



NCAR is sponsored by National Science Foundation



## Multi-GPU Programming, Part 2

By: Daniel Howard <u>dhoward@ucar.edu (mailto:dhoward@ucar.edu)</u>, Consulting Services Group, CISL & NCAR

Date: July 14th, 2022

In this notebook we explore the mini-app <u>MiniWeather</u> (<u>https://github.com/mrnorman/miniWeather</u>) to present techniques and code examples for implementing and assessing performance of various multi-GPU paradigms. We will cover:

1. Interoperability of OpenACC with MPI and NCCL GPU communication libraries 2. Hands-on implementation of MiniWeather with CUDA aware MPI and NCCL Head to the <u>NCAR JupyterHub portal (https://jupyterhub.hpc.ucar.edu/stable)</u> and **start a JupyterHub session on Casper login** (or batch nodes using 1 CPU, no GPUs) and open the notebook at 11\_MultiGPU/11\_multiGPU\_Part2.ipynb. Be sure to clone (if needed) and update/pull the NCAR GPU\_workshop directory.

# Use the JupyterHub GitHub GUI on the left panel or the below shell commands
git clone git@github.com:NCAR/GPU\_workshop.git
git pull

## Workshop Etiquette

- Please mute yourself and turn off video during the session.
- Questions may be submitted in the chat and will be answered when appropriate. You may also raise your hand, unmute, and ask questions during Q&A at the end of the presentation.
- By participating, you are agreeing to <u>UCAR's Code of Conduct</u> (<u>https://www.ucar.edu/who-we-are/ethics-integrity/codes-conduct/participants</u>)
- Recordings & other material will be archived & shared publicly.
- Feel free to follow up with the GPU workshop team via Slack or submit support requests to <u>rchelp.ucar.edu (https://support.ucar.edu)</u>
  - Office Hours: Asynchronous support via <u>Slack</u> (<u>https://ncargpuusers.slack.com</u>) or schedule a time with an organizer

### **Notebook Setup**

Set the PROJECT code to a currently active project, ie UCIS0004 for the GPU workshop, and QUEUE to the appropriate routing queue depending on if during a live workshop session (gpuworkshop), during weekday 8am to 5:30pm MT (gpudev), or all other times (casper).

The GPU\_TYPE=gp100 nodes are not configured for multi-GPU computing! Thus, the gpuworkshop queue is not useful for this session. Saying as much, please set GPU\_TYPE=v100 and use the gpudev both during the workshop and for independent work. See <u>Casper queue documentation</u> (<u>https://arc.ucar.edu/knowledge base/72581396#StartingCasperjobswithPBS-Concurrentresourcelimits</u>) for more info.

## What Have We Learned So Far?

In <u>Part 1 (Multi-GPU\_Programming\_for\_Earth\_Scientists\_Jiri\_Kraus\_NVIDIA.pdf)</u>, Jiri Kraus from NVIDIA shared many different approaches for Multi-GPU Programming.

- Non-CUDA Aware MPI
- CUDA Aware MPI
- NCCL (pronounced "nickel") NVIDIA Collective Communication Library
- NVSHMEM NVIDIA Shared Memory Library
- Other tips and backgrond information

Today, we will focus on hands-on implementation of **CUDA Aware MPI** and **NCCL** within MiniWeather.

### **Baseline Performance of Non-CUDA Aware MPI**

First, let's compile our baseline program miniWeather\_mpi\_openacc.F90. To note, I/O output has been disabled in all versions. Also, this version has already been partially modified to offload each MPI task to a distinct GPU.

Casper does not attempt to isolate GPUs between MPI tasks like other HPC centers may choose to do by default. On Casper, **every MPI task can access all GPUs available to the node** it is residing on.

**Question**: If this baseline code was not modified, why does MiniWeather's performance not improve with increasing the number of MPI tasks that reside on the same node?

Hint: Which GPU device is each MPI task using?

#### 

mpif90 -I\${PNETCDF\_INC} -Mextend -O0 -DNO\_INFORM -c miniWeather\_mpi\_openacc.F90 -o
miniWeather\_mpi\_openacc.F90.o \
-D\_NX=4096 -D\_NZ=2048 -D\_SIM\_TIME=10.0 -D\_OUT\_FREQ=10.0 -D\_DATA\_SPEC=DATA\_SPEC\_THE
RMAL \${OPENACC\_FLAGS}

```
mpif90 -Mextend -O3 miniWeather_mpi_openacc.F90.o -o openacc -L${PNETCDF_LIB} -lpn
etcdf ${OPENACC_FLAGS}
rm -f miniWeather mpi openacc.F90.o
```

Now, submit multi-GPU runs to get some performance benchmarks. We use a validation script to ensure the answer is correct. The validation script has the following usage syntax, where  $n_{tasks}$  is optional:

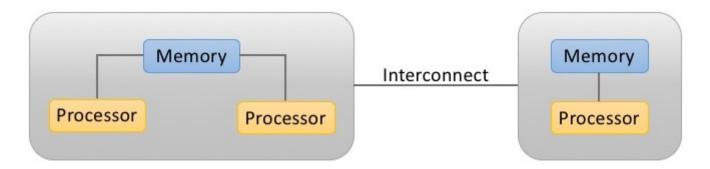
```
./check_output.sh executable mass_relative_tolerance
energy_relative_tolerance [n_tasks]
```

To note, Casper has nodes of 4 or 8 GPUs available and the main gpgpu queue allows up to 32 GPUs per job. The gpudev queue allows up to 4 GPUs per job.

```
In []: for S in 1  # Select number of nodes (Casper: gpgpu -> S*N <= 32, gpudev -> S
 *N <= 4 )
    do
    for N in 1 2 4  # Number of MPI tasks, CPUs, and GPUs per node (Casper: max(N)=
    8, 8-way nodes often busy )
        do
            qcmd -A $PROJECT -q $QUEUE -1 select=$S:ncpus=$N:ngpus=$N:mpiprocs=$N -1 gpu
        type=$GPU_TYPE -1 walltime=30 -- \
            $PWD/check_output.sh $PWD/openacc 1e-13 4.5e-5 $((S*N))
        done
        done</pre>
```

## **Basics of Communication with MPI**

The foundation to communicating data and messages for a **distributed-memory** computer is the **Message Passing Interface (MPI)** library. MPI consists of a collection of routines for exchanging data across distributed memory spaces in a parallel program, ie memory from one node to another node or one GPU to another GPU.



The MPI standard was first introduced in 1994 and has evolved many times over the years to a well established level of maturity across multiple library options, such as **OpenMPI**, **Intel MPI**, and **MVAPICH**.

A complete description of the MPI standard can be found on the <u>MPI Forum's</u> <u>Documentation Page (https://www.mpi-forum.org/docs/)</u>.

#### **Basic Structure of MPI Programs**

1. Initialize communications

- MPI\_INIT initializes the MPI environment
- MPI\_COMM\_SIZE returns the number of processes
- MPI\_COMM\_RANK returns this process's number (rank)
- 2. Communicate to share data between processes
  - MPI\_SEND sends a blocking message
  - MPI\_RECV receives a blocking message

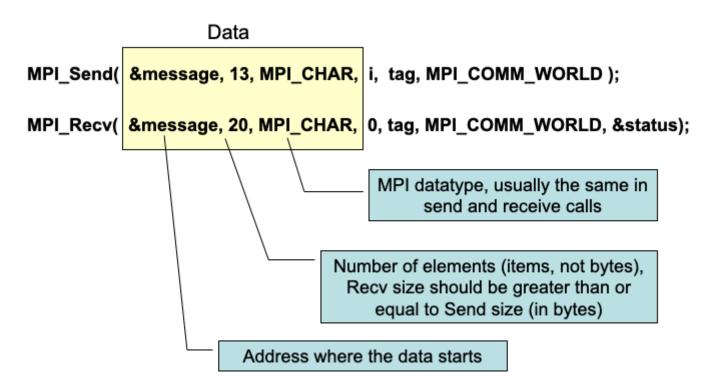
3. Exit from the message-passing system --

• MPI\_FINALIZE

There also exists collective operations such as MPI\_Bcast and MPI\_Allreduce.A primary concept to understand is **blocking** vs **non-blocking** communication, ie MPI\_Send vs MPI\_ISend.

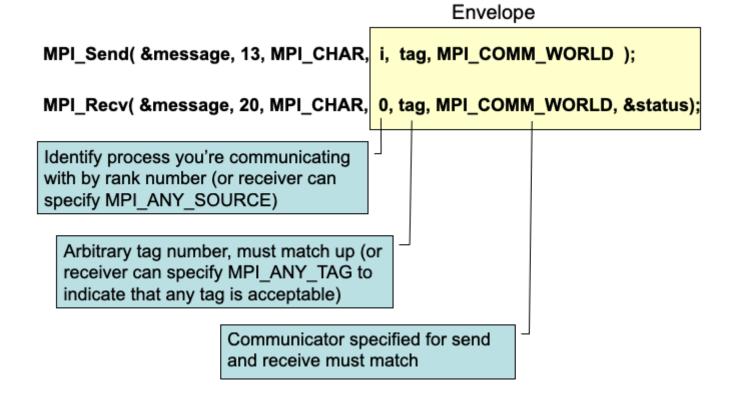
This concept is similar to **synchronous** vs **asynchronous** operations, discussed in earlier GPU sessions respectively.

#### Data Parameters - Example MPI\_Send and MPI\_Recv



Source: Cornell's <u>Message Passing Interface Virtual Workshop</u> (<u>https://cvw.cac.cornell.edu/MPI/messages</u>)

#### Envelope Parameters - Example MPI\_Send and MPI\_Recv



Source: Cornell's <u>Message Passing Interface Virtual Workshop</u> (<u>https://cvw.cac.cornell.edu/MPI/messages</u>)

#### Extension of MPI to Multi-GPU Communication

There is not time today to go into more details on MPI. Nonetheless, MPI is an important framework to understand and forms the basis of development for similar Multi-GPU communication patterns and developed libraries.

For example, the NCCL library utilizes the communication APIs ncclSend and ncclRecv, which are functionaly equivalent to MPI\_Send and MPI\_Recv. Thus, concepts for MPI communication are very useful for understanding related concepts in multi-GPU communication patterns. The only caveat is the additional separate memory space within the GPU alongside the CPU memory.

If you are not that familiar with MPI or want to review beginner/advanced concepts, you are encouraged to seek out additional learning material such as:

- Cornell's Virtual Workshop <u>5-part MPI Series</u> (<u>https://cvw.cac.cornell.edu/topics#MPI</u>)
- NCSA's and UIUC's <u>Introduction to MPI (https://www.hpc-training.org/xsede/moodle/enrol/index.php?id=34)</u> on the <u>hpc-training.org</u>
   (<u>https://www.hpc-training.org/xsede/moodle/)</u> HPC-Moodle platform
- XSEDE's <u>HPC Workshop: MPI (https://www.psc.edu/resources/training/xsede-hpc-workshop-may-2022-mpi/)</u> May 2022 offering

## Using CUDA Aware MPI for Multi-GPU Communication

Fortunately, <u>MiniWeather (https://github.com/mrnorman/miniWeather)</u> already provides an MPI implementation. With OpenACC, calls to MPI had to be surrounded by the directives !\$acc update host() and !\$acc update device() (Note: MPI\_ISend/MPI\_IRecv are non-blocking MPI calls).

```
!Prepost receives
```

```
call mpi_irecv(recvbuf_l,hs*nz*NUM_VARS,MPI_REAL8, left_rank,0,MPI_COMM_WORLD
,req_r(1),ierr)
```

call mpi\_irecv(recvbuf\_r,hs\*nz\*NUM\_VARS,MPI\_REAL8,right\_rank,1,MPI\_COMM\_WORLD
,req\_r(2),ierr)

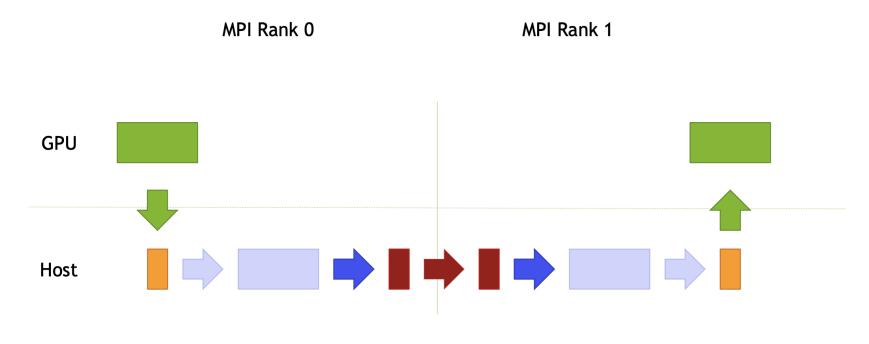
```
!OpeanACC GPU Kernel loading send buffers
!$acc update host(sendbuf_l,sendbuf_r) async
!$acc wait
```

```
!Fire off the sends
```

```
call mpi_isend(sendbuf_l,hs*nz*NUM_VARS,MPI_REAL8, left_rank,1,MPI_COMM_WORLD
,req_s(1),ierr)
    call mpi_isend(sendbuf_r,hs*nz*NUM_VARS,MPI_REAL8,right_rank,0,MPI_COMM_WORLD
,req_s(2),ierr)
    !Wait for receives to finish
    call mpi_waitall(2,req_r,status,ierr)
    ...
```

This approach works but is not most optimal given available communication routes between nodes.

Recall from the previous session how data must be copied from GPU memory to CPU memory to another node's CPU memory to that node's GPU memory.



MPI\_Send(s\_buf\_d, size, MPI\_BYTE, 1, tag, MPI\_COMM\_WORLD, ierr)
MPI\_Recv(r\_buf\_d, size, MPI\_BYTE, 0, tag, MPI\_COMM\_WORLD, ierr)

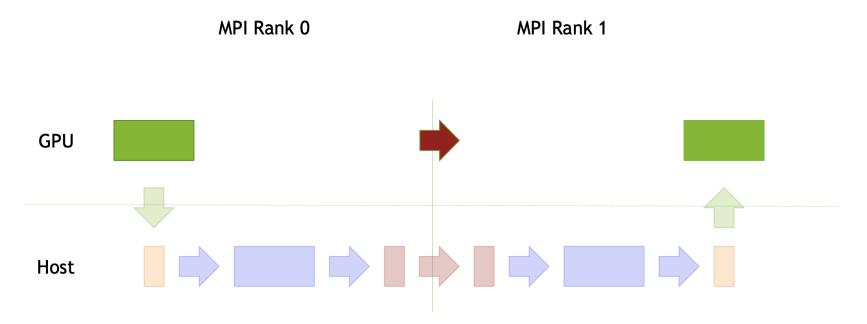
#### **OpenACC Interoperability and Implemenations for CUDA Aware MPI**

In order to redirect memory movement and avoid unecessary steps between the CPUs and GPUs, **MPI must be provided the GPU device location of data memory**. Here's an example in OpenACC:

```
!$acc host_data use_device(s_buf_d,r_buf_d)
...
!$acc end host_data
```

Essentialy, within any host\_data region in CPU code, data objects given in use\_device() will instead point to device/GPU memory. This simple directive should tightly encapsulate any MPI calls, allowing a CUDA Aware MPI library to directly reference memory on the GPU instead of memory on the CPU. If interested, see more OpenACC interoperability features at this GitHub (https://github.com/OpenACC/openacc-interoperability-examples) by Jeff Larkin.

For Casper, the default library OpenMPI enables CUDA aware features by default. However, different MPI libraries often require you to specify additional flags or environment variables to use CUDA aware features (slide 22 in <u>Part 1 (Multi-GPU Programming for Earth Scientists Jiri Kraus NVIDIA.pdf)</u>). Once the MPI library directly references GPU device memory when setting up communication, messages communicated across a HPC cluster can more directly travel to their destinations, shortening the time spent in communication.

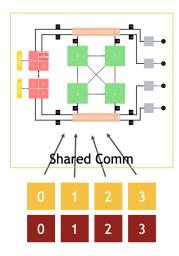


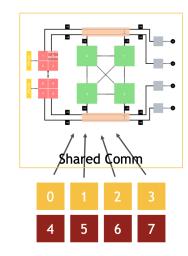
!\$acc host\_data use\_device(s\_buf\_d,r\_buf\_d)
MPI\_Send(s\_buf\_d, size, MPI\_BYTE, 1, tag, MPI\_COMM\_WORLD, ierr)
MPI\_Recv(r\_buf\_d, size, MPI\_BYTE, 0, tag, MPI\_COMM\_WORLD, ierr)
!\$acc end host data

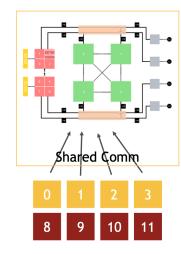
#### Using OpenACC to Assign GPU Devices to MPI Tasks

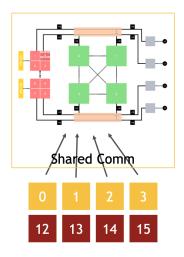
Parallel programs typically won't automatically know which GPU device it should be assigned to. Managing this is best left to the developer, which allows multiple arrangements, ie ...

- one process per MPI task per GPU
- one process managing multiple GPUs, etc.









A common technique to manage local GPU ranks across global MPI ranks utilizes a split MPI\_COMM\_TYPE\_SHARED communicator. This instantiates another MPI communicator that is local to an individual node, indexing a subset of processes across the local node's available MPI tasks.

With a split communicator, you can then use OpenACC Runtime API functions like acc\_get\_num\_devices() and acc\_set\_device() (must specify use openacc) to assign MPI tasks to specific GPUs given the devices available. An example initialization code snippet is below:

```
call MPI_Init(ierr)
    call MPI_Comm_size(MPI_COMM_WORLD, nranks, ierr)
    call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierr)
    call MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, myrank, MPI_IN
F0_NULL, local_comm, ierr)
    call MPI_Comm_rank(local_comm, local_rank, ierr)
    nGPUs_node = acc_get_num_devices(acc_get_device_type())
    call acc set device num(mod(local rank,nGPUs node), acc get device type())
```

## EXERCISE - Implement CUDA Aware MPI in miniWeather\_mpiAware\_openacc.F90

Following the direction of the TODO sections in <u>miniWeather mpiAware openacc.F90</u> (<u>miniWeather mpiAware openacc.F90</u>), create a CUDA aware MPI version of MiniWeather. This will involve the following changes:

- 1. <u>Line 78 & 80 (miniWeather mpiAware openacc.F90#L78)</u> Instantiate additional variables for the split local communicators and number of GPUs
- 2. <u>Line 401 & 423 (miniWeather mpiAware openacc.F90#L401)</u> Specify the send and receive buffers in MPI calls to use GPU device memory
- 3. <u>Line 505 & 525 (miniWeather mpiAware openacc.F90#L505)</u> Add a split communicator and assign GPUs per ranks local to each node

Once finished, use the cells below to compile the CUDA aware version, check for errors, and run it. If you get stuck, solutions are in the <u>solutions (solutions)</u> folder.

```
In [ ]: # Compiles the CUDA aware MPI version of MiniWeather using OpenACC, exec = ./opena
ccAware
OPENACC_FLAGS="-acc -gpu=cc70,lineinfo"
mpif90 -I${PNETCDF_INC} -Mextend -O0 -DNO_INFORM -c miniWeather_mpiAware_openacc.F
90 -o miniWeather_mpiAware_openacc.F90.o \
-D_NX=4096 -D_NZ=2048 -D_SIM_TIME=10.0 -D_OUT_FREQ=10.0 -D_DATA_SPEC=DATA_SPEC_THE
RMAL ${OPENACC_FLAGS}
mpif90 -Mextend -O3 miniWeather_mpiAware_openacc.F90.o -o openaccAware -L${PNETCDF
```

```
_LIB} -lpnetcdf ${OPENACC_FLAGS}
rm -f miniWeather mpiAware openacc.F90.0
```

```
In [ ]: # CUDA Aware MPI runs
S=1; N=4
    qcmd -A $PROJECT -q $QUEUE -1 select=$S:ncpus=$N:ngpus=$N:mpiprocs=$N -1 gpu_typ
e=$GPU_TYPE -1 walltime=30 -- \
    $PWD/check_output.sh $PWD/openaccAware 1e-13 4.5e-5 $((S*N))
```

## Using NCCL Library for Multi-GPU Communication

Leveraging the NVIDIA Collective Communication Library (NCCL) with OpenACC is relatively the same as CUDA Aware MPI. Below are some significant points to make:

## Function prototypes for calling NCCL only slightly differ from MPI functions By default, all NCCL functions are blocking within the provided CUDA stream

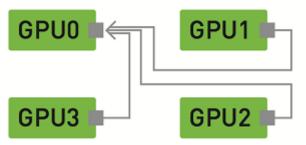
- Grouped non-blocking behavior can be achieved with ncclGroupStart() and ncclGroupEnd() regions
- 3. NCCL can directly leverage scheduling and overalapping of communication/compute on the GPU through effective CUDA stream selection while MPI cannot
- 4. Error handling is done via returned values from NCCL functions whereas MPI error handling is a passed argument
- 5. NCCL arguably should have better collective communication performance compared to MPI but point-to-point communication will likely not have demonstrable benefit
  - NCCL can achieve improved performance on a well configured system since it automatically can detect and optimize communication across given node topologies

#### Using the NCCL API

- Full documentation for NCCL is <u>here</u> (<u>https://docs.nvidia.com/deeplearning/nccl/user-guide/docs/index.html</u>)
- Listed functional prototypes and API specification is <u>here</u> (<u>https://docs.nvidia.com/deeplearning/nccl/user-guide/docs/api.html</u>)

When using any external library, it is highly encouraged to consult available documentation like the above to learn how to use a library.





In NCCL's case, the same <code>!\$acc host\_data use\_device()</code> approach is required alongside OpenACC code (or you can directly pass in a device memory pointer from your own CUDA kernel or other library).

Here are important data and function prototypes for NCCL useful for the next exercise:

- 1. Data prototypes for initializing NCCL
  - type(ncclUniqueId) :: nccl\_id A unique id for each group of communicators
  - type(ncclResult) :: nccl\_result A variable to store return values from NCCL functions, used for error handling
  - type(ncclComm) :: nccl\_comm The NCCL comunicator object
- 2. Function prototypes for initializing NCCL
  - ncclResult\_t ncclGetUniqueId(ncclUniqueId\* uniqueId) -Creates a nccl\_id for the communicators
  - ncclResult\_t ncclCommInitRank(ncclComm\_t\* comm, int nranks, ncclUniqueId commId, int rank) - Initializes NCCL, similar to MPI\_Init()
- 3. Function prototypes for Send/Recv communication
  - ncclResult\_t ncclSend(const void\* sendbuff, size\_t count, ncclDataType\_t datatype, int peer, ncclComm\_t comm, cudaStream\_t stream)
  - ncclResult\_t ncclRecv(void\* recvbuff, size\_t count, ncclDataType\_t datatype, int peer, ncclComm\_t comm, cudaStream\_t stream)

To enable runtime NCCL debugging, simply set NCCL\_DEBUG = WARN.

# EXERCISE - Implement NCCL Library in miniWeather\_mpiNCCL\_openacc.F90

Extending from the previous exercise, follow the TODO sections in <u>miniWeather\_mpiNCCL\_openacc.F90 (miniWeather\_mpiNCCL\_openacc.F90)</u> to create a NCCL version of Miniweather. Ideally, make this version portable by using the provided #ifdef\_NV\_GPU / #endif preprocessor sections.

- 1. <u>Line 14 (miniWeather mpiNCCL openacc.F90#L14)</u> Load the NCCL library module
- Line 93 (miniWeather mpiNCCL openacc.F90#L93) Instantiate NCCL variables needed for communicators
- 3. <u>Line 425 (miniWeather mpiNCCL openacc.F90#L425)</u> Setup a non-blocking group of sends and receives similar to the MPI sends and receives, also using OpenACC to reference GPU memory
- 4. <u>Line 560 (miniWeather mpiNCCL openacc.F90#L560)</u> Generate NCCL unique Id and use MPI\_Bcast to broadcast to all ranks and initialize NCCL communicators

Use the cells below to compile the NCCL version, check for errors, and run it. If you get stuck, solutions are in the <u>solutions (solutions)</u> folder.

```
In [ ]: # Compiles the NCCL version of MiniWeather using OpenACC, exec = ./openaccNCCL
OPENACC_FLAGS="-acc -gpu=cc70,lineinfo"
mpif90 -I${PNETCDF_INC} -I${NCCL_INC} -Mextend -O0 ${OPENACC_FLAGS} \
  -DNV_GPU -DNO_INFORM -D_NX=4096 -D_NZ=2048 -D_SIM_TIME=10.0 -D_OUT_FREQ=10.0 -D_DA
TA_SPEC=DATA_SPEC_THERMAL \
  -c miniWeather_mpiNCCL_openacc.F90 -o miniWeather_mpiNCCL_openacc.F90.o
mpif90 -Mextend -O3 ${OPENACC_FLAGS} miniWeather_mpiNCCL_openacc.F90.o -o openaccN
CCL \
  -L${PNETCDF_LIB} -lpnetcdf -L${NCCL_LIB} -lnccl
  rm -f miniWeather_mpiNCCL_openacc.F90.o
```

```
In [ ]: # NCCL runs
S=1; N=4
qcmd -A $PROJECT -q $QUEUE -1 select=$S:ncpus=$N:ngpus=$N:mpiprocs=$N -1 gpu_typ
e=$GPU_TYPE -1 walltime=30 -- \
$PWD/check_output.sh $PWD/openaccNCCL 1e-13 4.5e-5 $((S*N))
```

### Generate nsys Profiles of Multi-GPU Jobs

Use the below cells and included <u>nsysMPI\_pbs.sh</u> (<u>nsysMPI\_pbs.sh</u>) script to generate profile reports of each program.

- In [ ]: qsub -q gpudev -v EXEC=openacc,N=4 -1 select=1:ncpus=4:ngpus=4:mpiprocs=4 nsysMPI\_
  pbs.sh
- In [ ]: qsub -q gpudev -v EXEC=openaccAware,N=4 -1 select=1:ncpus=4:ngpus=4:mpiprocs=4 nsy
  sMPI\_pbs.sh
- In [ ]: qsub -q gpudev -v EXEC=openaccNCCL,N=4 -1 select=1:ncpus=4:ngpus=4:mpiprocs=4 nsys
  MPI\_pbs.sh

### **Additional Considerations**

The following UCX and OpenMPI environment variables are currently recommended for optimal performance of CUDA Aware MPI applications. Future testing and system adjustements may modify these recommendations. Notably, gdr\_copy is currently not incuded in UCX\_TLS.

```
export CUDA_LAUNCH_BLOCKING=0
export UCX_TLS=rc,sm,cuda_copy,cuda_ipc
export OMPI_MCA_pml=ucx
export OMPI_MCA_btl=self,vader,tcp,smcuda #openib
export UCX_RNDV_SCHEME=get_zcopy
export UCX_RNDV_THRESH=0
export UCX_MAX_RNDV_RAILS=1
export UCX_MEMTYPE CACHE=n
```

Add the following to qcmd to try it out.

-v

CUDA\_LAUNCH\_BLOCKING=0,"UCX\_TLS='rc,sm,cuda\_copy,cuda\_ipc'",OMPI\_MC

"OMPI\_MCA\_btl='self,vader,tcp,smcuda'",UCX\_RNDV\_SCHEME=get\_zcopy,UC UCX\_MAX\_RNDV\_RAILS=1,UCX\_MEMTYPE\_CACHE=n

## Resources

- MPI
- Cornell's Virtual Workshop <u>5-part MPI Series</u> (<u>https://cvw.cac.cornell.edu/topics#MPI</u>)
- NCSA's and UIUC's <u>Introduction to MPI (https://www.hpc-training.org/xsede/moodle/enrol/index.php?id=34)</u> on the <u>hpc-training.org</u>
   (<u>https://www.hpc-training.org/xsede/moodle/</u>) HPC-Moodle platform
- XSEDE's <u>HPC Workshop: MPI</u> (<u>https://www.psc.edu/resources/training/xsede-hpc-workshop-may-2022-mpi/</u>) May 2022 offering
- Multi-GPU
  - Condensed NVIDIA documentation on <u>NCCL Fortran API</u> (<u>https://docs.nvidia.com/hpc-sdk/compilers/fortran-cuda-interfaces/index.html#cfnccl-runtime</u>)
  - Full NVIDIA <u>NCCL Documentation</u> (<u>https://docs.nvidia.com/deeplearning/nccl/user-guide/docs/index.html</u>)
  - Julich Multi-GPU Tutorial (https://github.com/FZJ-JSC/tutorial-multi-gpu) material as provided at SC21 and ISC22
  - Cineca's <u>OpenACC Tutorial (https://github.com/romerojosh/cineca-openacc-tutorial)</u>, Conjugate Gradient solver using CUDA Aware MPI and NCCL
  - Jiri Kraus' <u>Multi-GPU Programming Model</u>