Best Practices for Jobs

NERSC New User Training
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CPU vs GPU

- Account (--account / -A)
  - -A <account> for CPU
  - -A <account_g> for GPU

- Constraints (--constraint / -C)
  - -C cpu
  - -C gpu

- Modules
  - Load `cpu`
  - Load `gpu` (default, CUDA aware MPI)
Always specify your account

Ensure the appropriate allocation is charged
● Default is set in iris, not always the one you want

```bash
#SBATCH --account=<NERSC Account>
```
Do not run production jobs in your home directory

Run in $SCRATCH
- Large, temporary storage
- Optimized for reads and writes

Install Software to Global Common
- /global/common/software
- Optimized for reads
- Mounted read-only to compute nodes via DVS (more later)
Set job time limits

Due to backfill scheduling, short and variable-length jobs generally start quickly resulting in much better job throughput

```bash
#SBATCH --time-min=<lower_bound>
#SBATCH --time=<upper_bound>
```
Set job filesystem licenses

A batch job will not start if any of the specified file systems are unavailable due to maintenance or an outage

#SBATCH --licenses=scratch,cfs
Specify the logical core per task

Each CPU core has two hardware threads

A CPU-only compute node has a total of 128 physical cores, or 256 logical CPUs total.

The GPU compute node has a total of 64 physical cores, or 128 logical CPUs total.

Why double? CPU-only compute nodes have two processors, GPU compute nodes have one.

More: https://docs.nersc.gov/jobs/affinity/#process-and-thread-affinity
Specify the logical core per task (CPU)

Logical cores per task (-c, --cpus-per-task)
- CPU: $2 \times \left\lfloor \frac{128}{\text{tasks per node}} \right\rfloor$
- GPU: $2 \times \left\lfloor \frac{64}{\text{tasks per node}} \right\rfloor$

Example: 5 MPI tasks per GPU node
- $2 \times \left\lfloor \frac{64}{5} \right\rfloor = 2 \times 12 = -c 24$

What is it for a CPU node?
- -c 50
And there’s more

https://docs.nersc.gov/jobs/best-practices/
- Some are more advanced than others
- Some require knowing more about your code
- Some require knowing more about the system

Thank you and welcome to NERSC!