Migrating From Cori to Perlmutter: GPU Codes

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Outline

● Perlmutter GPU Nodes.
● Programming Environment.
● Hands on Exercises walk through:
  ○ Launching Jobs
  ○ Building for GPUs
  ○ GPU Affinity
  ○ CUDA-Aware MPI
  ○ Other GPU Programming Models
GPU Nodes

- Perlmutter has 1792 GPU Nodes
  - 1536 Nodes with 40GB-A100
  - 256 Nodes with 80GB-A100

- Each GPU node has:
  - 64 core AMD Milan CPU (7763)
  - 4 NVIDIA A100 GPUs.

- Each Milan CPU core has two hardware threads.
GPU Nodes

- Each pair of GPUs is linked via NVLink.
- CPUs and GPUs communicate via PCIe Gen 4.
- SS11 NICs and CPU communicate via PCIe Gen 4.
- Each node has 256 GB of DDR4 Memory.
Programming Environment
GPU Programming Environment

• By default module `gpu` is loaded in your environment.

• This sets up the environment for applications being built for GPUs.

• By default `cudatoolkit` and `craype-accel-nvidia80` along with other GPU accelerated math libraries are loaded.

• Do note that default programming environment has GNU compilers. If NVIDIA compilers are required, switch to `PrgEnv-nvidia`. 
Currently Loaded Modules:

1) craype-x86-milan
2) libfabric/1.15.2.0
3) craype-network-ofi
4) xpmem/2.5.2-2.4_3.30__gd0f7936.shasta
5) PrgEnv-gnu/8.3.3
6) cray-dsmml/0.2.2
7) cray-libsci/23.02.1.1
8) cray-mpich/8.1.24
9) craype/2.7.19
10) gcc/11.2.0
11) perftools-base/23.02.0
12) cpe/23.02
13) xalt/2.10.2
14) Nsight-Compute/2022.1.1
15) Nsight-Systems/2022.2.1
16) cudatoolkit/11.7
17) craype-accel-nvidia80
18) gpu/1.0
GPU Programming Environment

Currently Loaded Modules:
1) craype-x86-milan  4) perftools-base/22.06.0  7) craype/2.7.16  10) cray-libsci/21.08.1 12) darshan/3.4.0  16) cudatoolkit/11.7
2) libfabric/1.15.0.0  5) xpmem/2.4.4-2.3_13.8_gff0e1d9.shasta  8) cray-dsmml/0.2.2  11) PrgEnv-gnu/8.3.3
3) craype-network-ofi  6) gcc/11.2.0  9) cray-mpich/8.1.17  12) xalt/2.10.2  13) darshan/3.4.0  14) Nsight-Compute/2022.1.1
17) craype-accel-nvidia80  18) Cray-Dsmml/0.2.2

mgawan@perlmutter:login37:~> ml

Cray PE Programming Environment

mgawan@perlmutter:login37:~> CC --version

**g++** (GCC) 11.2.0 20210728 (Cray Inc.)
Copyright (C) 2021 Free Software Foundation, Inc.
This is free software; see the source for copying conditions. There is NO warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

mgawan@perlmutter:login37:~> cc --version

**gcc** (GCC) 11.2.0 20210728 (Cray Inc.)
Copyright (C) 2021 Free Software Foundation, Inc.
This is free software; see the source for copying conditions. There is NO warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
GPU Programming Environment

mgawan@perlmutter:login37:~> module load PrgEnv-nvidia

Lmod is automatically replacing "gcc/11.2.0" with "nvidia/22.5".
Lmod is automatically replacing "PrgEnv-gnu/8.3.3" with "PrgEnv-nvidia/8.3.3".
Due to MODULEPATH changes, the following have been reloaded:
   1) cray-mpich/8.1.17

mgawan@perlmutter:login37:~> CC --version

nvc++ 22.5-0 64-bit target on x86-64 Linux -tp zen3-64
NVIDIA Compilers and Tools
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mgawan@perlmutter:login37:~> cc --version

nvc 22.5-0 64-bit target on x86-64 Linux -tp zen3-64
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### Available Programming Models

<table>
<thead>
<tr>
<th></th>
<th>Fortran/C/C++</th>
<th>CUDA</th>
<th>OpenACC 2.x</th>
<th>OpenMP 5.x</th>
<th>CUDA Fortran</th>
<th>Kokkos/Raja</th>
<th>MPI</th>
<th>HIP</th>
<th>DPC++/SYCL</th>
</tr>
</thead>
<tbody>
<tr>
<td>nvidia</td>
<td></td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>CCE</td>
<td></td>
<td>x</td>
<td></td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GNU</td>
<td></td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LLVM</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>x</td>
<td></td>
</tr>
</tbody>
</table>
## Recommended Environment

<table>
<thead>
<tr>
<th>Programming Model</th>
<th>Programming Environment</th>
</tr>
</thead>
<tbody>
<tr>
<td>CUDA</td>
<td>PrgEnv-nvidia/PrgEnv-gnu</td>
</tr>
<tr>
<td>Kokkos</td>
<td>PrgEnv-nvidia/PrgEnv-gnu</td>
</tr>
<tr>
<td>OpenMP offload</td>
<td>PrgEnv-nvidia/PrgEnv-cray</td>
</tr>
<tr>
<td>OpenACC</td>
<td>PrgEnv-nvidia</td>
</tr>
<tr>
<td>stdpar</td>
<td>PrgEnv-nvidia</td>
</tr>
</tbody>
</table>
Compiling

• *.c, *.cpp, *.f90 => CPU source code
  o may include MPI
  o may use directives for GPU
  o compile with regular compilers (Cray wrappers)
    • CC for C++
    • cc for C
    • ftn for Fortran
• *.cu => CUDA kernels
  o compile with nvcc
• (Note: With PrgEnv-nvidia, CUDA can be incorporated into same source files as CPU code, add "-cuda" or "-gpu" flag at compile time)
Hands on Exercises
Hands on Exercises

- Exercises along with instructions are available at: https://github.com/NERSC/Migrate-to-Perlmutter
- For GPU examples, move to the GPU folder.
- The README.md file details seven exercises and list steps to build and run them.
- It is suggested to go through these examples during the hands-on session to understand usage of different programming environments.
Hands on Exercises

What’s covered:

• Building and running CUDA, OpenACC and OpenMP codes for GPUs.
• Building and running GPU + MPI codes using NVIDIA and GNU programming environment.
• Building and running a CUDA-Aware MPI example.
• Understanding GPU affinity with an example.
Hands on Exercises

• For all the examples, build steps are provided in a Makefile within each exercise’s directory.

• Each exercise’s directory also contains a batch.sh file which the users can use to run.
Required SBATCH options (1)

```bash
#!/bin/bash

#SBATCH -q regular # "regular" QOS for most jobs
#SBATCH -N 2 # number of Nodes requested
#SBATCH -t 5 # max wallclock time (5 minutes)
#SBATCH -n 8 # number of MPI tasks
#SBATCH -c 32 # reserve 32 cpus per task
#SBATCH --ntasks-per-node=4 # 8 tasks / 4 per node = 2 nodes
#SBATCH --gpus-per-task=1 # reserve 1 GPU per task
#SBATCH -A ntrain8 # GPU version of your project/repo
#SBATCH -C gpu
#SBATCH –reservation=pm_gpu_mar10 # reservation

Each GPU node has 64 cores x 2 hyperthreads, so 128 CPUs => 32 cpus is 1/4th of a node
```
#!/bin/bash

#SBATCH -q regular
#SBATCH -N 2  # number of Nodes requested
#SBATCH -t 5  # max wallclock time (5 minutes)
#SBATCH -n 8  # number of MPI tasks
#SBATCH -c 32  # reserve 32 cpus per task
#SBATCH --ntasks-per-node=4  # 8 tasks / 4 per node = 2 nodes
#SBATCH --gpus-per-task=1  # reserve 1 (of four) GPUs per task
#SBATCH -A ntrain8  # GPU version of your project/repo
#SBATCH -C gpu  # use GPU nodes
#SBATCH –reservation=pm_gpu_mar10  # reservation

Specify a constraint of "run only on gpu nodes"
Useful Runtime Environment Variables

- Generates runtime debug info such as kernel launch and data transfers between host and device.
- PrgEnv-gnu (upcoming gcc/12 compiler)
  - % export GOMP_DEBUG=1
- PrgEnv-nvidia (Nvidia compiler)
  - % export NVCOMPILER_ACC_NOTIFY=<value>
  - where value can be:  1: kernel launches 2: data transfers
  - 4: region entry/exit  8: wait operations or synchronizations with the device
  - 16: device memory allocates and deallocates
- PrgEnv-cray (CCE compiler)
  - % export CRAY_ACC_DEBUG=<value>
  - where value can be 1, 2, 3
Exercise-1: Simple CUDA Kernel

- The source file contains a simple CUDA kernel that adds two vectors and stores the sum in third.
- *nvcc* by default identifies .cu files as containing CUDA.
  - `nvcc -arch=sm_80 vecAdd.cu -o vec_add`
  - `CC -cuda vecAdd.cpp -o vec_add`
- But this practice may not work for larger projects where rest of the code relies on a different compiler.
Exercise-2: CUDA separate compilation

- For complex projects where the host compiler does not recognize CUDA.
- Compile CUDA code separately (in separate files) and link to it later.

```
NVCCFLAGS = -arch=sm_80
vec_add: kernels.o kernels.h vecAdd.cpp
CC -o $@ vecAdd.cpp kernels.o
kernels.o: kernels.cu kernels.h
nvcc $(NVCCFLAGS) -c kernels.cu -o $@
```
Exercise-3: simple MPI + CUDA

- A simple example of MPI + CUDA in same source file is best built with “PrgEnv-nvidia”.
- The CC wrappers link with the MPI specifically built for “PrgEnv-nvidia”.
- When using “PrgEnv-nvidia” wrappers, –gpu flags need to be mentioned:

```bash
NVCCFLAGS = -arch=sm_80
NVCCFLAGS = -arch=sm_80
NVCFLAGS = -cuda -gpu=cc80
vec_add: vecAdd.cu
CC $(NVCFLAGS) vecAdd.cu -o $@
```
Exercise-4: separate compilation (MPI + CUDA)

- When using a programming environment other than "PrgEnv-nvidia", device code needs to be built separately.
- Load the programming environment of your choice, build the CUDA code separately and then link it with MPI wrappers.

```
NVCCFLAGS = -arch=sm_80
NVCCFLAGS = -gpu=cc80
vec_add: kernels.o kernels.h vecAdd.cpp
   CC -o $@ vecAdd.cpp kernels.o
kernels.o: kernels.cu kernels.h
   nvcc $(NVCCFLAGS) -c kernels.cu -o $@
```
## Compute Nodes Comparison for CPU Affinity

<table>
<thead>
<tr>
<th></th>
<th>Cori Haswell</th>
<th>Cori KNL</th>
<th>Perlmutter CPU</th>
<th>CPU on Perlmutter GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical cores</td>
<td>32</td>
<td>68</td>
<td>128</td>
<td>64</td>
</tr>
<tr>
<td>Logical CPUs per physical core</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Logical CPUs per node</td>
<td>64</td>
<td>272</td>
<td>256</td>
<td>128</td>
</tr>
<tr>
<td>NUMA domains</td>
<td>2</td>
<td>1</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>-c value for srun</td>
<td>2*floor(32/tpn)</td>
<td>4<em>floor(68/tpn), usually do 4</em>floor(64/tpn)</td>
<td>2* floor(128/tpn)</td>
<td>2*floor(64/tpn)</td>
</tr>
</tbody>
</table>

\[ tpn = \text{Number of MPI tasks per node} \]
Launch options and affinity (GPUs)

```bash
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --ntasks-per-node=64
#SBATCH --cpus-per-task=2
#SBATCH --gpus-per-node=4

export OMP_NUM_THREADS=1
srun -n 128 -cpu-bind=cores -gpus-bind=closest <executable>
```

- By default all processes will have access to all GPUs.
- A round robin assignment does not guarantee affinity.
- To guarantee that closest GPU is assigned: `-gpus-bind=closest`
- To bind ranks to individual cores: `-cpu-bind=cores`

\[ c = 2 \times \text{floor}(64/\text{tpn}) \]

Where:

\[ \text{tpn} = \text{ntasks-per-node} \]
Affinity and binding

Perlmutter GPU nodes are configured as "NPS4" => 4 NUMA nodes per socket. Each GPU is "closest" to certain cores.
Exercise-5: Rank to GPU binding

- This example prints out the cores each MPI rank is residing on along with the GPUs that are visible to each rank.
- By default all the MPI ranks will be able to view all the GPUs.
- Build and test the example by first running with `script_reg.sh` sbatch script.
- Then test with `script_close.sh` sbatch script.
- Notice that using the latter sbatch script each MPI rank can view only the GPU located closest to the corresponding NUMA node.
- The only difference was usage of `--gpu-bind=closest` flag. You can explore other ways this binding can be done, refer to: https://slurm.schedmd.com/srun.html
Launch options and affinity (GPUs)

```bash
srun -n8 --cpu-bind=cores ./vec_add
```

**Rank 1/8 (PID:73658 on Core: 16) from nid003497 sees 4 GPUs, GPU assigned to me is: 0000:41:00.0**
Other 3 GPUs are:
**rank = 0: 0000:03:00.0 **
**rank = 2: 0000:81:00.0 **
**rank = 3: 0000:C1:00.0 **

**Rank 5/8 (PID:73662 on Core: 17) from nid003497 sees 4 GPUs, GPU assigned to me is: 0000:41:00.0**
Other 3 GPUs are:
**rank = 0: 0000:03:00.0 **
**rank = 2: 0000:81:00.0 **
**rank = 3: 0000:C1:00.0 **

**Rank 0/8 (PID:73657 on Core: 0) from nid003497 sees 4 GPUs, GPU assigned to me is: 0000:03:00.0**
Other 3 GPUs are:
**rank = 1: 0000:41:00.0 **
**rank = 2: 0000:81:00.0 **
**rank = 3: 0000:C1:00.0 **

**Rank 2/8 (PID:73659 on Core: 32) from nid003497 sees 4 GPUs, GPU assigned to me is: 0000:81:00.0**
Other 3 GPUs are:
**rank = 0: 0000:03:00.0 **
**rank = 1: 0000:41:00.0 **
**rank = 3: 0000:C1:00.0 **
Launch options and affinity (GPUs)

NUMA node(s): 4
NUMA node0 CPU(s): 0-15,64-79
NUMA node1 CPU(s): 16-31,80-95
NUMA node2 CPU(s): 32-47,96-111
NUMA node3 CPU(s): 48-63,112-127

NUMANode L#0 (P#0 62GB)
  PCI c1:00.0 (3D)
NUMANode L#1 (P#1 63GB)
  PCI 82:00.0 (3D)
NUMANode L#2 (P#2 63GB)
  PCI 41:00.0 (3D)
NUMANode L#3 (P#3 63GB)
  PCI 03:00.0 (3D)

Rank 1/8 (PID:102481 on Core: 1) from nid001364 sees 1 GPUs, GPU assigned to me is: = 0000:C1:00.0
  Other 0 GPUs are:
Rank 0/8 (PID:102480 on Core: 0) from nid001364 sees 1 GPUs, GPU assigned to me is: = 0000:C1:00.0
  Other 0 GPUs are:
Rank 5/8 (PID:102486 on Core: 33) from nid001364 sees 1 GPUs, GPU assigned to me is: = 0000:41:00.0
  Other 0 GPUs are:
Rank 2/8 (PID:102482 on Core: 16) from nid001364 sees 1 GPUs, GPU assigned to me is: = 0000:82:00.0
  Other 0 GPUs are:
Rank 4/8 (PID:102485 on Core: 32) from nid001364 sees 1 GPUs, GPU assigned to me is: = 0000:41:00.0
  Other 0 GPUs are:
CUDA-aware MPI

Nvidia UVA (Unified Virtual Addressing) presents GPU device memory as part of the same address space as CPU main memory

- Allows a CUDA-aware MPI implementation (eg Cray-MPICH) to send and receive messages directly from/to GPU memory - no copy-to-main-memory needed

(from https://developer.nvidia.com/blog/introduction-cuda-aware-mpi/)
Example-6: CUDA-aware MPI

Make sure `gpu` module is loaded before trying this example as CUDA-aware MPI requires certain environment setup.

If your executable uses CUDA-aware MPI, `ldd` should show `libmpi_gtl_cuda.so.0`, eg:

```
libmpi_gtl_cuda.so.0 => /opt/cray/pe/lib64/libmpi_gtl_cuda.so.0
```
Exercise-7: OpenACC and OpenMP offload

• This example demonstrates building OpenACC and OpenMP offload codes.
• The example implements the same kernel from previous examples but this time using different programming models.
• Make sure that you have PrgEnv-nvidia loaded before trying out the example.

```
ifeq ($(OPENMP),y)
CXXFLAGS += -mp=gpu -gpu=cc80 -Minfo
EXE = vec_add.openmp
else ifeq ($(OPENACC),y)
CXXFLAGS += -acc -Minfo=accel
EXE = vec_add.openacc
```
Thank you!

More questions? Need help? ...
http://help.nersc.gov/