Joint CUDA-MPI Programming

Objective

- **To become proficient in writing a simple joint MPI-CUDA heterogeneous application**
  - Understand the key sections of the application
  - One-way communication

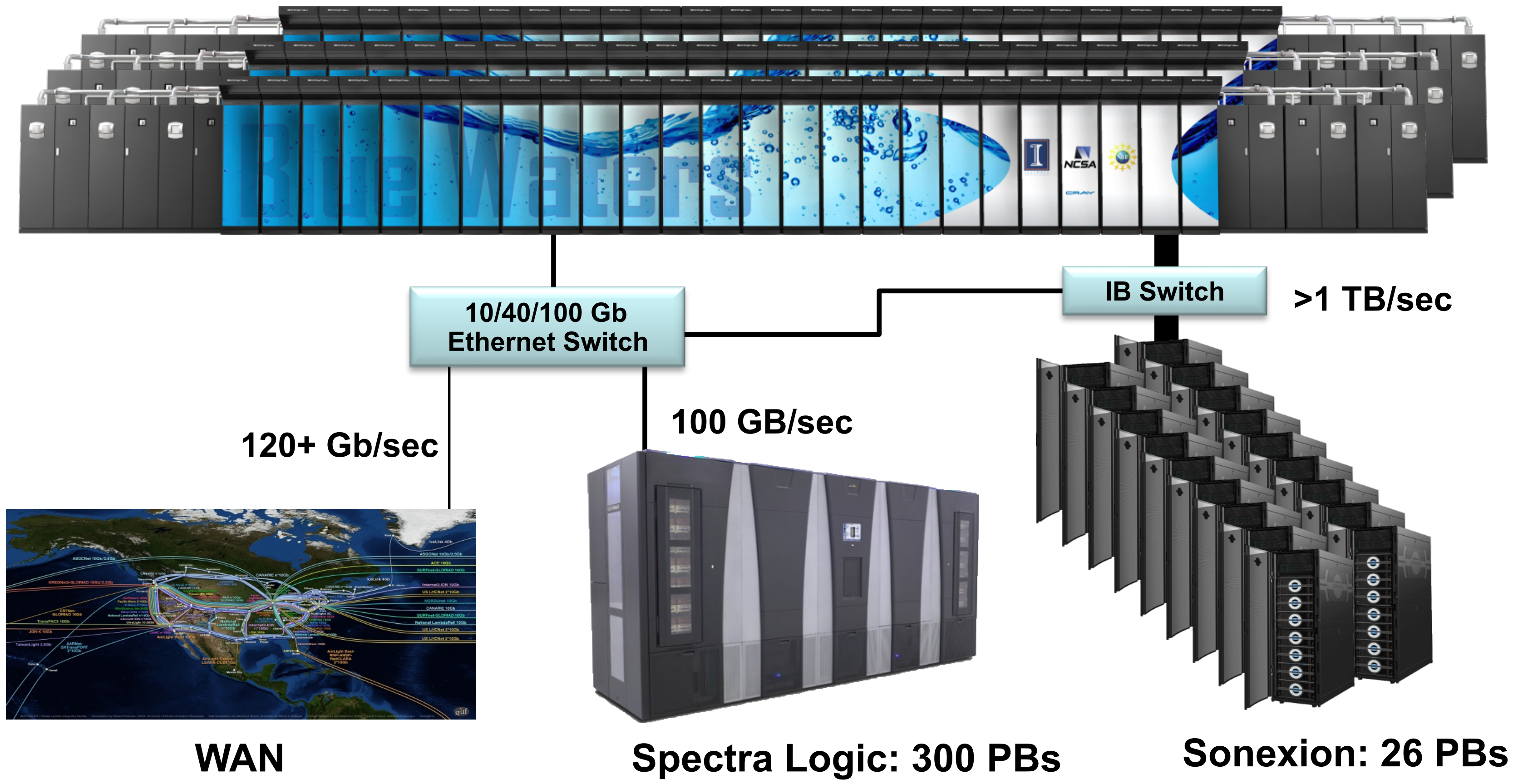
- **To become familiar with a more sophisticated MPI application that requires two-way data exchange**

Titan – the new ruler of TOP500

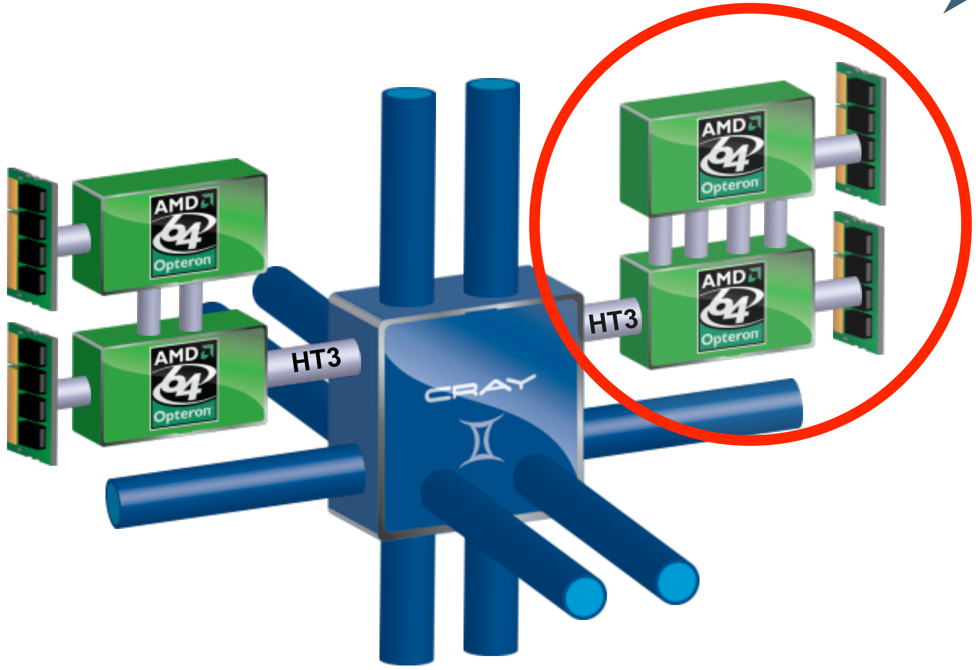
17.6 PF Sustained, 27.1 PF Peak

S3D – improve efficiency of biofuel combustion
WL-LSMS – interactions between electrons and atoms in magnetic materials
Denovo – improve efficiency and reduce waste in nuclear reactors
LAMMPS – improvements to semiconductors, biomolecules, polymers
CAM-SE – more accurate climate simulations
NRDF – laser fusion, fluid dynamics, medical imaging, nuclear reactors, …

Blue Waters Computing System



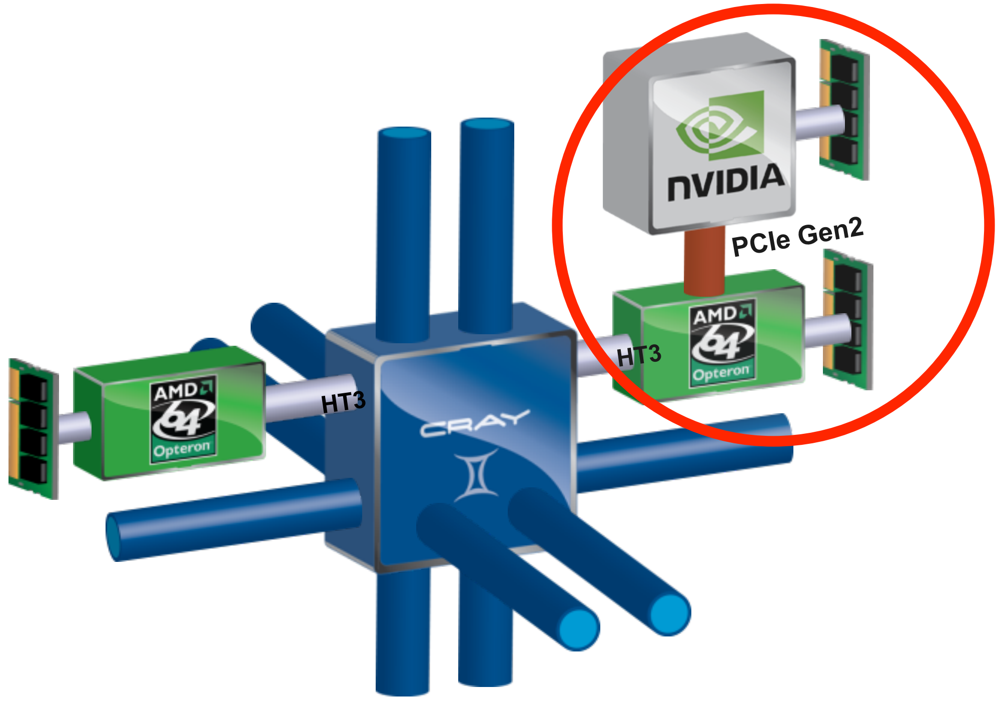
Cray XE6 Nodes



Blue Waters contains 22,640 Cray XE6 compute nodes.

- **Dual-socket Node**
  - Two AMD Interlagos chips
    - 16 core modules, 64 threads
    - 313 GFs peak performance
    - 64 GBs memory
      - 102 GB/sec memory bandwidth
  - Gemini Interconnect
    - Router chip & network interface
    - Injection Bandwidth (peak)
      - 9.6 GB/sec per direction

Cray XK7 Nodes

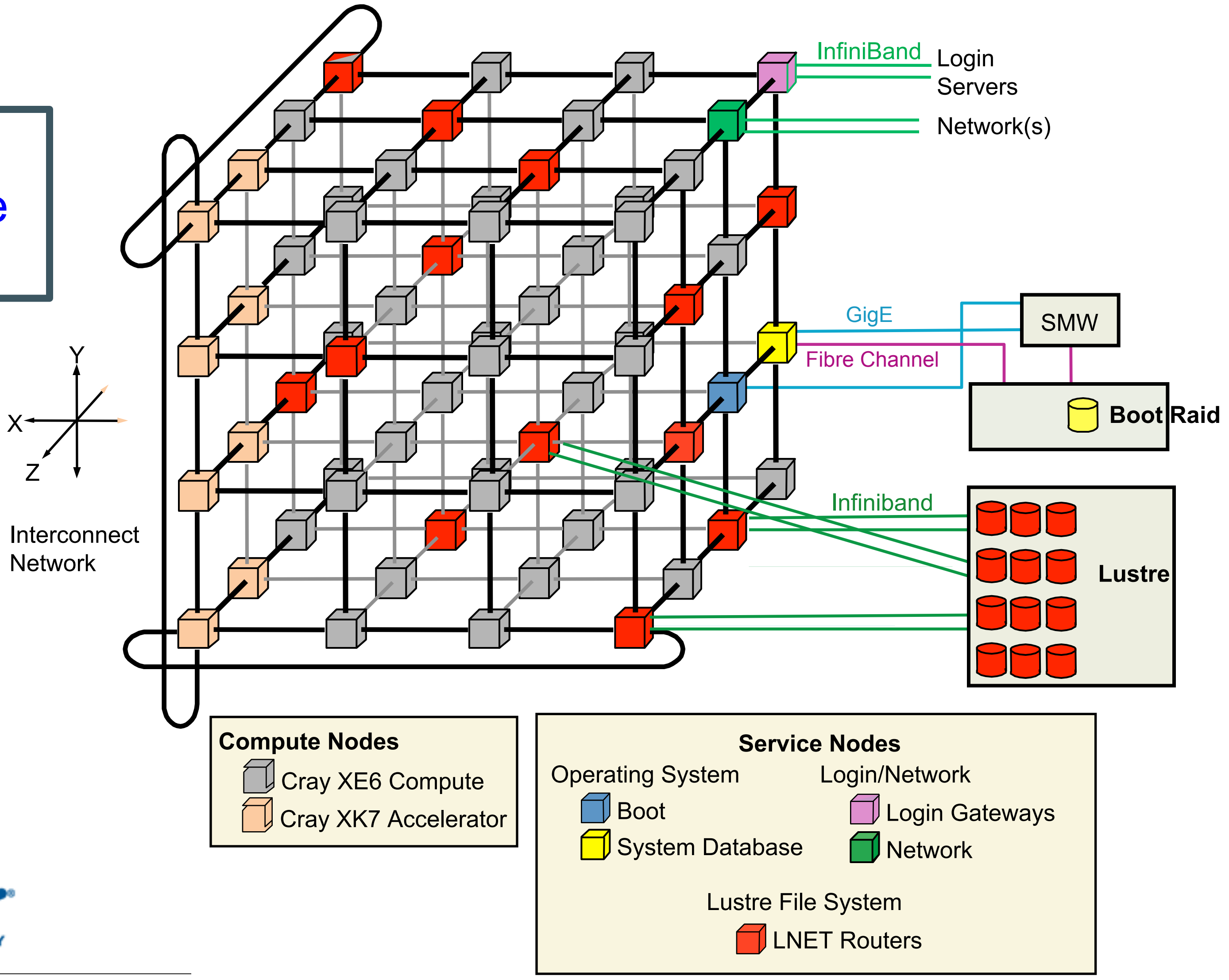


- **Dual-socket Node**
  - One AMD Interlagos chip
    - 8 core modules, 32 threads
    - 156.5 GFs peak performance
    - 32 GBs memory
      - 51 GB/s bandwidth
  - One NVIDIA Kepler chip
    - 1.3 TFs peak performance
    - 6 GBs GDDR5 memory
      - 250 GB/sec bandwidth
  - Gemini Interconnect
    - Same as XE6 nodes

Blue Waters contains 3,072 Cray XK7 compute nodes.

Gemini Interconnect Network

Blue Waters
3D Torus Size
23 x 24 x 24



Blue Waters and Titan Computing Systems

System Attribute	NCSA Blue Waters	ORNL Titan
Vendors	Cray/AMD/NVIDIA	Cray/AMD/NVIDIA
Processors	Interlagos/Kepler	Interlagos/Kepler
Total Peak Performance (PF)	11.5	27.1
Total Peak Performance (CPU/GPU)	7.1/4	2.6/24.5
Number of CPU Chips	48,352	18,688
Number of GPU Chips	3,072	18,688
Amount of CPU Memory (TB)	1511	584
Interconnect	3D Torus	3D Torus
Amount of On-line Disk Storage (PB)	26	13.6
Sustained Disk Transfer (TB/sec)	>1	0.4-0.7
Amount of Archival Storage	300	15-30
Sustained Tape Transfer (GB/sec)	100	7

Disconnect between TOP500 and usable performance

LINPACK is a **single test** that solves Ax=b
with **dense linear equations**
using Gaussian elimination with partial pivoting.
For matrix A, that is size MxM,
LINPACK requires 2/3 M^2 + $2M^2$ operations,
$O(N^2)$ memory and
$O(N^3)$ Floating Point operations

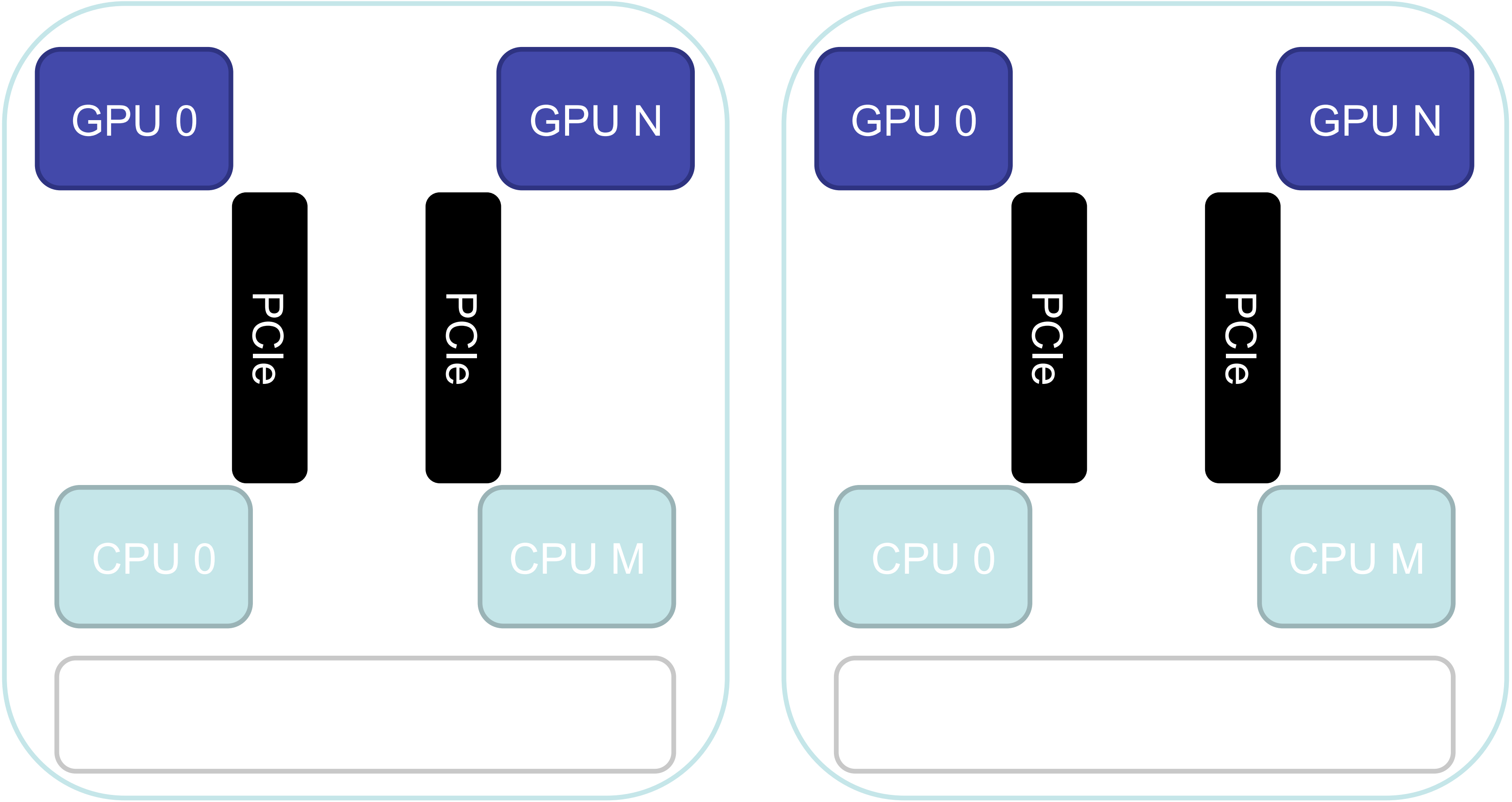
TOP500 Issues

• The TOP500 gives no indication of the cost or value of a system
• The TOP500 encourages organizations to make poor choices
• The TOP500 provides little historical value
• The TOP500 is dominated by who has the most money to spend – not what system is the best.
• The Linpack TOP500 measure takes too long to run and does not represent strong scaling
• The TOP500 metric has not kept up with changing algorithmic methods.
• The TOP500 Linpack performance test is dominated by single-core, dense linear algebra peak performance
• There is no relationship between the TOP500 ranking and real work potential, user productivity, system usability for real applications.
The TOP500 list disenfranchises many important application areas.
• The Linpack benchmark serves only one or two of the four purposes of a good benchmark.

Science Area	Number of Teams	Codes	Struct Grids	Unstruct Grids	Dense Matrix	Sparse Matrix	N-Body	Monte Carlo	FFT	PIC	Significant I/O
Climate and Weather	3	CESM, GCRM, CM1/WRF, HOMME	X	X		X		X			X
Plasmas/ Magnetosphere	2	H3D(M),VPIC, OSIRIS, Magtail/ UPIC	X				X		X		X
Stellar Atmospheres and Supernovae	5	PPM, MAESTRO, CASTRO, SEDONA, ChaNGa, MS-FLUKSS	X			X	X	X		X	X
Cosmology	2	Enzo, pGADGET	X			X	X				
Combustion/ Turbulence	2	PSDNS, DISTUF	X						X		
General Relativity	2	Cactus, Harm3D, LazEV	X			X					
Molecular Dynamics	4	AMBER, Gromacs, NAMD, LAMMPS				X	X		X		
Quantum Chemistry	2	SIAL, GAMESS, NWChem			X	X	X	X			X
Material Science	3	NEMOS, OMEN, GW, QMCPACK			X	X	X	X			
Earthquakes/ Seismology	2	AWP-ODC, HERCULES, PLSQR, SPECFEM3D	X	X			X				X
Quantum Chromo Dynamics	1	Chroma, MILC, USQCD	X		X	X					
Social Networks	1	EPISIMDEMICS									
Evolution	1	Eve									
Engineering/System of Systems	1	GRIPS,Revisit						X			
Computer Science	1			X	X	X			X		X

CUDA-based cluster

- Each node contains *N* GPUs

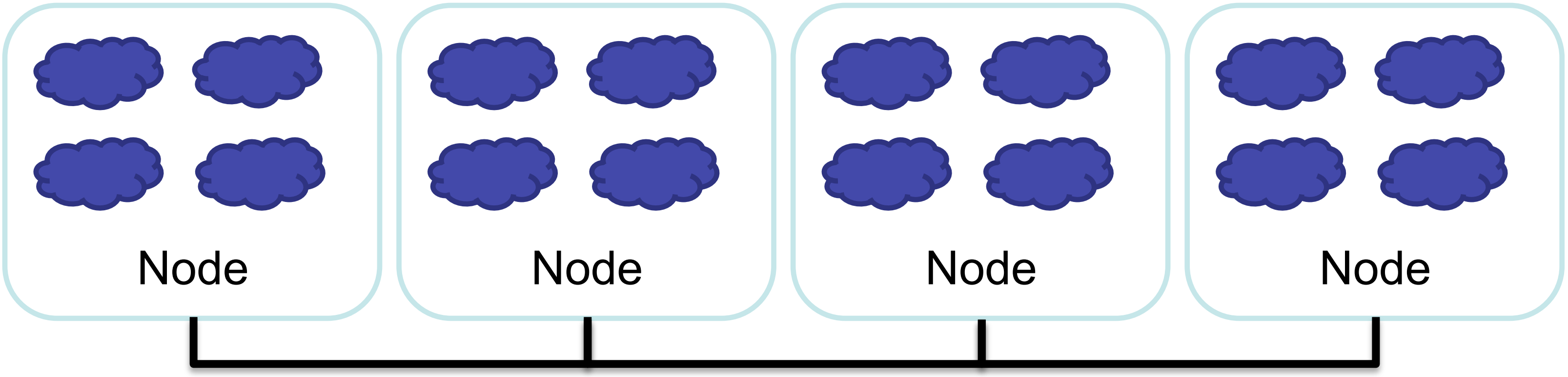


Message Passing Interface

- **MPI is a standard message passing API**
- **Oriented to cluster machines**
  - Distributed memory
  - Hides underlying interconnection network
- **Processes execute on different nodes of a network**

MPI Model

- Many processes distributed in a cluster



- Each process computes part of the output
- Processes communicate with each other
- Processes can synchronize

MPI Message Types

- **Point-to-point communication**
  - Send and Receive
- **Collective communication**
  - Barrier
  - Broadcast
  - Reduce
  - Gather and Scatter

MPI Initialization, Info and Sync

- `int MPI_Init(int *argc, char ***argv)`
  - Initialize MPI
- `MPI_COMM_WORLD`
  - MPI group with all allocated nodes
- `int MPI_Comm_rank (MPI_Comm comm, int *rank)`
  - Rank of the calling process in group of comm
- `int MPI_Comm_size (MPI_Comm comm, int *size)`
  - Number of processes in the group of comm
- `int MPI_Barrier (MPI_Comm comm)`
  - Blocks the caller until all group members have called it; returns at any process only after all group members have entered the call

Vector Addition: Main Process

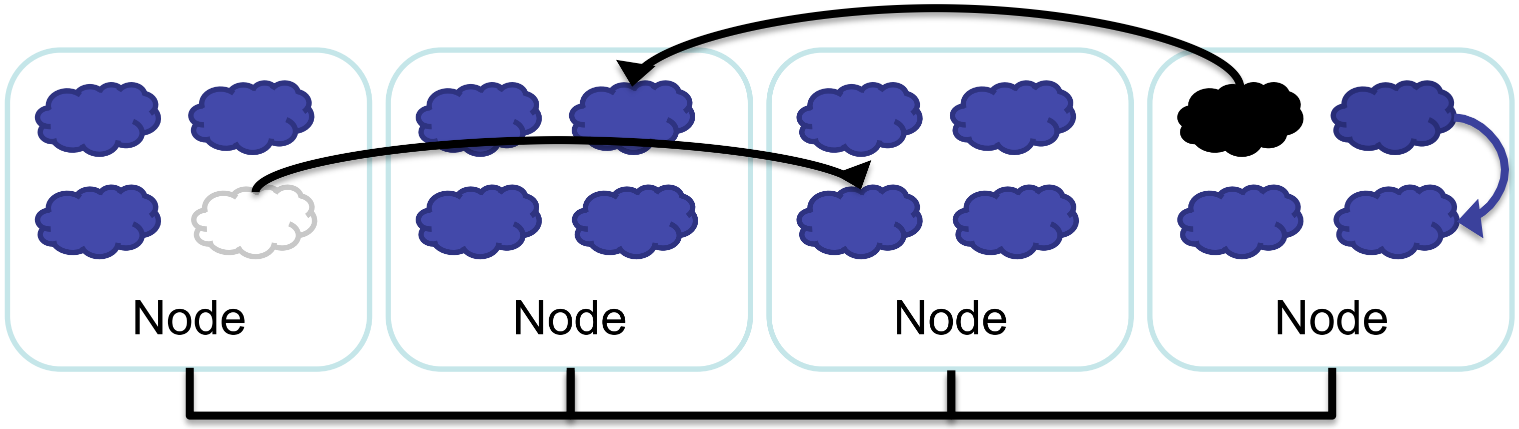
```
int main(int argc, char *argv[]) {
    int vector_size = 1024 * 1024 * 1024;
    int pid=-1, np=-1;
    // MPI Setup
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    if(np < 3) {
        if(0 == pid) printf("Needed 3 or more processes.\n");
        MPI_Abort( MPI_COMM_WORLD, 1 ); return 1;
    }
    if(pid < np - 1)
        compute_node(vector_size / (np - 1));
    else
        data_server(vector_size);

    MPI_Finalize();
    return 0;
}
```

MPI Sending Data

- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
  - buf: Initial address of send buffer (choice)
  - count: Number of elements in send buffer (nonnegative integer)
  - datatype: Datatype of each send buffer element (handle)
  - dest: Rank of destination (integer)
  - tag: Message tag (integer)
  - comm: Communicator (handle)

MPI Sending Data

- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
  - buf: Initial address of send buffer (choice)
  - count: Number of elements in send buffer (nonnegative integer)
  - datatype: Datatype of each send buffer element (handle)
  - dest: Rank of destination (integer)
  - tag: Message tag (integer)
  - comm: Communicator (handle)

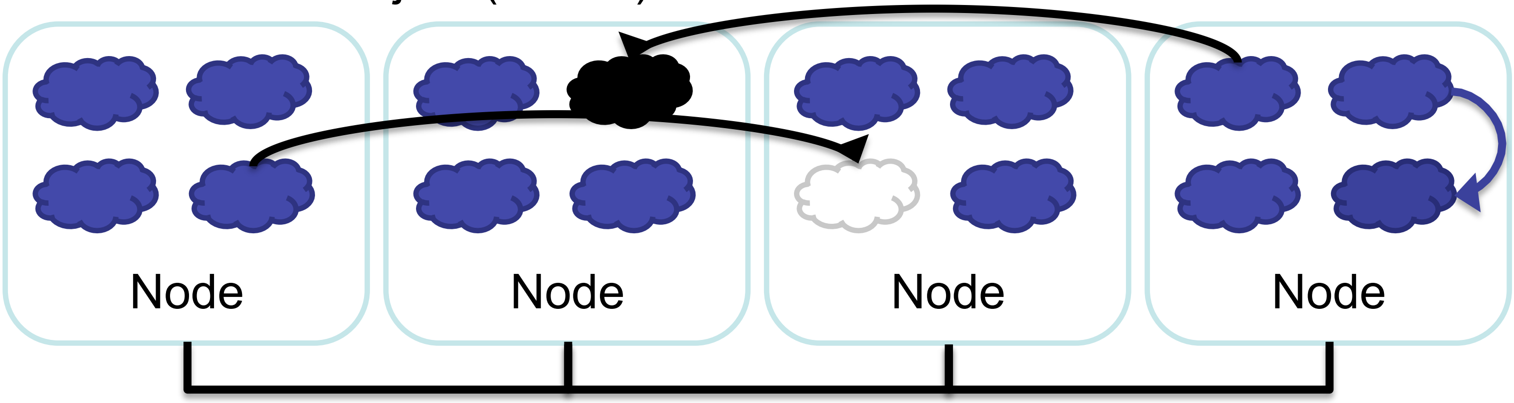


MPI Receiving Data

- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`
  - buf: Initial address of receive buffer (choice)
  - count: Maximum number of elements in receive buffer (integer)
  - datatype: Datatype of each receive buffer element (handle)
  - source: Rank of source (integer)
  - tag: Message tag (integer)
  - comm: Communicator (handle)
  - status: Status object (Status)

MPI Receiving Data

- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`
  - buf: Initial address of receive buffer (choice)
  - count: Maximum number of elements in receive buffer (integer)
  - datatype: Datatype of each receive buffer element (handle)
  - source: Rank of source (integer)
  - tag: Message tag (integer)
  - comm: Communicator (handle)
  - status: Status object (Status)



MPI Send and Receive Data

- `int MPI_Sendrecv(void *sendbuf, int sendcount, MPI_Datatype sendtype, int dest, int sendtag, void *recvbuf, int recvcount, MPI_Datatype recvtype, int source, int recvtag, MPI_Comm comm, MPI_Status *status)`
  - send/recvbuf: Initial address of send/receive buffer (choice)
  - send/recvcount: Number of elements in send/receive buffer (integer)
  - send/recvtype: Datatype of each send/receive buffer element (handle)
  - dest: Rank of destination (integer)
  - source: Rank of source (integer)
  - send/recvtag: Send/receive tag (integer)
  - comm: Communicator (handle)
  - status: Status object (Status). This refers to the receive operation.

Vector Addition: Server Process (I)

```
void data_server(unsigned int vector_size) {
    int np, num_nodes = np – 1, first_node = 0, last_node = np - 2;
    unsigned int num_bytes  = vector_size * sizeof(float);
    float *input_a = 0, *input_b = 0, *output = 0;

    // Set MPI Communication Size
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    // Allocate input and output data
    input_a = (float *)malloc(num_bytes);
    input_b = (float *)malloc(num_bytes);
    output = (float *)malloc(num_bytes);
    if(input_a == NULL || input_b == NULL || output == NULL) {
        printf(“Server couldn't allocate memory\n");
        MPI_Abort( MPI_COMM_WORLD, 1 );
    }
    // Initialize input data
    random_data(input_a, vector_size , 1, 10);
    random_data(input_b, vector_size , 1, 10);
```

Vector Addition: Server Process (II)

```
// Send data to compute nodes
      *ptr_a = input_a;
      *ptr_b = input_b;

for(int process = 1; process < last_node; process++) {
    MPI_Send(ptr_a, vector_size / num_nodes, MPI_FLOAT,
            process, DATA_DISTRIBUTE, MPI_COMM_WORLD);
    ptr_a += vector_size / num_nodes;

    MPI_Send(ptr_b, vector_size / num_nodes, MPI_FLOAT,
            process, DATA_DISTRIBUTE, MPI_COMM_WORLD);
    ptr_b += vector_size / num_nodes;
}
```

Vector Addition: Server Process (III)

```
    // Collect output data
    MPI_Status status;
    for(int process = 0; process < num_nodes; process++) {
        MPI_Recv(output + process * num_points / num_nodes,
            num_points / num_comp_nodes, MPI_REAL, process,
            DATA_COLLECT, MPI_COMM_WORLD, &status );
    }

    // Store output data
    store_output(output, dimx, dimy, dimz);

    // Release resources
    free(input);
    free(output);
}
```

Vector Addition: Compute Process (I)

```
void compute_node(unsigned int vector_size ) {
    int np;
    unsigned int num_bytes = vector_size * sizeof(float);
    float *input_a, *input_b, *output;
    MPI_Status status;

    MPI_Comm_size(MPI_COMM_WORLD, &np);
    int server_process = np - 1;

    // Alloc host memory
    input_a = (float *)malloc(num_bytes);
    input_b = (float *)malloc(num_bytes);
    output = (float *)malloc(num_bytes);

    // Get the input data from server process
    MPI_Recv(input_a, vector_size, MPI_FLOAT, server_process,
            DATA_DISTRIBUTE, MPI_COMM_WORLD, &status);
    MPI_Recv(input_b, vector_size, MPI_FLOAT, server_process,
            DATA_DISTRIBUTE, MPI_COMM_WORLD, &status);
```

Vector Addition: Compute Process (II)

```
    // Compute the partial vector addition
    for(int i = 0; i < vector_size; ++i) {
        output[i] = input_a[i] + input_b[i];
    }

    // Send the output
    MPI_Send(output, vector_size, MPI_FLOAT,
            server_process, DATA_COLLECT, MPI_COMM_WORLD);

    // Release memory
    free(input_a);
    free(input_b);
    free(output);
}
```

MPI + CUDA

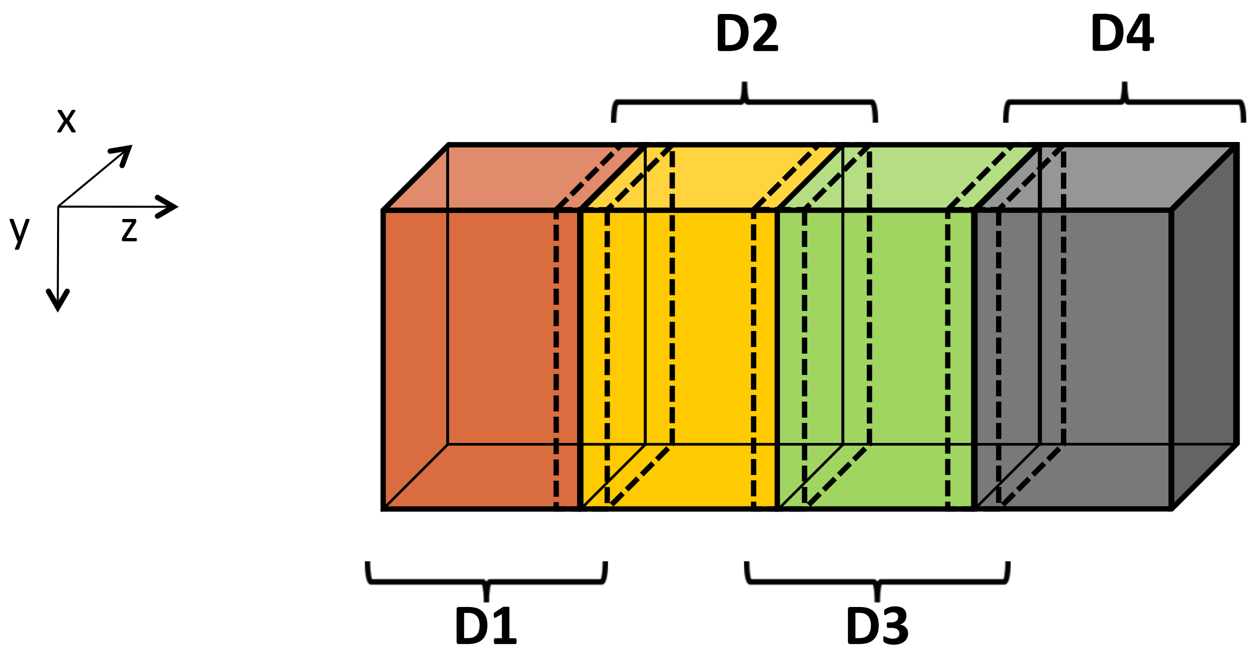
- The main challenge of MPI + CUDA is not integrating the two but overlapping communication and computation

Stencil Code: Main Process

```
int main(int argc, char *argv[]) {
    int pad = 0, dimx  = 480+pad, dimy  = 480, dimz  = 400, nreps = 100;
    int pid=-1, np=-1;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    if(np < 3) {
        if(0 == pid) printf("Needed 3 or more processes.\n");
        MPI_Abort( MPI_COMM_WORLD, 1 ); return 1;
    }
    if(pid < np - 1)
        compute_node_stencil(dimx, dimy, dimz / (np - 1), nreps);
    else
        data_server( dimx,dimy,dimz, nreps );

    MPI_Finalize();
    return 0;
}
```

Stencil Domain Decomposition

- Volumes are split into tiles (along the Z-axis)
  - 3D-Stencil introduces data dependencies



Stencil Code: Server Process (I)

```
void data_server(int dimx, int dimy, int dimz, int nreps) {
    int np, num_comp_nodes = np – 1, first_node = 0, last_node = np - 2;
    unsigned int num_points = dimx * dimy * dimz;
    unsigned int num_bytes  = num_points * sizeof(float);
    float *input=0, *output=0;
    /* Set MPI Communication Size */
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    /* Allocate input data */
    input = (float *)malloc(num_bytes);
    output = (float *)malloc(num_bytes);
    if(input == NULL || output == NULL) {
        printf("server couldn't allocate memory\n");
        MPI_Abort( MPI_COMM_WORLD, 1 );
    }
    /* Initialize input data */
    random_data(input, dimx, dimy ,dimz , 1, 10);
    /* Calculate number of shared points */
    int edge_num_points = dimx * dimy * (dimz / num_comp_nodes + 4);
    int int_num_points  = dimx * dimy * (dimz / num_comp_nodes + 8);
    float *send_address = input;
```

Stencil Code: Server Process (II)

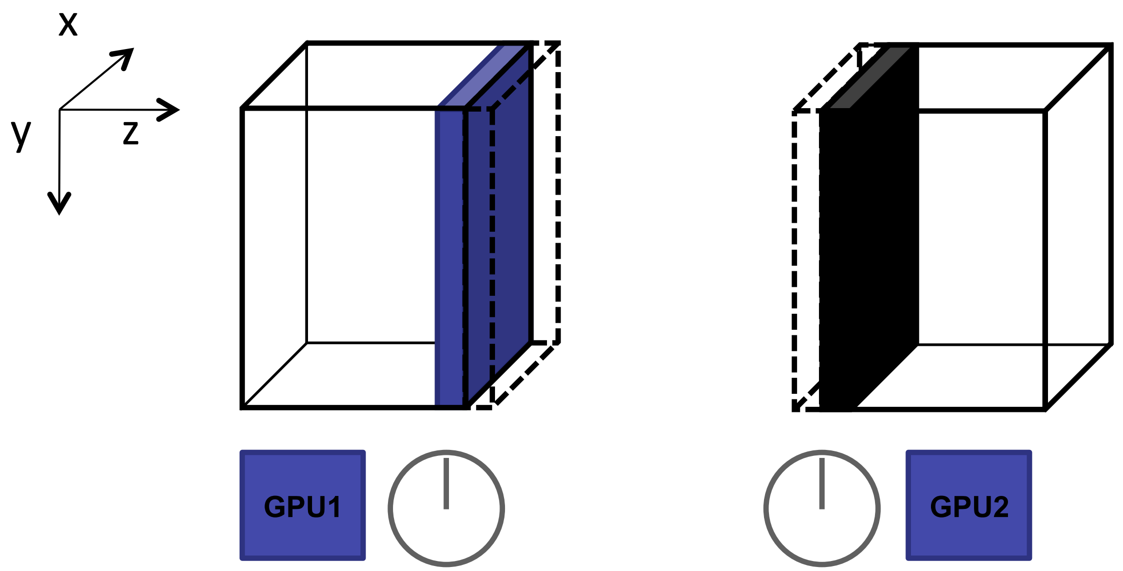
```
/* Send data to the first compute node */
MPI_Send(send_address, edge_num_points, MPI_REAL, first_node,
        DATA_DISTRIBUTE, MPI_COMM_WORLD );
send_address += dimx * dimy * (dimz / num_comp_nodes - 4);

/* Send data to "internal" compute nodes */
for(int process = 1; process < last_node; process++) {
    MPI_Send(send_address, int_num_points, MPI_REAL, process,
            DATA_DISTRIBUTE, MPI_COMM_WORLD);
    send_address += dimx * dimy * (dimz / num_comp_nodes);
}

/* Send data to the last compute node */
MPI_Send(send_address, edge_num_points, MPI_REAL, last_node,
        DATA_DISTRIBUTE, MPI_COMM_WORLD);
```

Stencil Code: Main Process (I)

```
    /* Wait for nodes to compute */
    // MPI_Barrier(MPI_COMM_WORLD);

    /* Collect output data */
    MPI_Status status;
    for(int process = 0; process < num_comp_nodes; process++)
        MPI_Recv(output + process * num_points / num_comp_nodes,
            num_points / num_comp_nodes, MPI_REAL, process,
            DATA_COLLECT, MPI_COMM_WORLD, &status );

    /* Store output data */
    store_output(output, dimx, dimy, dimz);

    /* Release resources */
    free(input);
    free(output);
}
```

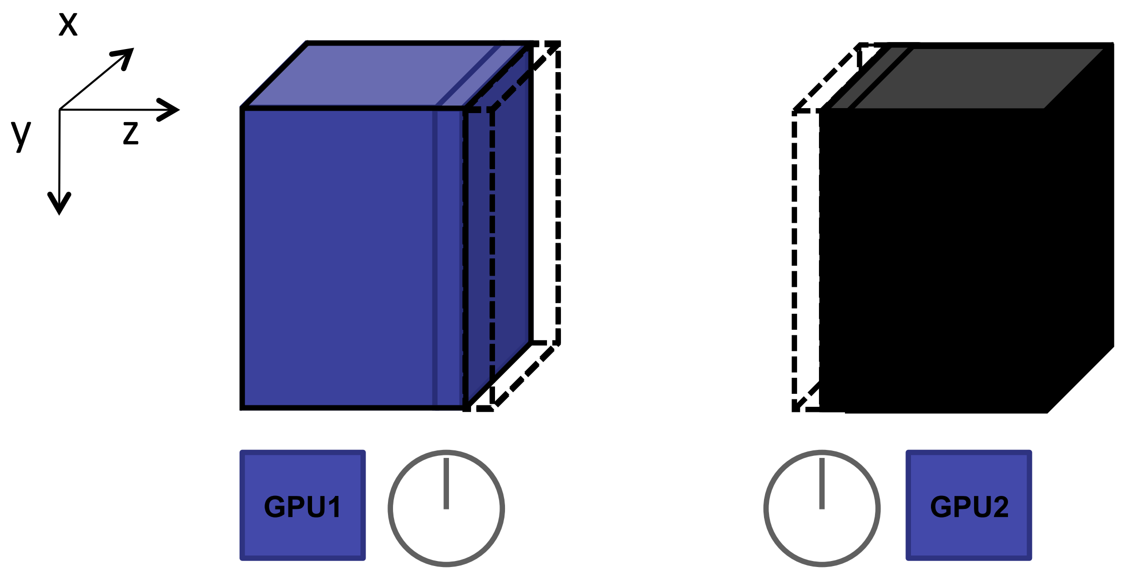
Boundary Exchange Example (I)

- **Approach: two-stage execution**
  - Stage 1: compute the field points to be exchanged



Boundary Exchange Example (II)

- **Approach: two-stage execution**
  - Stage 2: Compute the remaining points ***while*** exchanging the boundaries



Stencil Code: Compute Process (I)

```
void compute_node_stencil(int dimx, int dimy, int dimz, int nreps ) {
    int np, pid;
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    unsigned int num_points       = dimx * dimy * (dimz + 8);
    unsigned int num_bytes        = num_points * sizeof(float);
    unsigned int num_ghost_points = 4 * dimx * dimy;
    unsigned int num_ghost_bytes  = num_ghost_points * sizeof(float);

    int left_ghost_offset   = 0;
    int right_ghost_offset  = dimx * dimy * (4 + dimz);
    int left_stage1_offset  = 0;
    int right_stage1_offset = dimx * dimy * (dimz - 4);
    int stage2_offset       = num_ghost_points;
```

Stencil Code: Compute Process (II)

```
float *h_input = NULL, *h_output = NULL;
float *d_input = NULL, *d_output = NULL, *d_vsq = NULL;
float *h_left_ghost_own = NULL, *h_right_ghost_own = NULL;
float *h_left_ghost = NULL, *h_right_ghost = NULL;

/* Alloc host memory */
h_input  = (float *)malloc(num_bytes);
h_output = (float *)malloc(num_bytes);

/* Alloc pinned host memory for ghost data */
cudaMallocHost((void **)&h_left_ghost_own,  num_ghost_bytes );
cudaMallocHost((void **)&h_right_ghost_own, num_ghost_bytes );
cudaMallocHost((void **)&h_left_ghost,      num_ghost_bytes );
cudaMallocHost((void **)&h_right_ghost,     num_ghost_bytes );

/* Alloca device memory for input and output data */
cudaMalloc((void **)&d_input,  num_bytes );
cudaMalloc((void **)&d_output, num_bytes );
```

Stencil Code: Compute Process (III)

```
MPI_Status status;
int left_neighbor  = (pid > 0)    ? (pid - 1) : MPI_PROC_NULL;
int right_neighbor = (pid < np - 2) ? (pid + 1) : MPI_PROC_NULL;
int server_process = np - 1;

/* Get the input data from main process */
float *rcv_address = h_input + num_ghost_points * (0 == pid);
MPI_Recv(rcv_address, num_points, MPI_REAL, server_process,
        DATA_DISTRIBUTE, MPI_COMM_WORLD, &status );
cudaMemcpy(d_input, h_input, num_bytes, cudaMemcpyHostToDevice );

/* Upload stencil cofficients */
upload_coefficients(coeff, 5);

/* Create streams used for stencil computation */
cudaStream_t stream1, stream2;
cudaStreamCreate(&stream1);
cudaStreamCreate(&stream2);
```

Stencil Code: Compute Process (IV)

```
    // MPI_Barrier( MPI_COMM_WORLD );
    for(int i=0; i < nreps; i++) {
        /* Compute values needed by other nodes first */
        launch_kernel(d_output + left_stage1_offset,
            d_input + left_stage1_offset, dimx, dimy, 12, stream1);
        launch_kernel(d_output + right_stage1_offset,
            d_input + right_stage1_offset, dimx, dimy, 12, stream1);

        /* Compute the remaining points */
        launch_kernel(d_output + stage2_offset, d_input + stage2_offset,
                    dimx, dimy, dimz, stream2);

        /* Copy the data needed by other nodes to the host */
        cudaMemcpyAsync(h_left_ghost_own,
                d_output + num_ghost_points,
                num_ghost_bytes, cudaMemcpyDeviceToHost, stream1 );
        cudaMemcpyAsync(h_right_ghost_own,
                    d_output + right_stage1_offset + num_ghost_points,
                    num_ghost_bytes, cudaMemcpyDeviceToHost, stream1 );
        cudaStreamSynchronize(stream1);
```

Stencil Code: Compute Process (V)

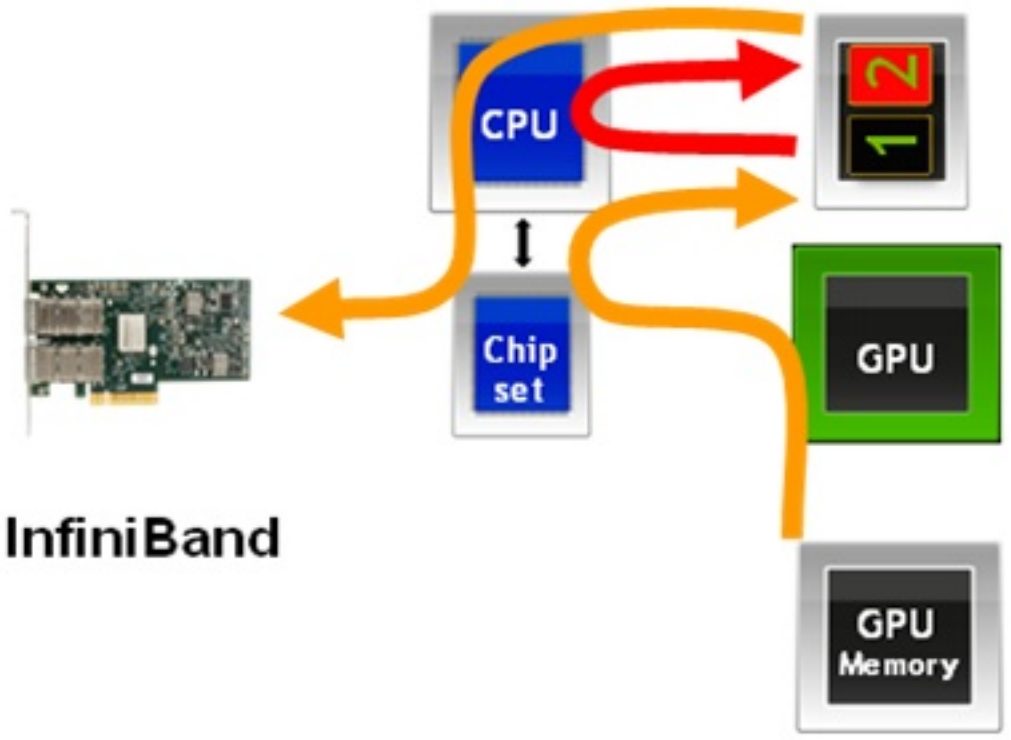
```
        /* Send data to left, get data from right */
        MPI_Sendrecv(h_left_ghost_own, num_ghost_points, MPI_REAL,
                     left_neighbor,  i, h_right_ghost,
                     num_ghost_points, MPI_REAL, right_neighbor, i,
                     MPI_COMM_WORLD, &status );
        /* Send data to right, get data from left */
        MPI_Sendrecv(h_right_ghost_own, num_ghost_points, MPI_REAL,
                     right_neighbor, i, h_left_ghost,
                     num_ghost_points, MPI_REAL, left_neighbor,  i,
                     MPI_COMM_WORLD, &status );

        cudaMemcpyAsync(d_output+left_ghost_offset,  h_left_ghost,
                     num_ghost_bytes, cudaMemcpyHostToDevice, stream1);
        cudaMemcpyAsync(d_output+right_ghost_offset, h_right_ghost,
                     num_ghost_bytes, cudaMemcpyHostToDevice, stream1 );
        cudaDeviceSynchronize();

        float *temp = d_output;
        d_output = d_input; d_input = temp;
    }
```

Stencil Code: Compute Process (VII)

```
    /* Wait for previous communications */
    // MPI_Barrier(MPI_COMM_WORLD);

    float *temp = d_output;
    d_output = d_input;
    d_input = temp;

    /* Send the output, skipping ghost points */
    cudaMemcpy(h_output, d_output, num_bytes, cudaMemcpyDeviceToHost);
    float *send_address = h_output + num_ghost_points;
    MPI_Send(send_address, dimx * dimy * dimz, MPI_REAL,
            server_process, DATA_COLLECT, MPI_COMM_WORLD);
    // MPI_Barrier(MPI_COMM_WORLD);

    /* Release resources */
    free(h_input); free(h_output);
    cudaFreeHost(h_left_ghost_own); cudaFreeHost(h_right_ghost_own);
    cudaFreeHost(h_left_ghost); cudaFreeHost(h_right_ghost);
    cudaFree( d_input ); cudaFree( d_output );
}
```

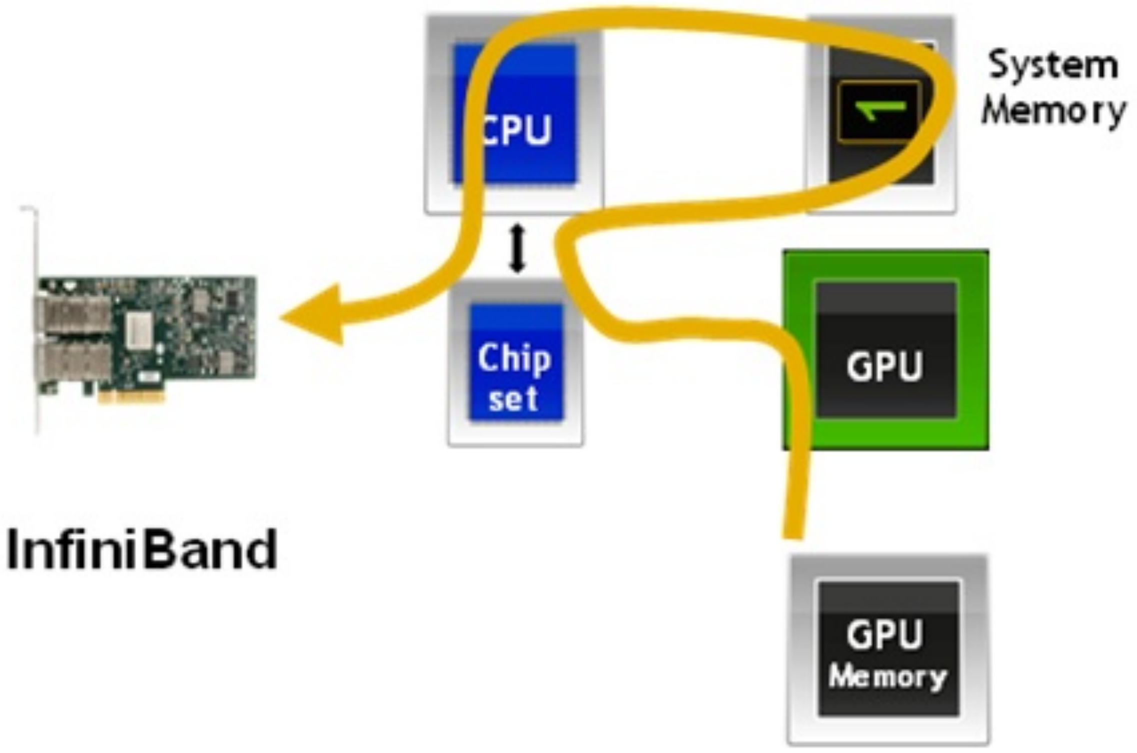
Without GPU Direct

- There is an internal copy (not seen by the user) between CUDA buffers and Infiniband buffers



With GPU Direct

- There is no internal copy, increasing performance
- The program code remains unchanged


CPU
System Memory
Chip set
GPU
GPU Memory
InfiniBand