Fakultät für **Mathematik und Informatik**

# NCCL and Host-Initiated NVSHMEM SC 2024

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## So far we learned about ..

- CUDA-Aware MPI
- What is behind (GPUDirect Technologies)
- How to debug, profile and trace your Code
- How to navigate in the traces
- How to overlap communication and computation on the GPUs
- Streams and priority streams

# Motivation

- MPI is **not** (yet [1] ) aware of CUDA streams
- Explicit synchronization between GPU-compute kernel and CPU communication calls is required
- CUDA-aware MPI is GPU-**memory**-aware communication
- For better efficiency: CUDA-**stream**-aware communication
    - Communication, which is aware of CUDA-streams or use CUDA streams
    - NCCL and (Host-API) of NVSHMEM

# What will you Learn?

- How to use NCCL inside an MPI Application to use CUDA-stream-aware P2P communication
- NVSHMEM memory model
- How to use stream-aware NVSHMEM communication operations in MPI Programs

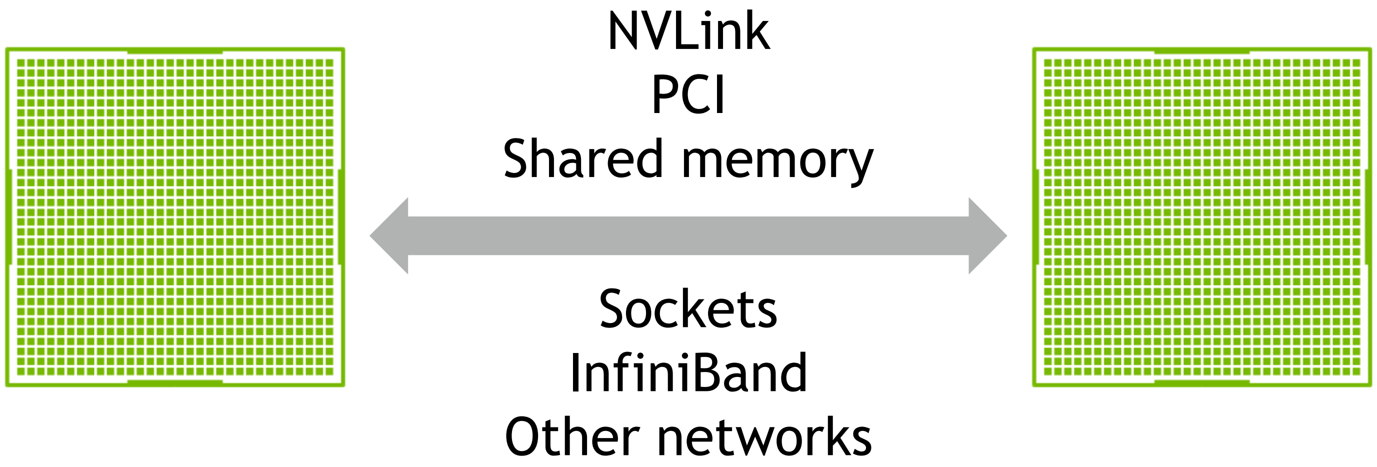
[1] *MPI Forum Hybrid Working Group - Stream and Graph Based MPI Operations: https://github.com/mpiwg-hybrid/hybrid-issues/issues/5*

## Optimized inter-GPU communication

### NCCL : NVIDIA Collective Communication Library

Communication library running on GPUs, for GPU buffers.

- Library for efficient communication with GPUs
- First: Collective Operations (e.g. Allreduce), as they are required for DeepLearning
- Since 2.8: Support for Send/Recv between GPUs
- Library running on GPU: Communication calls are translated to GPU a kernel (running on a stream)




Binaries : https://developer.nvidia.com/nccl and in NGC containers
Source code : https://github.com/nvidia/nccl
Perf tests : https://github.com/nvidia/nccl-tests

# NCCL-API (With MPI) - Initialization

First, we need a NCCL-Communicator for, this, wee need a NCCL UID

```
MPI_Init(&argc,&argv)
MPI_Comm_size(MPI_COMM_WORLD,&size);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);

ncclUniqueId nccl_uid;
if (rank == 0) ncclGetUniqueId(&nccl_uid);
MPI_Bcast(&nccl_uid, sizeof(ncclUniqueId), MPI_BYTE, 0, MPI_COMM_WORLD);

ncclComm_t nccl_comm;
ncclCommInitRank(&nccl_comm, size, nccl_uid, rank);
…
…
ncclCommDestroy(nccl_comm);
MPI_Finalize();
```

# Communication Calls

Supported for NCCL 2.8+

```
ncclSend(void* sbuff, size_t count, ncclDataType_t type, int peer, ncclComm_t comm, cudaStream_t stream);
ncclRecv(void* rbuff, size_t count, ncclDataType_t type, int peer, ncclComm_t comm, cudaStream_t stream);
```

```
    ncclAllReduce(void* sbuff, void* rbuff, size_t count, ncclDataType_t type, ncclRedOp_t op,           ncclComm_t comm, cudaStream_t stream);
    ncclBroadcast(void* sbuff, void* rbuff, size_t count, ncclDataType_t type,                 int root, ncclComm_t comm, cudaStream_t stream);
       ncclReduce(void* sbuff, void* rbuff, size_t count, ncclDataType_t type, ncclRedOp_t op, int root, ncclComm_t comm, cudaStream_t stream);
ncclReduceScatter(void* sbuff, void* rbuff, size_t count, ncclDataType_t type, ncclRedOp_t op,           ncclComm_t comm, cudaStream_t stream);
    ncclAllGather(void* sbuff, void* rbuff, size_t count, ncclDataType_t type,                           ncclComm_t comm, cudaStream_t stream);
```

# Fused Communication Calls

- Multiple calls to `ncclSend()` and `ncclRecv()` should be fused with `ncclGroupStart()` and `ncclGroupEnd()` to
  - Avoid deadlocks
    (if calls need to progress concurrently)
  - For more performance
    (can be more efficiently)

SendRecv:

```
ncclGroupStart();
 ncclSend(sendbuff, sendcount, sendtype, peer, comm, stream);
 ncclRecv(recvbuff, recvcount, recvtype, peer, comm, stream);
ncclGroupEnd();
```

Bcast:

```
ncclGroupStart();
if (rank == root) {
  for (int r=0; r<nranks; r++)
    ncclSend(sendbuff[r], size, type, r, comm, stream);}
ncclRecv(recvbuff, size, type, root, comm, stream);
ncclGroupEnd();
```

Neighbor exchange:

```
ncclGroupStart();
for (int d=0; d<ndims; d++) {
  ncclSend(sendbuff[d], sendcount, sendtype, next[d], comm, stream);
  ncclRecv(recvbuff[d], recvcount, recvtype, prev[d], comm, stream);
}
ncclGroupEnd();
```

# Jacobi solver communication with NCCL

```
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start, iy_end, nx, compute_stream);
ncclGroupStart();
ncclRecv(a_new,                   nx, NCCL_REAL_TYPE, top, nccl_comm, compute_stream);
ncclSend(a_new +(iy_end - 1)*nx, nx, NCCL_REAL_TYPE, btm, nccl_comm, compute_stream);
ncclRecv(a_new +(iy_end*nx),     nx, NCCL_REAL_TYPE, btm, nccl_comm, compute_stream);
ncclSend(a_new + iy_start * nx,  nx, NCCL_REAL_TYPE, top, nccl_comm, compute_stream);
ncclGroupEnd();
```

# Performance Improvement

- So far, no overlap of communication and computation
- Use techniques from previous session to overlap communication and computation
- Make sure that communication streams are scheduled
    - CUDA high priority streams!

```
int leastPriority = 0;
int greatestPriority = leastPriority;
cudaDeviceGetStreamPriorityRange(&leastPriority, &greatestPriority);

cudaStream_t compute_stream;
cudaStream_t push_stream;

cudaStreamCreateWithPriority(&compute_stream, cudaStreamDefault, leastPriority);
cudaStreamCreateWithPriority(&push_top, cudaStreamDefault, greatestPriority);
```

# Jacobi using NCCL and Overlapping Communication and Computation

```
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start,       iy_start + 1), nx, push_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_end - 1),   iy_end,        nx, push_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_start + 1), (iy_end - 1),  nx, compute_stream);

ncclGroupStart();
ncclRecv(a_new,                     nx, NCCL_REAL_TYPE, top, nccl_comm, push_stream);
ncclSend(a_new + (iy_end - 1) * nx, nx, NCCL_REAL_TYPE, btm, nccl_comm, push_stream);
ncclRecv(a_new + (iy_end * nx),     nx, NCCL_REAL_TYPE, btm, nccl_comm, push_stream);
ncclSend(a_new + iy_start * nx,     nx, NCCL_REAL_TYPE, top, nccl_comm, push_stream);
ncclGroupEnd();
```

# How to Compile an MPI+NCCL Application

- Include header files and link against CUDA NCCL library

```
#include <nccl.h>
```

```
MPICXX_FLAGS = -I$(CUDA_HOME)/include -I$(NCCL_HOME)/include
LD_FLAGS = -L$(CUDA_HOME)/lib64 -lcudart -lnccl

$(NVCC) $(NVCC_FLAGS) jacobi_kernels.cu –c –o jacobi.o
$(MPICXX) $(MPICXX_FLAGS)  jacobi.cpp jacobi_kernels.o $(LD_FLAGS) -o jacobi
```

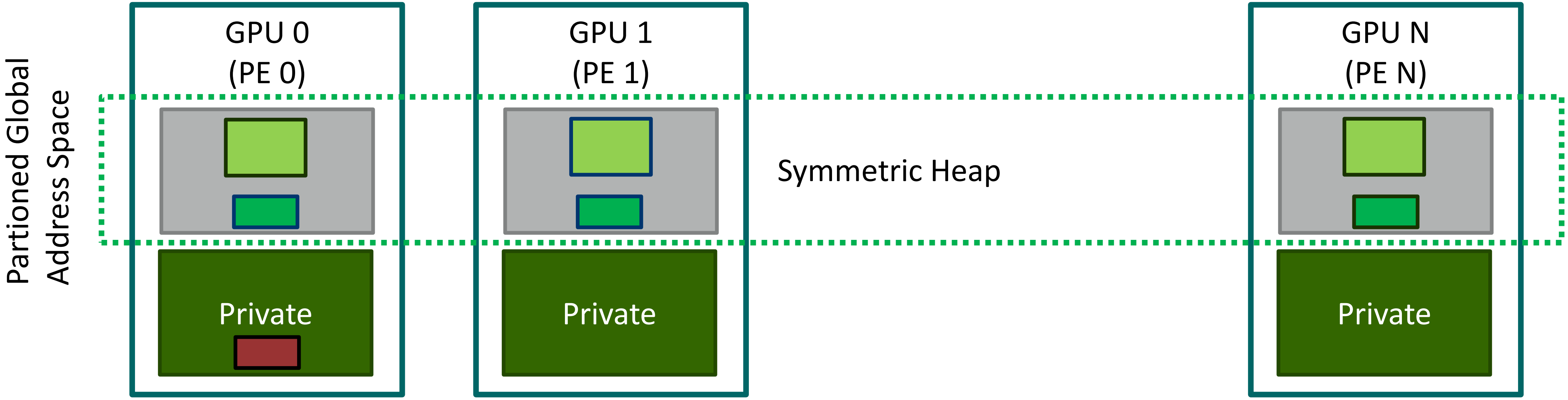
## NVSHMEM – Overview

- Implements the OpenSHMEM API for clusters of NVIDIA GPUs
- Partitioned Global Address Space (PGAS) programming model
  - One sided Communication with put/get
  - Shared memory Heap
- GPU Centric communication APIs
  - GPU Initiated: thread, warp, block
  - Stream/Graph-Based (communication kernel or cudaMemcpyAsync)
  - CPU Initiated
- prefixed with "*nvshmem*" to allow use with a CPU OpenSHMEM library
- Interoperability with OpenSHMEM and MPI

With some extensions to the API

# NVSHMEM Symmetric Memory Model






Symmetric objects are allocated collectively with the same size on every PESymmetric memory:

`nvshmem_malloc( shared_size);`

Must be the same on all PEs

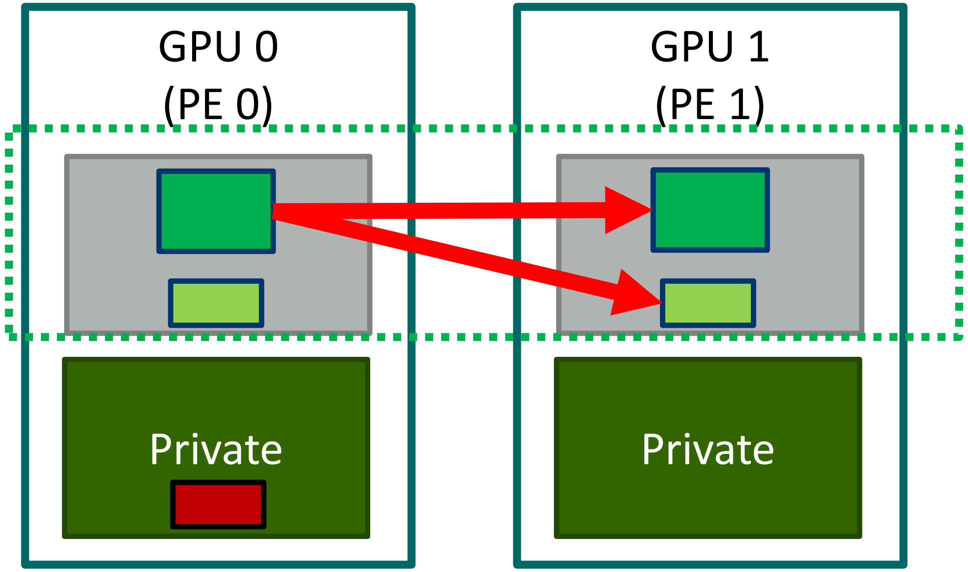
Private memory: `cudaMalloc(...)`

# Interoperability with MPI and OpenSHMEM

```
MPI_Init(&argc, &argv);
MPI_Comm mpi_comm = MPI_COMM_WORLD;
nvshmemx_init_attr_t attr;
attr.mpi_comm = &mpi_comm;
nvshmemx_init_attr(NVSHMEMX_INIT_WITH_MPI_COMM, &attr);
assert( size == nvshmem_n_pes() );
assert( rank == nvshmem_my_pe() );
…
nvshmem_finalize()
MPI_Finalize();
```

```
shmem_init();
nvshmemx_init_attr_t attr;
nvshmemx_init_attr(NVSHMEMX_INIT_WITH_SHMEM, &attr);
mype_node = nvshmem_team_my_pe(NVSHMEMX_TEAM_NODE);
…
```

## NVSHMEM Host API Put

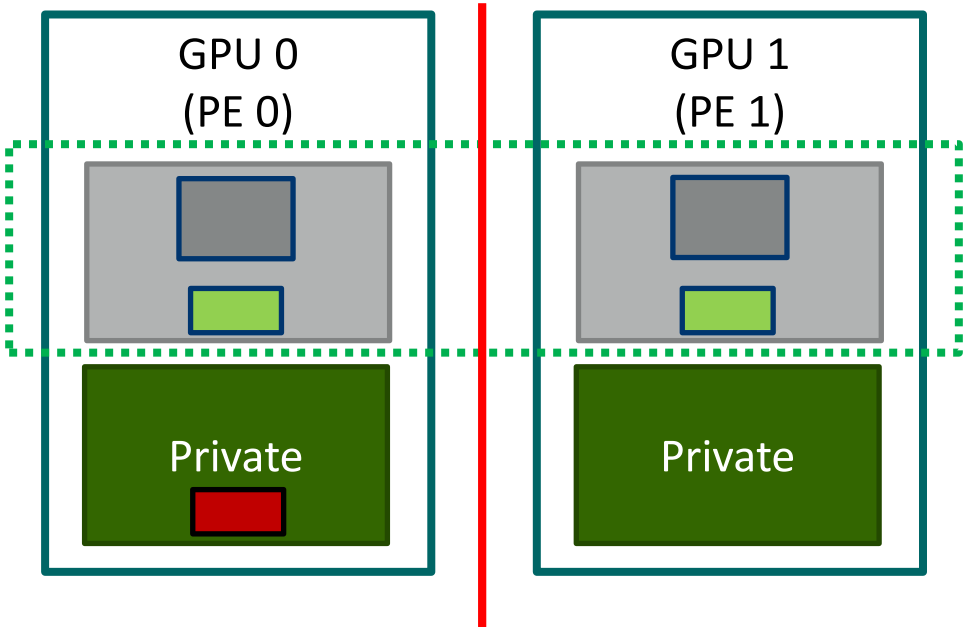



Copies *nelems* data elements of type *T* from symmetric objects *src* to *dest* on PE *pe*

```
void nvshmem_<T>_put(T*dest, const T*source, size_t nelems, int pe);
void nvshmemx_<T>_put_on_stream(T*dest, const T*src, size_t nelems, int pe, cudaStream_t stream);
```

The x marks extensions to the OpenSHMEM API

## NVSHMEM Barrier (on Host)




Synchronizes all PEs and ensures communication performed prior to the barrier has completed

```
void nvshmem_barrier_all(void);
void nvshmemx_barrier_all_on_stream(cudaStream_t stream)
```

## Jacobi solver communication with NVSHMEM

Chunk size must me the same on all PEs. Otherwise, you get **U**ndefined **B**ehavior!

```
real* a     = (real*) nvshmem_malloc(nx * (chunk_size+ 2) * sizeof(real));
real* a_new = (real*) nvshmem_malloc(nx * (chunk_size+ 2) * sizeof(real));
```

```
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start, iy_end, nx, compute_stream);
nvshmemx_float_put_on_stream(a_new, a_new +iy_end - 1) * nx, nx, btm, compute_stream);
nvshmemx_float_put_on_stream((a_new+iy_end)*nx, (ax_new+1)*nx,            nx, top, compute_stream);
nvshmemx_barrier_all_on_stream(compute_stream);
```

# Jacobi with NVSHMEM

Use high priority stream!

```
real* a =     (real*) nvshmem_malloc(nx * (chunk_size+ 2) * sizeof(real));
real* a_new = (real*) nvshmem_malloc(nx * (chunk_size+ 2) * sizeof(real));
```

```
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start,     iy_start + 1, nx, push_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_end - 1,   iy_end,       nx, push_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start + 1, iy_end - 1),  nx, compute_stream);

nvshmemx_float_put_on_stream(a_new,a_new + (iy_end-1) * nx,    nx, btm, push_stream);
nvshmemx_float_put_on_stream((a_new+iy_end)*nx, (ax_new+1)*nx, nx, top, push_stream);
nvhmemx_barrier_all_on_stream(push_stream);
```

## How to compile NVSHEM + MPI applications

- Compile CUDA-kernel
  - Use the -rdc=true compile flag due to the device interface
  - Link against the nvshmem libray -lnvshmem

```
#include <nvshmem.h>
#include <nvshmemx.h>
```

```
nvcc -rdc=true -ccbin g++ -gencode=$NVCC_GENCODE -I $NVSHMEM_HOME/include \
nvshmem_hello.cu -o nvshmem_hello  -L $NVSHMEM_HOME/lib -lnvshmem -lcuda
```

```
nvcc -rdc=true -ccbin g++ -gencode=$NVCC_GENCODE -I $NVSHMEM_HOME/include -c\
jacobi_kernels.cu -o jacobi_kernels.o

$mpixx  -I $NVSHMEM_HOME/include  jacobi.cpp jacobi_kernels.o -lnvshmem \
-lcuda  -o jacobi
```

## Summary

- NCCL and NVSHMEM support CUDA stream aware communication
- Both are interoperable with MPI
- NCCL support send/receive semantics
- NVSHMEM supports the OpenSHMEM library, supporting one sided communication operation
- Both allow to issue communication request asynchronous with respect to the CPU-thread, but synchronous to CUDA streams
- High priority streams are required to overlap communication and computation