

Using OpenMP Compilers on Perlmutter CPUs



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Using Perlmutter



System Specifications

Partition	# of nodes	CPU	GPU
GPU	1536	1x AMD EPYC 7763	4x NVIDIA A100 (40GB)
	256	1x AMD EPYC 7763	4x NVIDIA A100 (80GB)
CPU	3072	2x AMD EPYC 7763	-
Login	40	1x AMD EPYC 7713	1x NVIDIA A100 (40GB)

Access to Perlmutter

- NERSC users can use your existing account
- Non-users were sent instructions to get a training account
 - Project: ntrain8
 - Training accounts for Session 1 valid through May 15
- Login to Perlmutter: [ssh username@perlmutter.nersc.gov](ssh://username@perlmutter.nersc.gov)
- Getting homework exercises

```
% cd $SCRATCH
```

```
% git clone https://github.com/NERSC/openmp-series-2024
```

```
% cd openmp-series-2024
```

```
% cd Session-1-Introduction/exercises/cpp/0x_xx      (or: cd ../fortran/...)
```

```
% make
```

```
% sbatch xx.slurm
```

GCC is Default Compiler on Perlmutter

- PrgEnv-gnu is the default programming environment; GCC is the default compiler

```
[yunhe@perlmutter:login21:~> module list
```

Currently Loaded Modules:

1) craype-x86-milan	9) craype/2.7.30
2) libfabric/1.15.2.0	10) gcc-native/12.3
3) craype-network-ofi	11) perftools-base/23.12.0
4) xpmem/2.6.2-2.5 2.38 __gd067c3f.shasta	12) cpe/23.12
5) PrgEnv-gnu/8.5.0	13) cudatoolkit/12.2
6) cray-dsmml/0.2.2	14) craype-accel-nvidia80
7) cray-libsci/23.12.5	15) gpu/1.0
8) cray-mpich/8.1.28	

- User compiler wrappers to build: **cc** for C codes, **CC** for C++, and **ftn** for Fortran codes
 - It uses native gcc compilers (gcc, g++, and gfortran) underneath
- To compile an OpenMP code
 - **cc -fopenmp -O3 mycode.c -o mycode.exe**
 - **CC -fopenmp -O3 mycode.cc -o mycode.exe**
 - **ftn -fopenmp -O3 mycode.f90 -o mycode.exe**

Other Available Compilers on Perlmutter

- Besides GCC, there are Nvidia, CCE, and Intel compilers available on Perlmutter under [PrgEnv-gnu](#), [PrgEnv-nvidia](#), [PrgEnv-cray](#), and [PrgEnv-intel](#) respectively
- To use a different compiler, load the PrgEnv-xx module, and still use compiler wrappers to build, for example:

- `% module load PrgEnv-nvidia`

```
yunhe@perlmutter:login21:~> module list
```

```
[Currently Loaded Modules:
```

1) craype-x86-milan	9) gpu/1.0	
2) libfabric/1.15.2.0	10) nvidia/23.9	(g,c)
3) craype-network-ofi	11) craype/2.7.30	(c)
4) xpmem/2.6.2-2.5_2.38__gd067c3f.shasta	12) cray-dsmml/0.2.2	
5) perftools-base/23.12.0	13) cray-mpich/8.1.28	(mpi)
6) cpe/23.12	14) cray-libsci/23.12.5	(math)
7) cudatoolkit/12.2	15) PrgEnv-nvidia/8.5.0	(cpe)
8) craype-accel-nvidia80		

- `% cc -fopenmp -O3 mycode.c (or: cc -mp mycode.c)`
- `% module load PrgEnv-intel`
- `% ftn -fopenmp -O3 mycode.f90 (or: ftn -qomp mycode.f90)`

Running Jobs on Perlmutter CPUs

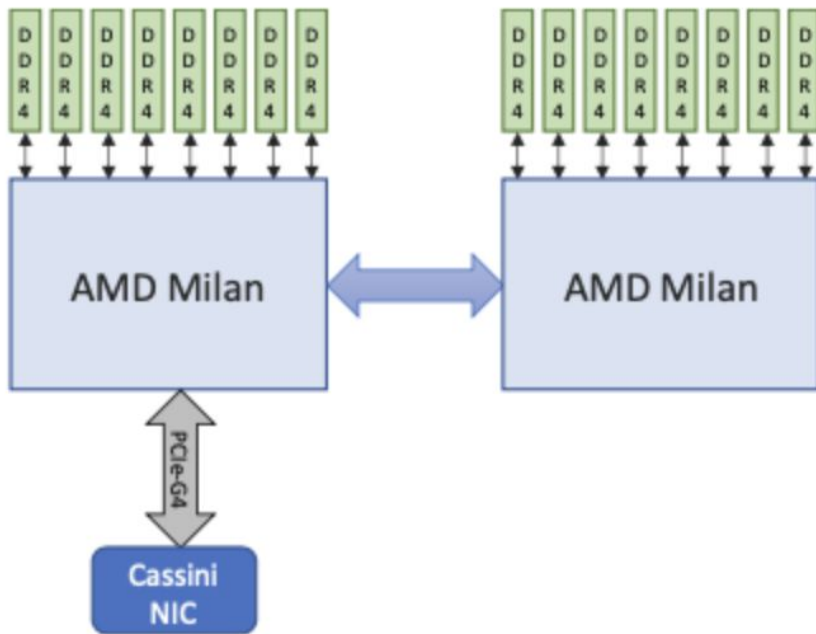
- Slurm batch scheduler is used to schedule jobs
- You can run a batch queue job:
prepare and submit a batch script
`% sbatch myjob.slurm`
- You can run an interactive batch job
`% salloc -N 1 -q interactive -C cpu -t 30:00`
<will land on a compute node>
`% export OMP_NUM_THREADS=8`
`% ./mycode.exe`

Sample pure OpenMP batch script

```
#!/bin/bash
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -t 10:00
#SBATCH -C cpu
#SBATCH -J mycode
#SBATCH -o mycode_%j.out

export OMP_NUM_THREADS=8
./mycode.exe
```

Perlmutter CPU nodes



- Each CPU node has: 2x AMD EPYC 7763 (Milan) CPUs, and 64 cores per CPU, meaning: 128 physical cores per CPU
- With 2 hyperthreads per core, meaning: 256 logical cores total (Slurm sees this when scheduling jobs)
- Without explicitly setting OMP_NUM_THREADS, you will see 256 threads running with most compilers