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Parallel programming with CUDA and MPI

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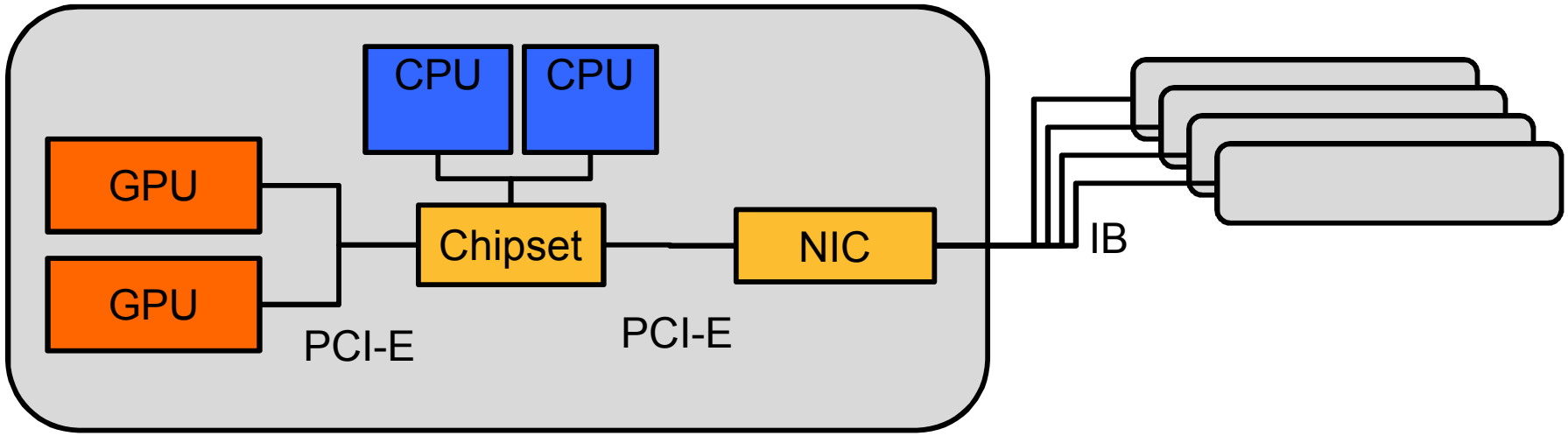
Content

- **Introduction**
- **MPI + CUDA programming**
- **MPI + OpenMP + CUDA programming**
- **Recent developments**
- **Summary**

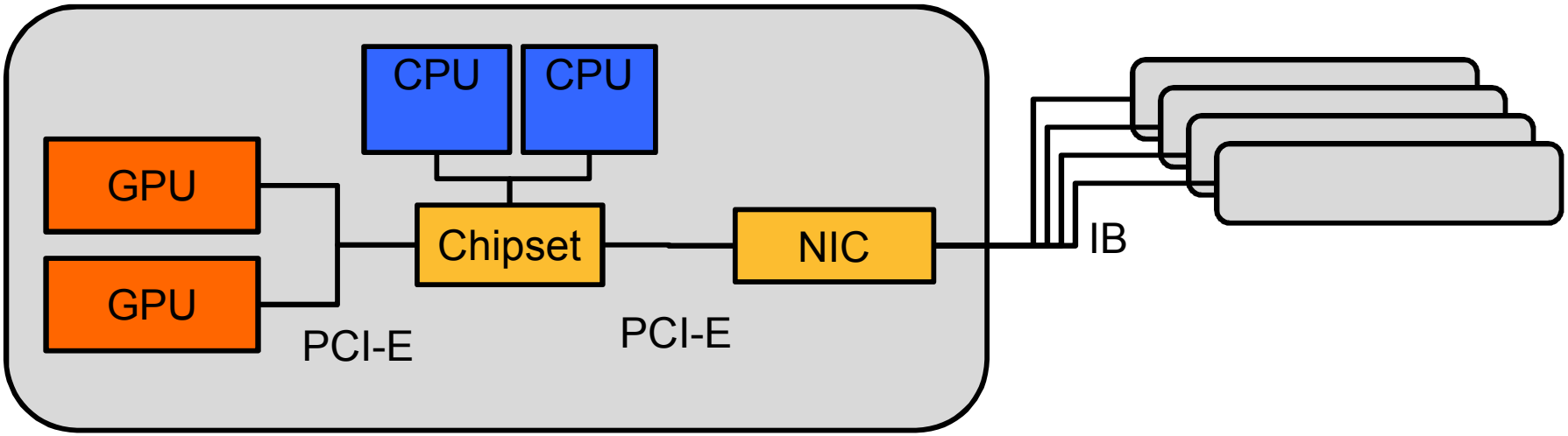
Introduction

- **Three levels of hardware parallelism**
  1. GPU - threads on the multiprocessors
  2. Node – Binding together GPU, CPU and NIC (network card)
  3. Machine - Several nodes connected with Infiniband



Introduction

- **Parallelization strategies**
  1. CUDA
  2. Threads (OpenMP, Pthreads) or MPI
  3. MPI



MPI + CUDA

MPI+CUDA topics

- **Introduction**
- **CUDA+MPI strategies: How to share the GPU resource**
- **Selecting GPU**
- **Combining MPI_Send and MPI_Receive with CUDA**

MPI + CUDA is easy

- **Cuda and MPI can be considered separate entities**
  - CUDA handles parallelization on GPU
  - MPI handles parallelization over nodes
- **Use one MPI process per GPU and accelerate the computational kernels with CUDA**
- **To transfer data between to devices**
  - Sender: Copy data from device to temporary host buffer
  - Sender: Send host buffer data
  - Receiver: Receive data to host buffer
  - Receiver: Copy data to device

MPI + CUDA is difficult: Portability

- **Technology is moving forward quickly**
  - Different compute capability generations
  - Different levels of support for GPUDirect v1 and v2
  - New MPI libraries with CUDA support are emerging
- **Machines differ from each other**
  - Number of GPUs and CPUs per node differ
    - 1 GPU per 2 processors to 8 GPUs per 2 processors
  - Selecting active GPU on multi GPU nodes

MPI + CUDA is difficult: Scalability

- **More challenging than for a traditional CPU machine**
  - Higher computational power per node
  - Higher latency for sending messages from one GPU to another one
- **Efficient device-to-device communication is non-trivial**
  - Hiding latencies through overlapping computation & communication
  - Pipelined sends and receives

MPI + CUDA is difficult: Scalability

- **New developments will make scaling easier**
  - Supercomputers with custom interconnects and system software: Cray XK6 with Gemini interconnect
  - GPUDirect v1: Avoids extra data copy in host memory when combining MPI + CUDA
  - GPUDirect v2: Efficient multi-GPU programming using threads; direct inter-node GPU-GPU transfers
  - Direct inter-node GPU-to-GPU transfers are under development
  - Work on GPU aware MPI implementations is ongoing

MPI + CUDA strategies

- **1. One MPI process per GPU**
  - GPU handling is straight forward
  - Wastes the other cores of the processor
- **2. Many MPI processes per GPU, only one uses it**
  - Poses difficult load balancing problems

MPI + CUDA strategies

- **3. Many MPI processes share a GPU**
  - Two processes cannot share the same GPU context, per process memory on GPU
  - Sharing may not always be possible
    - Limited memory on GPU
    - If GPUs are in exclusive mode
  - In some cases this strategy is more efficient as the idle time of the GPU decreases (e.g. NAMD)

Selecting GPU

- **To select a GPU for each process one needs to know which ranks are on the same node**
- **Simple approach**
  - You may assume MPI processes are assigned in a linear fashion to the cores
    - Node 1 ranks: 0 1 2 3 4 5
    - Node 2 ranks: 6 7 8 9 10 11 ….
  - You may also assume you know the number of processes per node to compute rank on node
    - int **nodeRank**=rank%processesPerNode

Selecting GPU

- **The simple approach is not very robust as it assumes the ranks have been placed in a specific fashion**
- **Advanced approach**
  - Get name of node using MPI_Get_processor_name()
  - Compute a hash (integer) value from the name
    - See google, e.g., http://www.cse.yorku.ca/~oz/hash.html
  - Create a intra-node communicator by using the hash value as the color for MPI_Comm_split()
  - Get **nodeRank** and **processesPerNode** from the new inter-node communicator using MPI_Comm_rank() and MPI_Comm_size()

Selecting GPUs

- **The number of active GPUs visible to the rank is**
  - cudaGetDeviceCount(&deviceCount);
- **Divide GPUs to processes (strategy 3)**

```
id= nodeRank%deviceCount;
cudaSetDevice(id);
```

- **One GPU per process (strategy 1)**

```
if(processesPerNode==deviceCount){
        id= nodeRank%deviceCount;
        cudaSetDevice(id);
        }
else //ERROR
```

MPI send & receive: Simple version

- **Time for one message is**
  - T_MPI(size) + 2 T_CUDA(size)
  - T_CUDA comparable to MPI (GB/s of transfer speed)
- **Simple to implement, but performance is not good for larger messages**

```
if (rank==0){
  cudaMemcpy(hBuffer,dBuffer,size,cudaMemcpyDeviceToHost);
  MPI_Send(hBuffer,size,MPI_BYTE,1,100,MPI_COMM_WORLD);
}
else if (rank==1){
  MPI_Recv(hBuffer,size,MPI_BYTE,
        0,100,MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  cudaMemcpy(dBuffer,hBuffer,size,cudaMemcpyHostToDevice);
}
```

MPI Send & receive: pipelined

- **The message is divided into chunks**
- **Using streams one can transfer data from GPU one chunk at a time using cudaMemcpyAsync**
- **Each chunk can be sent using non-blocking MPI_Isend once it has arrived into CPU memory**
- **At the receiver side the corresponding operation is performed**
- **Time is reduced as MPI and CUDA transfers are overlapped**
- **Requires platform dependent tuning of the chunksize, order of magnitude is 100KB**

MPI + OPENMP + CUDA

Introduction

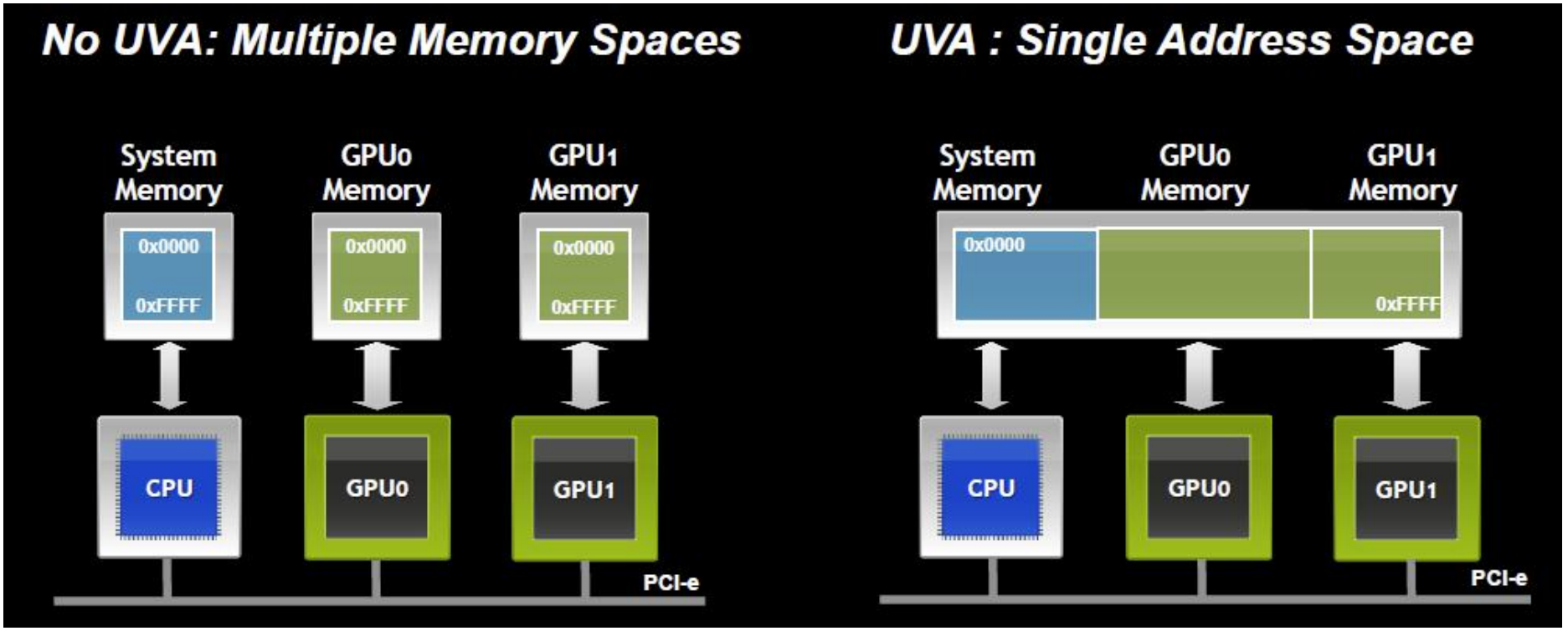
- **Each MPI process launches host level threads using, e.g., OpenMP**
- **Can match one MPI process per GPU and still use all cores**
- **Since CUDA 4 threads of the same process can share a GPU context**
  - Can use the same GPU buffers
  - Done simply by selecting the same device ID

MPI + OpenMP + CUDA

- **One MPI process per GPU**
  - Data parallel: All threads do computation and share the GPU. Since CUDA 4 they can share the same context
  - Task parallel: one handles GPU, one MPI, one IO the rest CPU computation, etc.
- **Several GPUs per MPI process**
  - Both data and task parallel approaches possible
  - Some performance benefit to be expected from GPU Direct v2, enables direct copies from GPU to GPU

RECENT DEVELOPMENTS

Unified Virtual Address (new in CUDA 4)



UVA

- **Same address space for both GPU and CPU**
  - Cannot automatically read data, transfers still needed
- **All memory must be allocated through CUDA library**
- **Enables one to find out where the memory is from the pointer value - easier interfaces possible**

Without UVA:

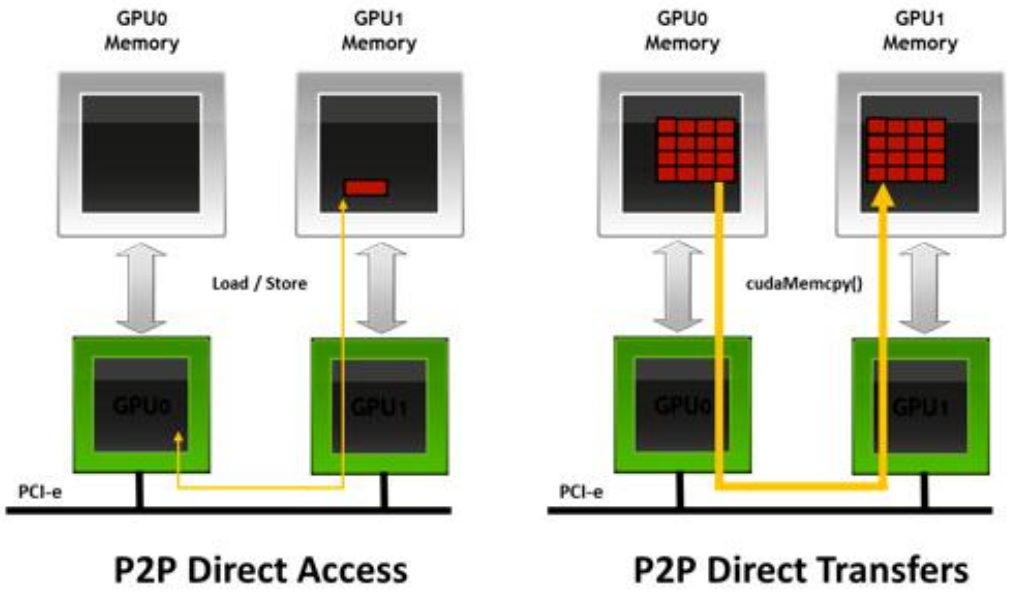
```
cudaMemcpy(dArray, hArray, SIZE, cudaMemcpyHostToDevice);
```

With UVA:

```
cudaMemcpy(dArray, hArray, SIZE, cudaMemcpyDefault);
```

GPU Direct v2 - Peer-to-peer communication

- **GPU Direct v2 only available for Tesla Fermi cards and Cuda 4 or later**
- **Direct access**
  - Can directly access memory on another GPU
- **Direct transfer**
  - Can copy data directly from one to the other
- **Works with one MPI process for all GPUs**
- **Easy to use with UVA**



GPU Direct v2 - Peer-to-peer communication

```
cudaSetDevice(ompThread);
if(ompThread == 0 )
  cudaMalloc((void**)&(dArray1), size);
else if(ompThread == 1 )
  cudaMalloc((void**)&(dArray2), size);
…
if( ompThread==0){
  cudaDeviceEnablePeerAccess(1,0);
  cudaMemcpy(dArray2, dArray1, size,cudaMemcpyDefault);
}
…
```

Enable efficient Peer-to-peer access using GPUDirect v2

- **Vuori.csc.fi device-to-device bandwidth**
  - With peer-to-peer more than 5GB/s
  - Without less than 4 GB/s

CUDA support in MPI libraries

- **MPI libraries where you can directly provide device pointers to the MPI calls**
  - MPI_Send(dBuffer,….)
  - UVA essential for these libraries, enables them to deduce where the buffer is
  - Handle data staging internally
- **OpenMPI**
  - CUDA support in current trunk version
- **MVAPICH2-GPU**
  - H. Wang et al., “MVAPICH2-GPU: optimized GPU to GPU communication for InfiniBand clusters”, Comput.Sci. Res.Dev, vol. 26, pp 257-266, 2011.
  - Will be in future versions

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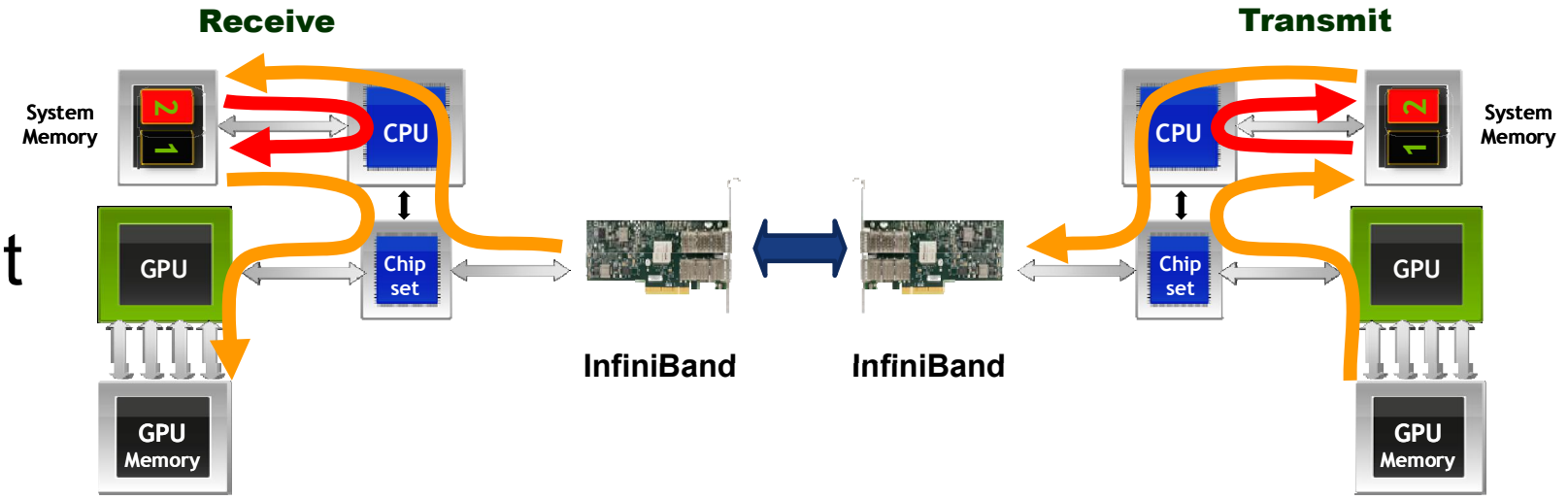
GPUDirect v1

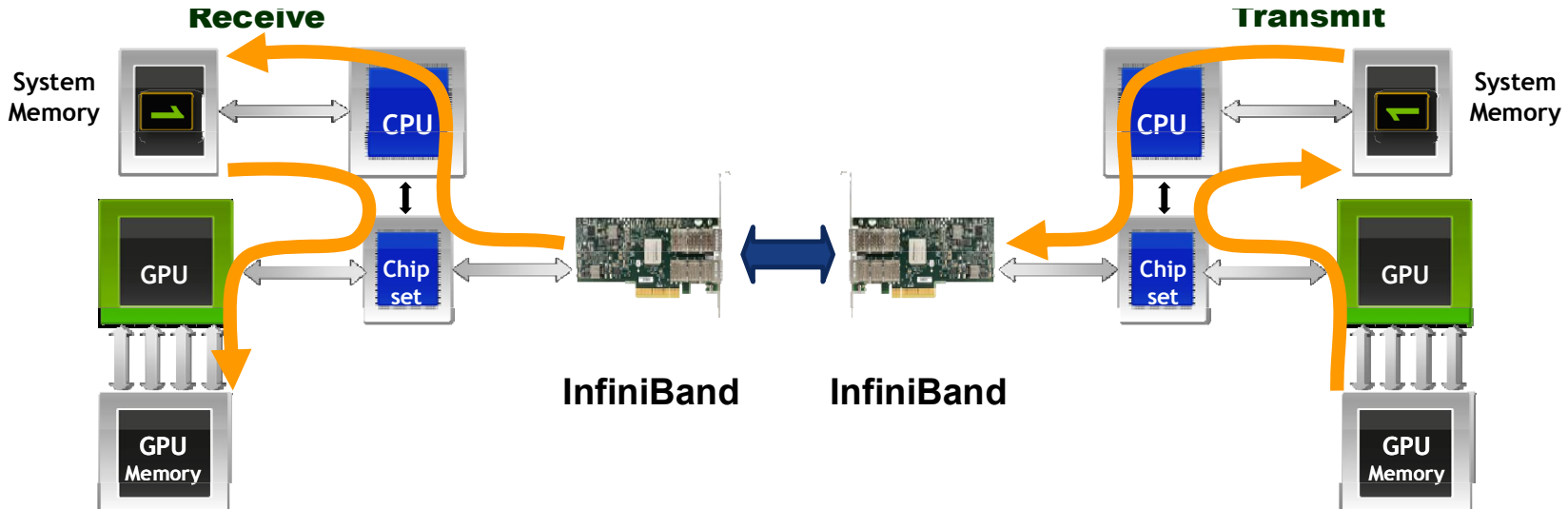
- **Infiniband network card and GPU can share the same pinned memory**
  - Infiniband uses pinned memory for RDMA transfers
  - CUDA also uses pinned memory for fast DMA transfers to/from card
- **Avoids one extra memory copy between GPU and Infiniband pinned memory**
- **Support by Mellanox and Qlogic**
- **No changes to user code necessary**

GPUDirect v1

Without



With



Summary

- **CUDA+MPI**
  - Naïve approach easy, getting good performance more tricky
  - Selecting GPU on multi-GPU nodes
- **CUDA+OpenMP+MPI**
  - Threads can share same GPU context
- **Recent developments**
  - MPI libraries with CUDA support will simplify things
  - Peer-to-peer access paves way for more efficient on-node multi-GPU parallelisation

references

- **Vlasov GPU paper**
- **CUDA and MPI, Dale Southard Senior Solution Architect NVIDIA**
- **An MPI-CUDA Implementation for Massively Parallel Incompressible Flow Computations on Multi-GPU Clusters**
- **Performance Analysis of a Hybrid MPI/CUDA Implementation of the NAS-LU Benchmark**
- **An MPI-CUDA implementation of an improved Roe method for two-layer shallow water systems**
- **GPUs for Molecular Dynamics (MD) Simulations: a user's perspective**
- **www2.fz-juelich.de/jsc/files/docs/vortraege/gpu/gpu-5-Multi_GPU.pdf**
- **people.maths.ox.ac.uk/gilesm/cuda/MultiGPU_Programming.pdf**
- **http://people.maths.ox.ac.uk/gilesm/cuda/lecs/lec6-2x2.pdf**
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- **http://developer.download.nvidia.com/compute/cuda/4_0/docs/GPUDirect_Technology_Overview.pdf**