Fakultät für
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NCCL and Host-Initiated NVSHMEM ISC 2024

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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*

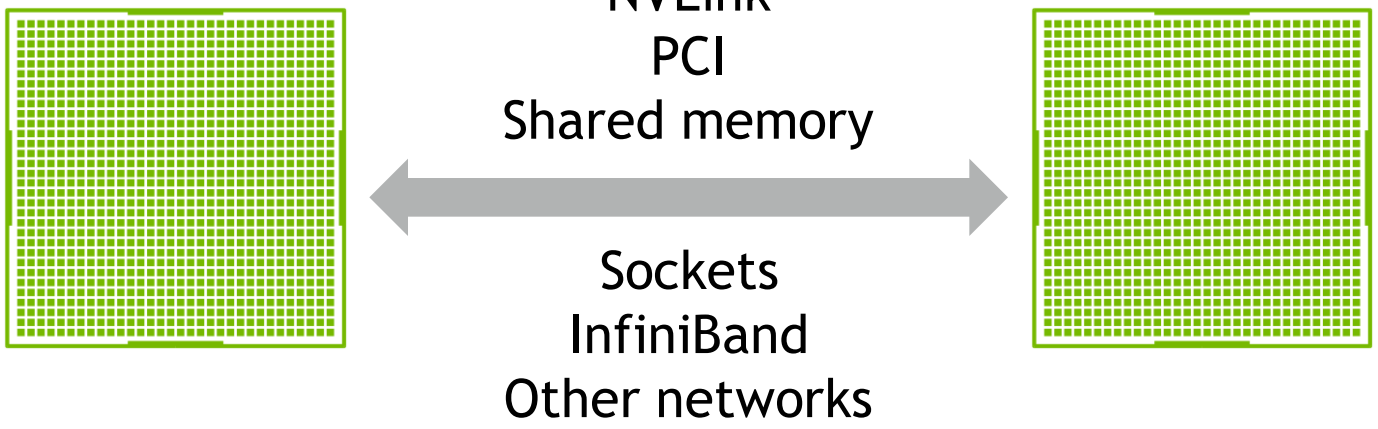
[1] MPI Forum Hybrid Working Group - Stream and Graph Based MPI Operations: https://github.com/mpiwg-hybrid/hybrid-issues/issues/5

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>
```

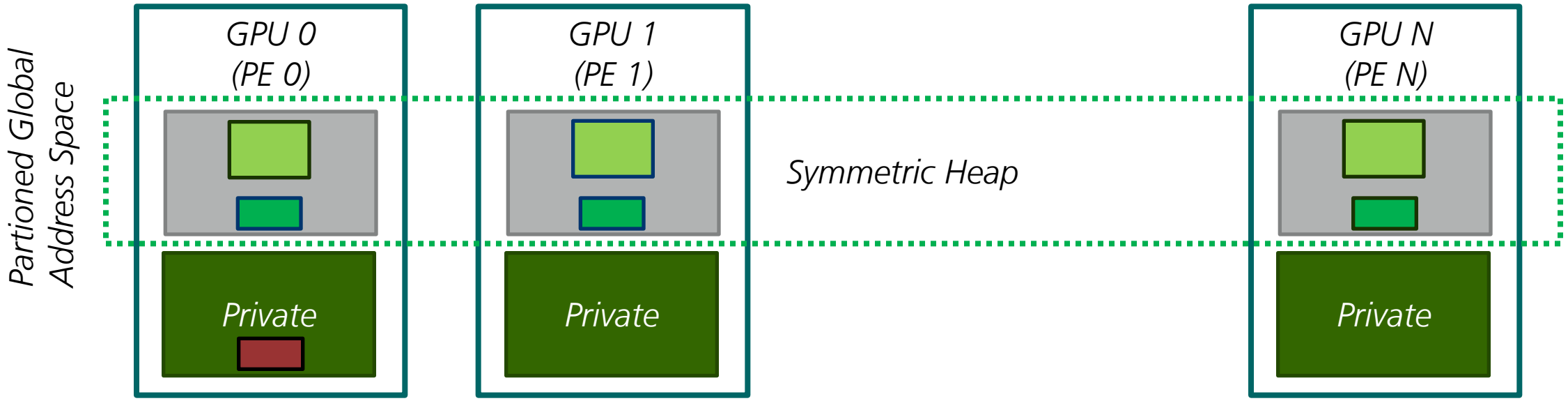
```
MPICXX_FLAGS = -I$(CUDA_HOME)/include -I$(NCCL_HOME)/include
LD_FLAGS = -L$(CUDA_HOME)/lib64 -lcudart -lnccl

$(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);
```

Private memory: `cudaMalloc(...)`

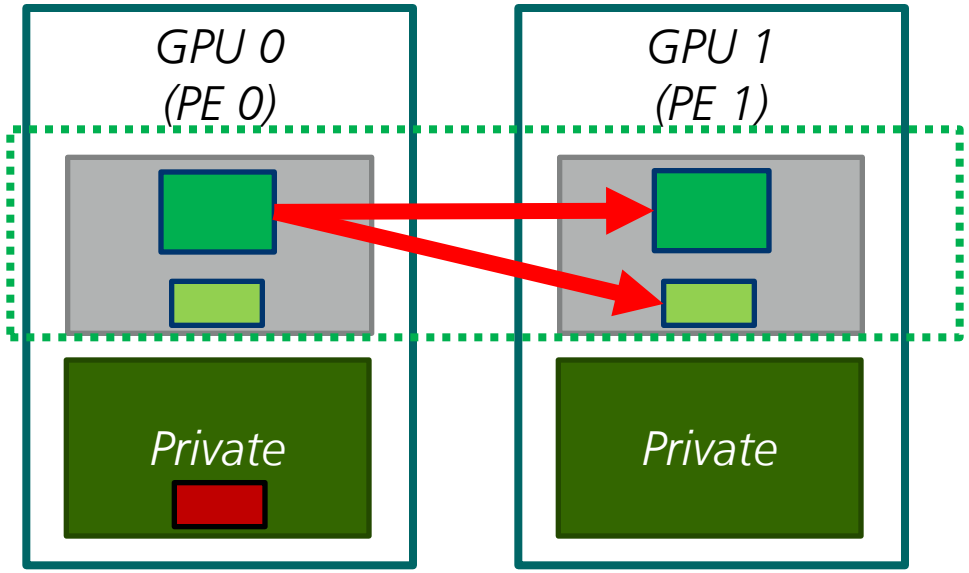
Must be the same on all PEs

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

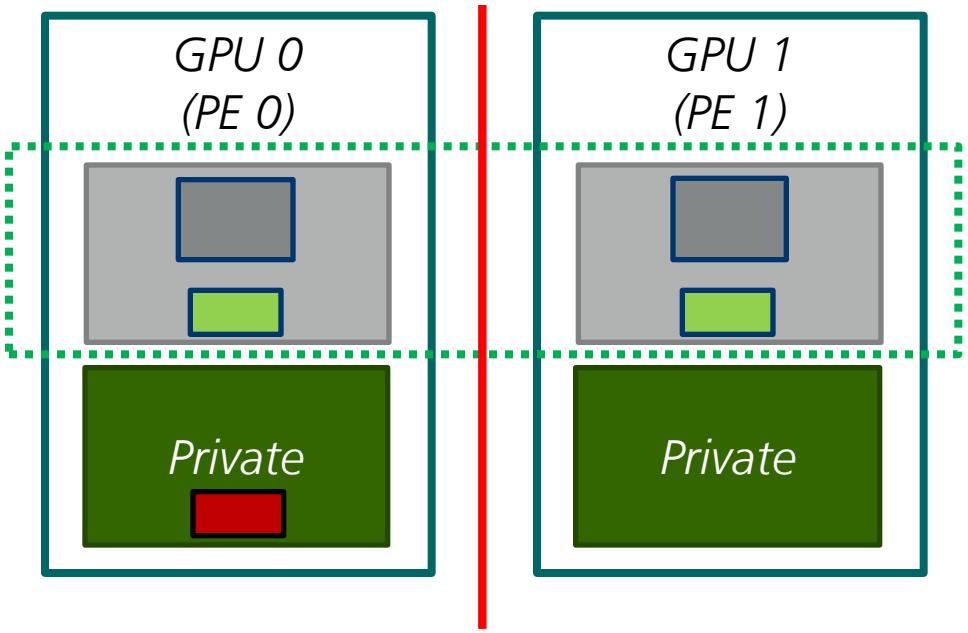


Copies nelems data elements of type T from symmetric objects src to dest on PE pe

```
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 againt 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
```

- *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*