NJIT
New Jersey Institute of Technology

High Performance Computing

NJIT High Performance Computing (HPC) Workshop: SLURM Batch system basics

Sep 18, 2024

Outline

- NJIT HPC Overview
- Batch Processing
- Example of Slurm Jobs
- Manage Slurm Jobs
- Troubleshooting Common Issues
- Slurm Interactive Jobs and Use GUI Apps
- Contact Us

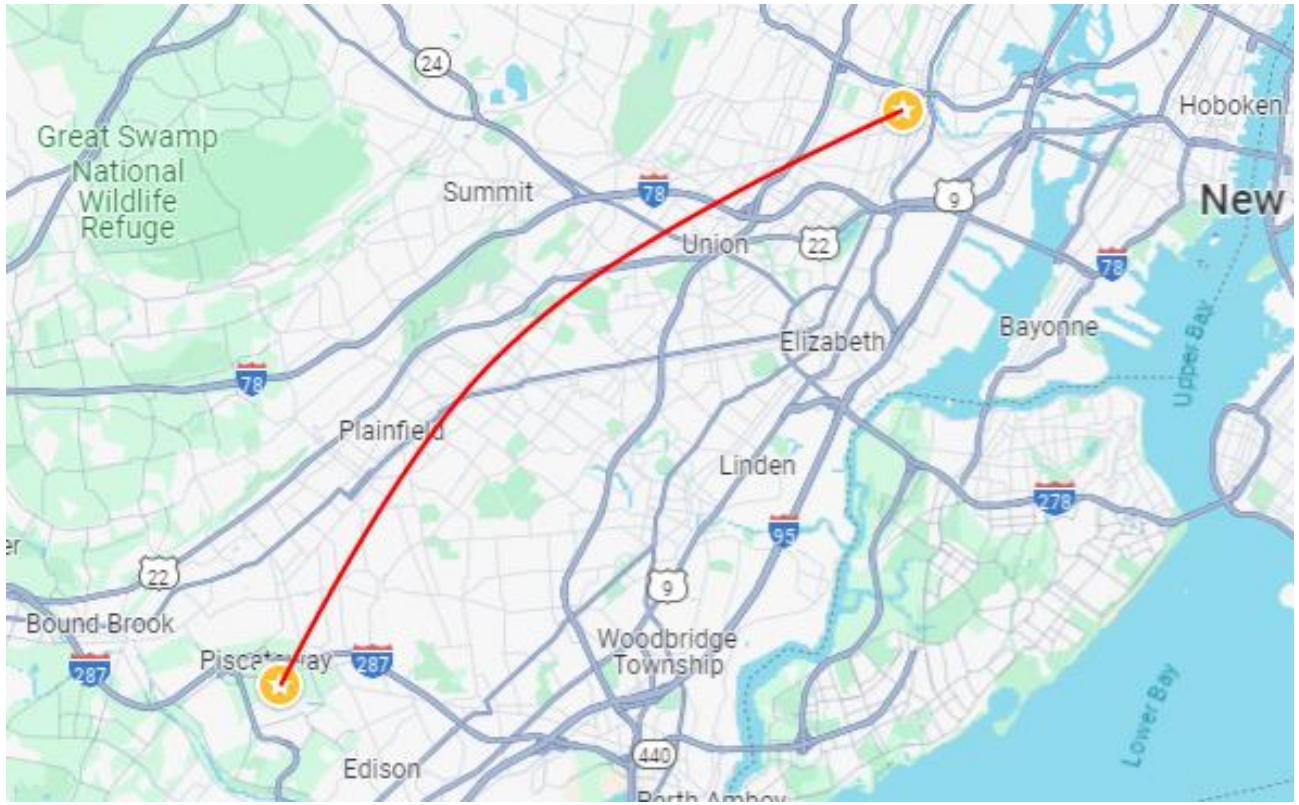
NJIT HPC Overview

About NJIT HPC

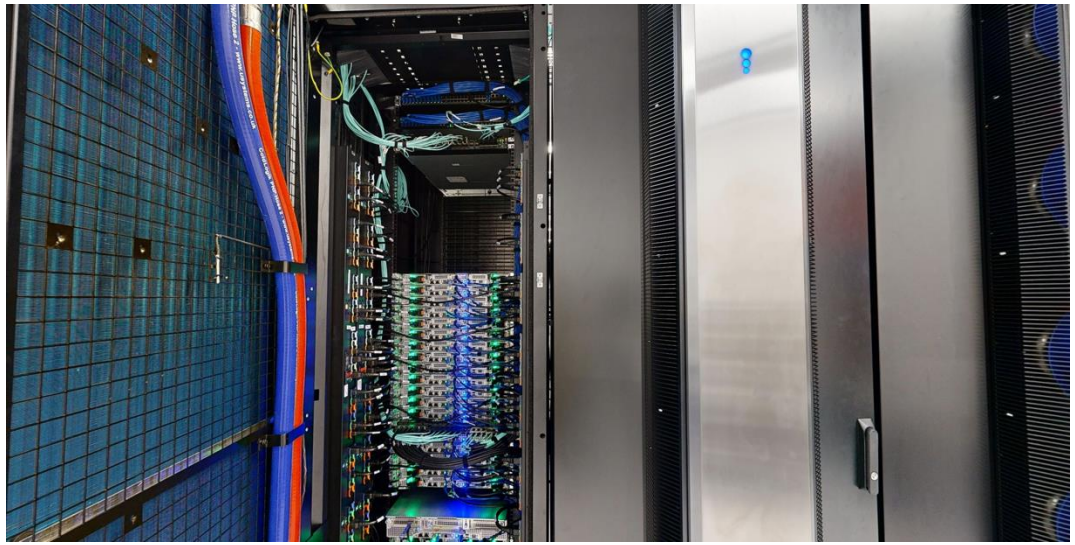
NJIT new high performance computing environment, built through a partnership with DataBank, a leading provider of enterprise-class colocation, connectivity and managed services, is live in DataBank's Piscataway, N.J. data center (EWR2) and will support NJIT's research efforts.

The services NJIT HPC provides

- High performance computing services
- Computational science expertise



Service Catalog



Cluster Computing

Built by Dell, the computing environment “Wulver” provides a total of 127 compute nodes or servers

Research Data Storage

High-performance, large capacity data storage spaces that are perfect for a wide variety of research data

Education

High performance computing and networking resources come together to create an exciting and innovative teaching and research environment

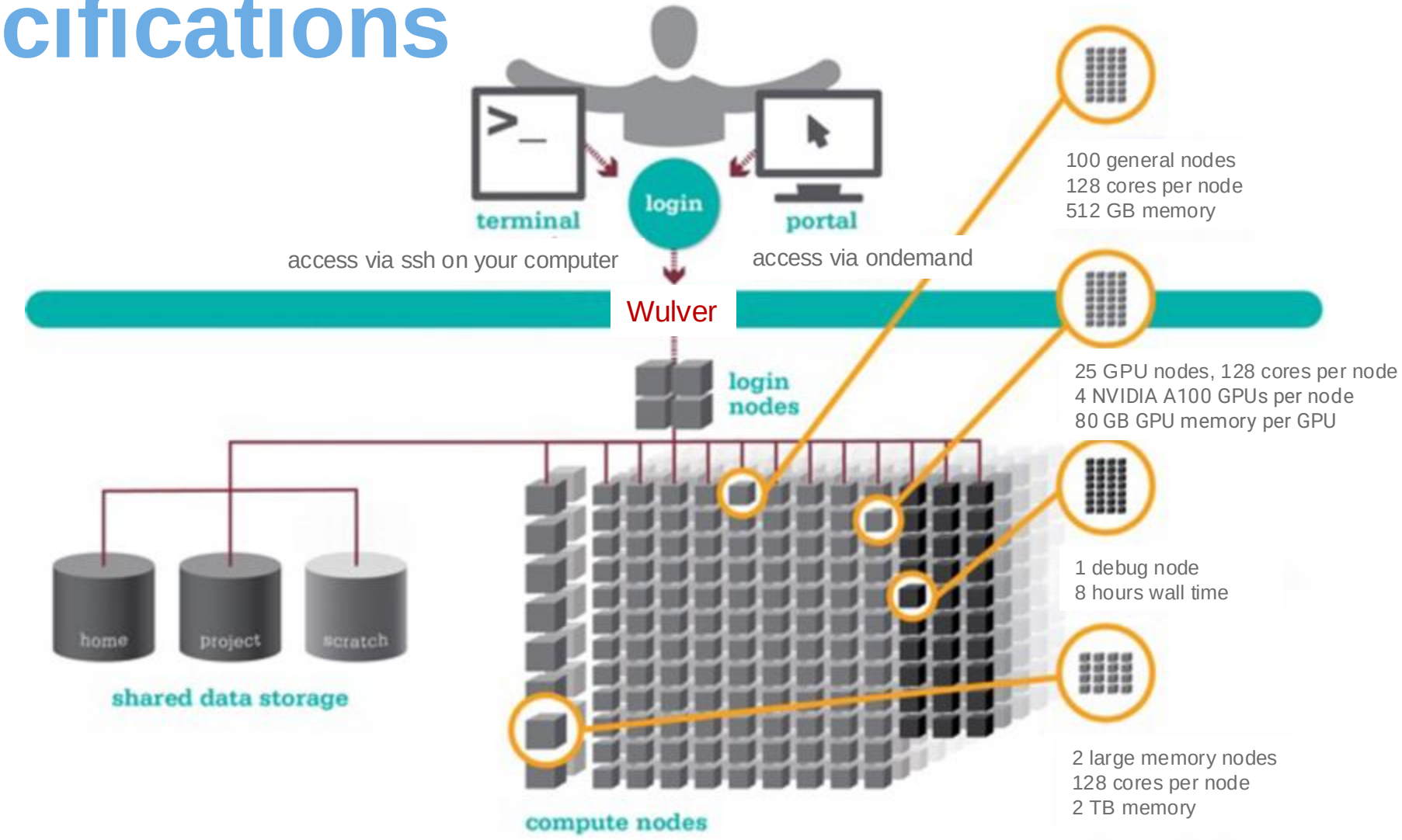
HPC Facilitation Service

Empowering users to perform essential research computing projects through training and effective user support

Scientific Software Development

Deep expertise in developing and deploying software

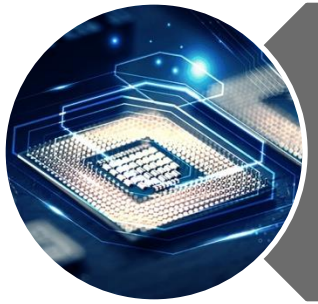
Wulver Cluster Specifications



hpc.njit.edu/clusters/get_started_on_Wulver

HPC Allocations

- Accounting of computational resources for research
- Standard annual allocation – 300,000 SU's per year
- Groups can purchase more if needed



Computing time

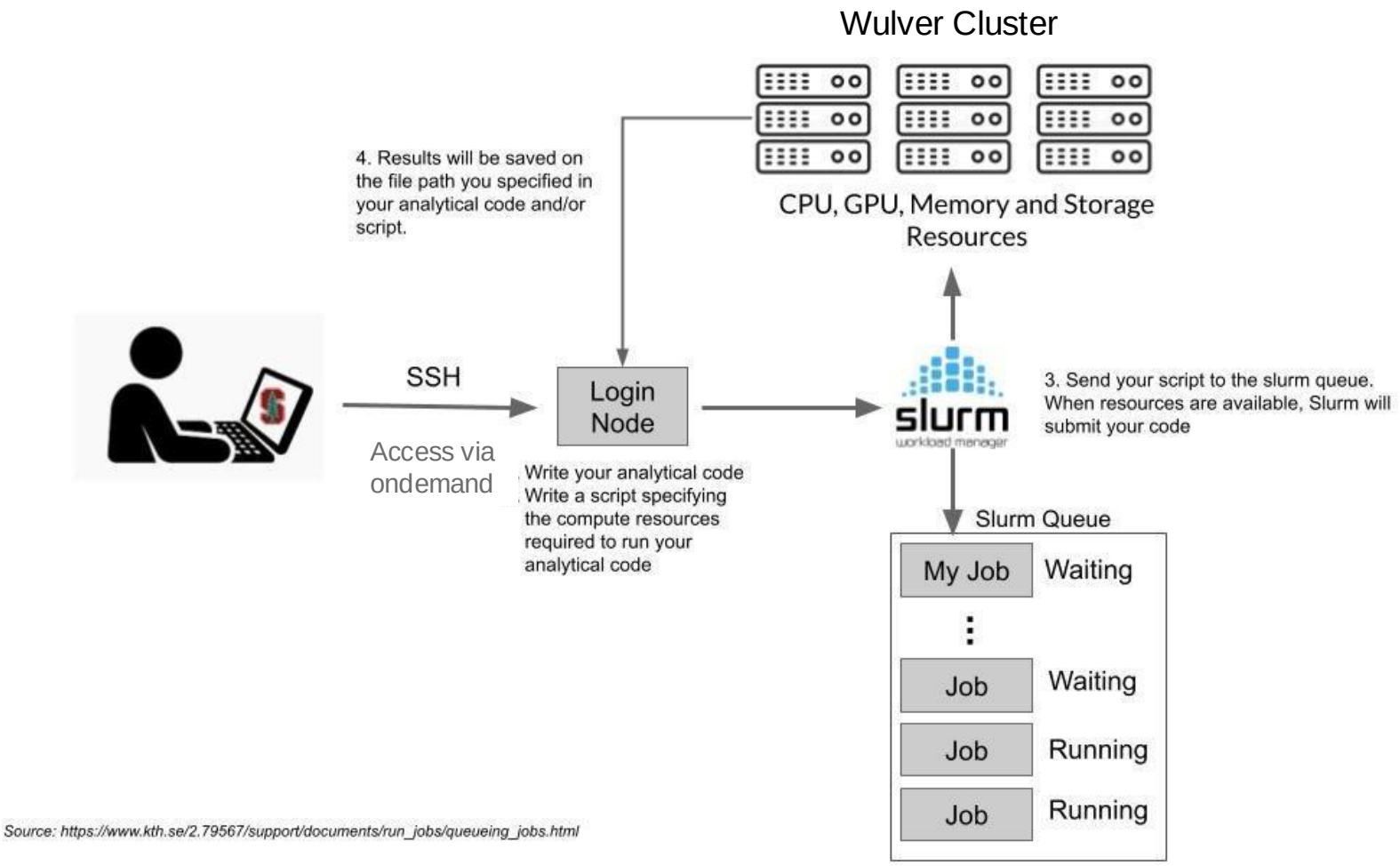
- Measured as CPU hours or SU (Service Units)
- 1 SU = Number of CPUs x Walltime in hours x usage factor

Storage

- Home (~50GB/user)
- Project (2TB/PI Group)
- Scratch (30+ days old files will be deleted)

Batch Processing

Why do supercomputers use queuing?



Source: https://www.kth.se/2.79567/support/documents/run_jobs/queueing_jobs.html

What is Slurm?

- Slurm is the predominant Open-Source scheduler for HPC compute
- Historically Slurm was an acronym standing for
  - **S**imple **L**inux **U**tility for **R**esource **M**anagement
- The Slurm scheduler provides three key functions:
  - it allocates access to resources (compute nodes) to users for some duration of time so they can perform work.
  - it provides a framework for starting, executing, and monitoring work (typically a parallel job such as MPI) on a set of allocated nodes.
  - it arbitrates contention for resources by managing a queue of pending jobs.

Manage Jobs – Options

Mandatory Options

Directive	Options	Description
--account=	account	PI's UCID
--partition=	Partition	Request a partition of resources for job allocation (queue)
--time=	Time [[d-]h:]m[:s]	Minimum time limit on job allocation
--qos=	Job Priorities	Define the job priority

see https://slurm.schedmd.com/srun.html for more details

HPC Partitions

- Example of SU charges: (20 cores with 4 GPU for 8 hours)
- SU = 20 x 8 x 3 = 480

Partition	Nodes	Cores /Node	CPU	GPU	Memory	SU charge
`--partition=general`	100	128	2.5G GHz AMD EPYC 7763 (2)	NA	512 GB	1 SU per hour per cpu
`--partition=debug`	1	4	2.5G GHz AMD EPYC 7763 (2)	NA	512 GB	No charges, must be used with `--qos=debug`
`--partition=gpu`	25	128	2.0 GHz AMD EPYC 7713 (2)	NVIDIA A100 GPUs (4)	512 GB	3 SU per hour per cpu
`--partition=bigmem`	2	128	2.5G GHz AMD EPYC 7763 (2)	NA	2 TB	1.5 SU per hour per cpu

https://hpc.njit.edu/Software/slurm/slurm/

Job Submission Time Interval Formats

- Valid time formats (with a few exceptions) for `-t / --time=` option

Minutes	(`-t 10` is 10 minutes)
Minutes:Seconds	(…`10:30` is 10 minutes & 30 secs)
Hours:Minutes:Seconds	(`1:0:0` is 1 hr + 0mins + 0secs)
Days-Hours:Minutes:Seconds	(`7-1:10:30` is 7days + 1hr + 10mins + 30secs)
Days-Hours	(`7-0` is 7days + 0hrs i.e. 7 days)
Days-Hours:Minutes	(`7-4:10` is 7days + 4hrs + 10mins)

QoS

- Standard Priority (`--qos=standard`)
  - Faculty PIs are allocated 300,000 Service Units (SU) per year on request at no cost
  - Additional SUs may be purchased at a cost of $0.005/SU.
  - The minimum purchase is 50,000 SU ($250)
  - Wall time maximum - 72 hours
- Low Priority (`--qos=low`)
  - Not charged against SU allocation
  - Wall time maximum - 72 hours
  - Jobs can be preempted by those with higher and standard priority jobs when they are in the queue
- High Priority (`--qos=high_$PI`)
  - Only available to owners/investors
  - Not charged against SU allocation
  - Wall time maximum - 72 hours – can be increased based on PI's request
  - Only available to contributors

Manage Jobs – Options

Additional Options

Directive	Options	Description
--ntasks=	Number of cpus	Number of CPUs (tasks) to be allocated
--nodes=	Node	Number of Nodes
--ntasks-per-node=	Numbers of cpus per node	Number of CPUs (tasks) per each node to be allocated
--mem=	Memory	Total memory of the job
--mem-per-cpu=	Memory per cpu	Memory to be allocated per each cpu
--gres=	Generic resources	Set the Number of gpus
--cpus-per-task=	Cpus per task	Number of CPUs per task
--requeue	Requeue	This is required when you want to continue the job after 72h walltime.

Directive	Options	Description
--error=	File	Define standard error file
--out=	File	Define standard output file
--input=	File	File used for standard input
--job	Name	Define job name
--mail-type=	ALL, BEGIN, END, FAIL, REQUEUE	Notify user by email when <type> event occurs
--mail-user=	Email address	Send email to this address for events specified with mail-type option (default is submitting user).
--dependency=	Job dependency	Set the job dependency when submitting multiple jobs

see https://slurm.schedmd.com/srun.html for more details

General Application Workflow

- Log into cluster with ucid and password
- Copy input files to new directory
- Change to copied directory via command line

  `cd /path/to/copied_directory`
- Copy job a template to the directory

  `cp /path/to/templates/`***`jobtemplate`***`.job` **`jobfile`**`.job`
- Modify the job file:
  - Change the number of resources to desired number
  - Change the module load command based on the application name and version
  - Update command line with commands required for job
  - Update the software modules
- Submit the job file using `sbatch`

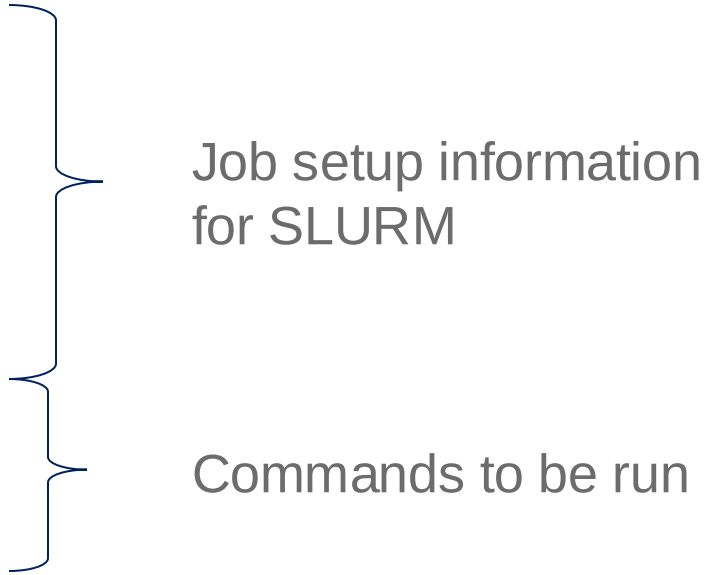
Examples of Slurm Jobs

Sample Simple Job Script

```
#!/bin/bash

#SBATCH --job-name=my_job
#SBATCH --partition=general
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --account=PI_UCID
#SBATCH --qos=low
#SBATCH --time=00:20:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --mail-type=ALL
#SBATCH –mail-user=ab1234@njit.edu

date
sleep 60
date
```



- This runs a batch job called “my_job” to the “general” partition, with 1 task, a wall time limit of 20 minutes.
- QOS is required. Account is recommended.
- `%x.%j` expands to JobName.JobID and prints this into a text file

Check sample job scripts in `/apps/testjobs/workshop`

Sample MPI Job script

```
#!/bin/bash

#SBATCH --job-name=mpi_test_job
#SBATCH --partition=general
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --account=PI_UCID
#SBATCH --qos=low
#SBATCH --time=00:10:00
#SBATCH --ntasks=256
#SBATCH --ntasks-per-node=128
#SBATCH --mem-per-cpu=2G

# Run application commands
srun /apps/testjobs/bin/mpihello
```

- This runs an MPI job named “mpi_test_job”, with 256 processes total, spread over 2 nodes. Default setting is 1 core per process/task, so this also allocates 512Gb memory total. Wall time is 10 minutes.

Check sample job scripts in `/apps/testjobs/workshop`

Sample Multi GPU Job script

```
#!/bin/bash

#SBATCH --job-name=test_gpu_job
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --partition=gpu
#SBATCH --account=PI_UCID
#SBATCH --qos=low
#SBATCH --time=00:20:00
#SBATCH --ntasks=2
#SBATCH --cpus-per-task=32
#SBATCH --gres=gpu:2

# Load application environment
module load CUDA

# Run application commands
nvidia-smi
```

- This runs a GPU job named “test_gpu_job”, with 64 cpus and full access to 2 GPUs. Wall time is 20 minutes.

Check sample job scripts in `/apps/testjobs/workshop`

Sample GPU Job script

```
#!/bin/bash

#SBATCH --job-name=test_gpu_job
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --partition=gpu
#SBATCH --account= PI_UCID
#SBATCH --qos=low
#SBATCH --time=00:20:00
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=8
#SBATCH --gpus-per-task=1

# Load application environment
module load CUDA

# Run application commands
nvidia-smi
```

- This runs a GPU job named “test_gpu_job”, with 8 cpus and 1 GPU

Check sample job scripts in `/apps/testjobs/workshop`

Manage Slurm Jobs

Manage Jobs - Overview

- SLURM documentation:
  - “User Manual” on head node (accessible through Web Portal)
  - The Source: SLURM Documentation
  - man pages (sbatch, squeue, etc.)

- Common job tasks
  - Submitting jobs
  - Running parallel jobs
  - Listing jobs
  - Resuming jobs
  - Canceling jobs

Manage Jobs – Submit via CLI

Submit a job script

- $ **sbatch my_script**
- Submitted batch job 1234

Listing jobs

- For current user in Pending, Running, Suspended states:
  - **$ squeue –u $LOGNAME**

```
JOBID PARTITION   NAME   USER ST TIME  NODES NODELIST(REASON)
1234   general uname.sh  test PD 0:00    2     (Priority)
```

For a more detailed query on active job:

- **$ scontrol show jobid=1234**

```
JobId=2 JobName=simple.job
UserId=test(1001) GroupId=test(1001) MCS_label=N/A
Priority=4294901759 Nice=0 Account=(null) QOS=standard
JobState=COMPLETED Reason=None Dependency=(null)
…
```

Canceling jobs

- $ **scancel 1234 -** Cancel job ID 1234

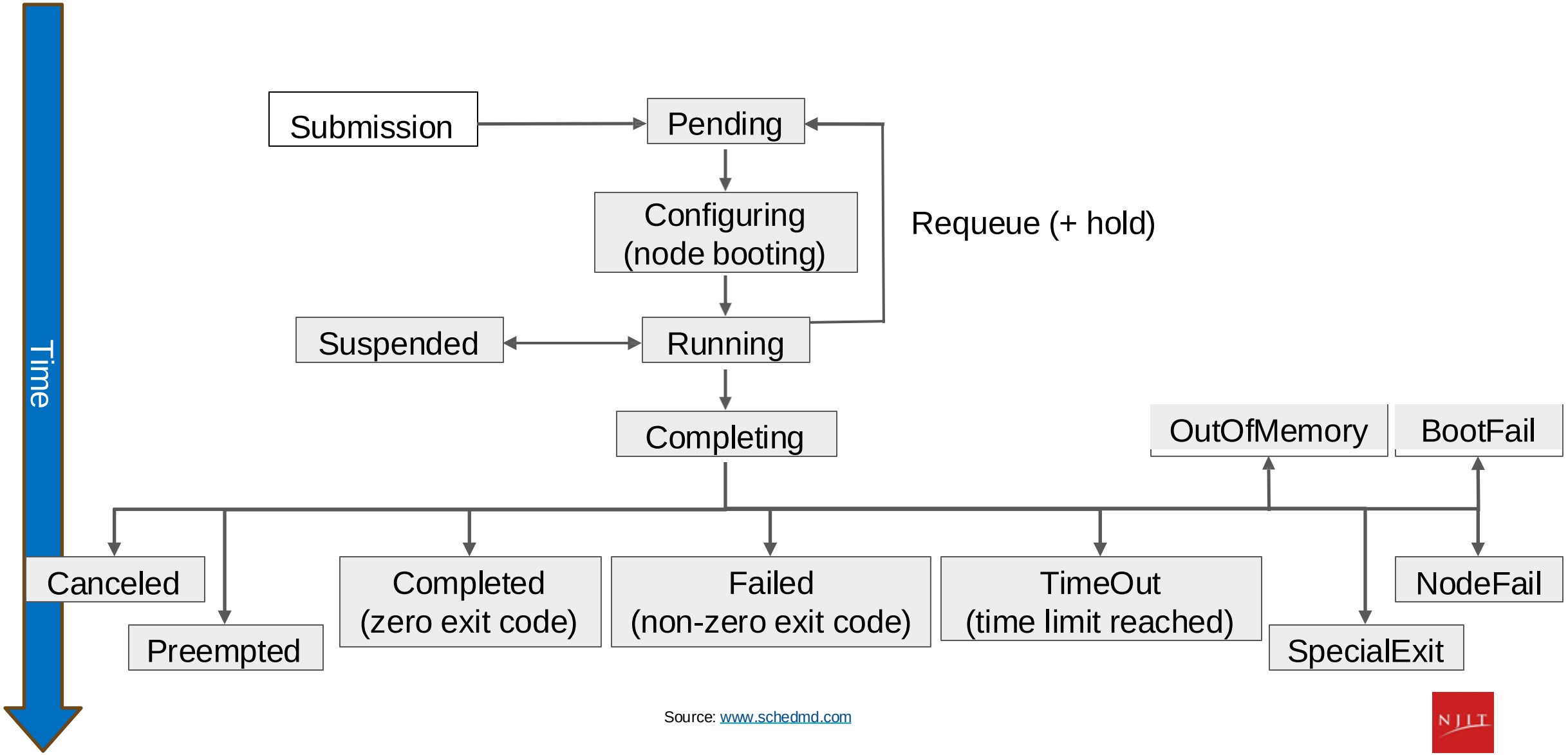
Show information about an active or completed job

- $ **slurm_jobid 1234**

Job States

- CA CANCELLED - Job was explicitly cancelled by the user or system administrator. The job may or may not have been initiated.
- **CD COMPLETED - Job has terminated all processes on all nodes with an exit code of zero.**
- CF CONFIGURING - Job has been allocated resources but are waiting for them to become ready for use (e.g. booting).
- **CG COMPLETING - Job is in the process of completing. Some processes on some nodes may still be active.**
- **F FAILED - Job terminated with non-zero exit code or other failure condition.**
- **NF NODE_FAIL** - Job terminated due to failure of one or more allocated nodes.
- **PD PENDING - Job is awaiting resource allocation.**
- **R RUNNING - Job currently has an allocation.**
- **RQ REQUEUED** - Completing job is being requeued.
- **PR PREEMPTED** - The job was terminated because of preemption by high priority job.
- ST STOPPED - Job has an allocation, but execution has been stopped with SIGSTOP signal. CPUS have been retained by this job.
- S SUSPENDED - Job has an allocation, but execution has been suspended and CPUs have been released for other jobs.
- TO TIMEOUT - Job terminated upon reaching its time limit.

Jobs Transition Through Various States



Source: www.schedmd.com

sbatch Example - Multiple apps in single script

Submit a batch job

```
> sbatch my_work2.bash
Submitted batch job 44005

> cat my_work2.bash
```

The ***srun*** commands utilize the resources in the allocation request.

The ***srun*** commands execute desired tasks **WITHIN** the set of requested resource.

They cannot use more/other than what was requested.

```
#!/bin/bash
#SBATCH --ntasks=128
#SBATCH --mem-per-cpu=4G
#SBATCH --time=60
...

srun -n100 app1 &
srun -n20 app2 &
srun -n8 app3 &
wait
bash my_cleanup_script.sh
...
```

Options used

```
--ntasks
--mem-per-cpu
--time
```

Number of tasks
Memory required per CPU
Wall time limit (minutes in our example)

Source: www.schedmd.com

sbatch Example : Requeuing job

```
#!/bin/bash -l
#SBATCH --job-name=dam-break
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err
#SBATCH --partition=general
#SBATCH --nodes=1
#SBATCH --open-mode=append
#SBATCH --ntasks-per-node=32
#SBATCH --qos=standard
#SBATCH --mem-per-cpu=4G
#SBATCH --account=PI_ucid
#SBATCH --time=3-00:00:00
#SBATCH --requeue
#SBATCH --mail-type=ALL
#SBATCH --mail-user=ab1234@njit.edu

# Load the modules
module load foss/2022b OpenFOAM
source $FOAM_BASH

# Run the job using
requeue_job mpirun interFoam -parallel
```

Append the output to an exiting output file once requeued

Sample job script in /apps/testjobs/requeue

sbatch Example - Job Dependencies

Submit sequence of three batch jobs

```
> sbatch --ntasks=1  --parsable  pre_process.bash
45001
> sbatch --ntasks=128 --parsable --dependency=afterok:45001 do_work.bash
45002
> sbatch --ntasks=1  --parsable  --dependency=afterok:45002  post_process.bash
45003
```

Options used

`--ntasks`	Number of tasks and by default the number of cores
`--dependency`	Job dependency

https://slurm.schedmd.com/sbatch.html#OPT_dependency

sbatch Example - Environment Variables

```
> sbatch --nodes=1 --export=ALL,EDITOR=/bin/vim my.bash
```

`--export`

Specify environment variables to be exported.
Supported options include “ALL”, “NONE”, and “name=value” pairs.
Default is “ALL”.If any “name=value” pairs are included, they are **added** to the existing Environment.
If “NONE”, then environment variables are set (e.g. “SLURM_JOB_ID”, “SLURM_SUBMIT_DIR”, etc.)

Waiting for Your Job To Run

- Queue wait time depends on many factors
  - System load
  - Resources requested
    - nodes, cores, large memory, gpus
    - **reduced priority for users or groups using a lot of resources**
- Check the running jobs in QoS
  - `squeue -q [QoS]`

Troubleshooting Common Issues

Common inquiries

checkload	• sinfo but more details
checkq	• squeue but more details
slurm_jobid	• Show information about a running or queued job
sq	• Display pending job/queue info in a helpful way, You can also check the last job details with `sq`
squeue --start	• Jobs will be listed in order expected start time • Times are only estimates and subject to change
quota_info	• Show space and SU quotas for self or others
listqos	• Show all QOSes or members of QOSes

Some Common Problems

After using sbatch, the job disappears in 30 seconds and there's no result output.

- Check the details with slurm_jobid [JOBID], use --err and --out
- Use sq if you are unsure about the job id.

Invalid account or account/partition combination specified.

- Check --account
- Use quota_info $LOGNAME

```
JOBID PARTITION   NAME   USER ST TIME  NODES NODELIST(REASON)
1234    general uname.sh  xiss PD 0:00   2 (ReqNodeNotAvail, Reserved for
maintenance)
```

- Jobs that do not end before the maintenance window begins will be held until the maintenance is complete

```
JOBID PARTITION   NAME   USER ST TIME  NODES NODELIST(REASON)
1234    general uname.sh  xiss PD 0:00   2 (MaxCpuPerAccount)
```

- listqos high_$PI
- squeue -q high_$PI

Some Common Problems(contd)

```
JOBID PARTITION   NAME    USER ST TIME  NODES
NODELIST(REASON)
1234    general uname.sh  xiss PD 0:00      2
(AssocGrpBillingMinutes)
```

- Your PI group have reached the limit of SU in standard
- `scontrol update JobId=Job_ID QOS=low`

Error message: cggroup out of memory handler

- Check the memory requirement
- You probably need to increase memory on --mem or the number of cpus from --mem-per-cpu
- If nothing works, then the problem is likely due to incorrect setup of the problem.

```
JOBID PARTITION   NAME    USER ST TIME  NODES NODELIST(REASON)
1234    general uname.sh  xiss PD 0:00    2 (MaxMemPerAccount)
```

- listqos high_$PI
- squeue -q high_$PI

Slurm Interactive Jobs and Use GUI Apps

Interactive Batch Jobs

Interactive, but handled through batch system

Resource limits same as standard batch limits
Use `srun` or `salloc` command

Useful for tasks forbidden on login nodes

Debug parallel programs
Quickly test your code

May not be practical when system load is high

Long wait, same as standard batch job

To submit an interactive batch job (example)

srun -p general -n 1 --ntasks-per-node=8 --qos=standard --account=PI_ucid --mem-per-cpu=2G --time=59:00 --pty bash

Using Applications with GUI on OnDemand

Login to ondemand.njit.edu

Go to “Interactive Apps” and select the application from the list.

If you don’t find the app, select Linux Desktop

Once are you connected, select “Terminal Emulator” from “Applications” option from top left

Reminder: Wulver Monthly Maintenance

- Wulver will be temporarily out of service for maintenance once a month, specifically on the 2nd Tuesday, to perform updates, repairs, and upgrades.
- During the maintenance period, the logins will be disabled
- Jobs that do not end before the maintenance window begins will be held until the maintenance is complete

Resources to get your questions answered

Getting Started: Access to Wulver

List of Software: Wulver Software

HOW TOs: Conda Documentation

Installing Python packages via Conda

Request Software: HPC Software Installation

Access to OnDemand Open OnDemand

Contact: Please visit HPC Contact

Open a ticket: email to hpc@njit.edu

Consult with Research Computing Facilitator: HPC User Assistance

System updates

- Read Message of the Day on login
- Visit NJIT HPC News

NJIT

hpc@njit.edu

hpc.njit.edu

twitter.com/njit

facebook.com/NewJerseyInstituteofTechnology

linkedin.com/school/njit/