Migrating From Cori to Perlmutter: GPU Codes

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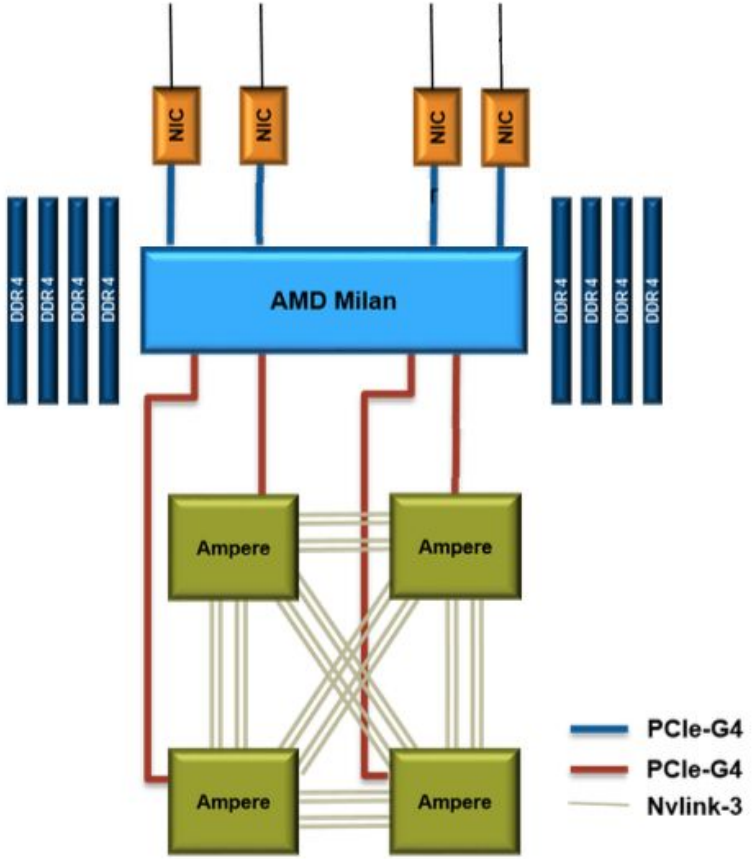
Outline

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

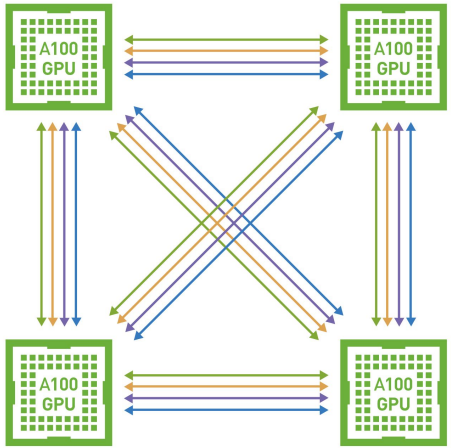
GPU Nodes

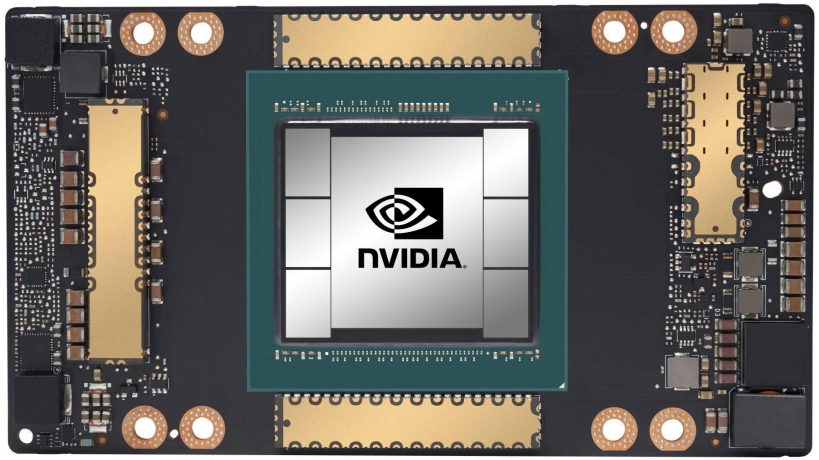
- Perlmutter has 1536 GPU Nodes and 3072 CPU nodes.
- Each GPU node has a 64 core AMD Milan CPU (7763) and 4 NVIDIA A100 GPUs.
- Each CPU node has two 64 core AMD Milan CPUs.
- Each Milan CPU core has two hardware threads.

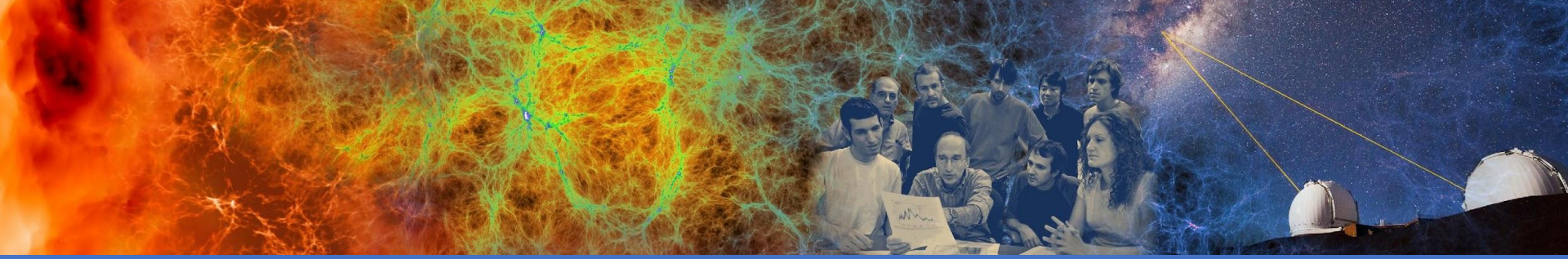


GPU Nodes

- A100 GPUs on Perlmutter have 40 GBs of HBM each.
- Each A100 GPU can perform 9.7 TFlops (FP64).
- Each pair of GPUs have NVLink connections.
- CPUs and GPUs communicate with PCIe Gen 4.







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.

GPU Programming Environment

```
mgawan@perlmutter:login37:~> ml

Currently Loaded Modules:
  1) craype-x86-milan     4) perftools-base/22.06.0      7) craype/2.7.16      10) cray-libsci/21.08.1.2  13) 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       14) Nsight-Compute/2022.1.1   17) craype-accel-nvidia80
  3) craype-network-ofi   6) gcc/11.2.0                  9) cray-mpich/8.1.17  12) xalt/2.10.2            15) Nsight-Systems/2022.2.1   18) gpu/1.0
```

GPU Programming Environment

```
mgawan@perlmutter:login37:~> ml

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  1) craype-x86-milan     4) perftools-base/22.06.0      7) craype/2.7.16      10) cray-libsci/21.08.1.2  13) darshan/3.4.0          16) cudatoolkit/11.7
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  3) craype-network-ofi   6) gcc/11.2.0                  9) cray-mpich/8.1.17  12) xalt/2.10.2           15) Nsight-Systems/2022.2.1   18) gpu/1.0


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.)
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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
NVIDIA Compilers and Tools
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```
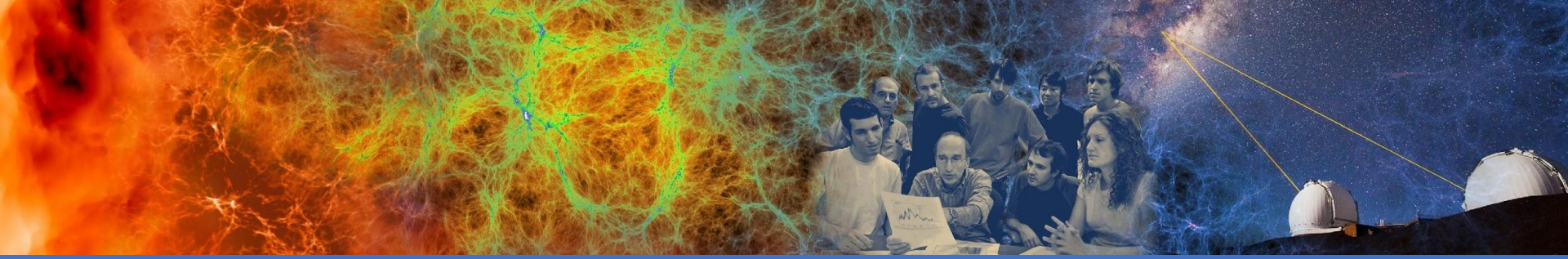

Recommended Environment

Programming Environment	Programming Model
PrgEnv-nvidia/PrgEnv-gnu	CUDA
PrgEnv-nvidia/PrgEnv-gnu	Kokkos
PrgEnv-nvidia/PrgEnv-cray	OpenMP offload
PrgEnv-nvidia	OpenACC
PrgEnv-nvidia	stdpar

Compiling

- *.c, *.cpp, *.f90 => CPU source code
  - may include MPI
  - may use directives for GPU
  - **compile with regular compilers (Cray wrappers)**
    - **CC for C++**
    - **cc for C**
    - **ftn for Fortran**
- *.cu => CUDA kernels
  - **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.

Necessary SBATCH options (1)

```
#!/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-ta                                    task
#SBATCH -A ntrain2                                       project/repo
#SBATCH -C gpu
#SBATCH -reservation=pm_gpu_dec1   # reservation
```

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

Necessary SBATCH options (2)

```
#!/bin/bash
#SBATCH -q regular                  # regular QOS
#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 ntrain2                 # GPU                          po
#SBATCH -C gpu                     #
#SBATCH -reservation=pm_gpu_dec1   # 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:

```
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.
- In such a scenario “cudart” library needs to be linked in as well

```
NVCCFLAGS = -arch=sm_80
NVCFLAGS = -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

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

tpn = Number of MPI tasks per node

Launch options and affinity (GPUs)

```
#!/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>
```

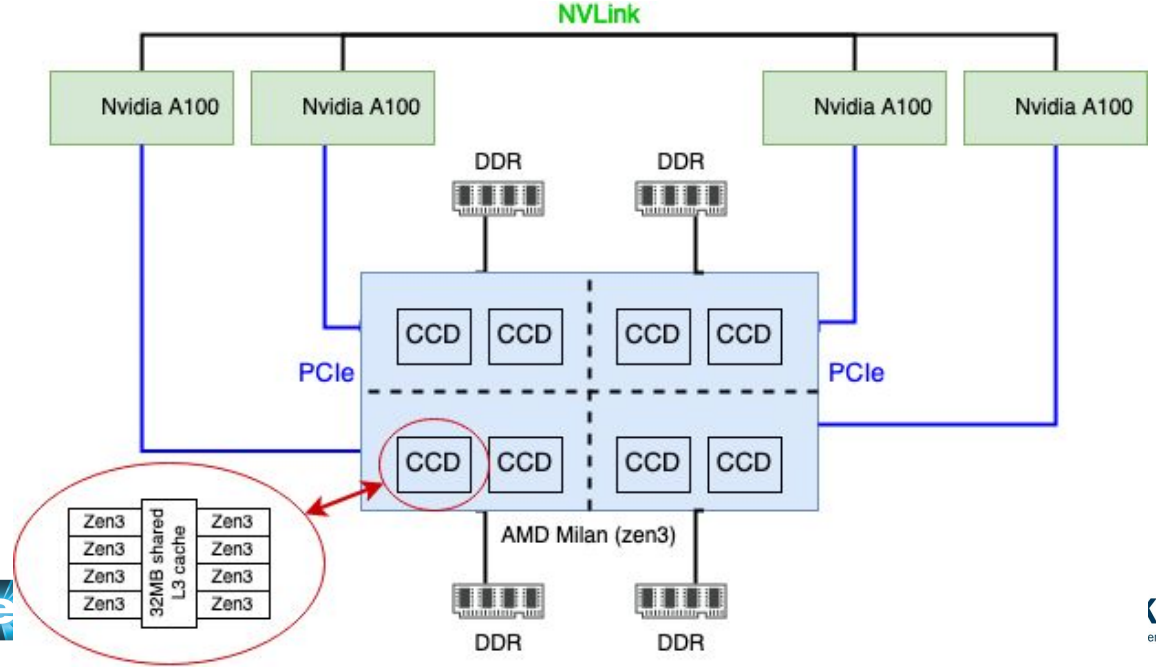
c = 2*(64/k)

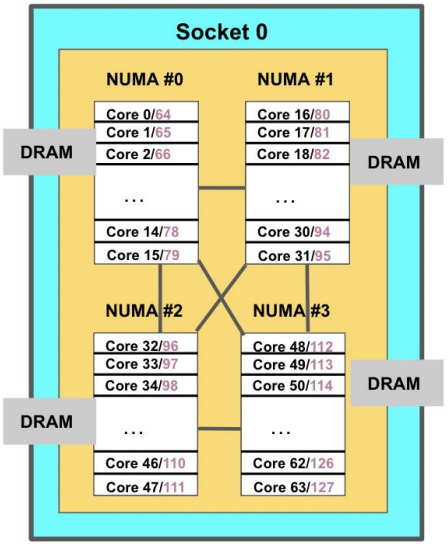
where:
k = ntasks-per-node

- 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

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)

```
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 **
```

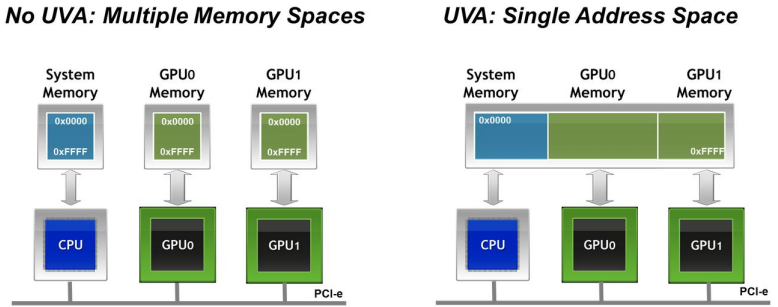
Launch options and affinity (GPUs)

```
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:
```

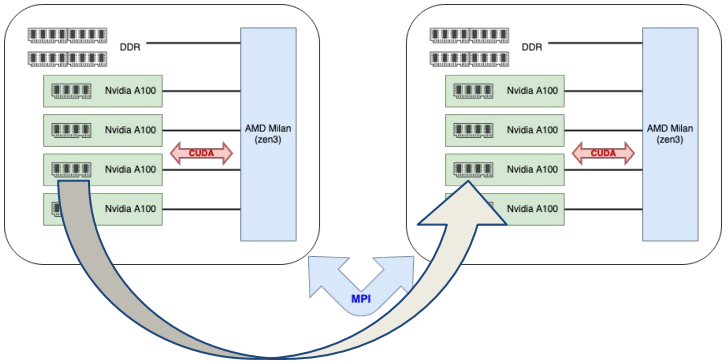
CUDA-aware MPI

Nvidia UVA 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.

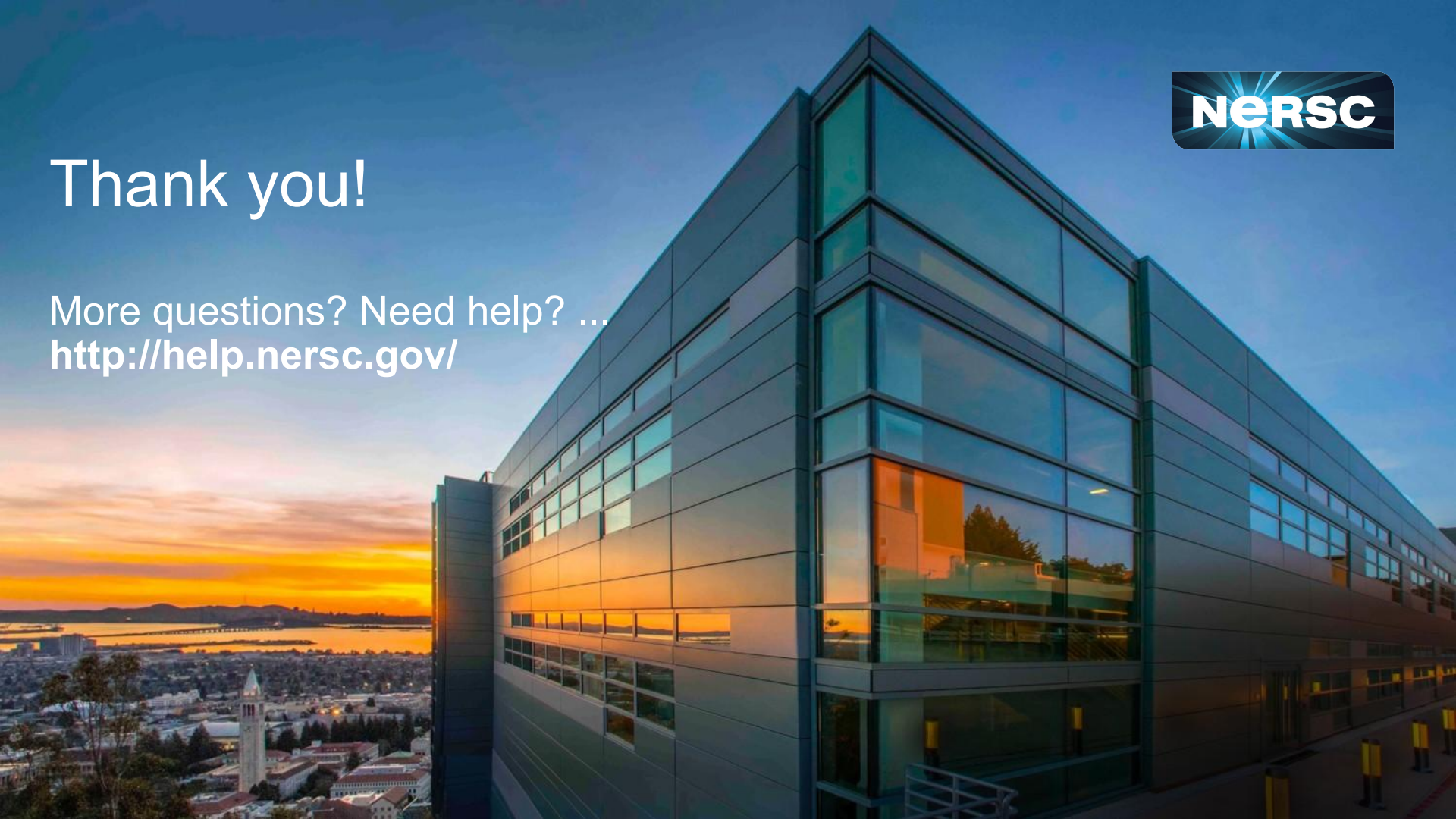
If your executable uses CUDA-aware MPI, **`ldd`** should show `libmpi_gtl_cuda.so.0`, eg:

```
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
```


NERSC
Thank you!
More questions? Need help? ...
http://help.nersc.gov/