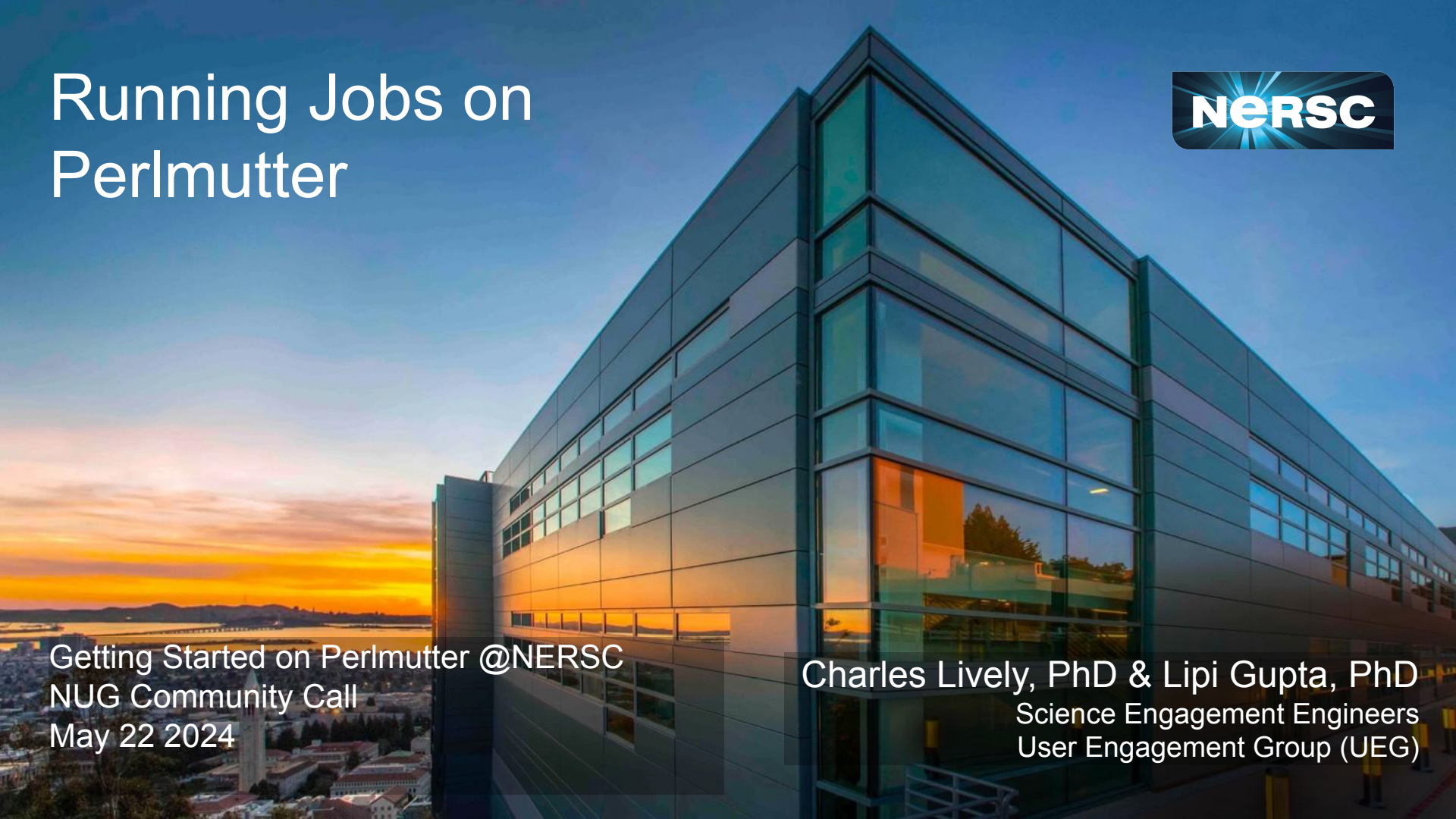
Running Jobs on Perlmutter



Getting Started on Perlmutter @NERSC
NUG Community Call
May 22 2024

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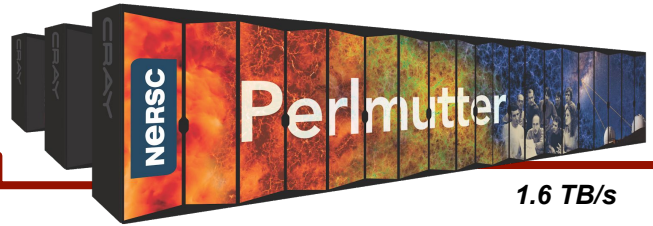
Science Engagement Engineers
User Engagement Group (UEG)

Agenda

- Perlmutter System Overview
- Perlmutter Software and Programming Environment Overview
- Running Jobs on Perlmutter
- Slurm Commands
- Best Practices on Perlmutter Job Submissions

Perlmutter System Overview

NERSC Systems Ecosystem



TOP500 The List.
#8, 93.8PF Peak

>5 *TB/s*

35 PB All-Flash Scratch

HPE Slingshot 11 interconnect
4 NICs/GPU node,
1 NIC/CPU node

1.6 TB/s

1,792 GPU-accelerated nodes
4 NVIDIA A100 GPUs+1 AMD "Milan" CPU
448 TB (CPU) + 320 TB (GPU) memory

3,072 CPU-only nodes
2 AMD "Milan" CPUs
1,536 TB CPU memory

Off-Platform Storage

50 GB/s — HPSS Tape Archive ~300 PB

100 GB/s — Common File System 130 PB

5 GB/s — /home 450 TB

DTNs, Gateways

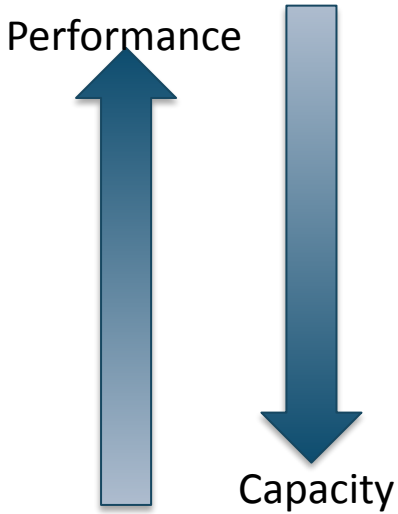
Spin edge services

Ethernet
Science Friendly Security
Production Monitoring
Power Efficiency
LAN

ESnet ENERGY SCIENCES NETWORK
2 x 400 Gb/s
2 x 100 Gb/s

Experimental Facility | ASCR Facility | Home Institution | Cloud | Edge

Simplified NERSC File Systems



Memory

Lustre Scratch — local file system

GPFS Community — global file system

Tape Archive HPSS — longer term storage

Global Common — shared software

Global Home — individual home directories

Perlmutter File Systems

Global Home

- Permanent, relatively small storage
- NOT tuned to perform well for parallel jobs
- Snapshot backups
- **Perfect for storing data such as source codes, shell scripts**
- **cd $HOME**

Global Community File System (CFS)

- Permanent, larger storage
- Medium performance for parallel jobs
- Snapshot backups
- **Perfect for sharing data within research group**
- **cd $CFS**

Local Scratch

- Large, temporary storage
- Optimized for read/write operations, NOT storage
- Not backed up
- Purge policy (8 weeks)
- **Perfect for staging data and performing computations**
- **cd $SCRATCH**

Long-Term Storage System

HPSS

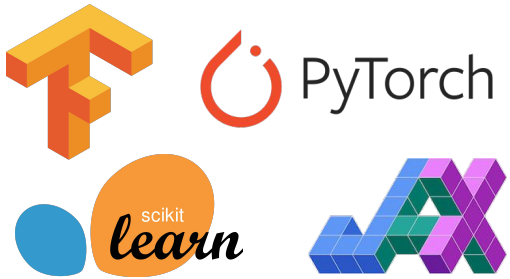
- High-Performance Storage System
- Archival storage of infrequently accessed data
- Hierarchical storage:
  - Data first ingested onto high-performance disk arrays
  - Migrated to large enterprise tape subsystem for long-term retention

NERSC has a rich data ecosystem!

data transfer and access

data management

data analytics



machine learning

visualization

containers

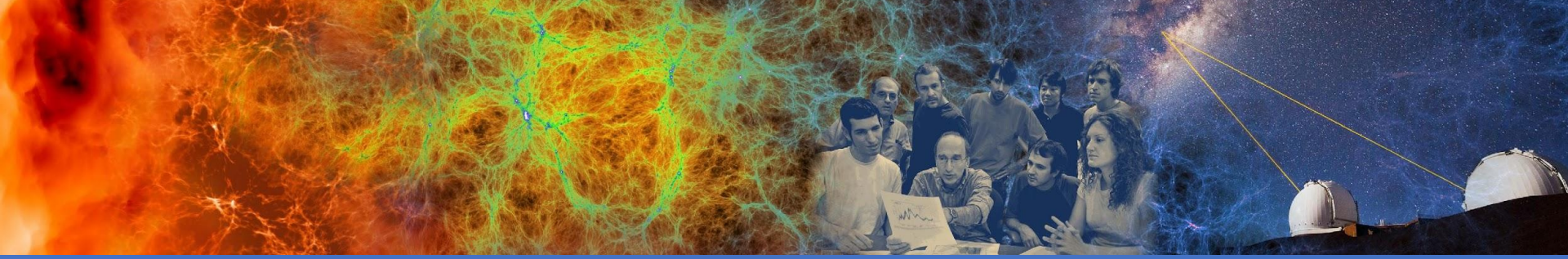
workflows

Perlmutter Supports Multiple Compilers and Every GPU Programming Model

	Fortran/ C/C++	CUDA	OpenACC 2.x	OpenMP 5.x	CUDA Fortran	Kokkos / Raja	MPI	HIP	DPC++ / SYCL
NVIDIA									
CCE									
GNU									
LLVM									
Intel									

Vendor Supported

NERSC Supported



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

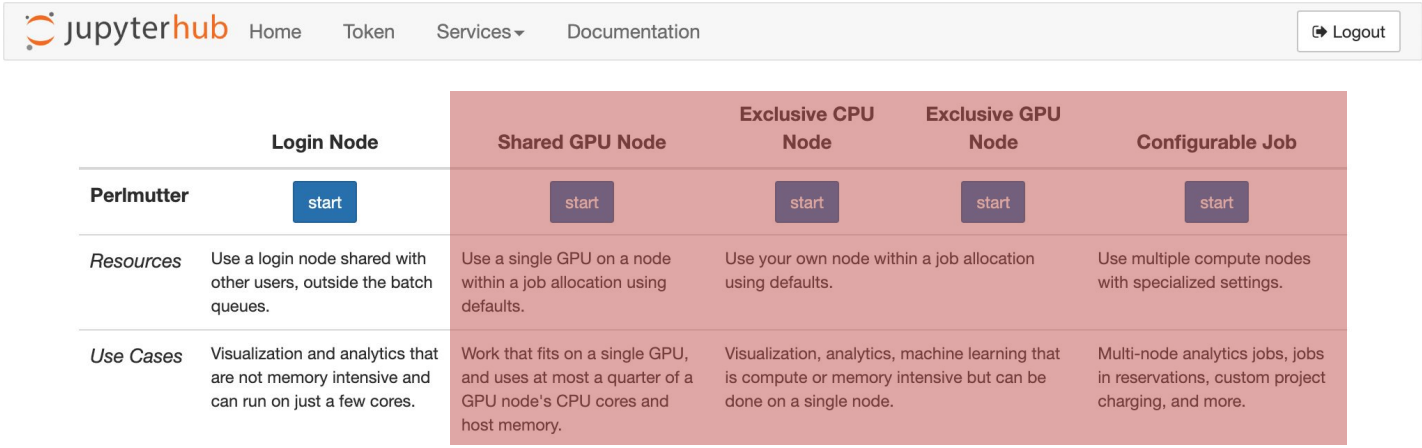
```
clively@nid001465:/global/u1/c/clively> salloc -A m4388 -N 1 -t 10:00 -C gpu
salloc: Pending job allocation 25915811
salloc: job 25915811 queued and waiting for resources
salloc: job 25915811 has been allocated resources
salloc: Granted job allocation 25915811
salloc: Waiting for resource configuration
salloc: Nodes nid004053 are ready for job
clively@nid004053:/global/u1/c/clively>
```

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



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

```
clively@nid004053:/global/u1/c/clively> sbatch job_script.sh
Submitted batch job 25916143
clively@nid004053:/global/u1/c/clively>
```

How do I submit a batch job?

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

```
clively@nid004053:/global/u1/c/clively> sbatch job_script.sh
Submitted batch job 25916143
clively@nid004053:/global/u1/c/clively>
```

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 ./a.out
```

- 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
#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 ./a.out
```

- 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

```
clively@nid001465:/global/u1/c/clively> sqs
JOBID             ST USER      NAME              NODES TIME_LIMIT       TIME  SUBMIT_TIME          QOS             START_TIME          FEATURES       NODELIST(REASON
24125002          PD clively   /global/cfs/      1          10:00       0:00  2024-05-22T03:31:22  cron            2024-05-29T03:31:00 cron           (BeginTime)
24125000          PD clively   /global/cfs/      1          10:00       0:00  2024-05-22T02:12:08  cron            2024-05-23T02:11:00 cron           (BeginTime)
24125001          PD clively   /global/cfs/      1          10:00       0:00  2024-05-22T00:21:49  cron            2024-05-23T00:21:00 cron           (BeginTime)
25915811          CG clively   interactive       1          10:00      10:17  2024-05-22T07:29:14  gpu_debug       2024-05-22T07:30:26 gpu&a100       nid004053
25915593          R  clively   interactive       1        1:00:00      15:47  2024-05-22T07:25:48  gpu_interactive 2024-05-22T07:26:16 gpu&a100       nid001465
```

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!

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

```
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
```

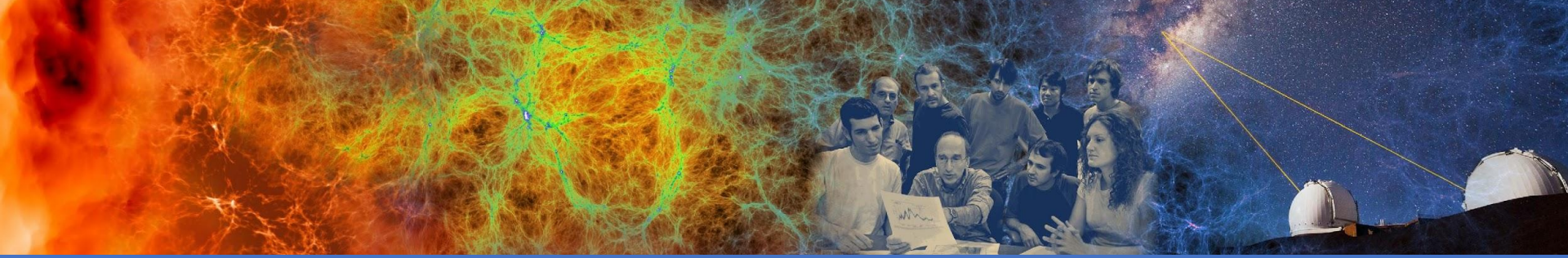
How to look at completed jobs?

- `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 …`

```
#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
```

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?

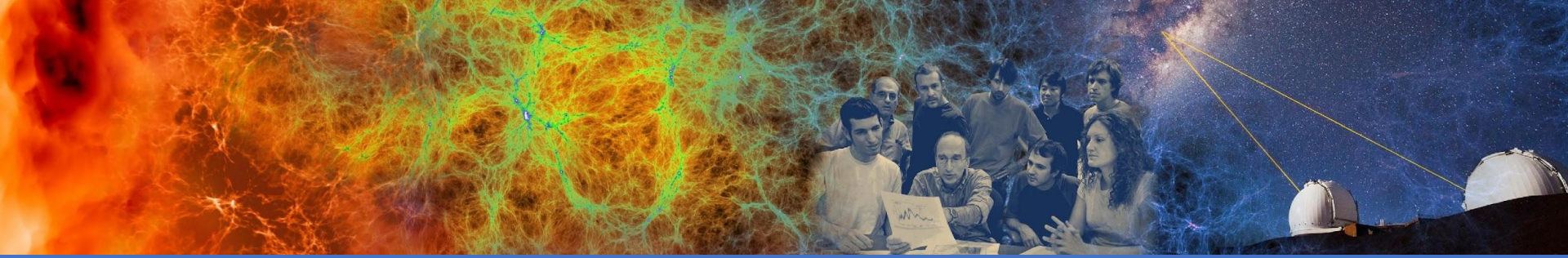
- Pull your image before you start your job
  - `podman-hpc pull registry/image:tag`

```
#!/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
```

podman

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

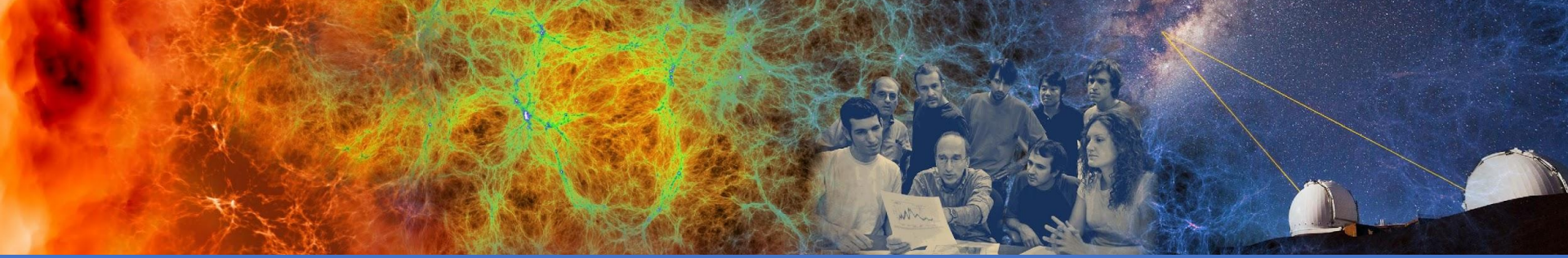
Using GNU Parallel

```
#!/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

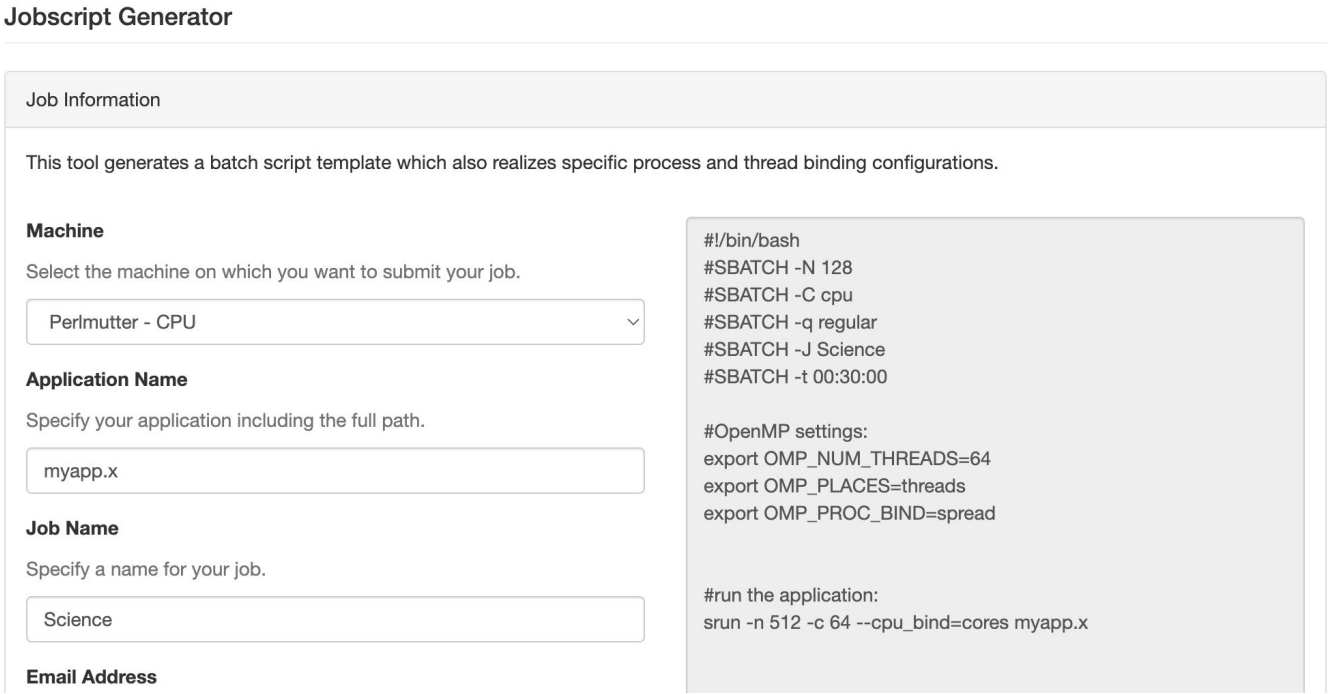
Jobs Scheduling

- 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



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

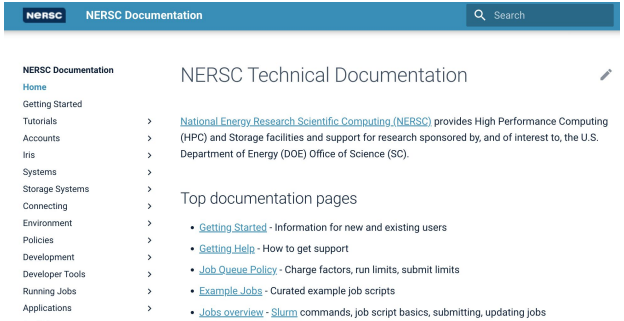
```
#!/bin/bash
#SBATCH -A m0000
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 8:00:00
#SBATCH -C gpu
#SBATCH -J science
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err

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`

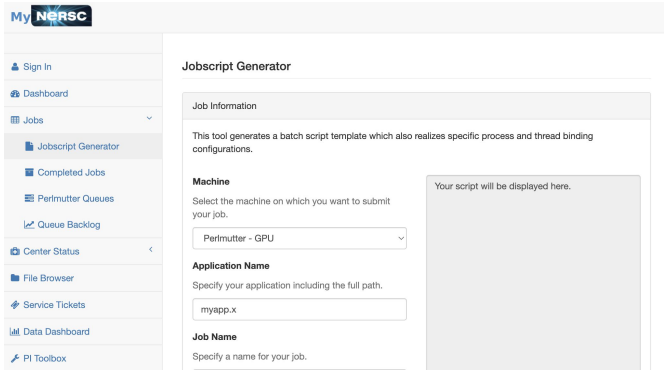
What did we cover?

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

https://docs.nersc.gov



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



Resources

- **Self Help**

https://ercap.nersc.gov
https://iris.nersc.gov
https://iris.nersc.gov/add-user
http://www.nersc.gov/users/accounts/
http://www.nersc.gov/users/accounts/allocations/
http://www.nersc.gov/users/accounts/user-accounts/
http://www.nersc.gov/users/accounts/user-accounts/how-usage-is-charged
http://www.nersc.gov/users/connecting-to-nersc/mfa/
https://docs.nersc.gov/connect/federatedid/
https://docs.nersc.gov/filesystems/archive/#hpss-usage-charging

Resources cont.

- **NERSC Account Support**
  - http://help.nersc.gov
  - accounts@nersc.gov

- **NERSC Allocation Support**
  - http://help.nersc.gov
  - allocations@nersc.gov


Thank You for listening and Welcome to NERSC!
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