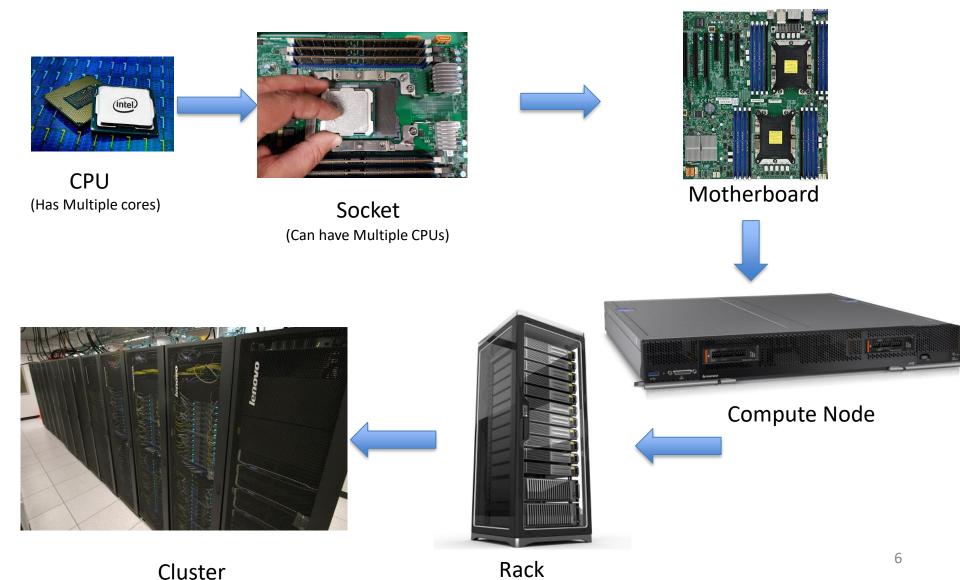
#### Hardware Infrastructure building blocks



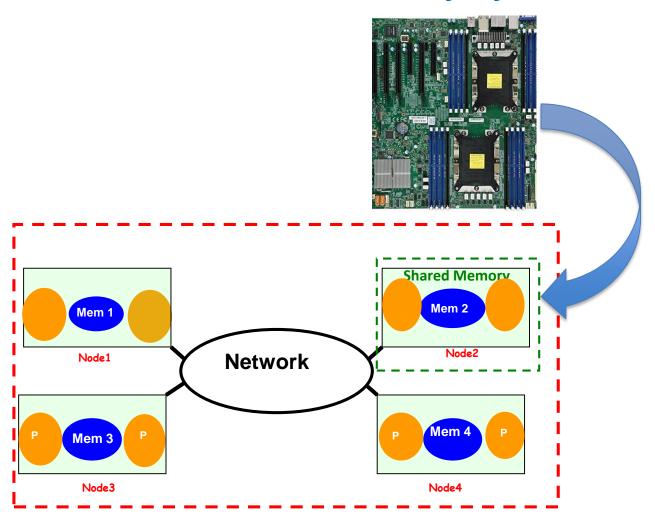
#### Some definitions

- A processor is a small chip that <u>responds to</u> and <u>processes</u> 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



#### **Distributed vs Shared Memory Systems**



**Distributed Shared Memory** 

#### The RCC compute cluster

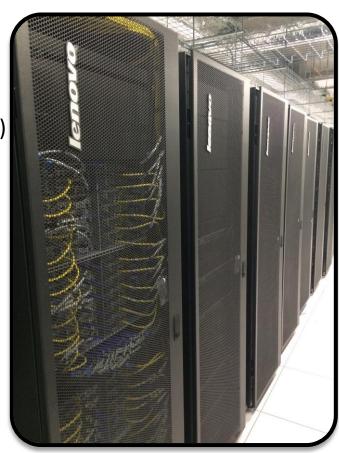
#### **Computing hardware**

#### 367 nodes total

- 342 tightly coupled Broadwell nodes (10,360 cores)
   Two intel E5-2680v4 processors per node (14 core/proc)
   155 nodes have EDR network card
   187 nodes have FDR network card
- 6 NVidia Tesla K80 GPU nodes (4 GPU cards/node)
- 5 large shared memory nodes (512GB each)
- 14 dual socket loosely-coupled Broadwell nodes

#### **Cluster Partnership Program: 1000+ nodes**

- 900+ tightly coupled infiniband nodes
- **20+** Big memory nodes
- 100+ Nvidia GPU nodes



RCC Manages 1515 nodes (35,904 cores)

#### RCC Hardware: Midway2 (Shared)

Cores(Nodes)	CPU	Memory	Network
5236 (187)	2.4GHz Intel Broadwell	64GB	EDR 100Gbit/s InfiniBand
4,340 (155)	2.4GHz Intel Broadwell	64GB	FDR14 56Gbit/s InfiniBand
140 (5)	2.4GHz Intel Broadwell	512GB	FDR14 56Gbit/s InfiniBand
504 (14)	2.4GHz Intel Broadwell	64GB	1 GigE

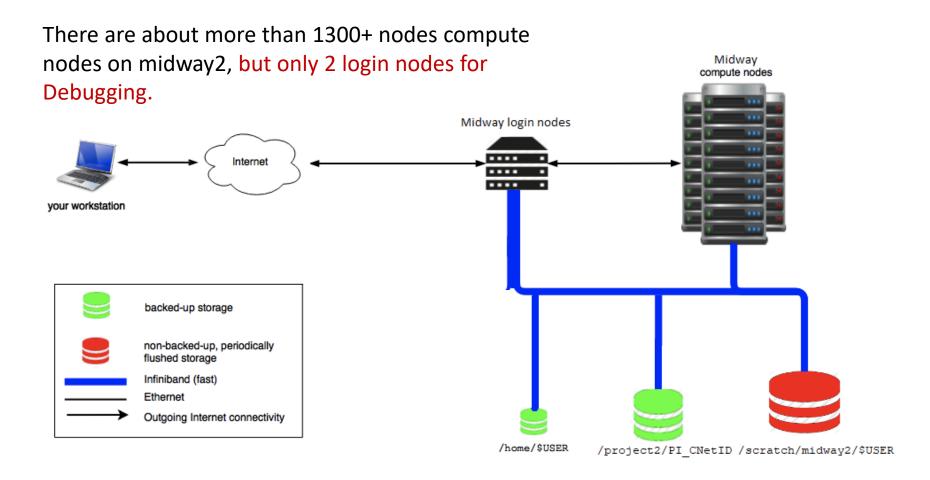
Cores (Nodes)	CPU Accelerator	Memory	Network
168 (6)	2.4GHz Intel Broadwell NVIDIA Tesla K80	128GB	FDR14 56bit/s InfiniBand

#### RCC Hardware: Midway2 (Shared)

Cores(No	des) CPU	Memory	Slurm Queue
5180 (18	2.4GHz Intel Broadwe	ell 64GB	broadwl
5180 (18	5) 2.4GHz Intel Broadwe	ell 64GB	broadwl
168 (6)	2.4GHz Intel Broadwe	ell 512GB	bigmem2
504 (18	3) 2.4GHz Intel Broadwo	ell 64GB	broadwl-lc

Cores (Nodes)	CPU Accelerator	Memory	Queue
168 (6)	2.4GHz Intel Broadwell NVIDIA Tesla K80	128GB	gpu2

## Schematic of the Midway Cluster



#### Midway2 Storage

#### **High Capacity storage: /project2**

- **3.8 PB** of storage
- Backed up to tape system
- 7 daily and 4 weekly snapshots located at /snapshots/project2
- 7 day grace period on over quota

#### **High Performance storage: /scratch/midway2**

- **190 TB** usable
- Not backed up
- 100 GB user soft quota
- 30 day grace period on over quota

#### Home directory space: /home

- **61 TB** of capacity
- Each user has 30 GB quota
- 7 day grace period on over quota
- 7 daily and 2 weekly snapshots located at /snapshots/home



# How to Run jobs at RCC

- Interactively
- Submitting jobs to a queue using SLURM

#### Repository

Please clone the Github repo at:

https://github.com/rcc-uchicago/SLURM WORKSHOP.git

[tszasz@midway2-login1 Intro\_SLURM]\$ git clone https://github.com/rcc-uchicago/SLURM\_WORKSHOP.git

#### A Key point to remember

There are about more than 1300+ nodes compute nodes on midway2, but only 2 login nodes.

This means you are sharing the login nodes with many other users at once. Running intensive programs on the login nodes causes the login nodes to be slow for all other users.

- login nodes are for editing files, compiling, moving files, changing permissions, and other non-intensive tasks.
- We recommend to use sinteractive for interactive runs
- For long running jobs => submit them to the priority queue through SLURM

#### Running Interactive jobs

- Login directly to a node
  - -Login to midway2.rcc.uchicago.edu

• Run interactively using sinteractive

```
sinteractive --time=01:00:00 --nodes=1
--ntasks=2 --mem-per-cpu=1000 --
partition=broadwl --reservation=slurm-
workshop
```

## Summary of partitions and nodes on sinfo -s Midway2

```
[rajshukla@midway2-login1 ~]$ sinfo -s
PARTITION
               AVAIL TIMELIMIT
                                 NODES(A/I/O/T)
                                                 NODELIST
                      infinite
                                                 dali-login[1-2],midway-login[1-2]
cron
                                      0/28/1/29 midway[002-030]
                      infinite
westmere
                 up
                      infinite
                                     49/24/2/75 midway[044,069-073,089,109,112,193-197,216-226,398-414,417-445,448-451]
sandyb
mfj
                      infinite
                                      1/11/0/12 midway2-[0489-0500]
                      infinite
                                        0/1/0/1 midway397
test
                      infinite
                                      16/0/1/17 midway2-[0217-0220,0409-0410,0427-0436],midway2-bigmem05
cobey
inovembre
                 up infinite
                                        4/4/0/8 midway2-[0401-0408]
tas1
                    infinite
                                      0/19/5/24 midway[783-806]
                      infinite
                                        0/8/1/9 midway[230-232,493-494],midway-134-[01-04]
gpu
viz
                      infinite
                                        0/1/0/1 midway229
mic
                      infinite
                                        0/0/2/2 midway-mic[01-02]
                     infinite
                                        0/3/0/3 midway[453-454,590]
sepalmer
kicp
                      infinite
                                     0/20/11/31 midway[159-188,191]
                     infinite
                                     0/20/11/31 midway[159-188,191]
kicp-long
                      infinite
                                        0/4/0/4 midway[151-152,189-190]
kicp-ht
surph
                      infinite
                                       0/7/7/14 midway[143-150,153-158]
                 up
                                     0/27/18/45 midway[143-150,153-188,191]
surph-large
                      infinite
xenon1t
                      infinite
                                      14/2/0/16 midwav2-Γ0411-04267
```

⇒ NODES(A/I/O/T) : Nodes (Allocated/Idle/Other/Total) e.g: To check the broadwl partition: sinfo –s |grep broadwl

midway2-[0203-0216]

midway2-[0002-0133,0137-0190,0221-0280,0282-0299,0301,0311-0398,0461-0466,0612]

infinite

infinite

up

up

214/133/13/360

12/0/2/14

## **SLURM: Some key terms to remember**

A **job defines** 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, use the command:

squeue

To see your jobs in the queue

squeue -u <cnetid>

or

myq

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
```

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
```

This #! is a shebang

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

# is a comment everything after # is ignored by bash

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
```

**#SBATCH** is a directive

It is a comment in Bash

**#SBATCH** is only relevant to SLURM:

sbatch my\_script.sh

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
```

**#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

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

#### 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

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.

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
```

```
=> 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.
- module load <module name> => 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):

```
#!/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

Your Job

Your Job

Your Job

Your Job

#SBATCH --time=00:30:00

Your Job

Your Job

#SBATCH --time=00:30:00
```

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

## Please do the 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.

## Please do the 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

## Please do the Exercise; Ex-3 in Repo

#### How to submit GPU jobs?

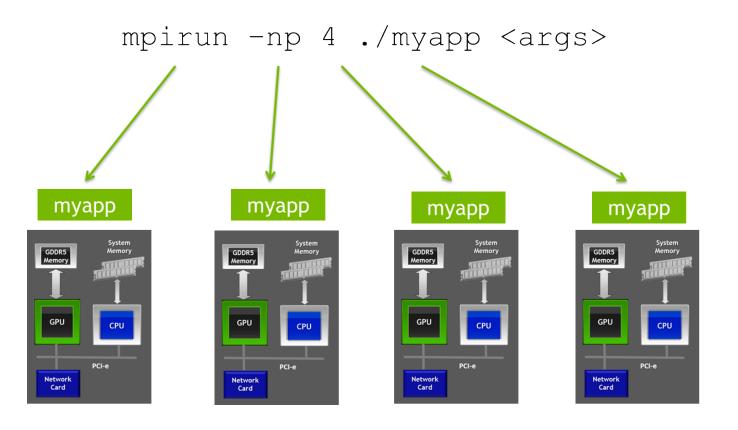
```
#!/bin/bash
#Here is a comment
#SBATCH --time=1:00:00
#SBATCH -partition=gpu2
#SBATCH -gres=gpu:1
#SBATCH -nodes=1
#SBATCH –ntasks-per-node=8
#SBATCH --mem-per-cpu=2000
#SBATCH -job-name=MyJob
#SBATCH -output= MyJob-%j.out
#SBATCH -error=MyJob-%j.err
module load <module name>
#Run your code
./my executable
```

Specify partition gpu2
Specify number of gpus, like *qpu*:1

## Please do the Exercise; Ex-4 in Repo

#### How to submit MPI + GPU jobs?

**CUDA Aware MPI** 



## How to submit MPI + GPU jobs?

#### Compilation

Job Submission

```
#!/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
```

```
#!/bin/bash brown.edu/oscar/gpu-computing/mpi-cuda

#SBATCH -t 00:30:00

#SBATCH --nodes=2

#SBATCH --ntasks-per-node=4 slide show Review

#SBATCH --partition=gpu2

#SBATCH --gres=gpu:2dd-ins Shapes lone 30 Models

#SBATCH --job-name=MyJob

#SBATCH --job-name=MyJob

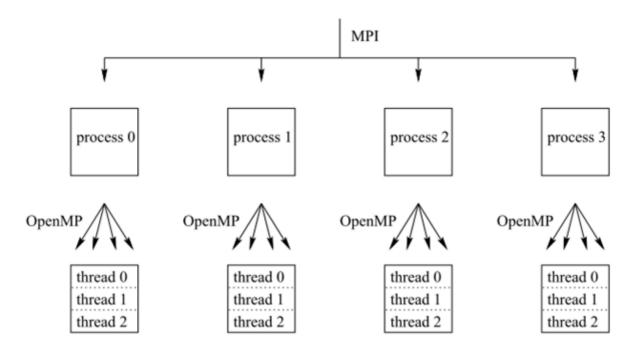
#SBATCH --output=MyJob-%j.out

#SBATCH --qos=stafftest

mpirun ./HostMap
```

## Please do the 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 --aos=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
```

## Please do the 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))
echo "Running job array number: "$SLURM ARRAY TASK ID "input " $input
```

## Please do the Exercise; Ex-6 in Repo

### How to submit dependent jobs

#### **SLURM Rule:**

sbatch --dependency=type:job\_id jobfile

```
# first the job re-us now dependencies

jobID_1=$(sbatch preprocessing the processing the proces
```

### 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				

## Please do the 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**

Please do the Exercise; Ex-8 in Repo

This depends on the code you are running

This depends on the code you are running

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

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.

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

Lrajsnukla⊕mi	away2-Log	ini ~j\$ nodestatus ***			/ F	eatu	ires	n 	<b>&gt;</b>
Northead comments Normal comments Normal comments Normal comments	Basic	Status of nodes:	o Background Image vay2				Solid fill  Cradient fill  Cradient fill  Cradient fill  Cradient fill  Cradient fill  Cradient fill		5 AM
NODES S	CPU Homebrew	MEM Features	hange	STATUS	CORES	IN USE	Pic MEM as	IN USE	PURPOSE
	Man Page	Text Antialies text	I Text				Color	und Graphics	Jul 2
midway2-0002	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	in[1-2] <b>mix</b>	16	57.1%	24GB	41.9%	broadwl
midway2-0003	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	alloc 10,0427-0436],midway2-bigme	28	100%	5GB	9%	broadwl
midway2-0004	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	twoy-134-[01-04]alloc	28	100%	15GB	26.7%	broadwl
midway2-0005	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	alloc	28	100%	7GB	12.4%	broadwl
midway2-0006	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	mix	25	89.2%	16GB	28.7%	broadwl
midway2-0007	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	mix	16	57.1%	4GB	8.2%	broadwl
midway2-0008	28-core	58GB tc,e5-2680v4,64	GB,ib,fdr,ibspine-d9b	mix	19	67.8%	19GB	33.1%	broadwl

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. Midway2 has a script to display the resources a job used:

Replace 99999 with the job ID of the job you are interested in.

### 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
- => For node failure please email <a href="help@rcc.uchicago.edu">help@rcc.uchicago.edu</a>, if this happens

You can fix these

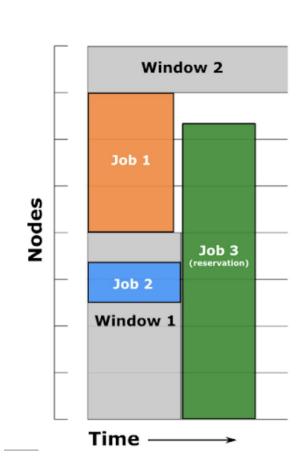
## **Job Priority**

- 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**

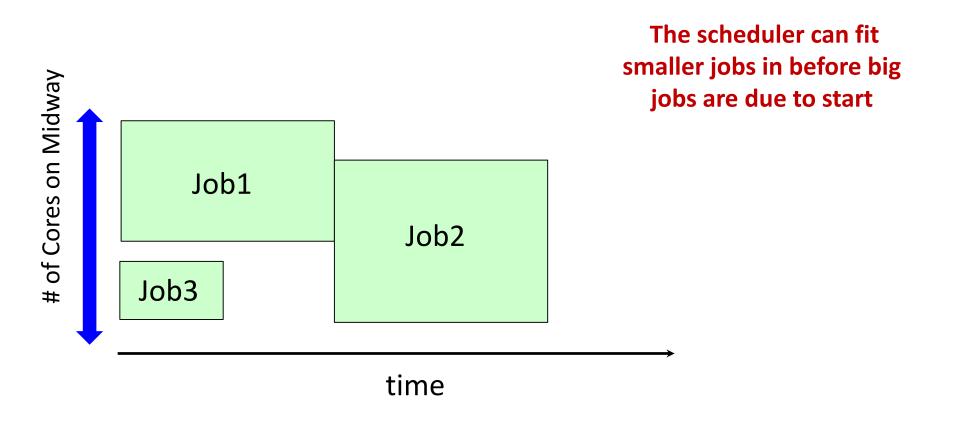
#### **Backfill**

This blue line represents all the cores on Midway



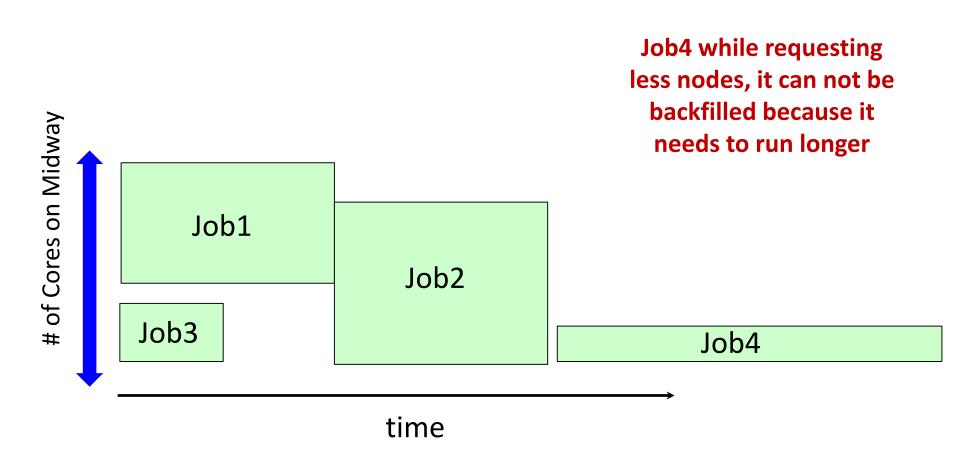
the x axis is time

# Job Priority Backfill



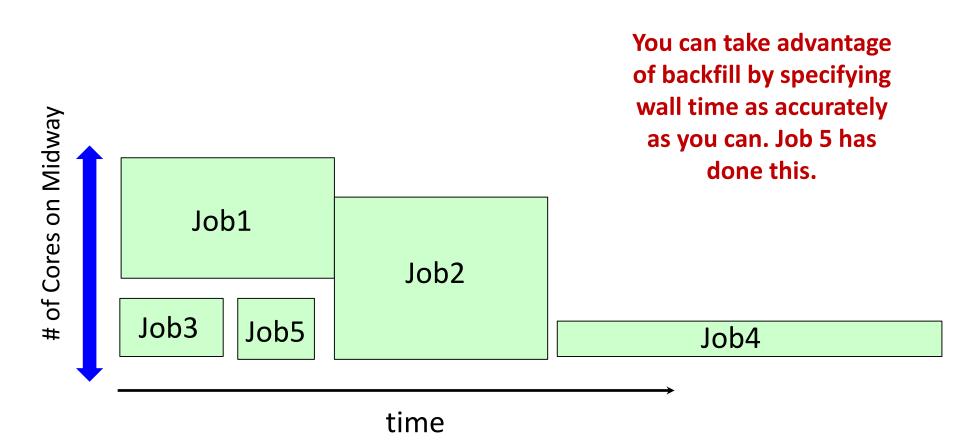
## **Job Priority**

#### **Backfill**

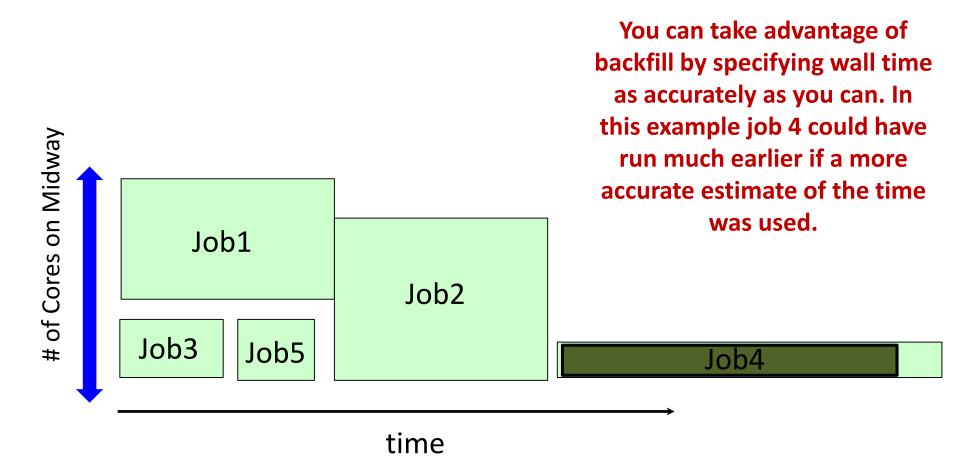


## **Job Priority**

#### **Backfill**



# Job Priority Backfill



## 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

#### Recommended online resources

- User guide on running jobs on Midway
  - https://rcc.uchicago.edu/docs/runningjobs/index.html
- Details Slurm documentation
  - https://slurm.schedmd.com/sbatch.html
- SLURM Cheat Sheet
  - https://slurm.schedmd.com/pdfs/summary.pdf

#### RCC Help

#### Contact:

A bottom—up approach to supporting research computing

- By email: help@rcc.uchicago.edu
- Web: rcc.uchicago.edu
- Phone: 773-795-2667
- In person:
  - 5607 S Drexel Avenue
  - Regenstein Room 216
- Workshops and Tutorials:
- http://rcc.uchicago.edu/services/training.html

## Thank You!