Introduction to MPI-Distributed Computing with GPUs.

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Multi-GPU Computing: What you will learn

- CUDA-aware MPI
- Example: Jacobi-Solver
- Under the hood (why you should use CUDA-aware MPI)
  - GPUs in Clusters
  - CUDA Unified Virtual Addressing
  - GPUDirect P2P and GPUDirect RDMA

Message Passing Interface - MPI

- Standard to exchange data between processes via messages
  - Defines API to exchange messages
    - Point to Point: e.g. `MPI_Send`, `MPI_Recv`
    - Collectives: e.g. `MPI_Reduce, MPI_Allreduce, MPI_Bcast`
- Multiple implementations (open source and commercial)
  - Bindings for C/C++, Fortran, Python, …
  - e.g. MPICH, OpenMPI, MVAPICH, IBM Spectrum MPI, Cray MPT, ParaStation MPI, …

Example MPI Program

```c
#include <mpi.h>

#include <stdio.h>


int main(int argc, char** argv) {

    // Initialize the MPI environment

    MPI_Init(NULL, NULL);

    int size;

    MPI_Comm_size(MPI_COMM_WORLD, &size);

    int world_rank;

    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);

    MPI_Finalize();

}
```

```
mpicc -o hello_mpi.out hello_mpi.c
mpirun -n 4 ./hello_mpi.out
```

CUDA-aware MPI

CUDA-aware MPI allows you to use Pointers to GPU-Memory as source and destination

```
//MPI rank 0
MPI_Send(s_buf_d,n,MPI_BYTE,size-1 ,tag,MPI_COMM_WORLD);


//MPI size-1
MPI_Recv(r_buf_d,n,MPI_BYTE,0,tag,MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

Pointer to GPU memory!

LAUNCH MPI+CUDA

- Launch one process per GPU
- How to use CUDA-aware MPI
  - *MVAPICH*: `$`**`MV2_USE_CUDA=`**`1 mpirun -np ${np} ./myapp <args>`
  - *Open MPI: CUDA-aware features are enabled per default (using UCX)*
  - *Cray:* `MPICH_RDMA_ENABLED_CUDA`
  - *IBM Spectrum MPI*: `$mpirun` **`-gpu`** `-np ${np} ./myapp <args>`
  - *ParaStation MPI* (using UCX): `$`**`PSP_CUDA=`**`1 mpirun -np ${np} ./myapp <args>`
- On JUWELS Booster:
  - Load CUDA-aware OpenMPI or ParaStation MPI modules
  - GPU-tuning is done via module loading
  - `srun  --gres=gpu:4 -n {np} ./myapp <args>`

How to compile

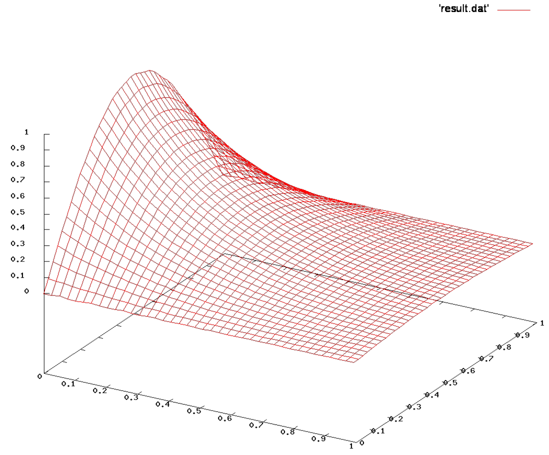
```
nvcc -o my_kernel.o $(NVCC_FLAGS) my_kernels.cu -c

mpicc -o my_multiGPUapp -lcudart my_kernel.o my_multiGPUapp.c
```

Example: Jacobi Solver

- Solves the 2D-Laplace Equation on a rectangle
- $\Delta \boldsymbol{u}(\boldsymbol{x}, \boldsymbol{y}) = \mathbf{0} \; \forall \; (\boldsymbol{x}, \boldsymbol{y}) \in \Omega \backslash \boldsymbol{\delta}\Omega$

- Dirichlet boundary conditions on left/right boundaries (constant values on boundaries)
- Reflecting boundaries on top and bottom
- Iterative solver:
  u(t+1) = f(u(t))

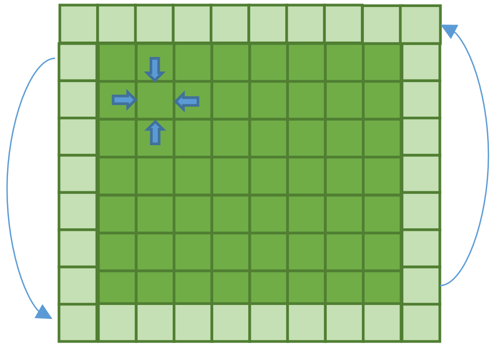


Example: Jacobi solver

While not converged

do Jacobi step:

```
int iy = blockIdx.y * blockDim.y + threadIdx.y
int ix = blockIdx.x * blockDim.x + threadIdx.x
if (iy < ny-1 && ix < nx-1) {
    new_val =
          0.25 * (a[iy * nx + ix + 1] + a[iy * nx + ix - 1
                  a[(iy + 1) * nx + ix] + a[(iy - 1  * nx + ix]);
     a_new[iy * nx + ix] = new_val;
```

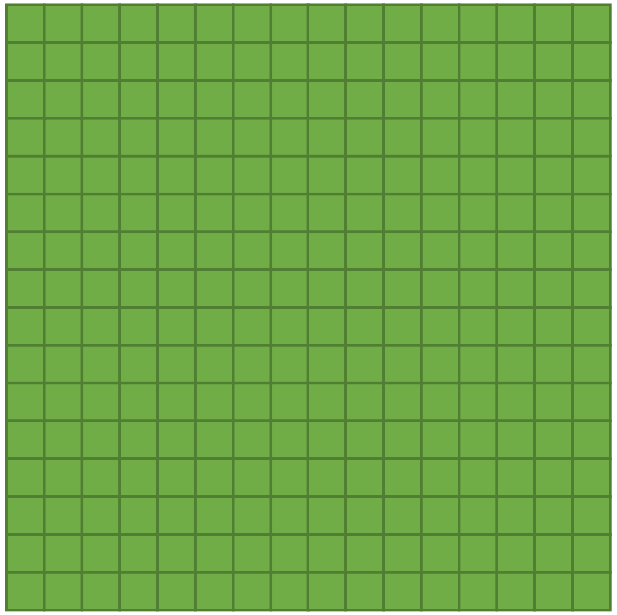


apply boundary Condition

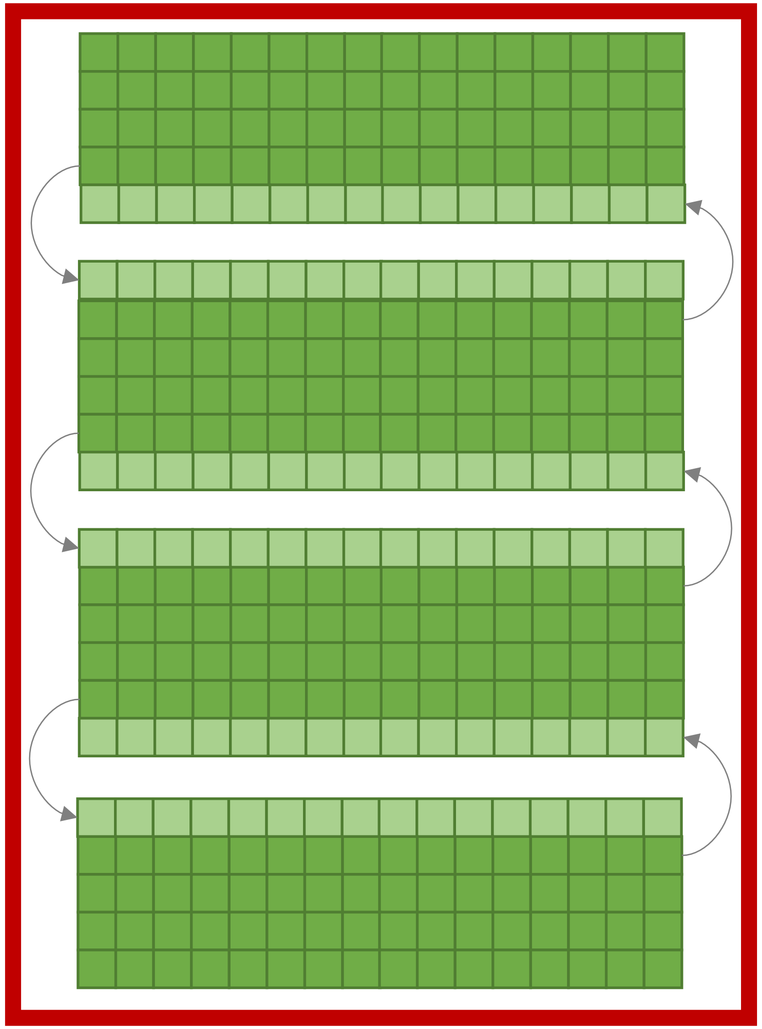
swap `a_new` and `a`

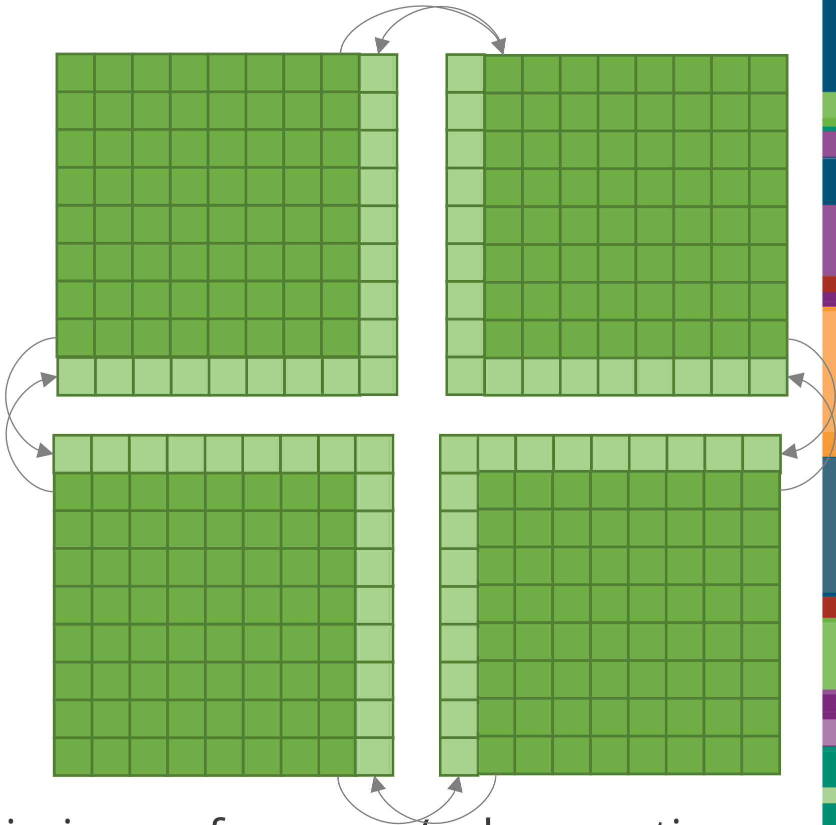
next iteration

Domain Decomposition



Minimize number of neighbors:
Communicate to less neighbors
Optimal for latency bound communication,
Continuous Transfers





Minimize surface area/volume ratio:
Communicate less data
Optimal for bandwidth bound communication
Non-Continuous Transfers

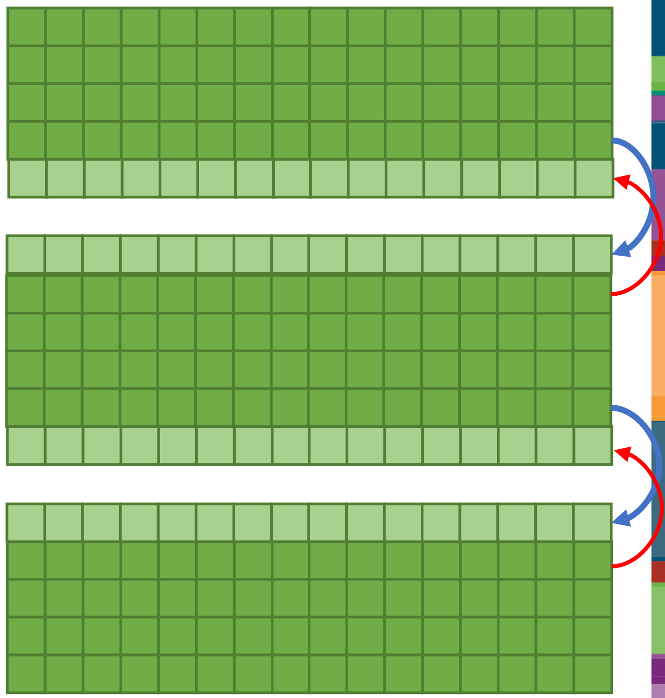
Jacobi example: Top and Bottom Boundaries

bottom neighbor

```
MPI_Sendrecv(a_new_d+offset_last_row, m-2, MPI_DOUBLE,
             b_nb, 1,a_new_d+offset_top_boundary, m-2,
             MPI_DOUBLE, t_nb, 1, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
```

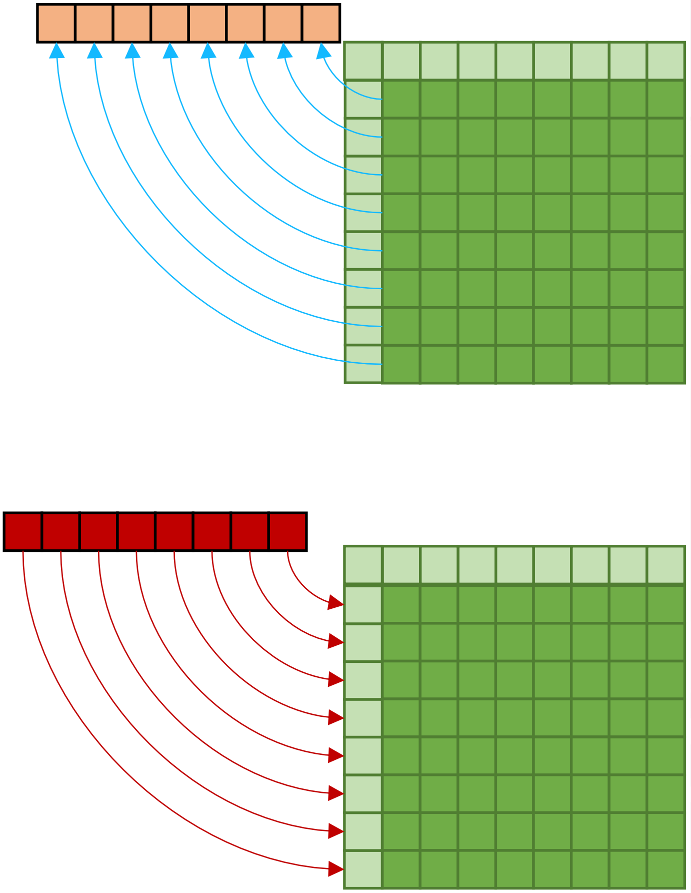
top neighbor

```
MPI_Sendrecv(a_new_d+offset_first_row, m-2, MPI_DOUBLE,
             t_nb,0,a_new_d+offset_bottom_boundary, m-2,
             MPI_DOUBLE,b_nb,  0, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
```



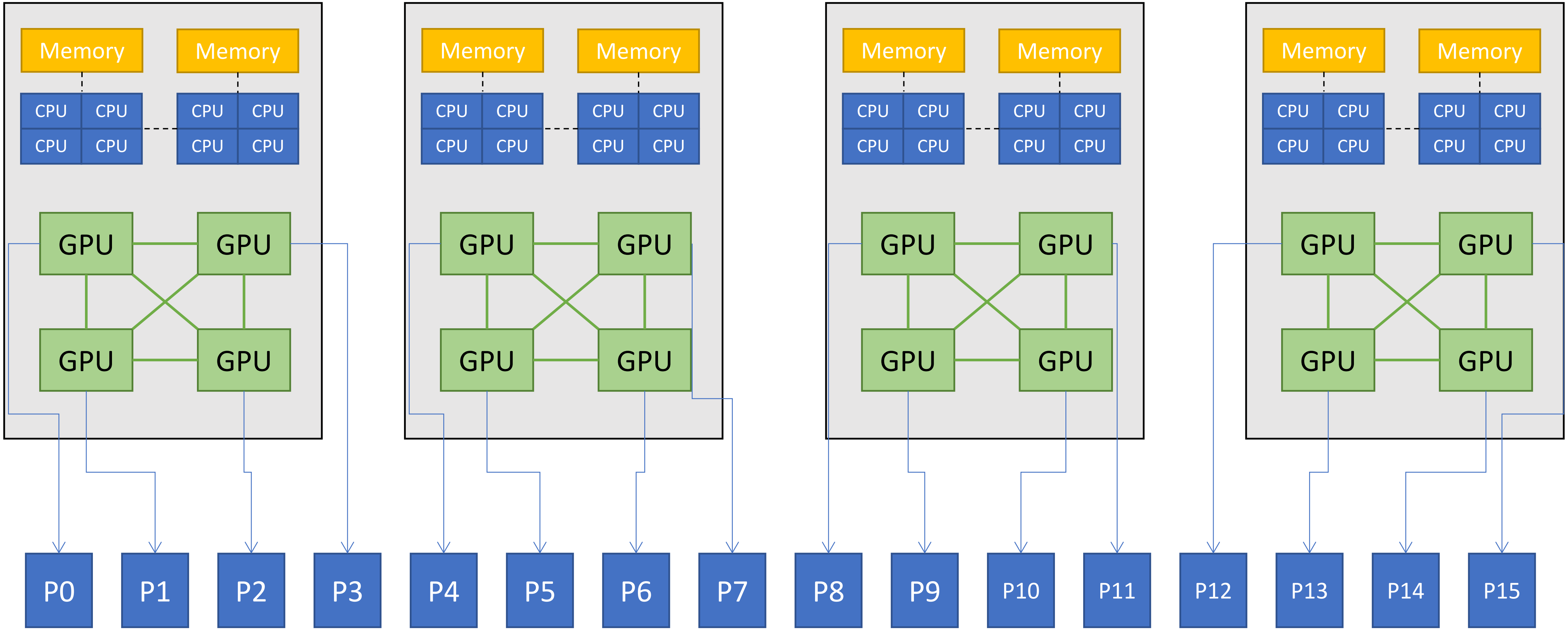
Jacobi: Left (and right) neighbours

```
//right neighbor omitted
pack<<<gs,bs,0,s>>>(to_left_d, u_new_d, n, m);
cudaStreamSynchronize(s);
MPI_Sendrecv(to_left_d, n-2, MPI_DOUBLE, l_nb, 0,
             from_right_d, n-2, MPI_DOUBLE, r_nb, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE );
unpack<<<gs,bs,0,s>>>(u_new_d, from_right_d, n, m);
cudaStreamSynchronize(s);
```



Process Mapping on Multi GPU Systems

One GPU per Process



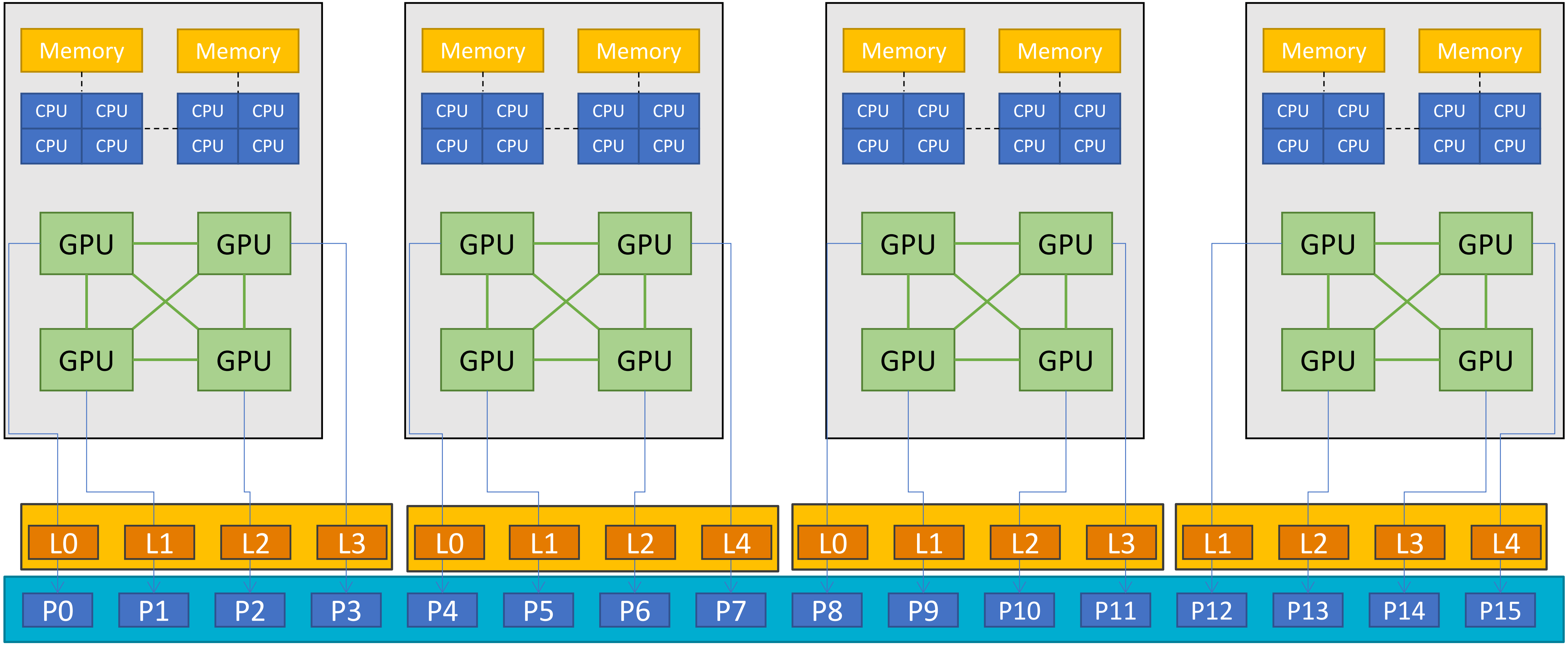
Distribute GPUs to local Nodes

```
MPI_Comm local_comm;
MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, rank,
                    MPI_INFO_NULL, &local_comm);
int local_rank = -1;
MPI_Comm_rank(local_comm,&local_rank);
MPI_Comm_free(&local_comm);

int num_devs = 0;
cudaGetDeviceCount(&num_devs);
cudaSetDevice(local_rank%num_devs);
```

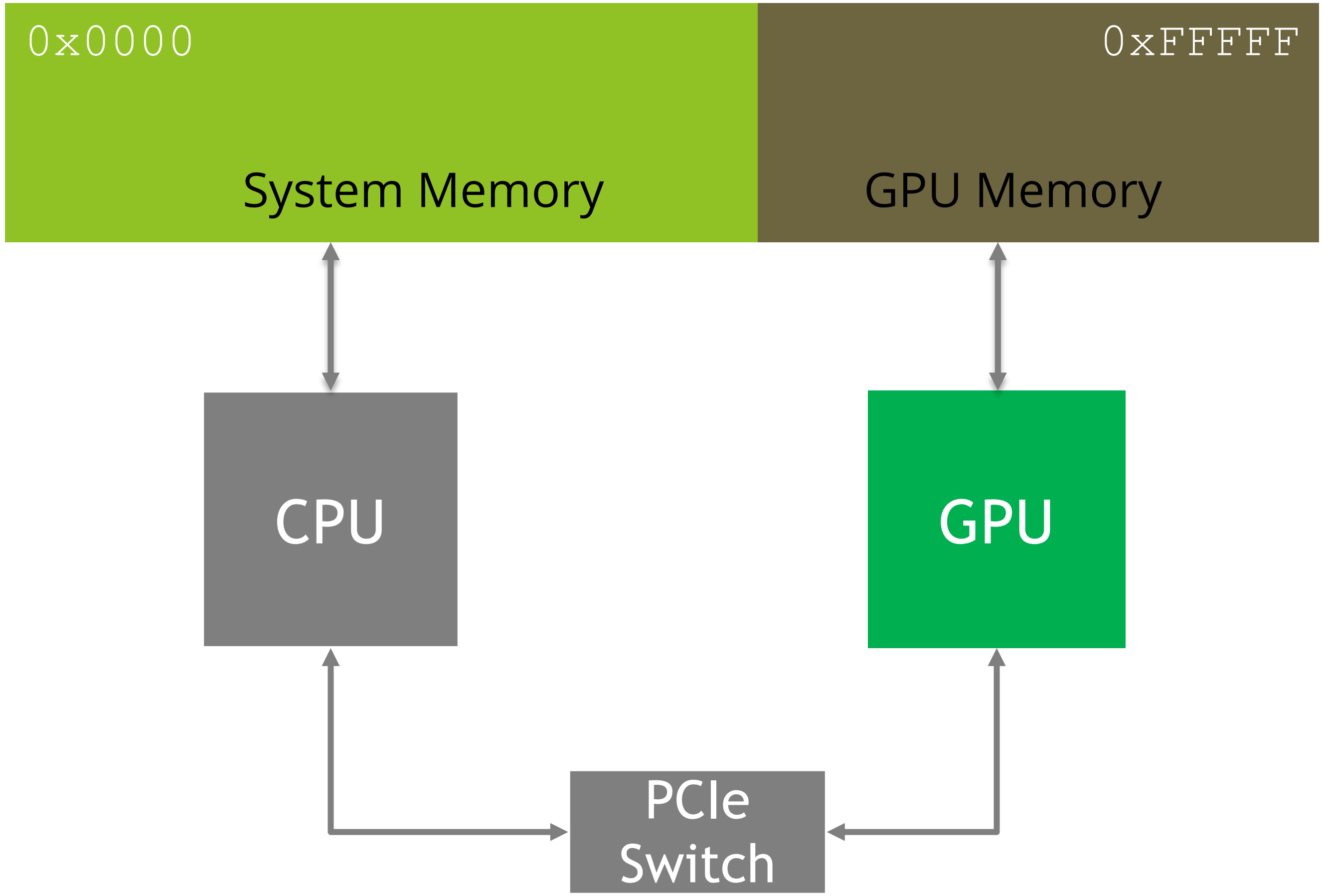
Needed, if resource manager handles GPU-affinity

Process Mapping on Multi GPU Systems
One GPU per Process

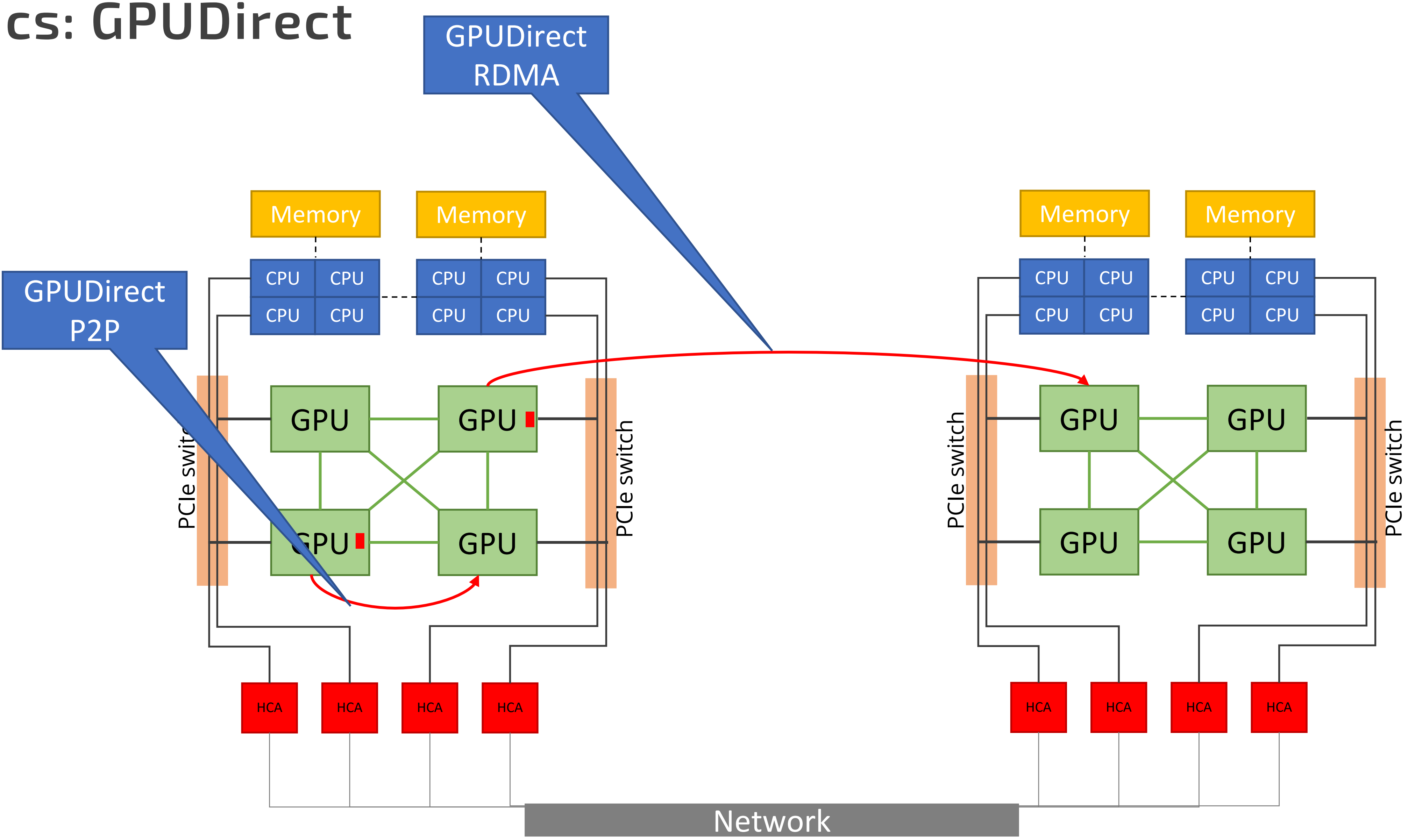


CUDA Unified Virtual Addressing

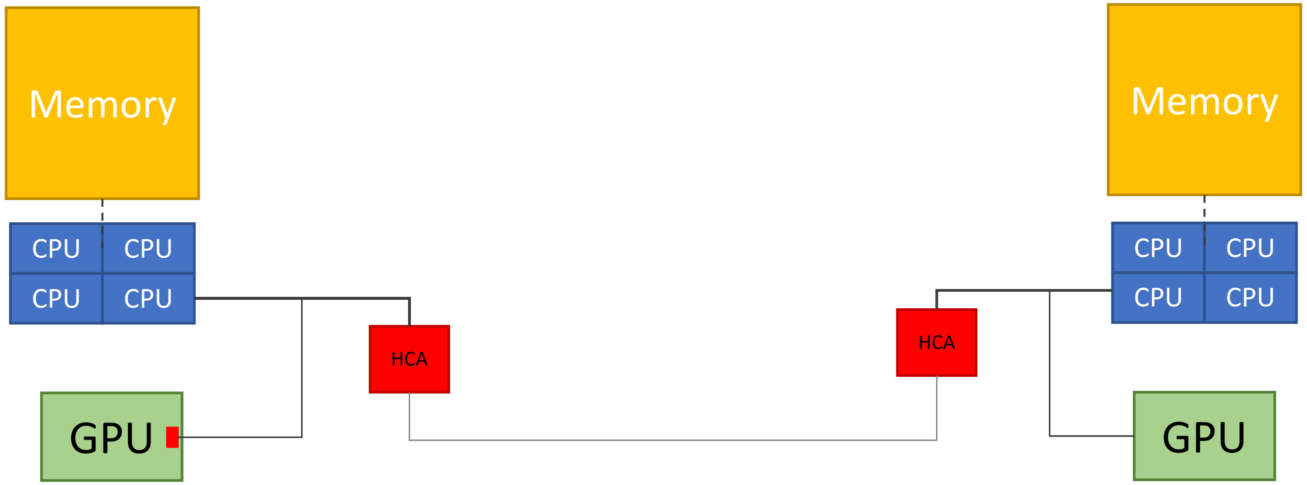
- One address space for all CPU and GPU memory
  - Determine physical memory location from a pointer value
  - Enable libraries to simplify their interfaces (e.g. MPI)
- Supported on devices with compute capability 2.0+ for
  - 64-bit applications on Linux and Windows (+TCC)



Basics: GPUDirect

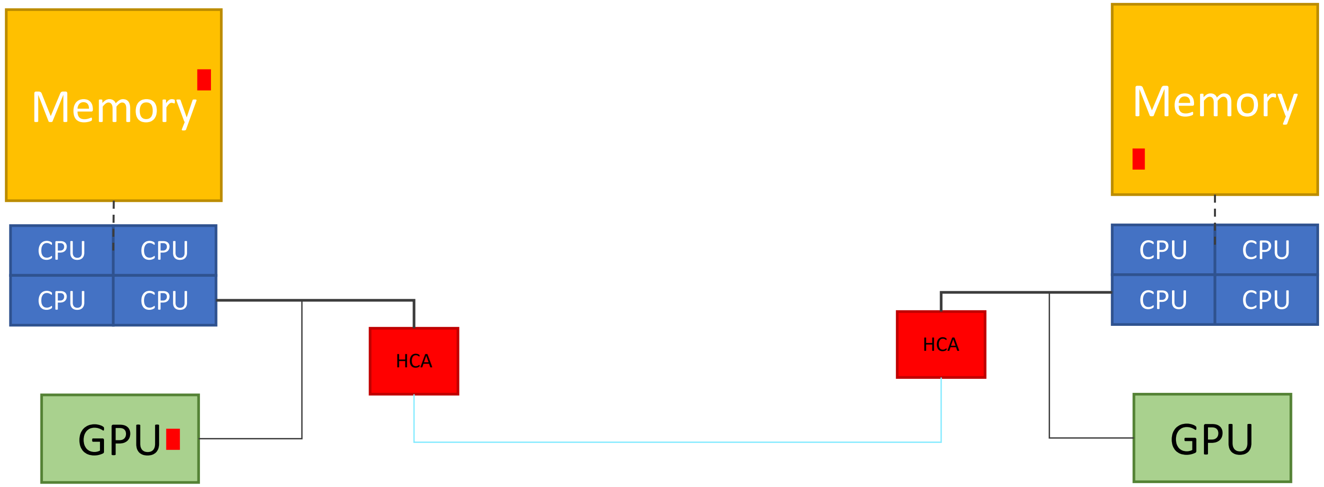


CUDA-aware MPI with GPUDirect RDMA



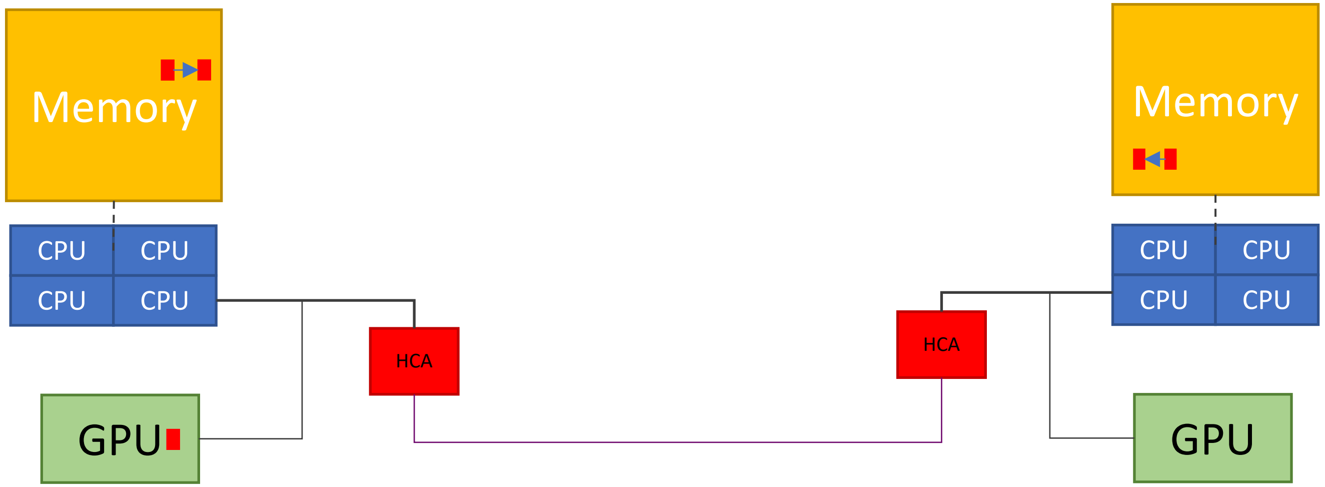
```
MPI_Send(s_buf_d,size,MPI_BYTE,1,tag,MPI_COMM_WORLD);
MPI_Recv(r_buf_d,size,MPI_BYTE,0,tag,MPI_COMM_WORLD,&stat);
```

CUDA-aware MPI without GPUDirect RDMA



```
MPI_Send(s_buf_d,size,MPI_BYTE,1,tag,MPI_COMM_WORLD);
MPI_Recv(r_buf_d,size,MPI_BYTE,0,tag,MPI_COMM_WORLD,&stat);
```

Regular MPI

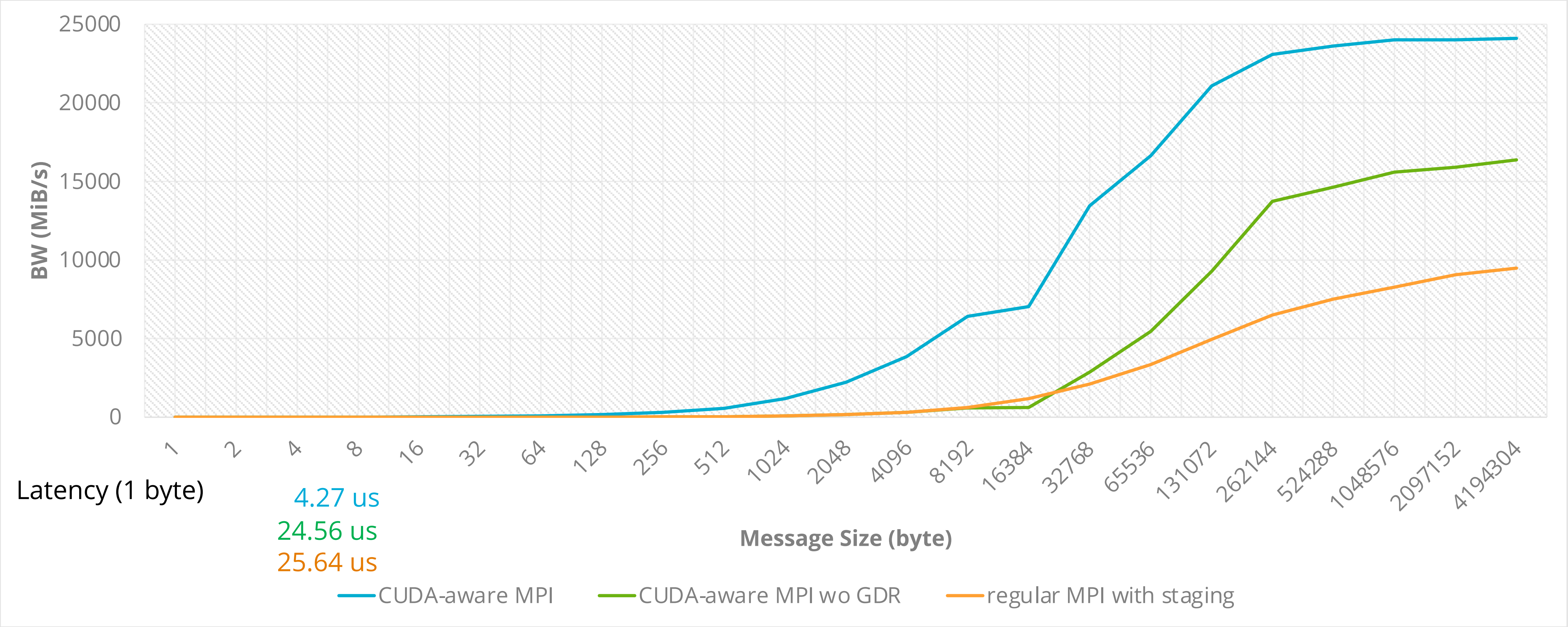


```
cudaMemcpy(s_buf_h,s_buf_d,size,cudaMemcpyDeviceToHost);
MPI_Send(s_buf_h,size,MPI_BYTE,1,tag,MPI_COMM_WORLD);

MPI_Recv(r_buf_h,size,MPI_BYTE,0,tag,MPI_COMM_WORLD,&stat);
cudaMemcpy(r_buf_d,r_buf_h,size,cudaMemcpyHostToDevice);
```

Performance Results GPUDirect RDMA

OpenMPI 4.1.0RC1 + UCX 1.9.0 on JUWELS Booster



Latency (1 byte)

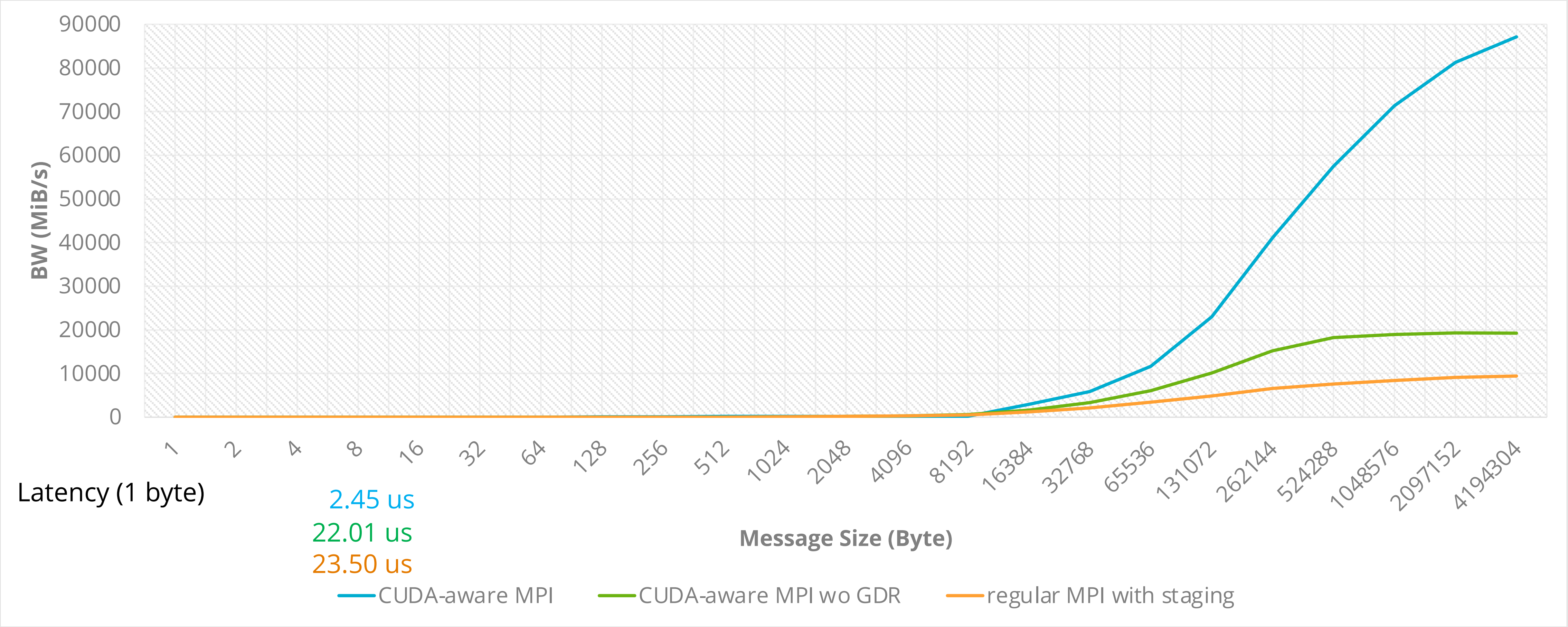
4.27 us

24.56 us

25.64 us

Performance Results GPUDirect P2P

OpenMPI 4.1.0RC1 + UCX 1.9.0 on JUWELS-Booster



Latency (1 byte)

2.45 us

22.01 us

23.50 us

Summary

- CUDA-aware MPI allows efficient communication for multi-GPU applications
  - Allows MPI-communication operations from GPU memory buffers
  - Simplified programming
  - Use GPUDirect technologies for performance
  - Minimizes data copies
- Most MPI versions have support for CUDA-aware MPI
- Best practice: One process per rank
  - Use local communicator in MPI