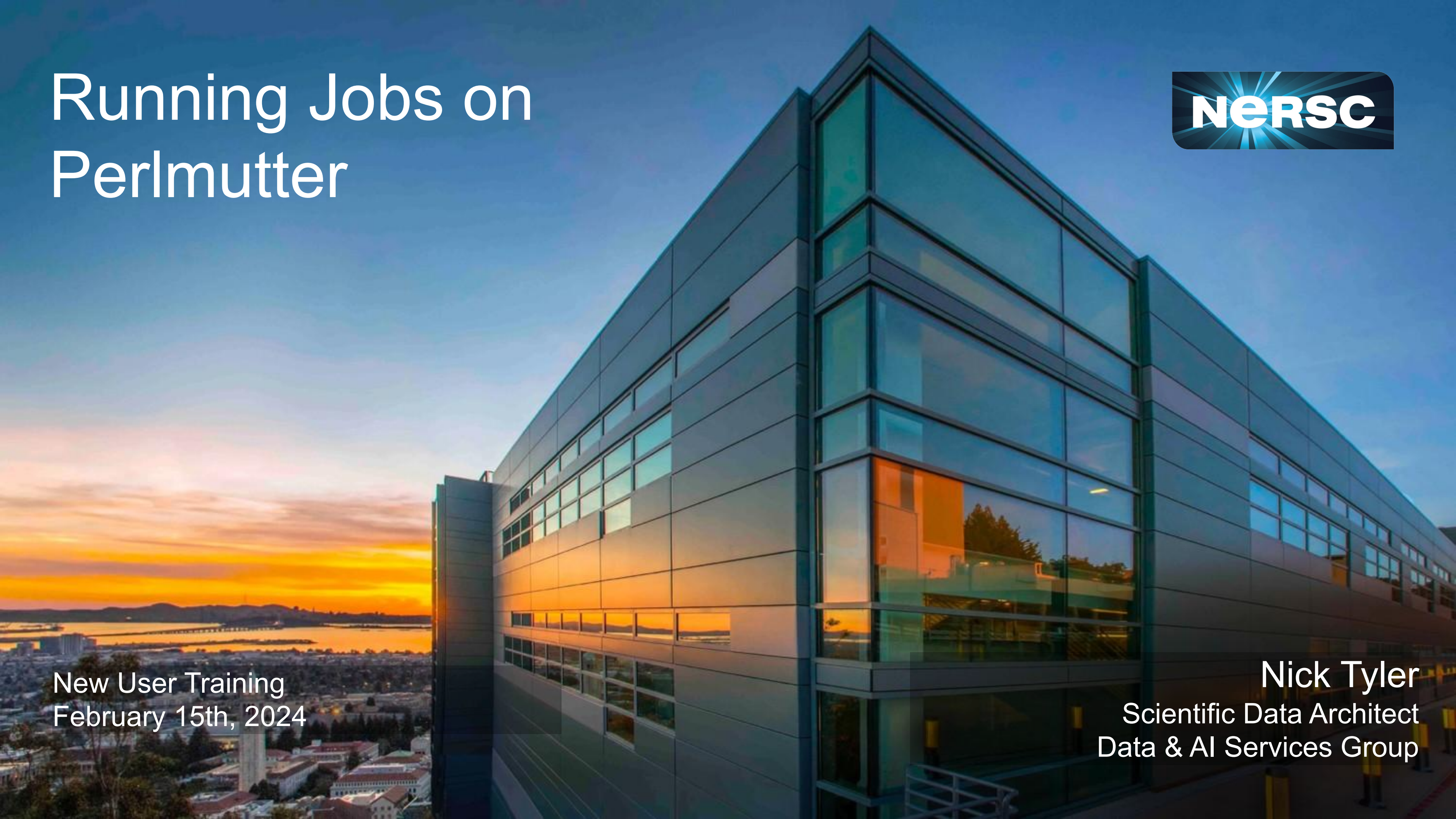
Running Jobs on Perlmutter



New User Training
February 15th, 2024

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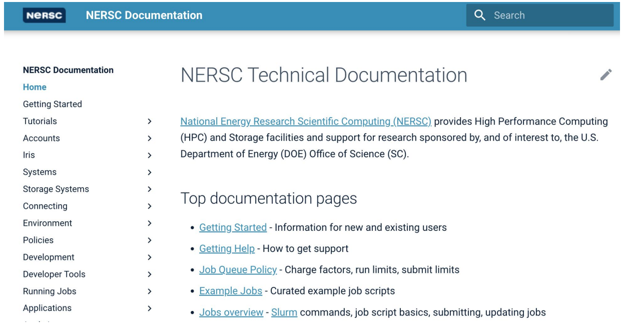
Data & AI Services Group

I’ll be covering a lot

- If you’re brand new to HPC, Welcome!
  - What is a job?
  - How to run your code as a job?
- If you’re just new to NERSC, Also Welcome!
  - Get to more advanced topics later
    - Running a job in container
    - Workflows
- Docs and Script Generator
- Job performance and profiling
  - Tomorrow - 10am PT

https://docs.nersc.gov



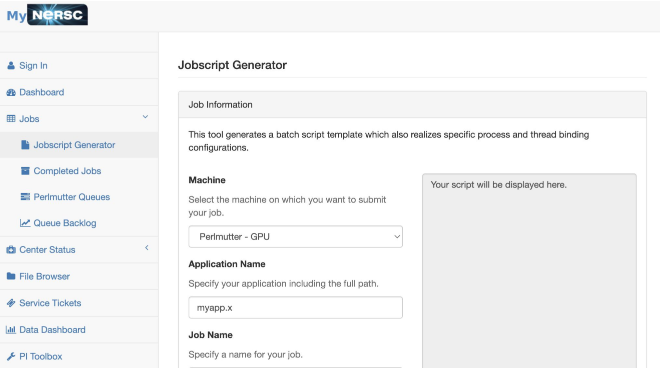
NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- Getting Started - Information for new and existing users
- Getting Help - How to get support
- Job Queue Policy - Charge factors, run limits, submit limits
- Example Jobs - Curated example job scripts
- Jobs overview - Slurm commands, job script basics, submitting, updating jobs

https://my.nersc.gov/script_generator.php



Jobscript Generator

Job Information

This tool generates a batch script template which also realizes specific process and thread binding configurations.

Machine

Select the machine on which you want to submit your job.

Perlmutter - GPU

Application Name

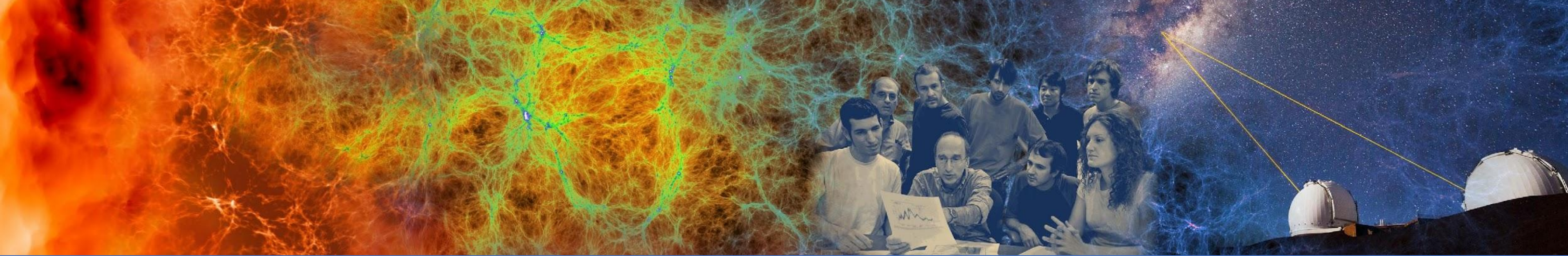
Specify your application including the full path.

myapp.x

Job Name

Specify a name for your job.

Your script will be displayed here.



Basic Job Submission

What is a Job? How do I get one?

- When you connect to Perlmutter you are on a login node
  - This includes Jupyter sessions
- Login nodes are **NOT** meant for large computing tasks!
  - They are shared by all users
  - Be kind to your fellow user
  - We only have 40 login nodes
- So where does my computation go?
  - On a compute node!
  - Perlmutter has 4864 compute nodes
    - 1792 GPU nodes, 3072 CPU nodes

What is a Job? How do I get one?

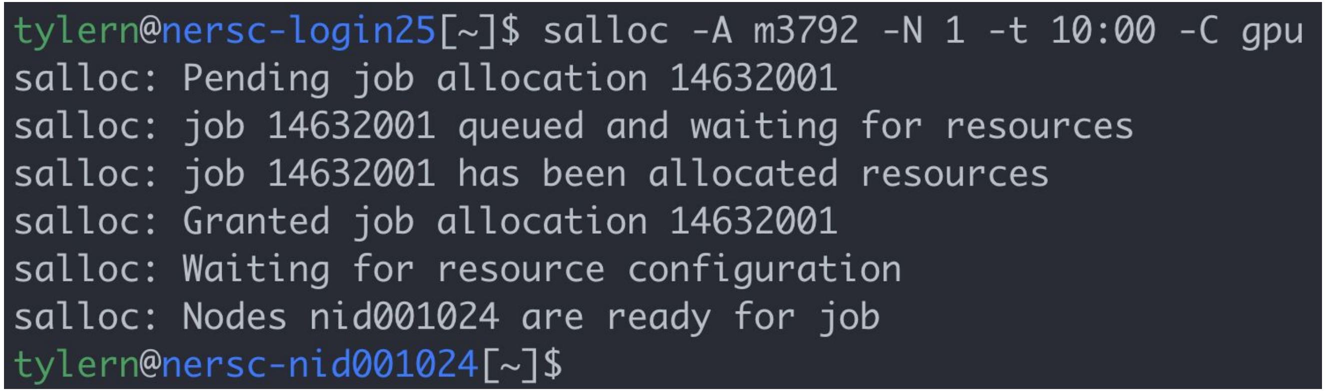
- There are two ways to access a compute node
  - Interactive job
    - Directly connect to the compute node
    - Through a command line interface
    - Have a jupyter notebook on a compute node
  - Batch job
    - Place the work you want to do in a script
    - Submit the script to a queue
    - Wait for the work to be done

How are jobs managed?

- Perlmutter uses Slurm workload manager
  - Slurm is an open source tool that performs job scheduling
- Slurm takes care of three key responsibilities
  - Allocating computer resources to jobs
  - Executes and monitors all jobs
  - Managing priorities of the jobs
- Even if you’re familiar with Slurm it is configured differently per site

How do I get a job from Slurm?

- Interactive
  - `salloc` - Slurm allocation
    - Gets an allocation on a node or set of nodes
  - At NERSC this defaults to running your login shell on a node in the allocation



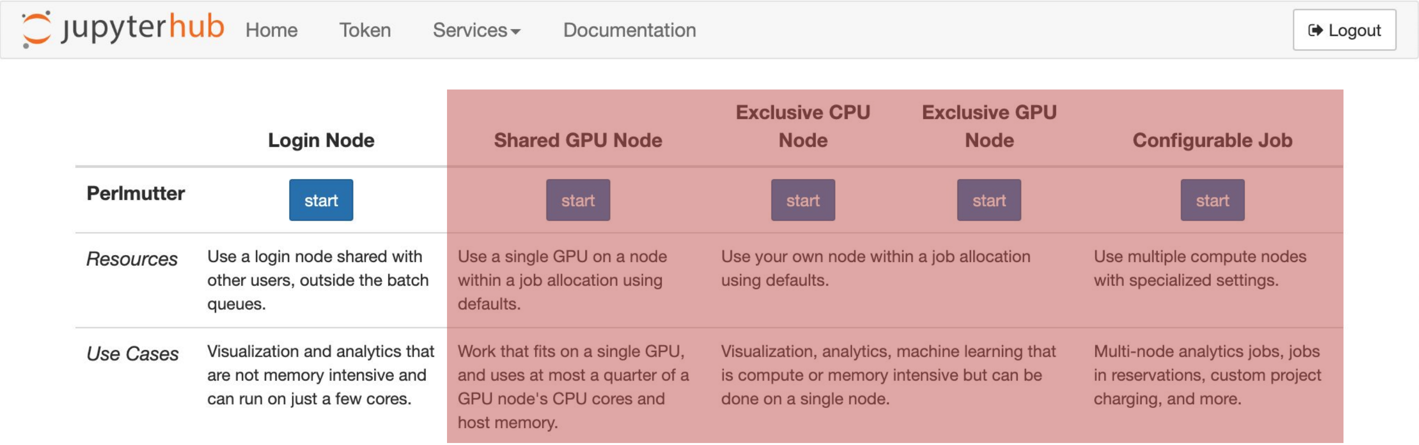
```
tylern@nersc-login25[~]$ salloc -A m3792 -N 1 -t 10:00 -C gpu
salloc: Pending job allocation 14632001
salloc: job 14632001 queued and waiting for resources
salloc: job 14632001 has been allocated resources
salloc: Granted job allocation 14632001
salloc: Waiting for resource configuration
salloc: Nodes nid001024 are ready for job
tylern@nersc-nid001024[~]$
```

What did I ask Slurm to do?

- `salloc -A m0000 -N 1 -t 10:00 -C gpu`
- `salloc`
  - Give me some compute nodes to use
- `-A m0000 | --account=m0000`
  - Charge to this NERSC account (usually starts with `m`)
- `-N 1 | --nodes=1`
  - Get 1 compute node to work on
- `-t 10:00 | --time=10:00`
  - Give me that node for 10 minutes
- `-C gpu | --constraint=gpu`
  - The type of node you want, either `cpu` or `gpu`

How do I get a job from Slurm?

- Interactive allocations in Jupyter
    - These options can get you on a compute node
    - Come tomorrow to learn more about Jupyter!



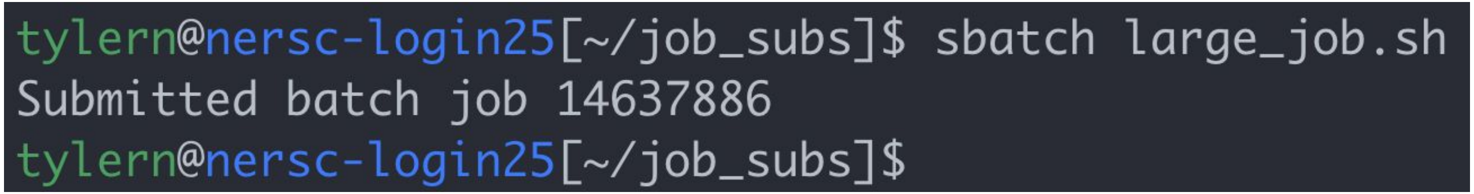
	Login Node	Shared GPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable Job
Perlmutter	start	start	start	start	start
Resources	Use a login node shared with other users, outside the batch queues.	Use a single GPU on a node within a job allocation using defaults.	Use your own node within a job allocation using defaults.		Use multiple compute nodes with specialized settings.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Work that fits on a single GPU, and uses at most a quarter of a GPU node's CPU cores and host memory.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.		Multi-node analytics jobs, jobs in reservations, custom project charging, and more.

When do I use an interactive job?

- Use interactive jobs to test and debug code
  - Also good option for profiling code
- Jobs in the interactive queue have limits
  - `-q interactive | --qos=interactive`
    - 1-4 nodes && 4 hours max walltime
  - `-q shared_interactive | --qos=shared_interactive`
    - ½ node max && 4 hours max walltime
      - 2 GPUs, 32 cores, 64 threads, ~120GB ram
      - 64 cores, 128 threads, ~250GB ram

I need more time and nodes!

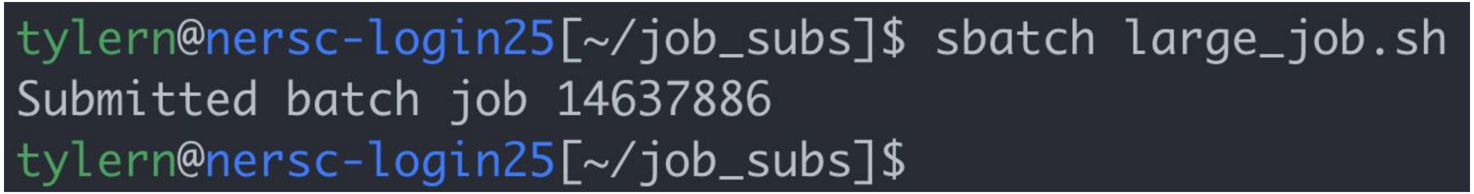
- Use a batch job
  - Submits the work you want to do into a queue
  - Lets Slurm schedule your work
    - Allows Slurm to give your job more time
    - Allows Slurm to schedule more compute nodes



```
tylern@nersc-login25[~/job_subs]$ sbatch large_job.sh
Submitted batch job 14637886
tylern@nersc-login25[~/job_subs]$
```

How do I submit a batch job?

- `sbatch` - Slurm Batch
    - Submit a batch script to Slurm
  - `sbatch script.sh`
  - Slurm gives you back a job id



```
tylern@nersc-login25[~/job_subs]$ sbatch large_job.sh
Submitted batch job 14637886
tylern@nersc-login25[~/job_subs]$
```

What does script.sh look like?

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 4
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err


srun -n $SLURM_NNODES hostname
```

- Similar options to `salloc`
- Add the special `#SBATCH` comment
- Slurm reads options from script
- Ask for 4 nodes for 8 hours
  - `-J science | --job-name=science`
  - Organize slurm outputs
    - `%x` - job name
    - `%j` - job id

What does script.sh look like?

```
#!/bin/bash
#SBATCH -A m0000
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#SBATCH -C cpu
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#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err


srun -n $SLURM_NNODES hostname
```

- Slurm adds environment variables to your job
    - Use the `$SLURM_NNODES` to get number of nodes requested
- Slurm run - `srun`
    - Run parallel jobs
        - Use this instead of `mpirun`
- This will run one `hostname` per node

Helpful Slurm environment variables

```
SLURM_JOB_NUM_NODES # -N/--nodes=
SLURM_NTASKS_PER_NODE # --ntasks-per-node=
SLURM_CPUS_ON_NODE # Set by Slurm
SLURM_GPUS_ON_NODE # Set by Slurm
```

```
Total CPUs: $((SLURM_JOB_NUM_NODES * SLURM_CPUS_ON_NODE))

Total Tasks: $((SLURM_JOB_NUM_NODES * SLURM_NTASKS_PER_NODE))

CPUs per Task: $(((SLURM_JOB_NUM_NODES * SLURM_CPUS_ON_NODE) / SLURM_NTASKS))

Total GPUs: $((SLURM_JOB_NUM_NODES * SLURM_GPUS_ON_NODE))

GPUs per Task: $(((SLURM_JOB_NUM_NODES * SLURM_GPUS_ON_NODE) / SLURM_NTASKS))
```

What does the -q option do?

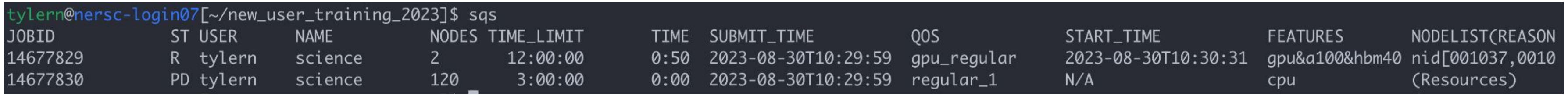
- Different queues with different limits
- `-q qebug    | --qos=debug`
  - 1-8 nodes && 30 minute max walltime
  - Test your script
  - Scaling before running larger jobs
- `regular` and `shared`
  - Where science gets done!
  - 24 hour max walltime, 5000 max job submissions
  - `-q regular | --qos=regular`
  - `-q shared  | --qos=shared`
    - ½ node max per job

How do I debug my script?

- Override options in the script with CLI options
- Helpful for debugging or scaling tests
  - Use the debug queue
    - `sbatch -q debug -t 10 script.sh`
  - Scale testing
    - `sbatch -N 2 script.sh`
    - `sbatch -N 20 script.sh`

How do I see if my jobs working?

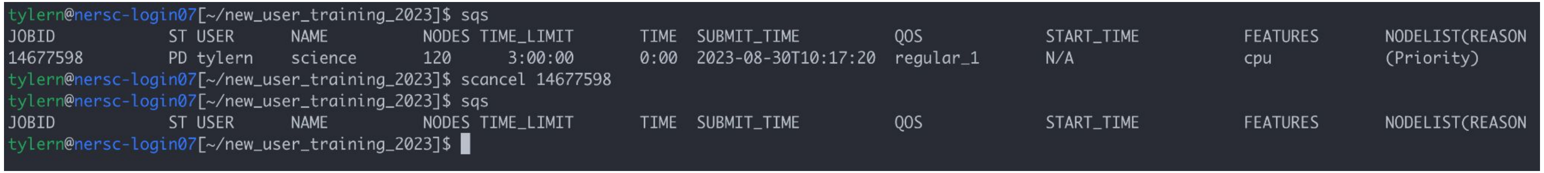
- `squeue` - Slurm queue
  - view information about jobs in the Slurm queue
  - Returns information from all jobs
    - Can be a lot on a big system like Perlmutter
- `sqs`
  - NERSC shortcut with some helpful output options
- Shows job state `R` - Running, `PD` - Pending
- `TIME` - How long the job has been running



```
tylern@nersc-login07[~/new_user_training_2023]$ sqs
JOBID            ST USER      NAME         NODES TIME_LIMIT       TIME  SUBMIT_TIME          QOS             START_TIME           FEATURES      NODELIST(REASON
14677829         R  tylern    science      2         12:00:00     0:50  2023-08-30T10:29:59  gpu_regular     2023-08-30T10:30:31  gpu&a100&hbm40 nid[001037,0010
14677830         PD tylern    science      120        3:00:00     0:00  2023-08-30T10:29:59  regular_1       N/A                  cpu           (Resources)
```

How do I end a job?

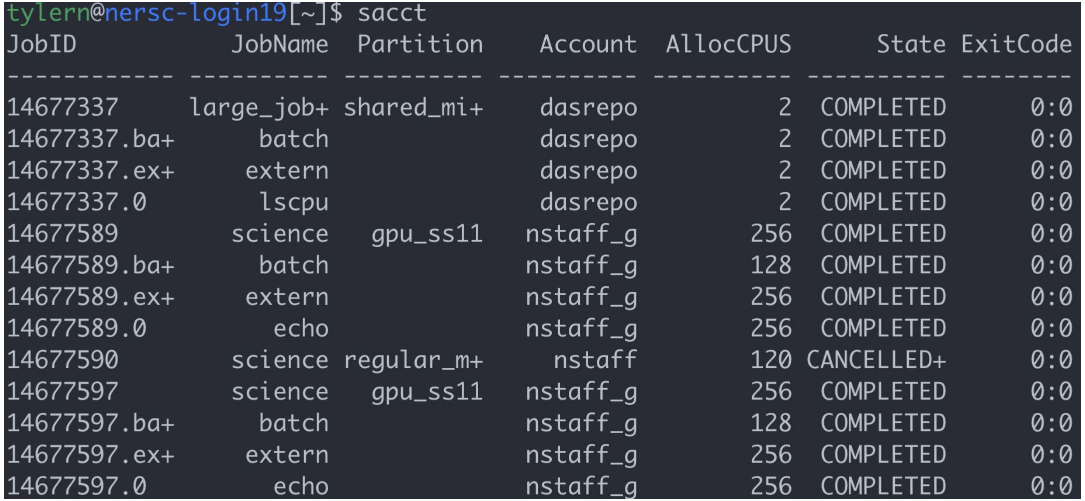
- `scancel` - Slurm cancel
  - Send stop signal to jobs or job steps managed by Slurm
    - Stop job running too long or with the wrong parameters
    - Conserve your NERSC hours if you made a mistake!



```
tylern@nersc-login07[~/new_user_training_2023]$ sqs
JOBID            ST USER      NAME          NODES TIME_LIMIT       TIME  SUBMIT_TIME          QOS            START_TIME           FEATURES       NODELIST(REASON
14677598         PD tylern    science       120      3:00:00       0:00  2023-08-30T10:17:20  regular_1      N/A                  cpu            (Priority)
tylern@nersc-login07[~/new_user_training_2023]$ scancel 14677598
tylern@nersc-login07[~/new_user_training_2023]$ sqs
JOBID            ST USER      NAME          NODES TIME_LIMIT       TIME  SUBMIT_TIME          QOS            START_TIME           FEATURES       NODELIST(REASON
tylern@nersc-login07[~/new_user_training_2023]$
```

How to look at completed jobs?

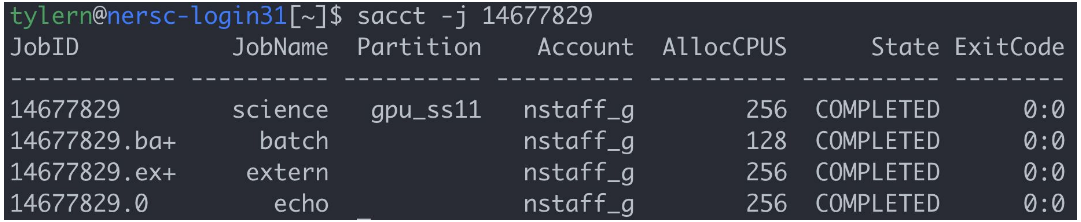
- `sacct` - Slurm accounting
  - Accounting data for all jobs and job steps in the Slurm job accounting log or Slurm database
  - By default shows jobs completed in the last day



```
tylern@nersc-login19[~]$ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
14677337     large_job+ shared_mi+    dasrepo          2  COMPLETED      0:0
14677337.ba+      batch               dasrepo          2  COMPLETED      0:0
14677337.ex+     extern               dasrepo          2  COMPLETED      0:0
14677337.0        lscpu               dasrepo          2  COMPLETED      0:0
14677589        science    gpu_ss11  nstaff_g        256  COMPLETED      0:0
14677589.ba+      batch              nstaff_g        128  COMPLETED      0:0
14677589.ex+     extern              nstaff_g        256  COMPLETED      0:0
14677589.0         echo              nstaff_g        256  COMPLETED      0:0
14677590        science regular_m+     nstaff        120 CANCELLED+      0:0
14677597        science    gpu_ss11  nstaff_g        256  COMPLETED      0:0
14677597.ba+      batch              nstaff_g        128  COMPLETED      0:0
14677597.ex+     extern              nstaff_g        256  COMPLETED      0:0
14677597.0         echo              nstaff_g        256  COMPLETED      0:0
```

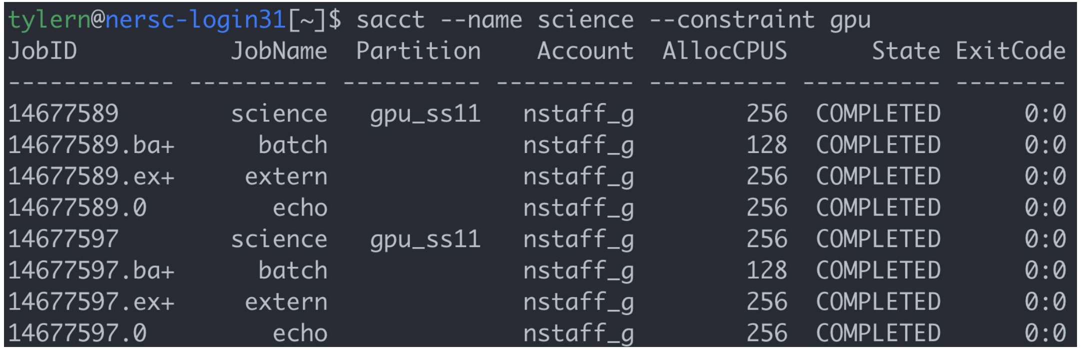
How to look at completed jobs?

- `sacct -j jobid`
  - ○ Shows information about one jobid

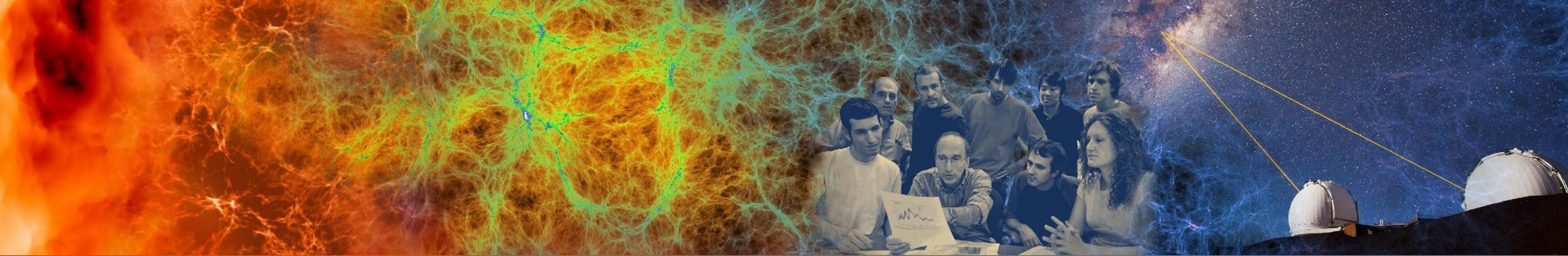


```
tylern@nersc-login31[~]$ sacct -j 14677829
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
14677829        science   gpu_ss11   nstaff_g        256  COMPLETED      0:0
14677829.ba+      batch              nstaff_g        128  COMPLETED      0:0
14677829.ex+     extern              nstaff_g        256  COMPLETED      0:0
14677829.0         echo              nstaff_g        256  COMPLETED      0:0
```

- `sacct --name science --constraint gpu`
  - ○ Search through jobs by other attributes



```
tylern@nersc-login31[~]$ sacct --name science --constraint gpu
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
14677589        science   gpu_ss11   nstaff_g        256  COMPLETED      0:0
14677589.ba+      batch              nstaff_g        128  COMPLETED      0:0
14677589.ex+     extern              nstaff_g        256  COMPLETED      0:0
14677589.0         echo              nstaff_g        256  COMPLETED      0:0
14677597        science   gpu_ss11   nstaff_g        256  COMPLETED      0:0
14677597.ba+      batch              nstaff_g        128  COMPLETED      0:0
14677597.ex+     extern              nstaff_g        256  COMPLETED      0:0
14677597.0         echo              nstaff_g        256  COMPLETED      0:0
```



Jobs in containers

Running jobs in containers

- Containers are a great
  - Make your software portable between systems
  - Decrease start time of large jobs
    - python
- NERSC Supports two container technologies
  - Shifter
  - podman-hpc - ***New***
    - Can build images on login nodes!

- We don’t support Singularity/Apptainer on Perlmutter

What is a container?

- A way to pack up all your software
- Docker is just one technology
- On your personal computer
  - Build
    - `docker build …`
  - Ship
    - `docker push …`
  - Run
    - `docker run …`

docker

```
#Dockerfile
FROM ubuntu:latest

RUN apt-get update &&
    apt-get install -y \
    cmake python3-pip

RUN pip install pandas

COPY code /mycode
WORKDIR /mycode
RUN cmake --build .
```

Where do I ship it?

- NERSC has a registry
  - `registry.nersc.gov`
  - Build

    -
      ```
      docker build -t registry.nersc.gov/m0000/test:v1.0 .
      ```
  - Ship

    -
      ```
      docker login registry.nersc.gov
      ```

    -
      ```
      docker push registry.nersc.gov/m0000/test:v1.0
      ```
  - Run with Shifter or Podman-HPC

How do I run a Shifter container?

- Pull your image before you start your job
  - `shifterimg pull registry/image:tag`

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 4
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err
#SBATCH --image=registry/image:tag

srun -n $SLURM_NNODES shifter hostname
```

SHIFTER

How do I run a Shifter container?

- Extra options for `shifter`
  - `--volume=/pscratch/sd/u/user:/scratch`
  - `--env=MYENV=1234`
  - `--clearenv`
  - `--workdir=/work`
  - `--module=...`
    - `none`
    - `mpich`
    - `cvmfs`
    - `gpu`
    - `cuda-mpich`
    - `nccl-2.15`
    - `network`

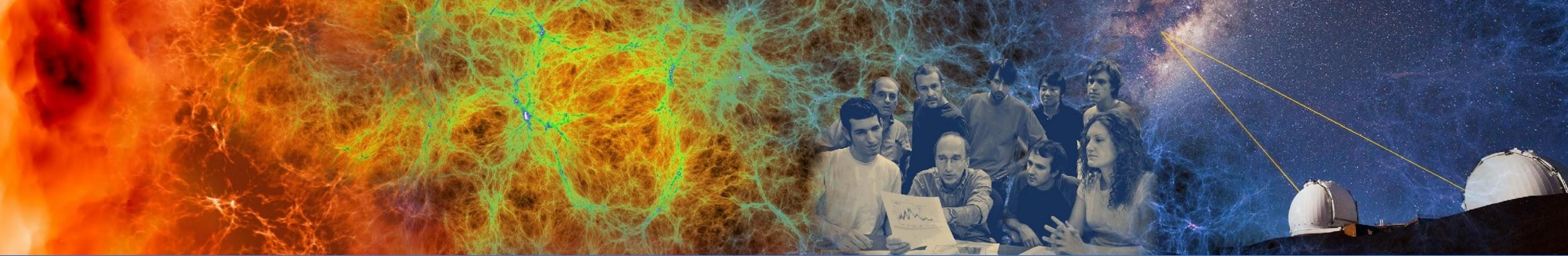
How do I run a podman-hpc container?

- Pull your image before you start your job
  - `podman-hpc pull registry/image:tag`

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 4
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

srun -n $SLURM_NNODES \
    podman-hpc run registry/image:tag hostname
```

How do I run a podman-hpc container?

- Pull, Or build images on login nodes, then migrate to scratch
  - `podman-hpc build -t image_name:tag .`
  - `podman-hpc migrate image_name:tag`
- Docker/Podman options work
  - `--volume=/pscratch/sd/u/user:/scratch`
  - `--net host`
- Extra options similar to shifter modules
  - `--mpi`
  - `--gpu`
  - `--cuda-mpi`



Multiple jobs and Workflows

I have multiple things I need to do

- Bundling jobs with slurm
    - Run multiple executables sequentially or simultaneously
- Use a Slurm job array
    - Same job task with different inputs
- Workflow tools
    - GNU Parallel
        - Many small tasks, fit onto one node
    - More complex tasks
        - Parsl, Fireworks, etc.

Bundling work into one job

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 4
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

srun -n 128 -c 8  --cpu_bind=cores ./a.out
srun -n 64 -c 16  --cpu_bind=cores ./b.out
srun -n 32 -c 32  --cpu_bind=cores ./c.out
```

- Bundling jobs with slurm
  - ○ Programs run **sequentially**
  - ○ Only have to wait for scheduler once
    - Reuse the same allocated nodes for different steps in your workflow

Bundling work into one job

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 4
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

srun -N 1 -n 256 ./a.out input0 &
srun -N 1 -n 256 ./a.out input1 &
srun -N 1 -n 256 ./a.out input3 &
srun -N 1 -n 256 ./a.out input4 &
wait
```

- Bundling jobs with slurm
  - ○ Programs run **simultaneously**
  - ○ Only have to wait for scheduler once
    - This example runs same program with different inputs per `srun`

Using Job Arrays

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err
#SBACTH --array=1-4

echo $SLURM_ARRAY_JOB_ID

srun -n 256 ./a.out $SLURM_ARRAY_JOB_ID
```

- Slurm manages each job independently
  - If one task fails it won’t affect others
- Good option for getting
  - Large statistics on same inputs
  - Parameter sweep over input files

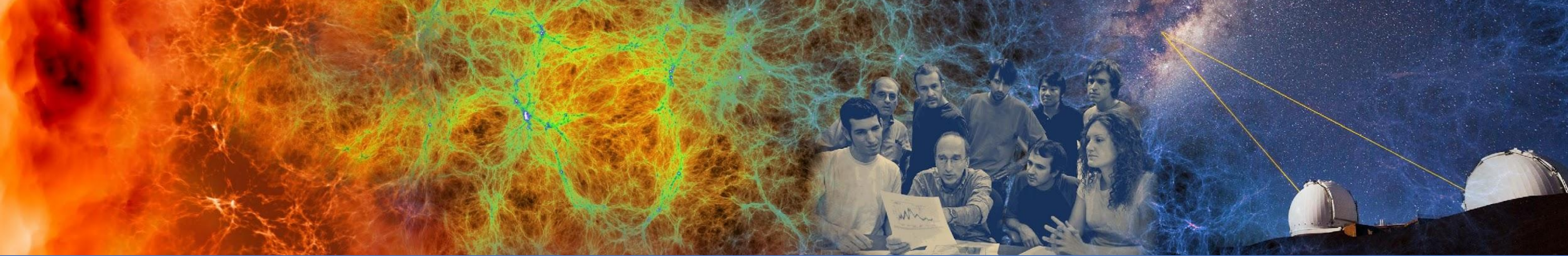
Using GNU Parallel

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

module load parallel

parallel -j256 ./a.out {} ::: inputs*
```

- You manage tasks inside of allocation
  - Great for many small tasks
    - Faster start times than `sruns`
  - Reuse allocation for all your tasks
- As tasks finish the next one starts
  - Use allocation efficiently

More complex workflows with dependencies

- Use a workflow management system
    - Parsl/FuncX/Globus Compute
    - Fireworks
    - Many more…
  - ○ Write code to define workflow
  - ○ Often written in python
  - ○ Handle dependencies between different types of tasks
  - ○ github.com/CrossFacilityWorkflows/DOE-HPC-workflow-training
    - Resources from previous training with ALCF and OLCF
- Reach out at `help.nersc.gov` with more questions



Best Practices

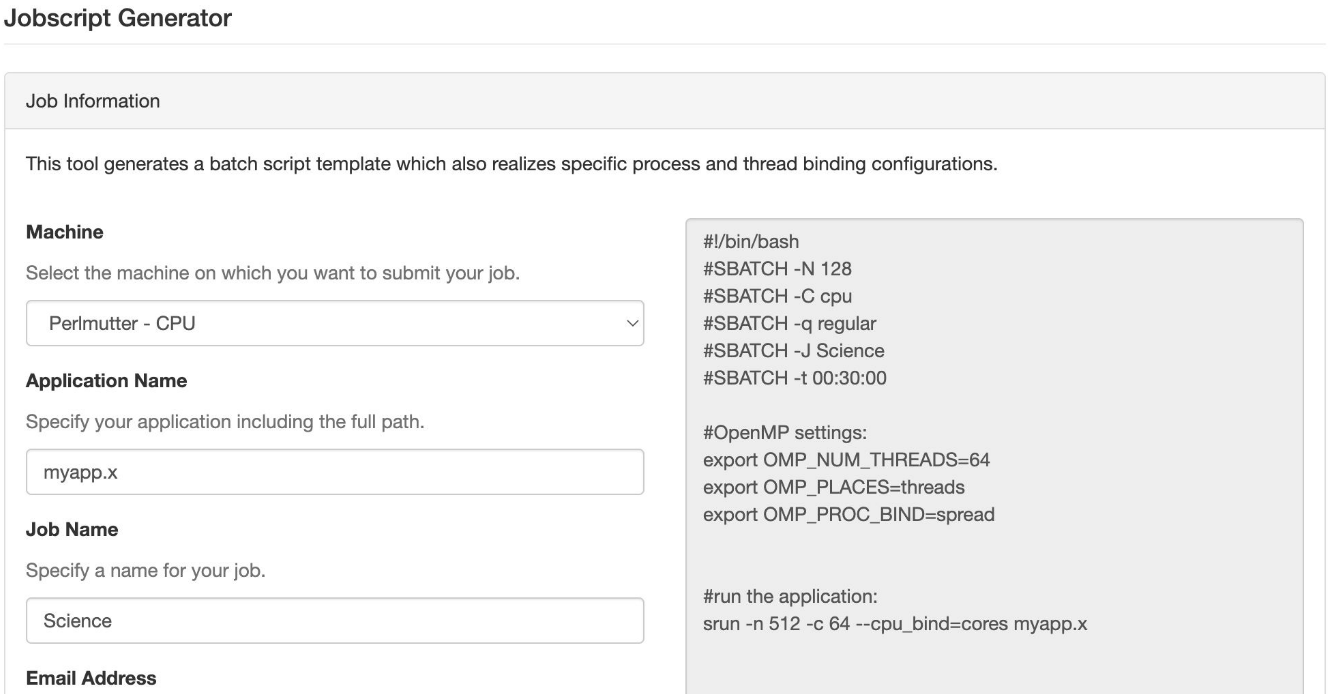
Jobs Scheduling

- Each job has a priority value
  - Grouped by user, QOS, and account
  - Only two jobs per these groupings gain priority at a time
    - More jobs can run, only two will age
- Main scheduler uses priority list
  - Schedules a few days in the future
- Backfill scheduler puts shorter jobs in “holes”
  - Prioritize utilization

Jobs Scheduling Tips

- One job with a large allocation
  - Per node priority ageing is the highest
  - Can get scheduled first
- Shorter time length jobs
  - Easier to schedule as backfill
  - Use a workflow manager
- Choose the right time from Slurm
  - Balance between enough runtime
  - Waiting in the queue for a long job

Job script generator: More advanced threading options



Jobscript Generator

Job Information

This tool generates a batch script template which also realizes specific process and thread binding configurations.

Machine

Select the machine on which you want to submit your job.

Perlmutter - CPU

Application Name

Specify your application including the full path.

myapp.x

Job Name

Specify a name for your job.

Science

Email Address

```
#!/bin/bash
#SBATCH -N 128
#SBATCH -C cpu
#SBATCH -q regular
#SBATCH -J Science
#SBATCH -t 00:30:00

#OpenMP settings:
export OMP_NUM_THREADS=64
export OMP_PLACES=threads
export OMP_PROC_BIND=spread


#run the application:
srun -n 512 -c 64 --cpu_bind=cores myapp.x
```

Options for OpenMP Code

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

export OMP_NUM_THREADS=8
export OMP_PLACES=cores
export OMP_PROC_BIND=spread

srun -n 256 ./a.out $SLURM_ARRAY_JOB_ID
```

- OpenMP
  - config through env variables
- Some libraries use OpenMP by default
  - BLAS/LAPACK
  - numpy in python
    - Small numpy arrays can be faster with less threads

Options for MPI codes

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err


srun -n 32 -c 16 --cpu_bind=cores ./a.out
```

- Settings to Address NUMA Performance
  - Use `--cpu_bind=cores` when
    - `#MPI tasks ≤ #cores`
  - Use `--cpu_bind=threads` when
    - `#MPI tasks > #cores`

Options for Hybrid OpenMP/MPI codes

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 8:00:00
#SBATCH -C cpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

export OMP_NUM_THREADS=8
export OMP_PLACES=cores
export OMP_PROC_BIND=spread

srun -n 32 -c 16 --cpu_bind=cores ./a.out
```

- Hybrid MPI/OpenMP code
  - ○ Number of cores per task `-c`
  - ○ `-c` ≥ `OMP_NUM_THREADS`
  - ○ Give enough cpus to be able to use OpenMP threads efficiently

Options for gpu codes

```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 8:00:00
#SBATCH -C gpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

export OMP_NUM_THREADS=8
export OMP_PLACES=cores
export OMP_PROC_BIND=spread

srun -n 8 -c 8 --gpus-per-task=1 \
    --cpu_bind=cores ./a.out
```

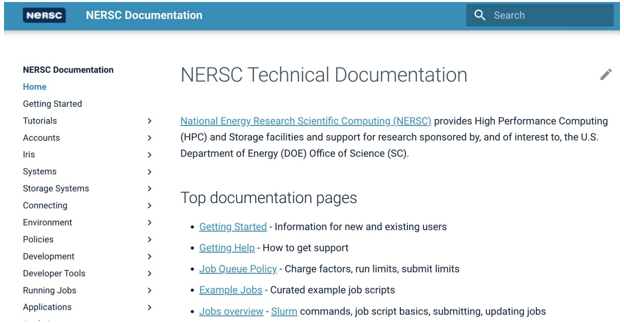
- GPU codes
  - Can specify the number of gpus per task
    - `--gpus-per-task=n`
- More advanced
  - Specific gpu mapping
    - `--gpu-bind`

What did we cover?

- What is a job?
- How to run your code as a job?
- Running a job in container
- Workflows
- Docs and Script Generator

- Jupyter for interactive jobs
  - Tomorrow - 9:30am PT
- Job performance and profiling
  - Tomorrow - 10am PT

https://docs.nersc.gov



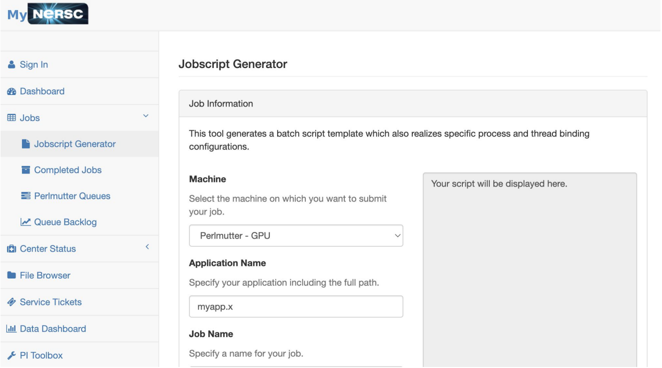
NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- Getting Started - Information for new and existing users
- Getting Help - How to get support
- Job Queue Policy - Charge factors, run limits, submit limits
- Example Jobs - Curated example job scripts
- Jobs overview - Slurm commands, job script basics, submitting, updating jobs

https://my.nersc.gov/script_generator.php



Jobscript Generator

Job Information

This tool generates a batch script template which also realizes specific process and thread binding configurations.

Machine

Select the machine on which you want to submit your job.

Perlmutter - GPU

Application Name

Specify your application including the full path.

myapp.x

Job Name

Specify a name for your job.

Your script will be displayed here.

Thank You for listening and Welcome to NERSC!