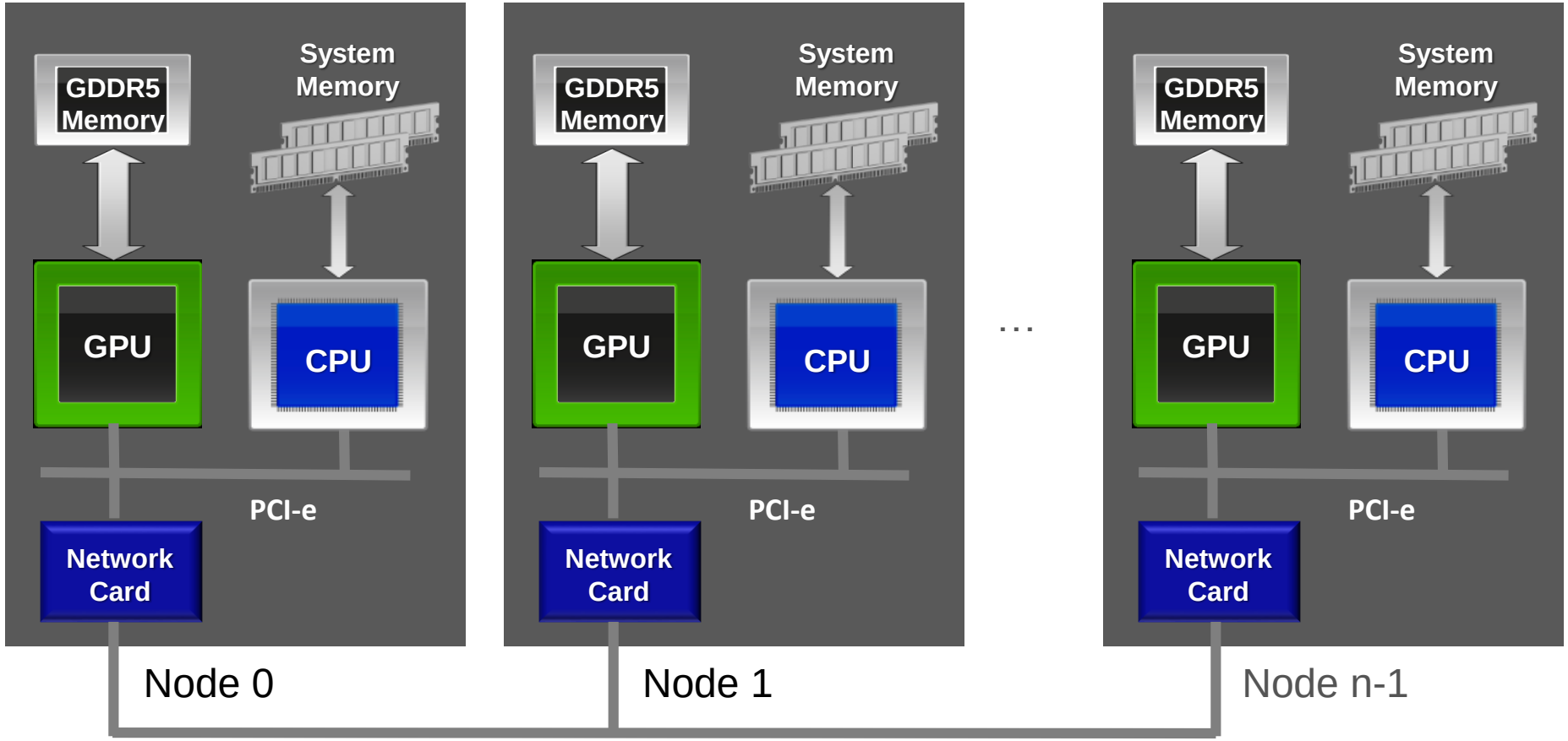
GPU TECHNOLOGY CONFERENCE

NVIDIA

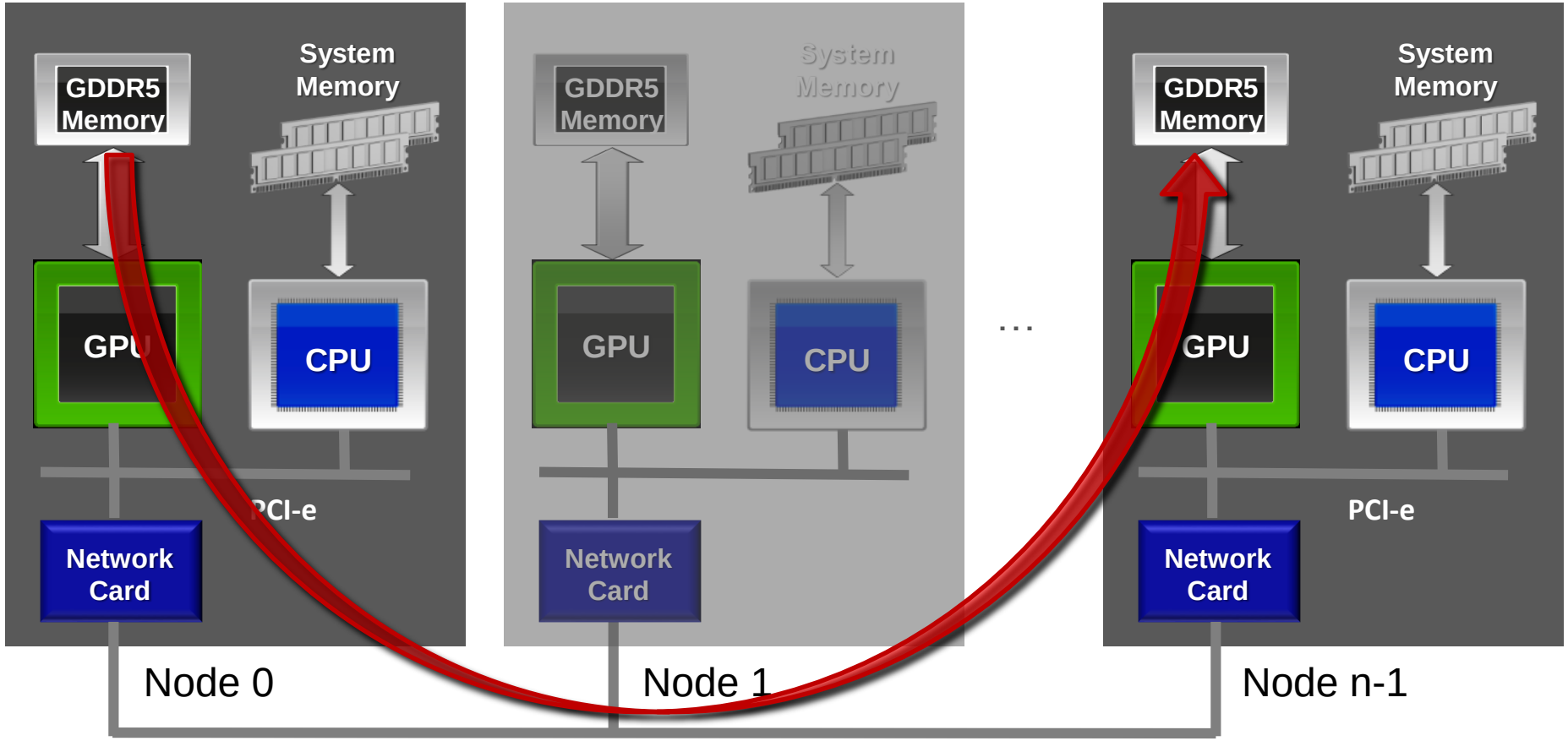
MULTI GPU PROGRAMMING WITH MPI

Jiri Kraus and Peter Messmer, NVIDIA

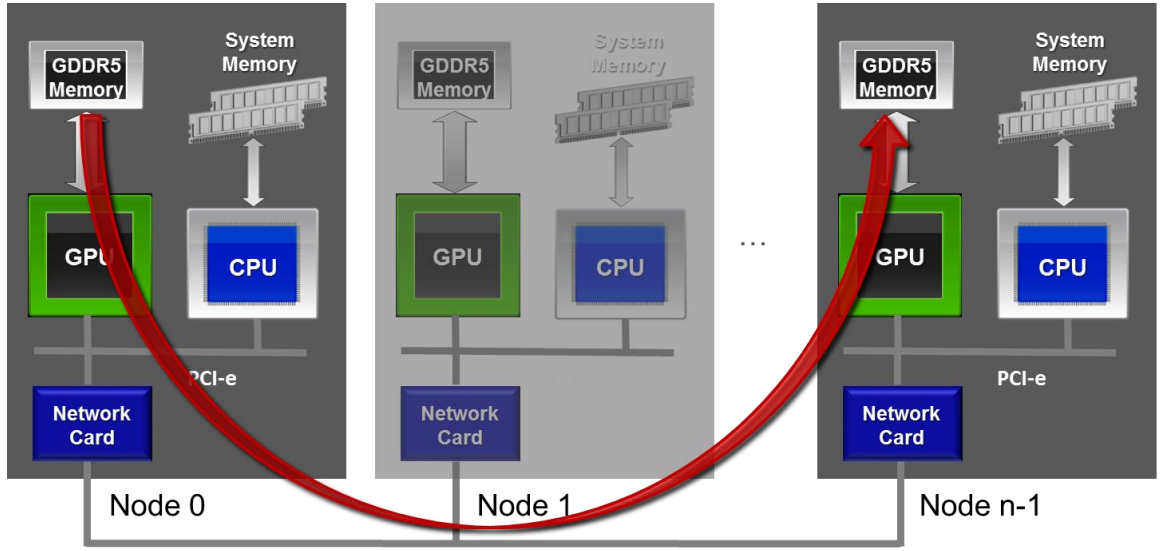
MPI+CUDA



MPI+CUDA


GDDR5 Memory
System Memory
GPU
CPU
PCI-e
Network Card
Node 0
GDDR5 Memory
System Memory
GPU
CPU
Network Card
Node 1
...
GDDR5 Memory
System Memory
GPU
CPU
PCI-e
Network Card
Node n-1

MPI+CUDA




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

//MPI rank n-1
MPI_Recv(r_buf_d,size,MPI_CHAR,0,tag,MPI_COMM_WORLD,&stat);
```

WHAT YOU WILL LEARN

- What MPI is
- How to use MPI for inter GPU communication with CUDA and OpenACC
- What CUDA-aware MPI is
- What Multi Process Service is and how to use it
- How to use NVIDIA Tools in an MPI environment
- How to hide MPI communication times

MESSAGE PASSING INTERFACE - MPI

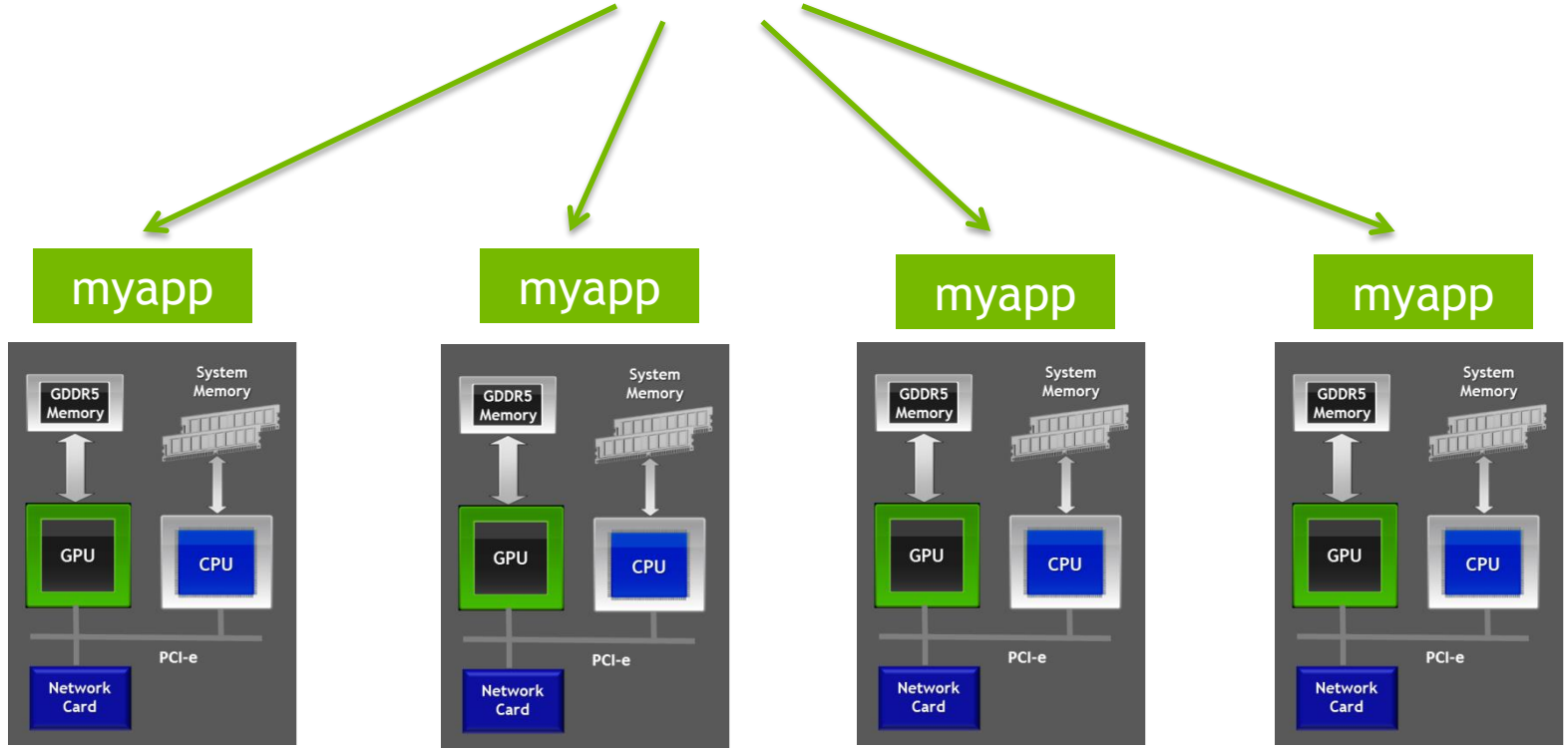
- Standard to exchange data between processes via messages
  - Defines API to exchanges messages
    - Pt. 2 Pt.: e.g. MPI_Send, MPI_Recv
    - Collectives, e.g. MPI_Reduce
- Multiple implementations (open source and commercial)
  - Binding for C/C++, Fortran, Python, …
  - E.g. MPICH, OpenMPI, MVAPICH, IBM Platform MPI, Cray MPT, …

MPI - A MINIMAL PROGRAM

```
#include <mpi.h>
int main(int argc, char *argv[]) {
    int rank,size;
    /* Initialize the MPI library */
    MPI_Init(&argc,&argv);
    /* Determine the calling process rank and total number of ranks */
    MPI_Comm_rank(MPI_COMM_WORLD,&rank);
    MPI_Comm_size(MPI_COMM_WORLD,&size);
    /* Call MPI routines like MPI_Send, MPI_Recv, ... */
    ...
    /* Shutdown MPI library */
    MPI_Finalize();
    return 0;
}
```

MPI - COMPILING AND LAUNCHING

```
$ mpicc -o myapp myapp.c
$ mpirun -np 4 ./myapp <args>
```



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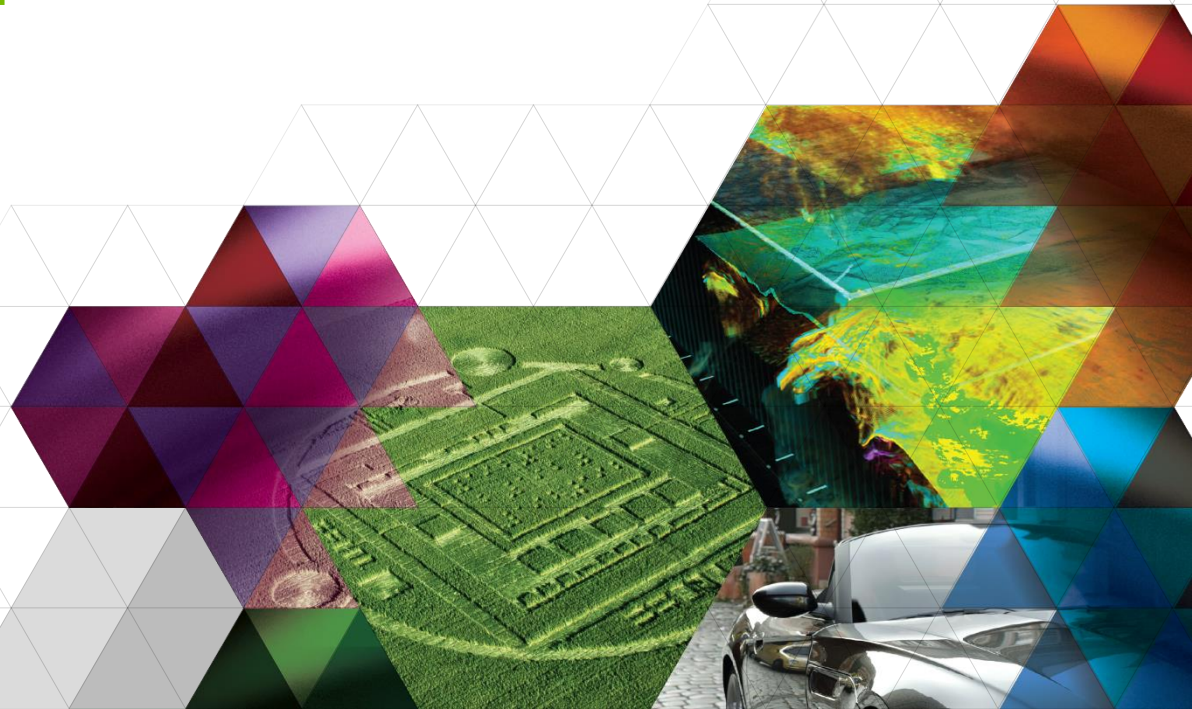
A SIMPLE EXAMPLE

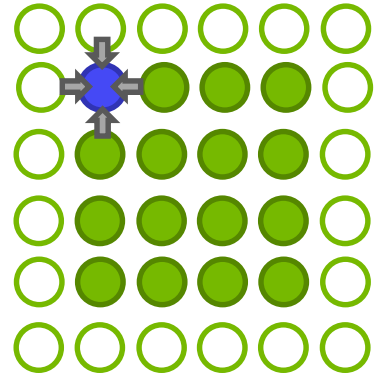


EXAMPLE: JACOBI SOLVER – SINGLE GPU

While not converged

- Do Jacobi step:

```
for (int i=1; i < n-1; i++)
   for (int j=1; j < m-1; j++)
     u_new[i][j] = 0.0f - 0.25f*(u[i-1][j] + u[i+1][j]
                                 + u[i][j-1] + u[i][j+1])
```



- Swap `u_new` and `u`
- Next iteration

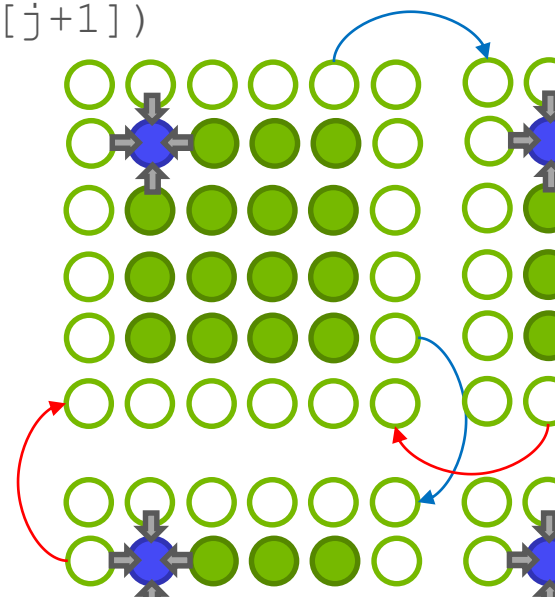
EXAMPLE: JACOBI SOLVER – MULTI GPU

While not converged

- Do Jacobi step:

```
for (int i=1; i < n-1; i++)
  for (int j=1; j < m-1; j++)
    u_new[i][j] = 0.0f - 0.25f*(u[i-1][j] + u[i+1][j]
                                + u[i][j-1] + u[i][j+1])
```

- Exchange halo with 2 4 neighbor
- Swap `u_new` and `u`
- Next iteration



EXAMPLE: JACOBI SOLVER

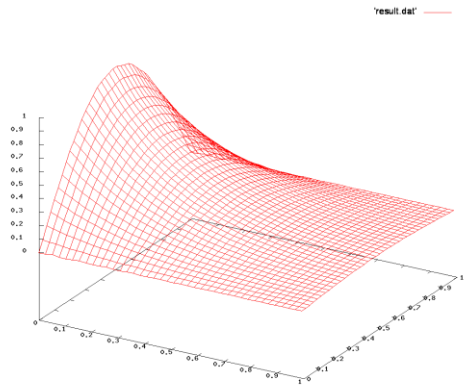
- Solves the 2D-Laplace equation on a rectangle

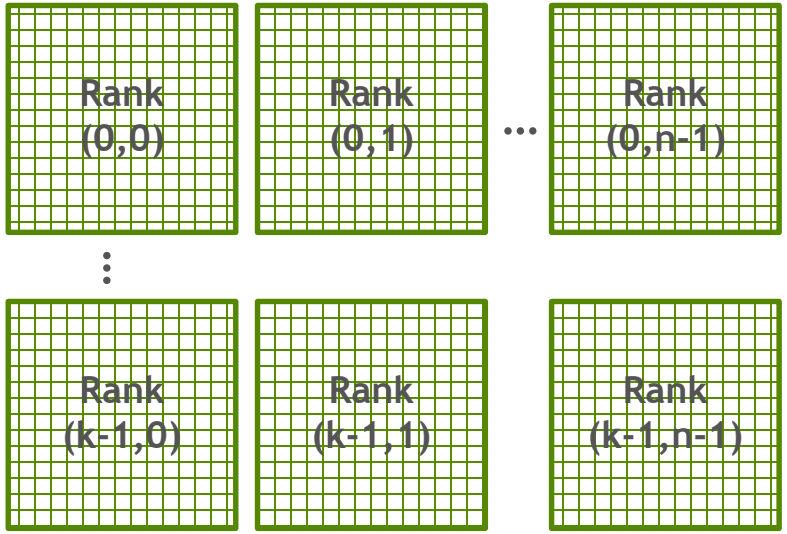
$$\Delta u(x,y) = 0 \; \forall \; (x,y) \in \Omega \backslash \delta\Omega$$

  - Dirichlet boundary conditions (constant values on boundaries)

$$u(x,y) = f(x,y) \in \delta\Omega$$

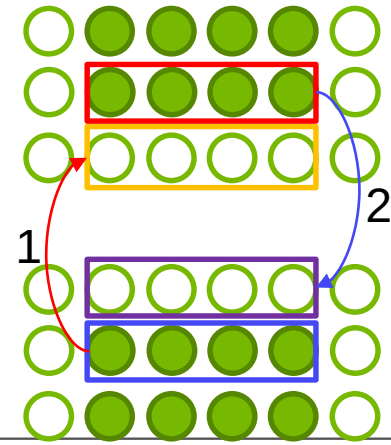
- 2D domain decomposition with n x k domains



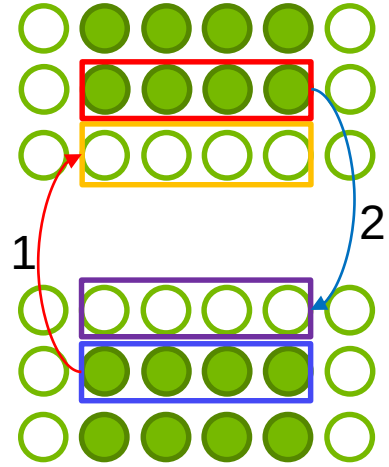


EXAMPLE: JACOBI – TOP/BOTTOM HALO UPDATE

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



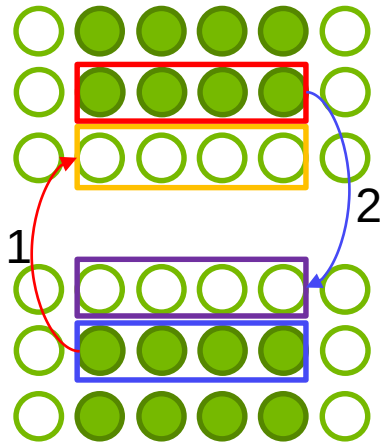

```
MPI_Sendrecv(u_new+offset_last_row, m-2, MPI_DOUBLE, b_nb, 1,
             u_new+offset_top_bondary, m-2, MPI_DOUBLE, t_nb, 1,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```



EXAMPLE: JACOBI – TOP/BOTTOM HALO UPDATE

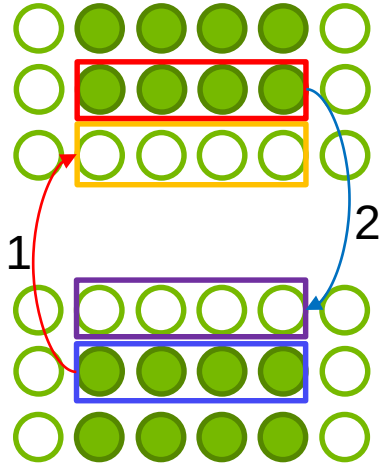
OpenACC

```
#pragma acc host_data use_device ( u_new ) {
  MPI_Sendrecv(u_new+offset_first_row, m-2, MPI_DOUBLE, t_nb, 0,
               u_new+offset_bottom_bondary, m-2, MPI_DOUBLE, b_nb, 0,
               MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  MPI_Sendrecv(u_new+offset_last_row, m-2, MPI_DOUBLE, b_nb, 1,
               u_new+offset_top_bondary, m-2, MPI_DOUBLE, t_nb, 1,
               MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```



CUDA

```
MPI_Sendrecv(u_new_d+offset_first_row, m-2, MPI_DOUBLE, t_nb, 0,
             u_new_d+offset_bottom_bondary, m-2, MPI_DOUBLE, b_nb, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
MPI_Sendrecv(u_new_d+offset_last_row, m-2, MPI_DOUBLE, b_nb, 1,
             u_new_d+offset_top_bondary, m-2, MPI_DOUBLE, t_nb, 1,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```



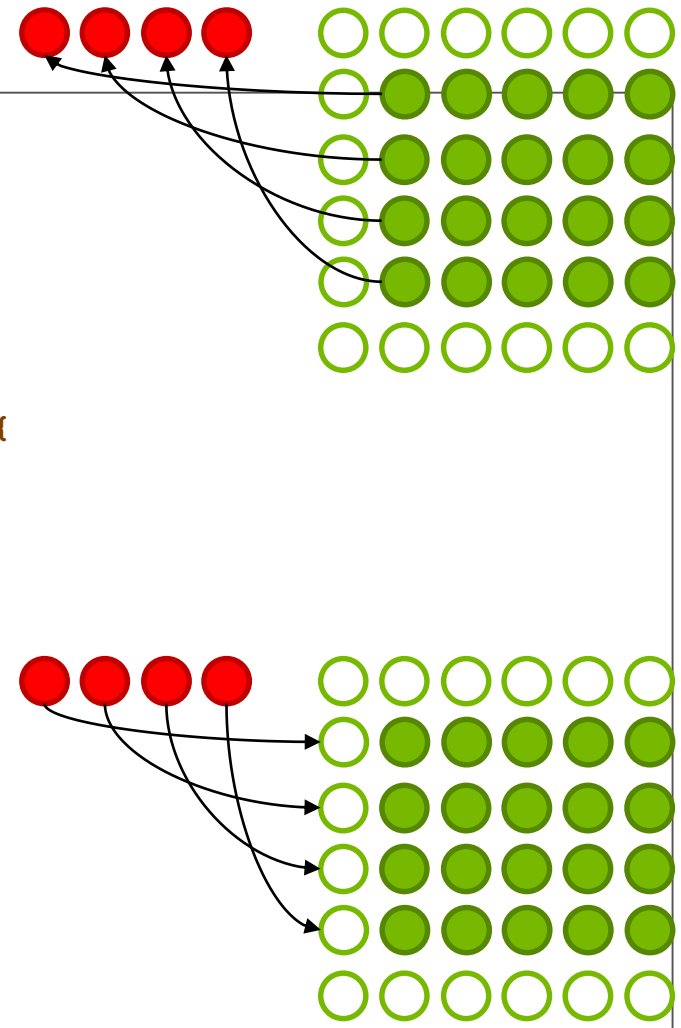
EXAMPLE: JACOBI – LEFT/RIGHT HALO UPDATE

OpenACC

```
//right neighbor omitted
#pragma acc parallel loop present ( u_new, to_left )
for ( int i=0; i<n-2; ++i )
     to_left[i] = u_new[(i+1)*m+1];

#pragma acc host_data use_device ( from_left, to_left ) {
  MPI_Sendrecv( to_left, n-2, MPI_DOUBLE, l_nb, 0,
                from_left, n-2, MPI_DOUBLE, l_nb, 0,
                MPI_COMM_WORLD, MPI_STATUS_IGNORE );
}

#pragma acc parallel loop present ( u_new, from_left )
for ( int i=0; i<n-2; ++i )
     u_new[(i+1)*m] = from_left[i];
```



EXAMPLE: JACOBI – LEFT/RIGHT HALO UPDATE

CUDA

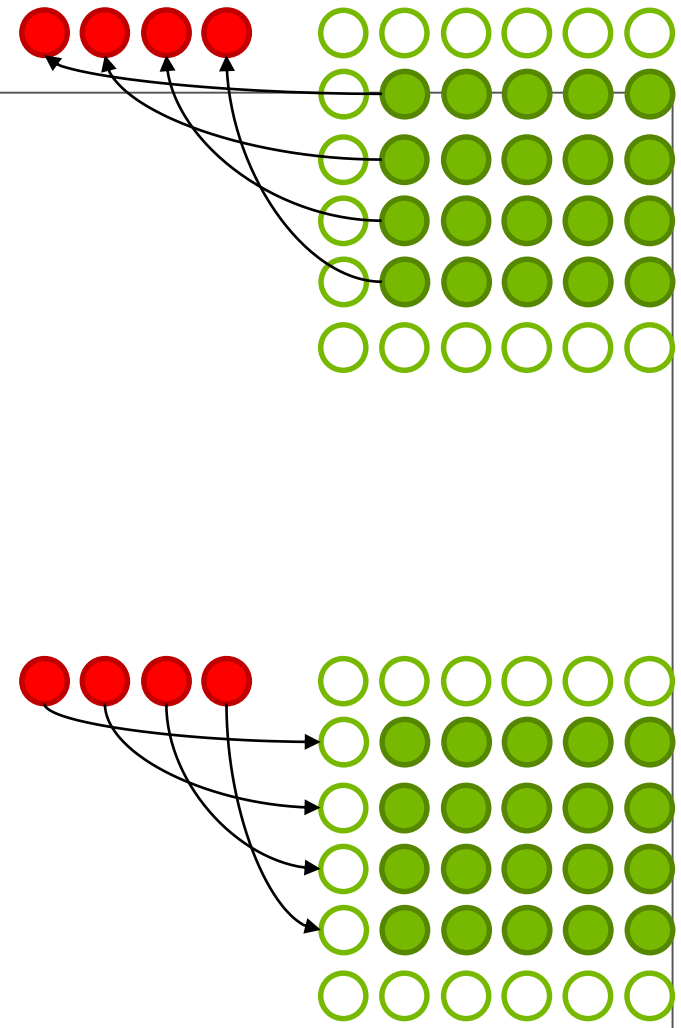
```
//right neighbor omitted
pack<<<gs,bs,0,s>>>(to_left_d, u_new_d, n, m);
cudaStreamSynchronize(s);




MPI_Sendrecv( to_left_d, n-2, MPI_DOUBLE, l_nb, 0,
              from_left_d, n-2, MPI_DOUBLE, l_nb, 0,
              MPI_COMM_WORLD, MPI_STATUS_IGNORE );




unpack<<<gs,bs,0,s>>>(u_new_d, from_left_d, n, m);
```



STARTING MPI+CUDA/OPENACC PROGRAMS

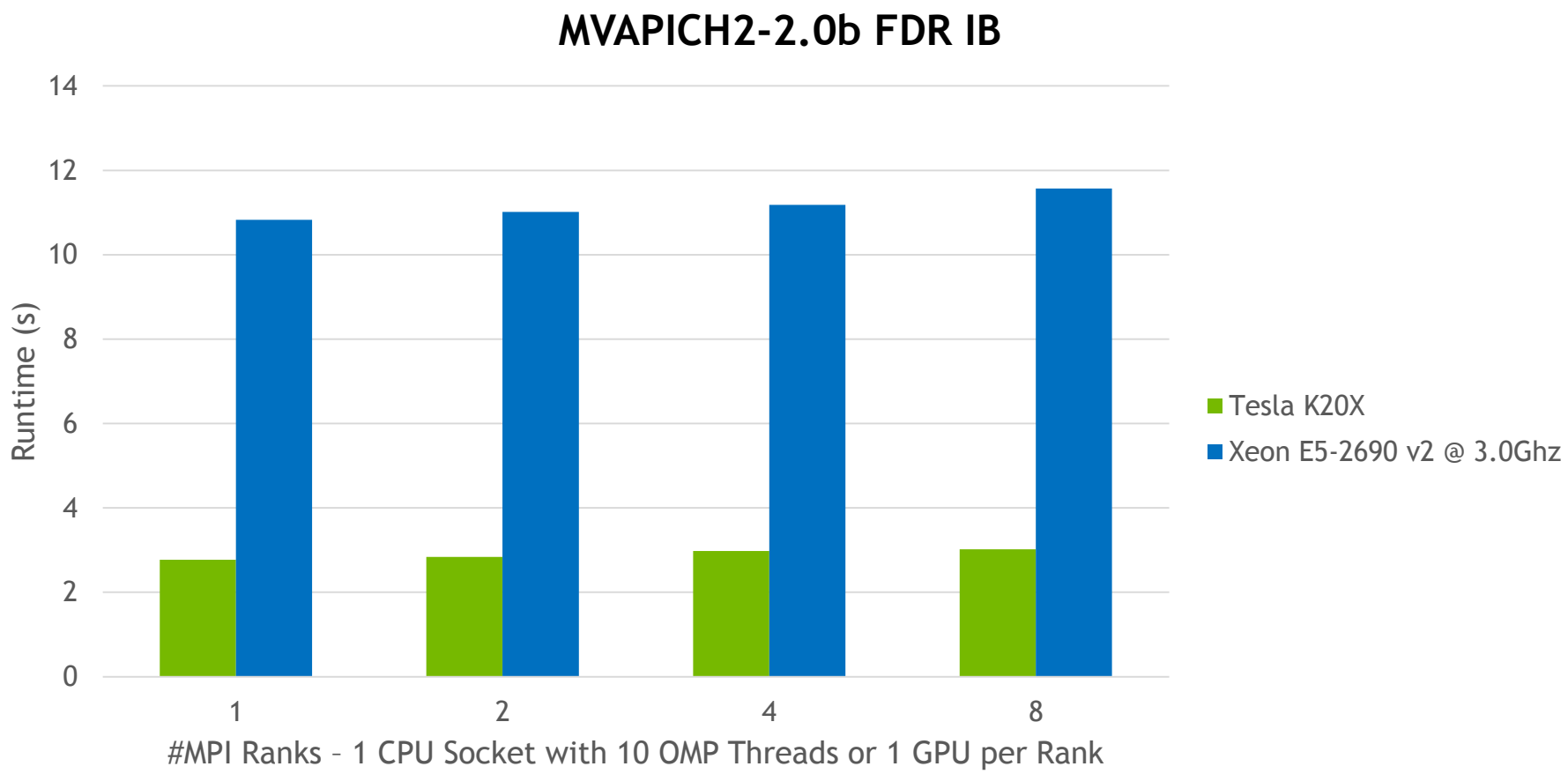
- Launch one process per GPU
  - MVAPICH: `MV2_USE_CUDA`

```
$ MV2_USE_CUDA=1 mpirun -np ${np} ./myapp <args>
```

  - Open MPI: CUDA-aware features are enabled per default
  - Cray: `MPICH_RDMA_ENABLED_CUDA`
  - IBM Platform MPI: `PMPI_GPU_AWARE`

JACOBI RESULTS (1000 STEPS)

WEAK SCALING 4K X 4K PER PROCESS



EXAMPLE: JACOBI – TOP/BOTTOM HALO UPDATE – WITHOUT CUDA-AWARE MPI

OpenACC

```
#pragma acc update host( u_new[1:m-2], u_new[(n-2)*m+1:m-2] )
MPI_Sendrecv(u_new+offset_first_row, m-2, MPI_DOUBLE, t_nb, 0,
             u_new+offset_bottom_bondary, m-2, MPI_DOUBLE, b_nb, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
MPI_Sendrecv(u_new+offset_last_row, m-2, MPI_DOUBLE, b_nb, 1,
             u_new+offset_top_bondary, m-2, MPI_DOUBLE, t_nb, 1,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
#pragma acc update device( u_new[0:m-2], u_new[(n-2)*m:m-2] )
```

CUDA

```
//send to bottom and receive from top - top bottom omitted

cudaMemcpy(u_new+1, u_new_d+1, (m-2)*sizeof(double), cudaMemcpyDeviceToHost);
MPI_Sendrecv(u_new+offset_first_row, m-2, MPI_DOUBLE, t_nb, 0,
             u_new+offset_bottom_bondary, m-2, MPI_DOUBLE, b_nb, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
cudaMemcpy(u_new_d, u_new, (m-2)*sizeof(double), cudaMemcpyDeviceToHost);
```

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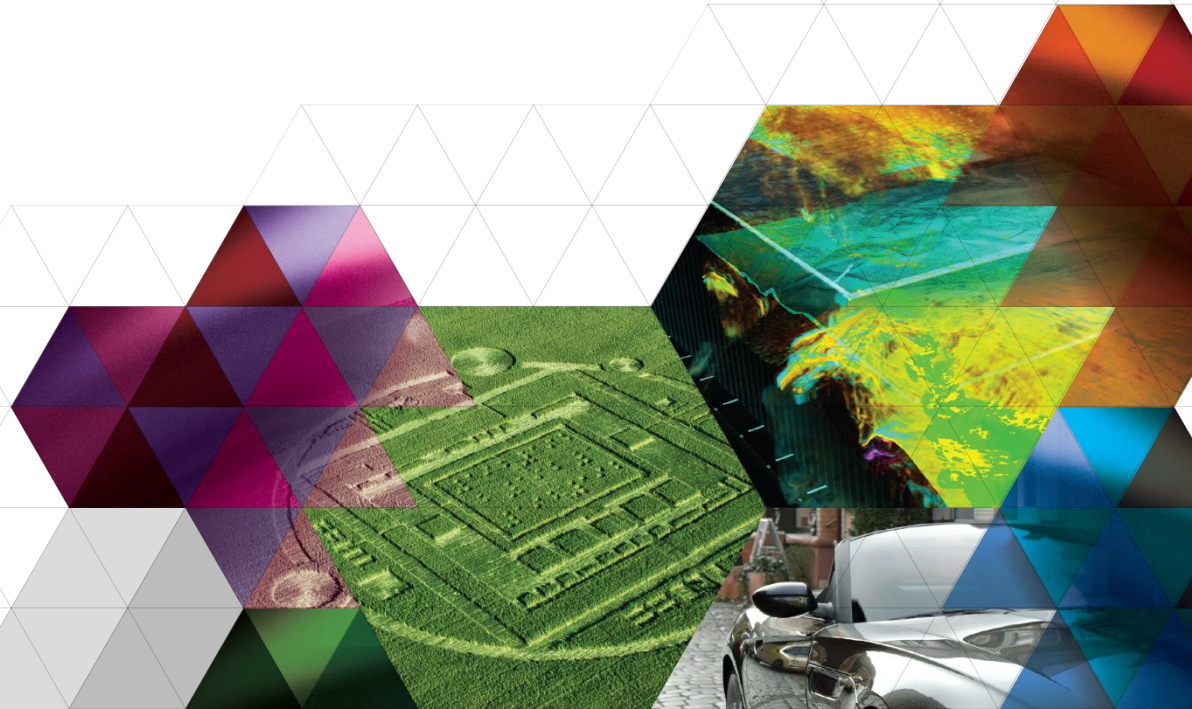
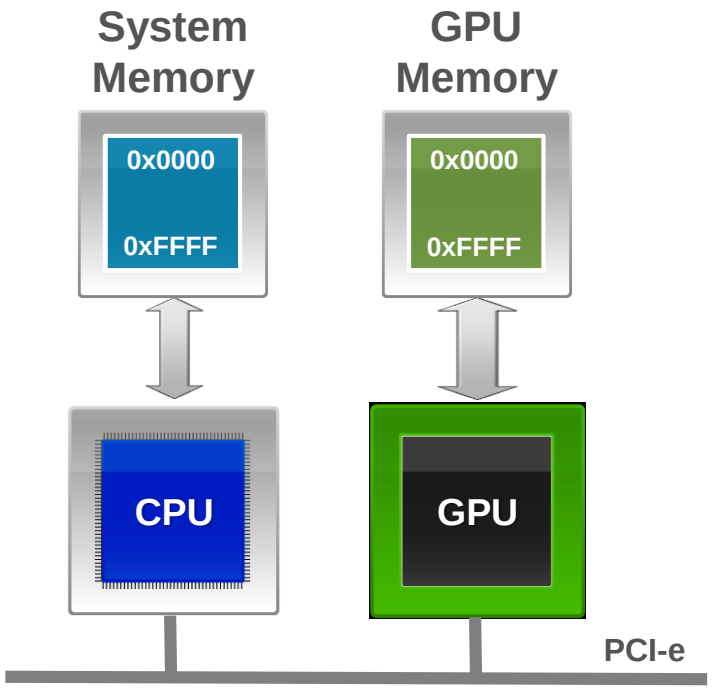
THE DETAILS

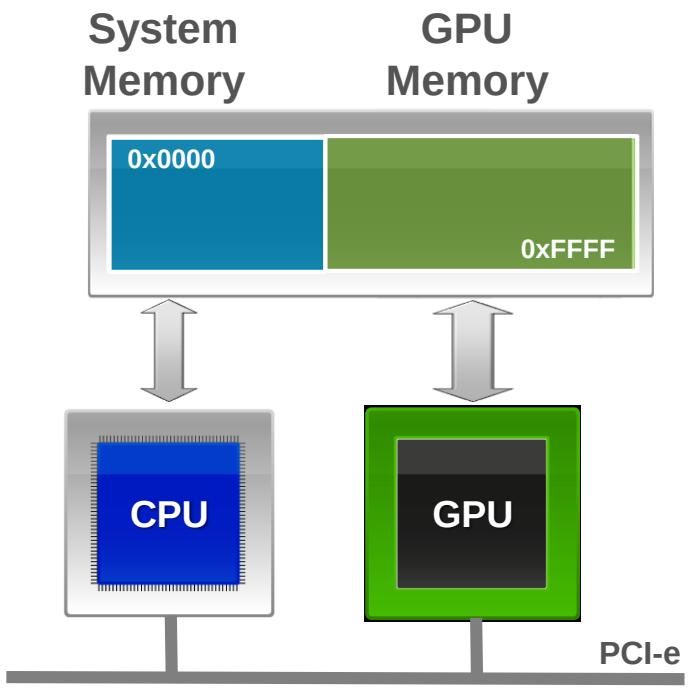


UNIFIED VIRTUAL ADDRESSING

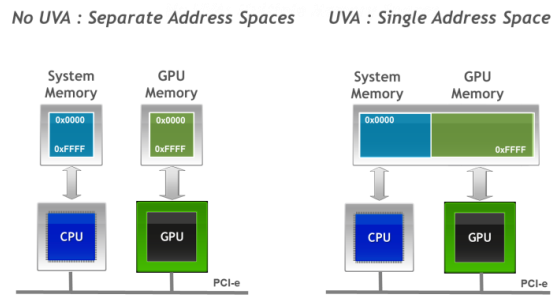
No UVA : Separate Address Spaces



UVA : Single Address Space

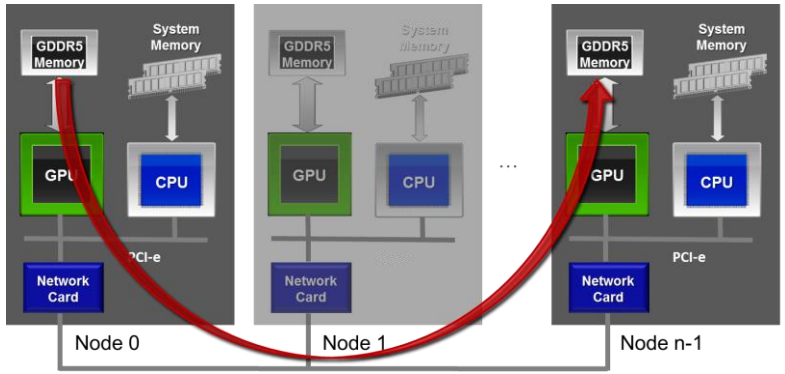


UNIFIED VIRTUAL ADDRESSING



- 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 and cudaMemcpy)
- Supported on devices with compute capability 2.0 for
  - 64-bit applications on Linux and on Windows also TCC mode

MPI+CUDA



With UVA and CUDA-aware MPI

```
//MPI rank 0
MPI_Send(s_buf_d,size,…);

//MPI rank n-1
MPI_Recv(r_buf_d,size,…);
```

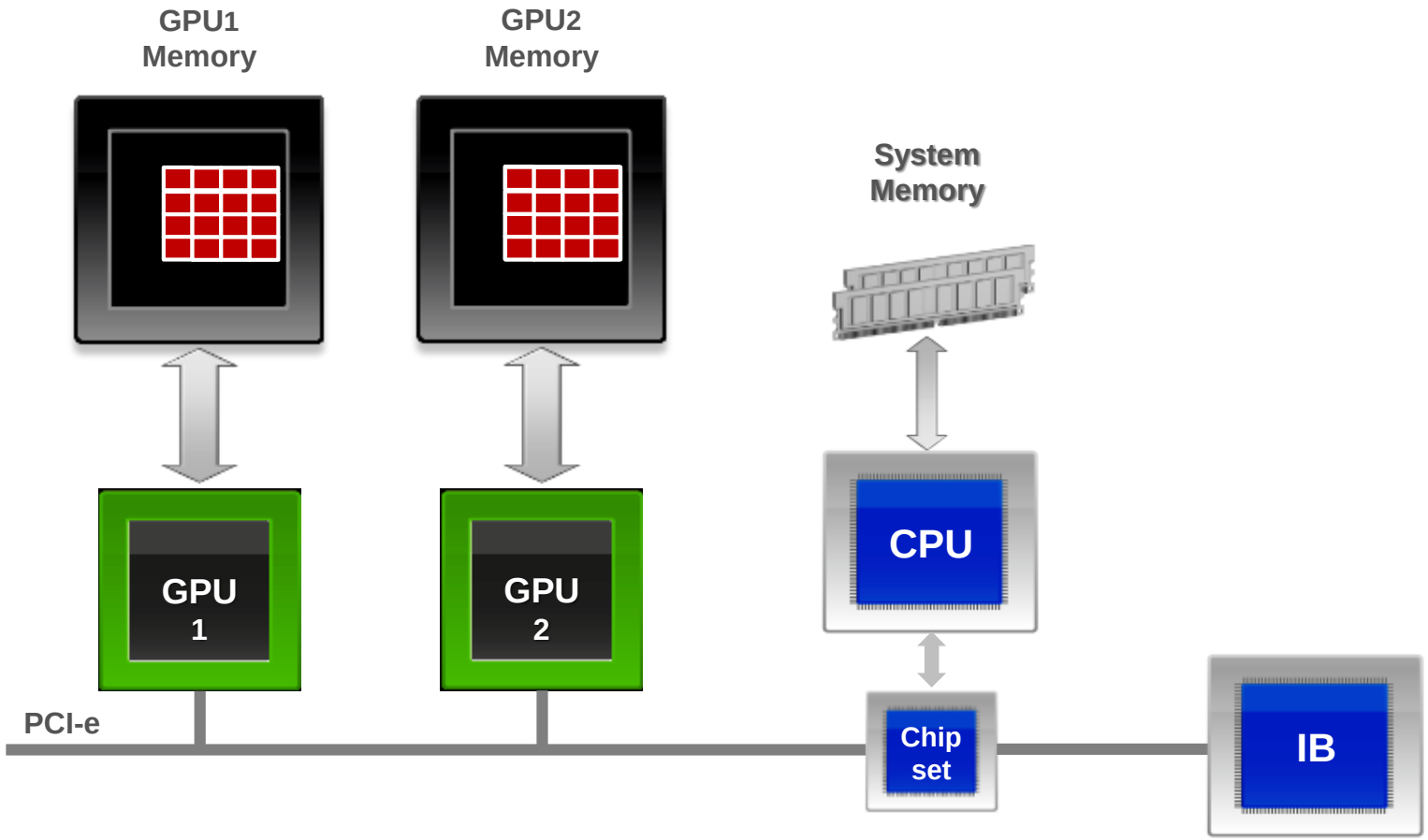
No UVA and regular MPI

```
//MPI rank 0
cudaMemcpy(s_buf_h,s_buf_d,size,…);
MPI_Send(s_buf_h,size,…);

//MPI rank n-1
MPI_Recv(r_buf_h,size,…);
cudaMemcpy(r_buf_d,r_buf_h,size,…);
```

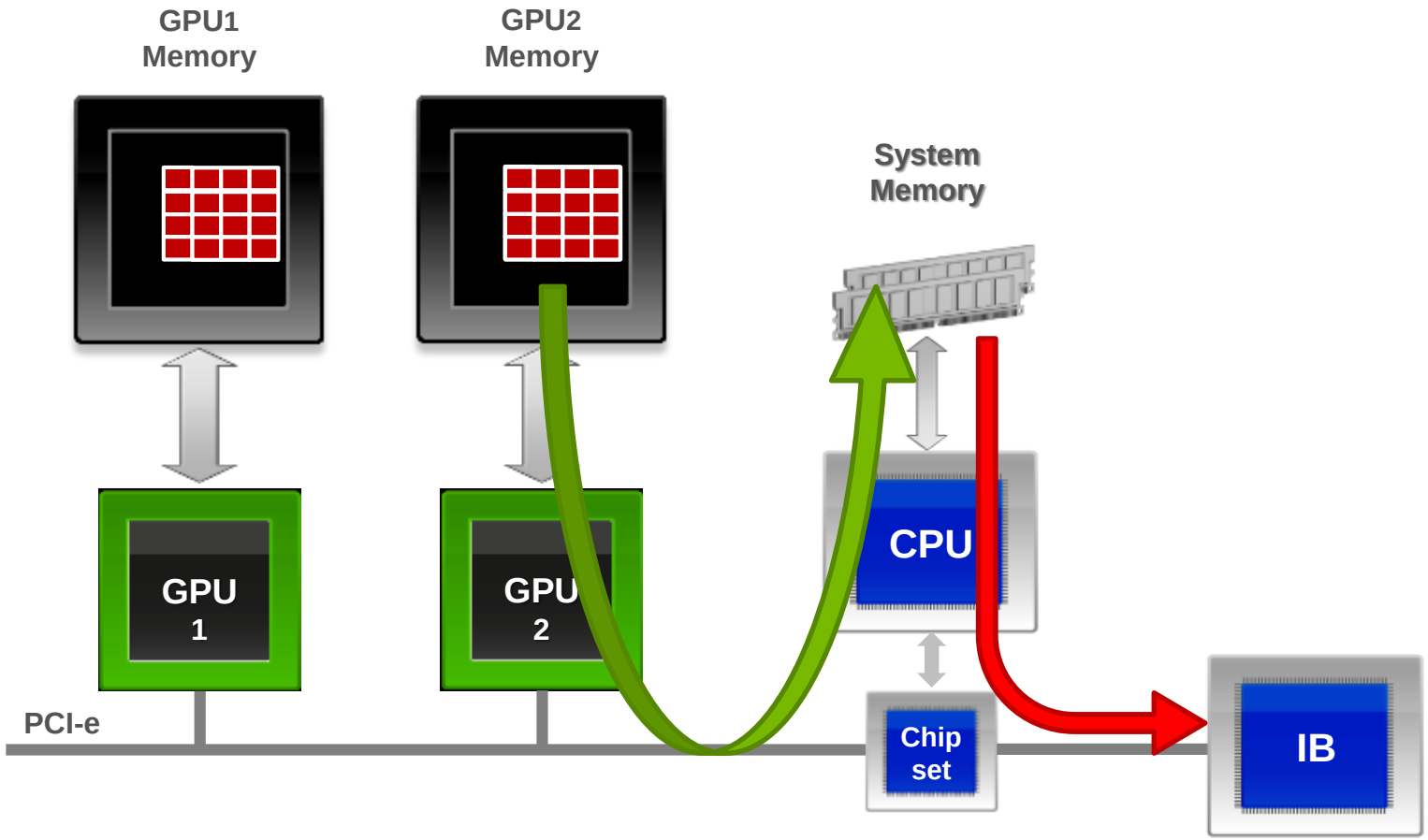
NVIDIA GPUDIRECT™

ACCELERATED COMMUNICATION WITH NETWORK & STORAGE DEVICES



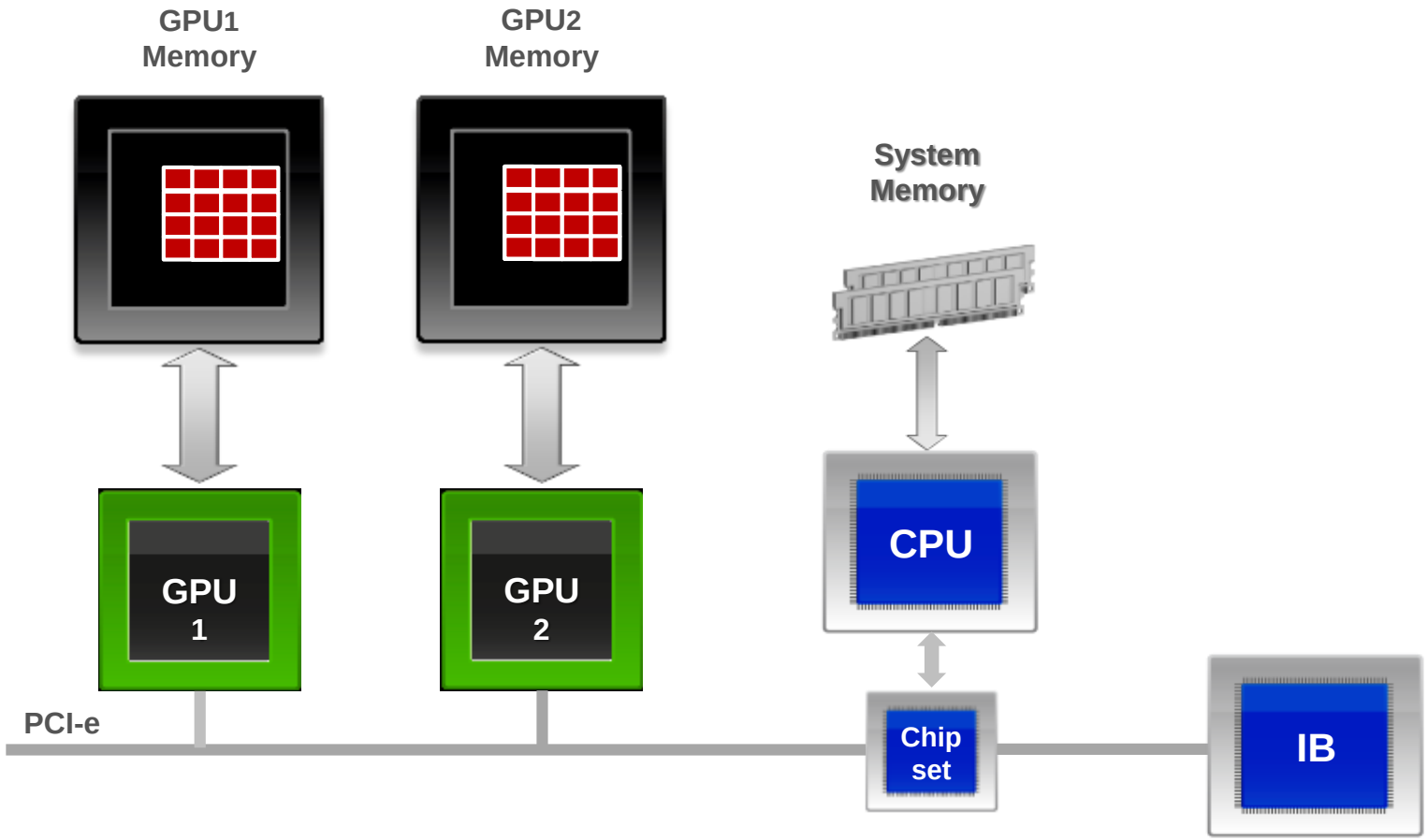
NVIDIA GPUDIRECT™

ACCELERATED COMMUNICATION WITH NETWORK & STORAGE DEVICES



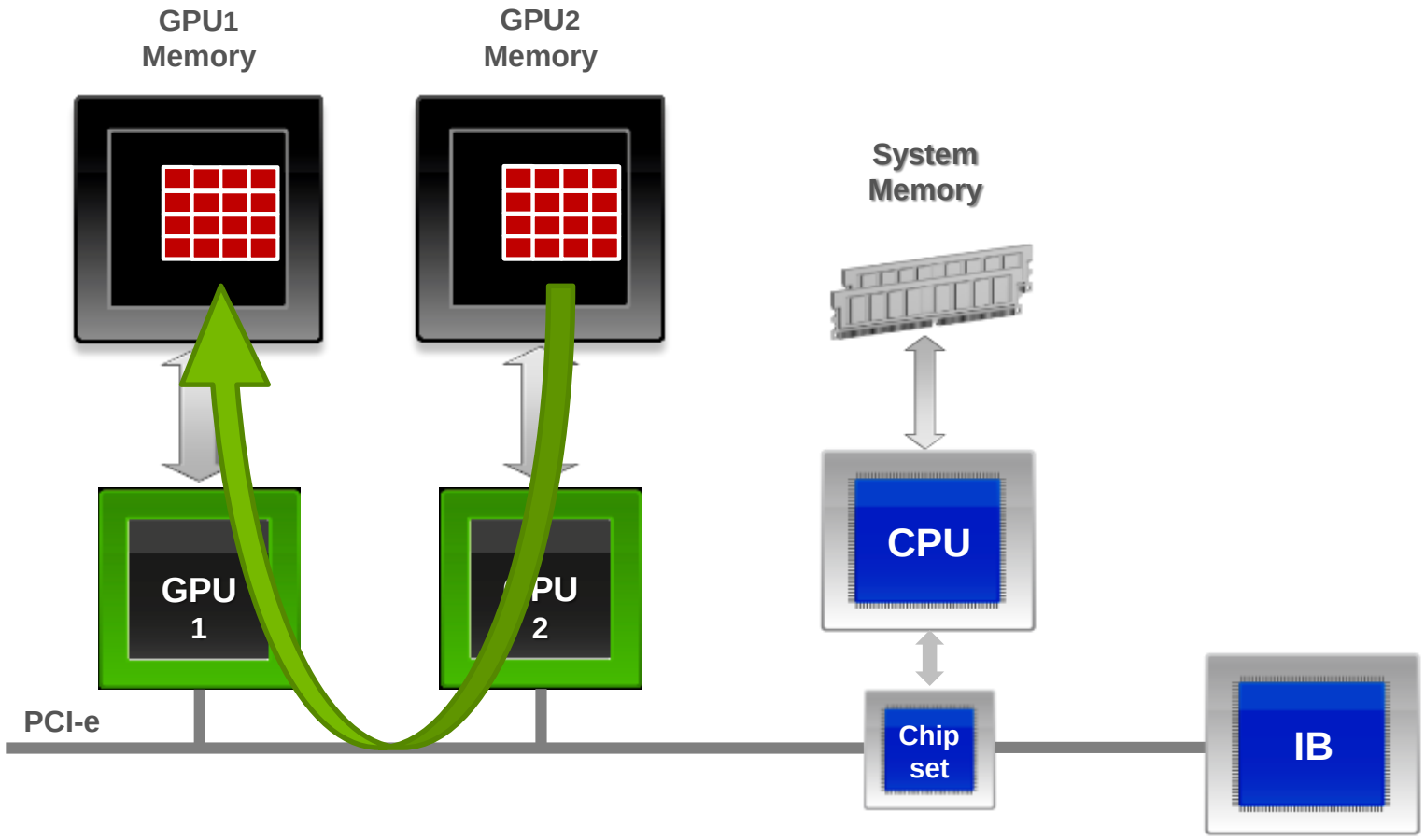
NVIDIA GPUDIRECT™

PEER TO PEER TRANSFERS



NVIDIA GPUDIRECT™

PEER TO PEER TRANSFERS



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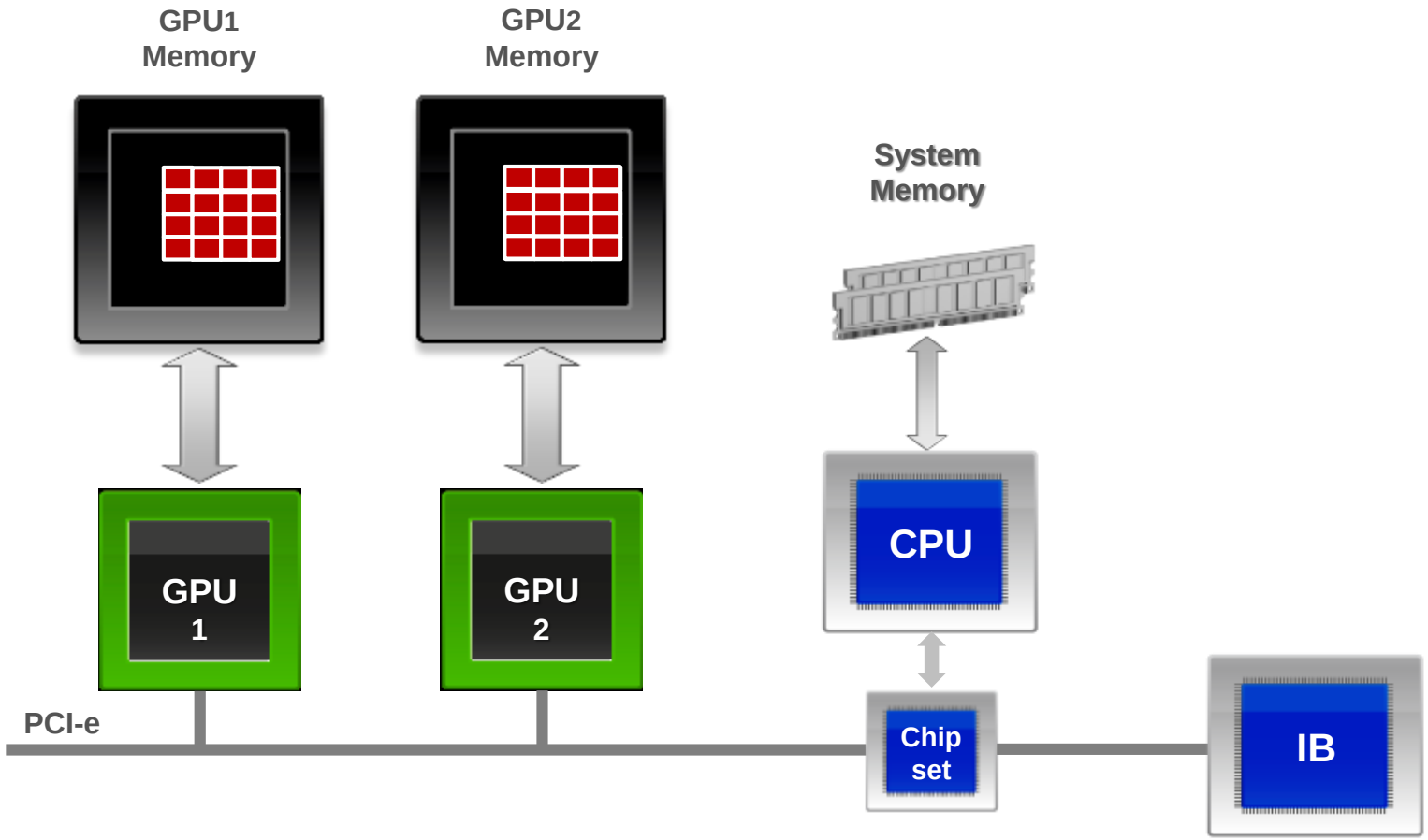
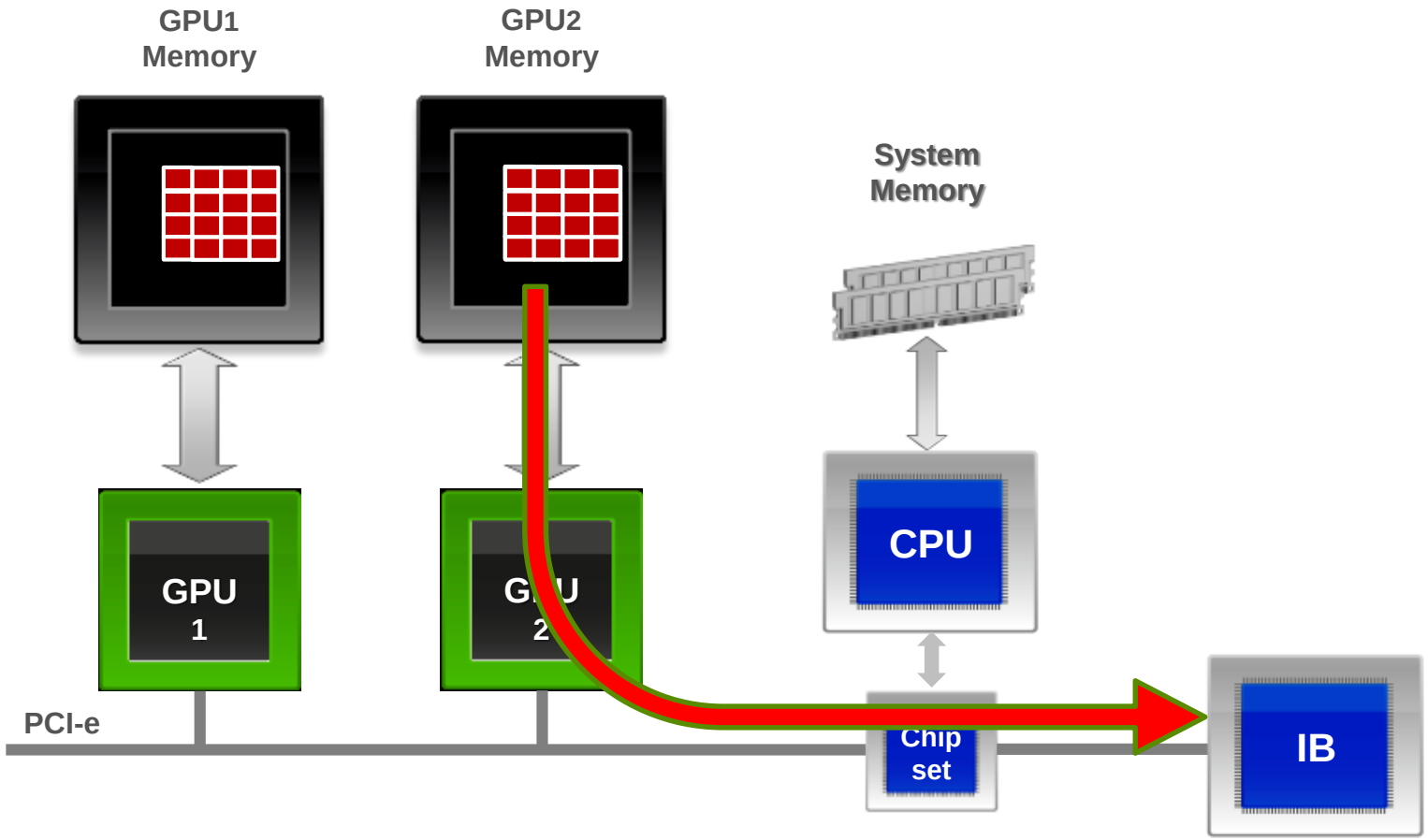
SUPPORT FOR RDMA



NVIDIA GPUDIRECT™

SUPPORT FOR RDMA



CUDA-AWARE MPI

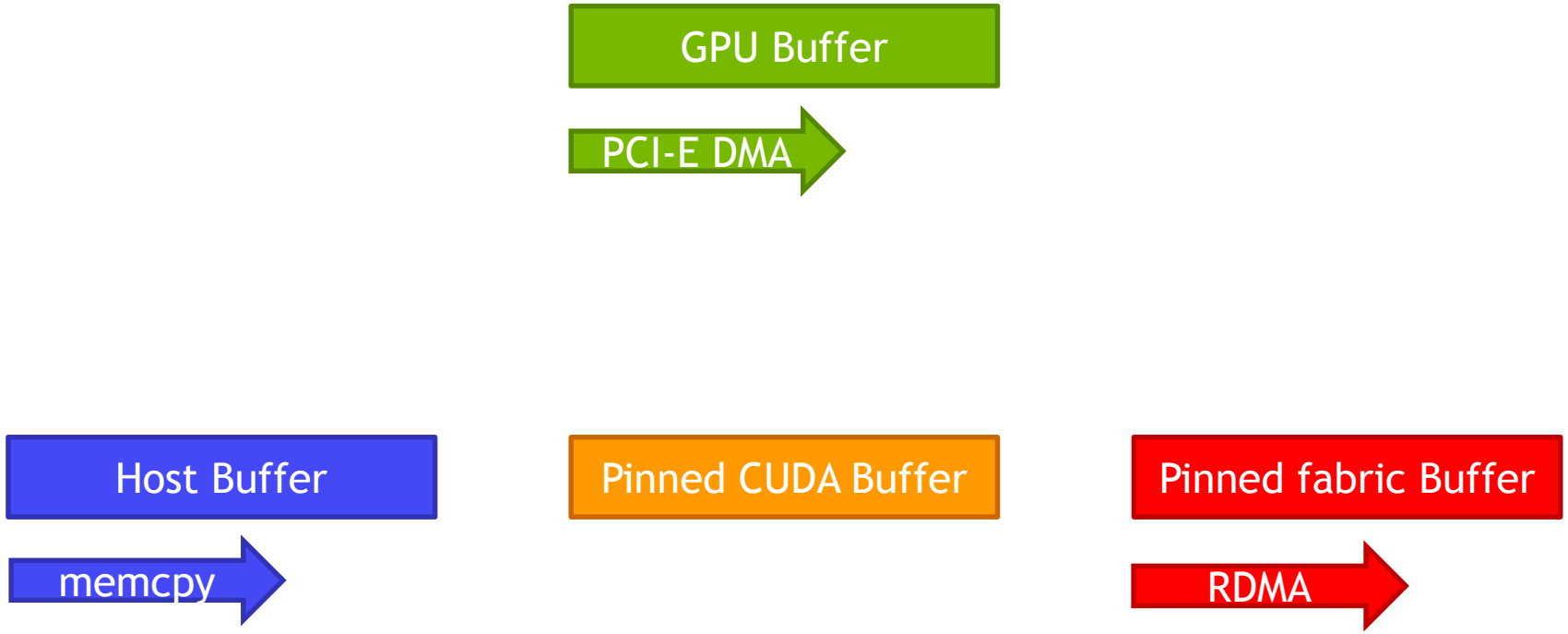
Example:

MPI Rank 0 MPI_Send from GPU Buffer

MPI Rank 1 MPI_Recv to GPU Buffer

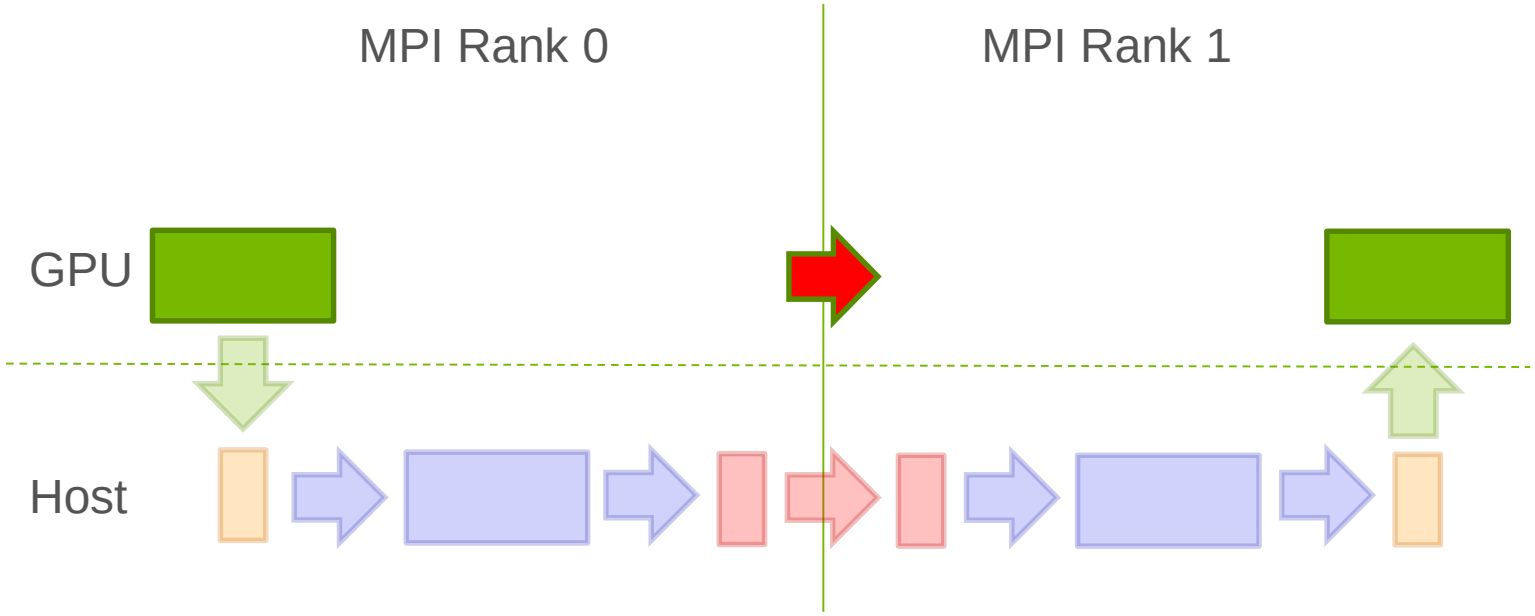
- Show how CUDA+MPI works in principle
  - Depending on the MPI implementation, message size, system setup, … situation might be different
- Two GPUs in two nodes

CUDA-AWARE MPI



MPI GPU TO REMOTE GPU

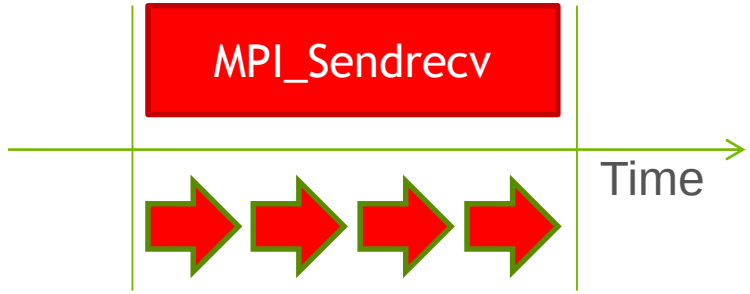
GPUDIRECT SUPPORT FOR RDMA



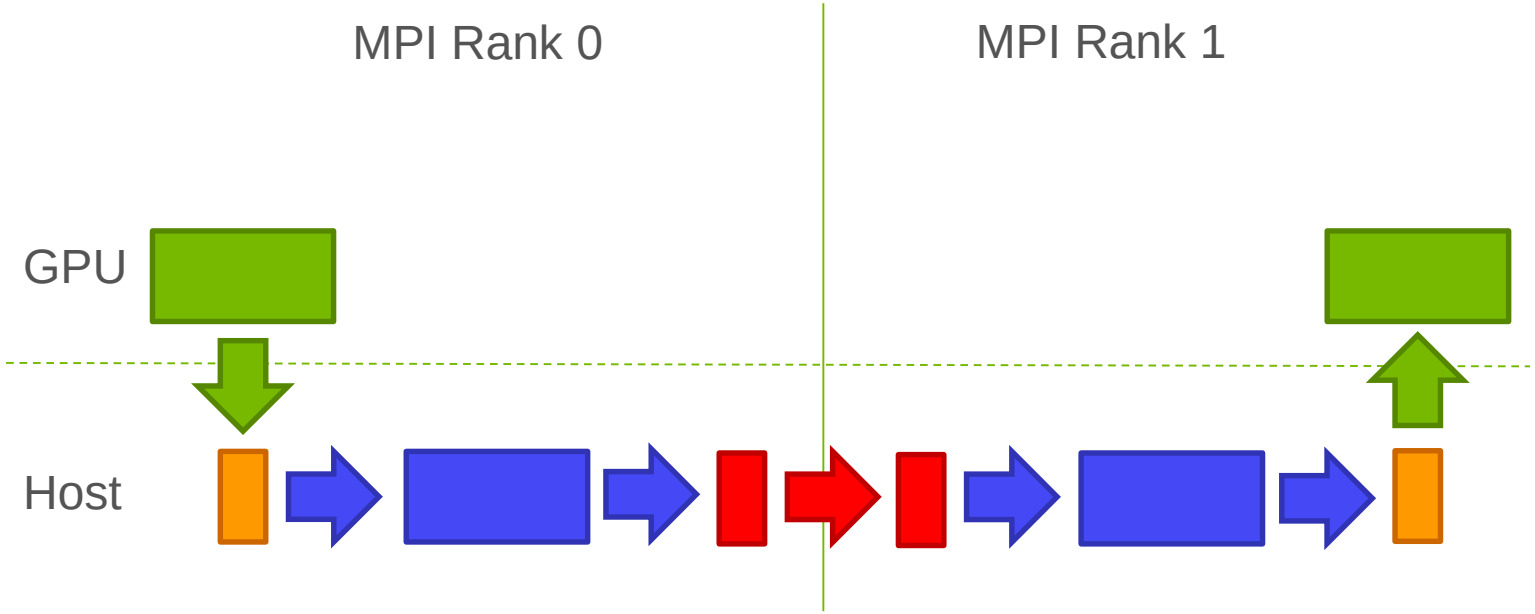

```
MPI_Send(s_buf_d,size,MPI_CHAR,1,tag,MPI_COMM_WORLD);

MPI_Recv(r_buf_d,size,MPI_CHAR,0,tag,MPI_COMM_WORLD,&stat);
```

MPI GPU TO REMOTE GPU

GPUDIRECT SUPPORT FOR RDMA

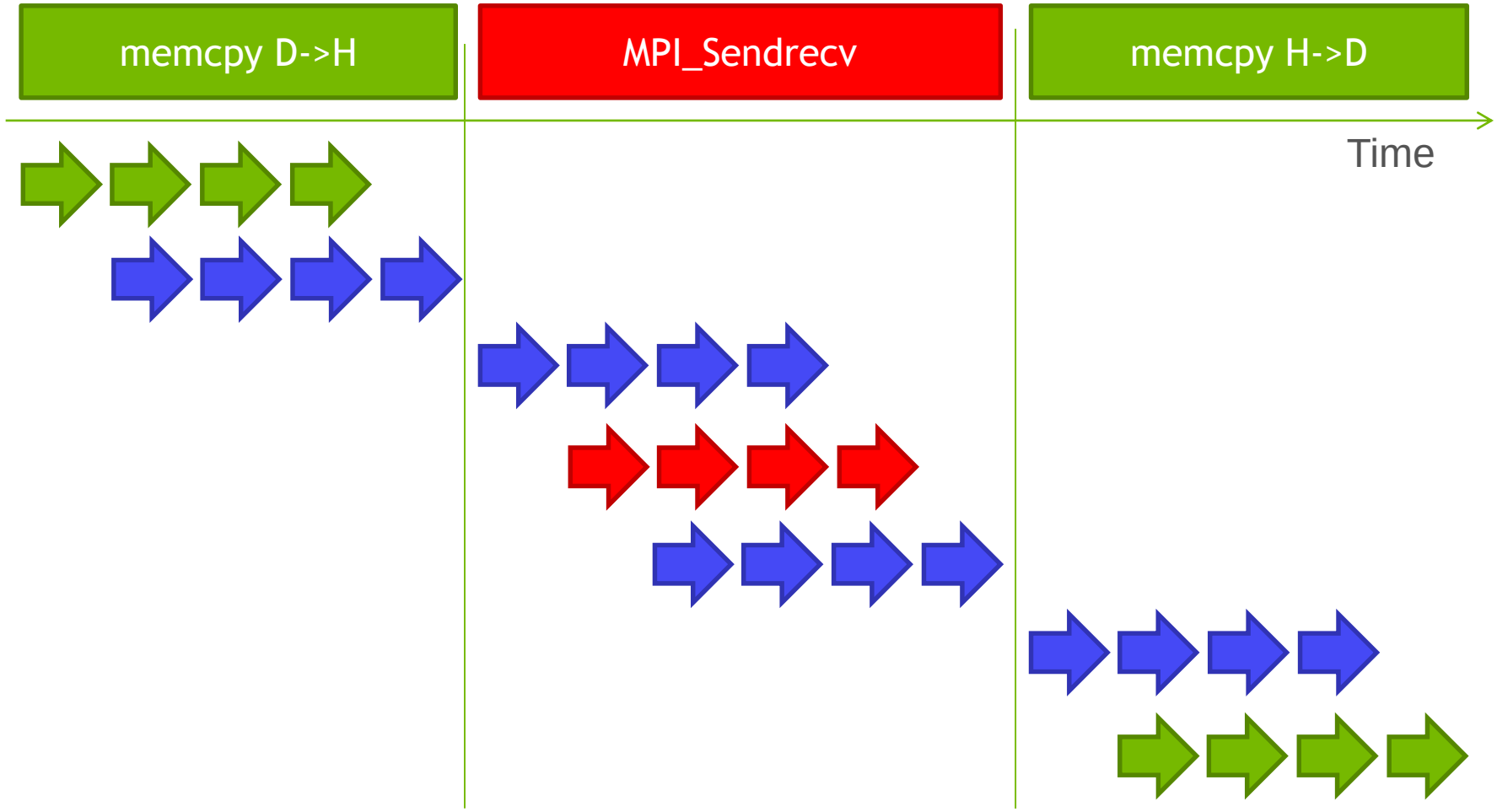


REGULAR MPI GPU TO REMOTE GPU



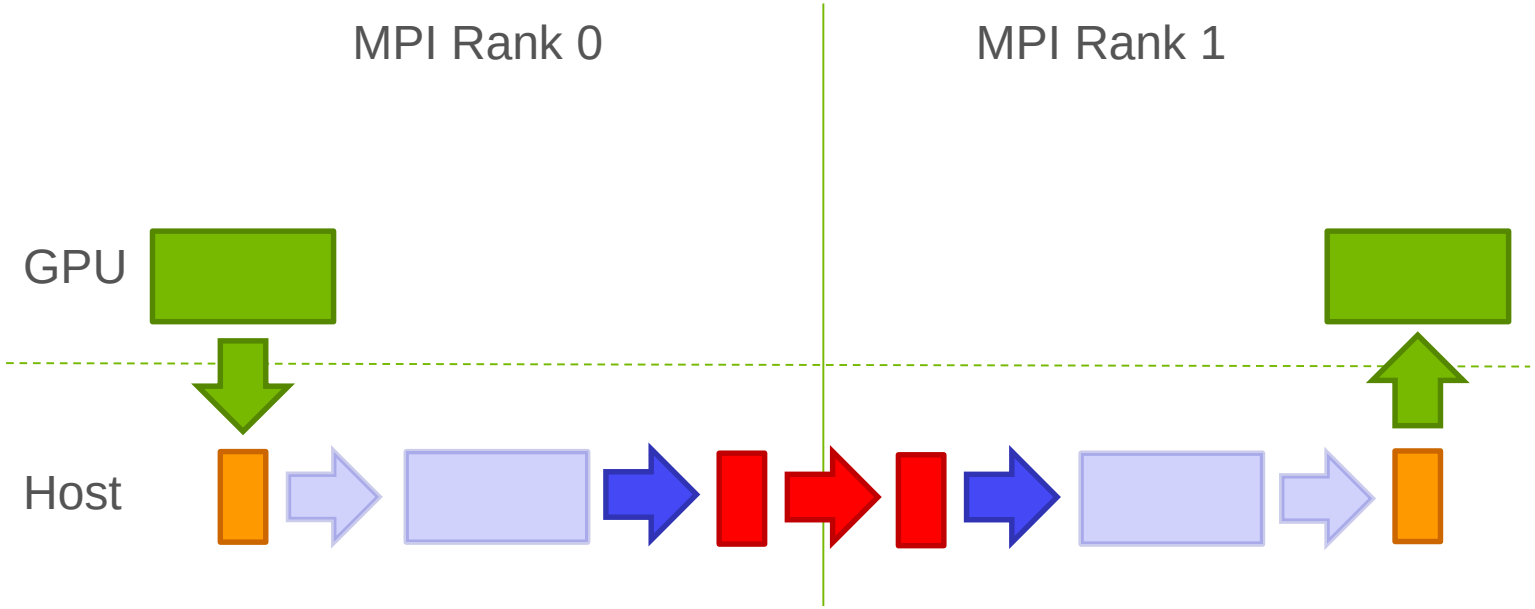

```
cudaMemcpy(s_buf_h,s_buf_d,size,cudaMemcpyDeviceToHost);
MPI_Send(s_buf_h,size,MPI_CHAR,1,tag,MPI_COMM_WORLD);

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

REGULAR MPI GPU TO REMOTE GPU



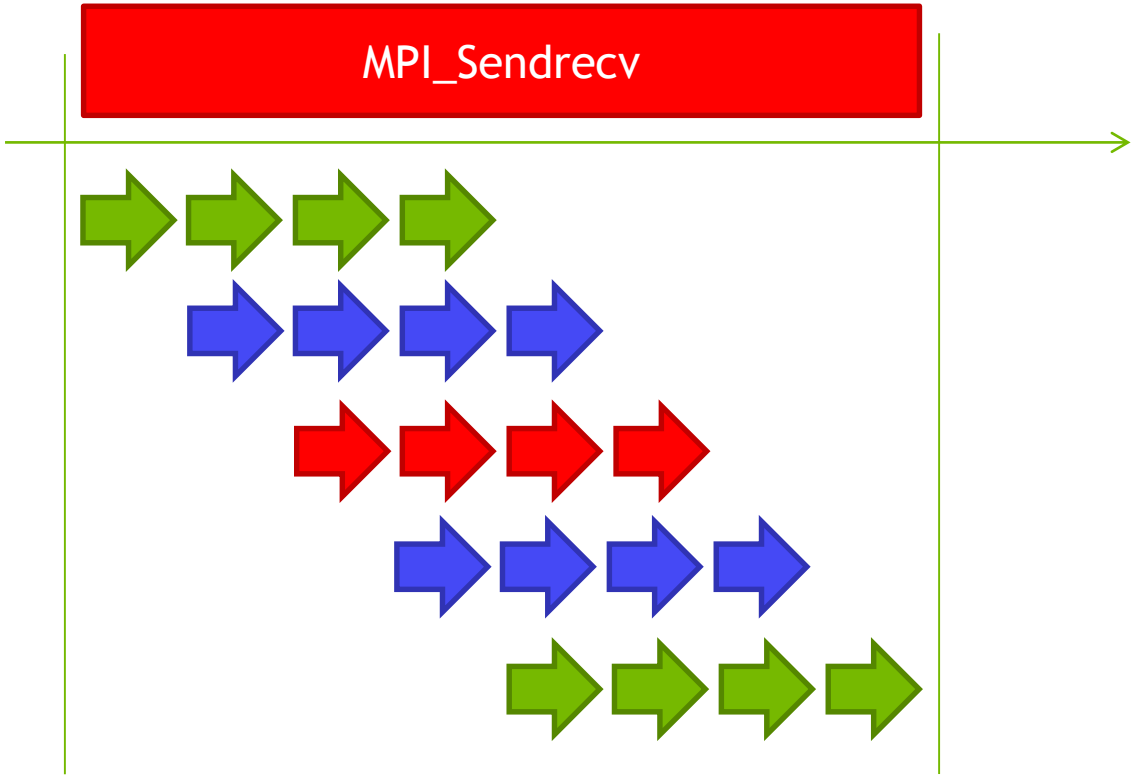
MPI GPU TO REMOTE GPU

WITHOUT GPUDIRECT

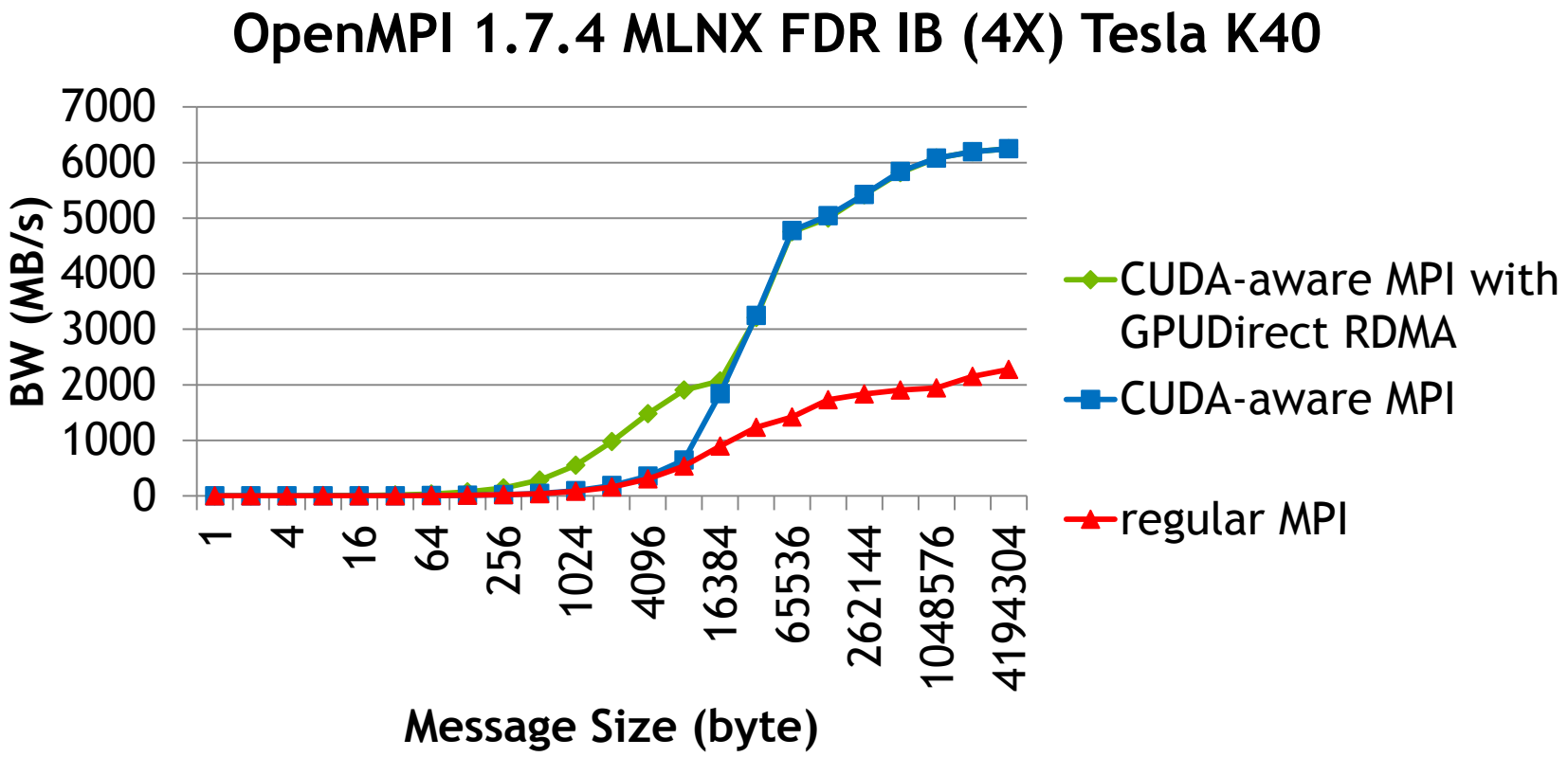



```
MPI_Send(s_buf_h,size,MPI_CHAR,1,tag,MPI_COMM_WORLD);

MPI_Recv(r_buf_h,size,MPI_CHAR,0,tag,MPI_COMM_WORLD,&stat);
```

MPI GPU TO REMOTE GPU
WITHOUT GPUDIRECT



PERFORMANCE RESULTS TWO NODES



Latency (1 byte)	19.04 us	16.91 us	5.52 us

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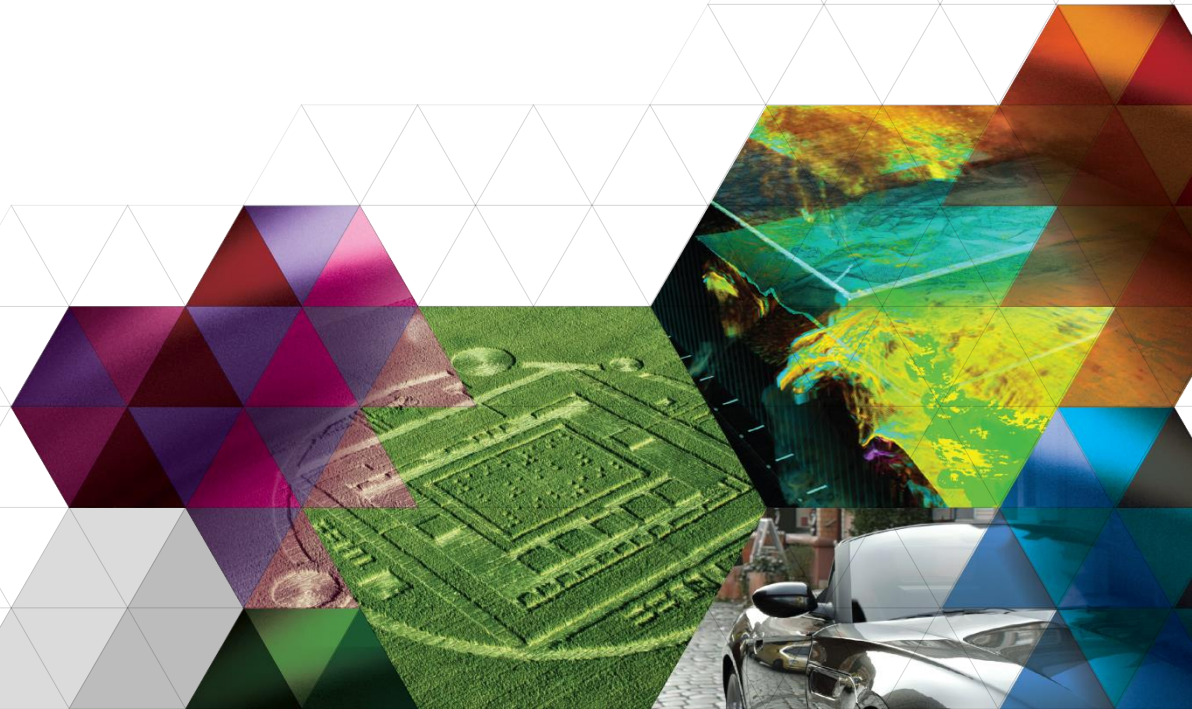
MULTI PROCESS SERVICE (MPS) FOR MPI APPLICATIONS



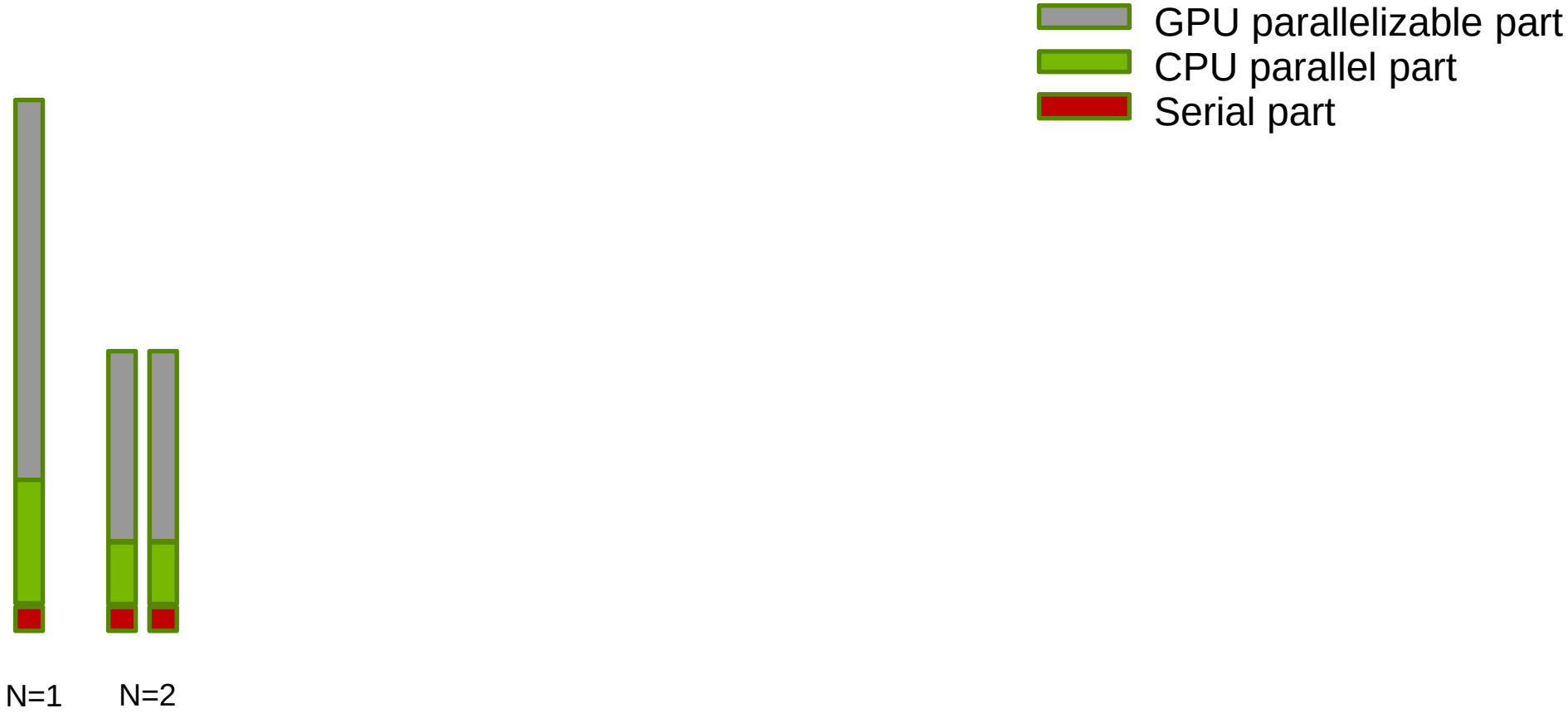
GPU ACCELERATION OF LEGACY MPI APPLICATION

- Typical legacy application
  - MPI parallel
  - Single or few threads per MPI rank (e.g. OpenMP)
- Running with multiple MPI ranks per node
- GPU acceleration in phases
  - Proof of concept prototype, ..
  - Great speedup at kernel level
- Application performance misses expectations

N=1

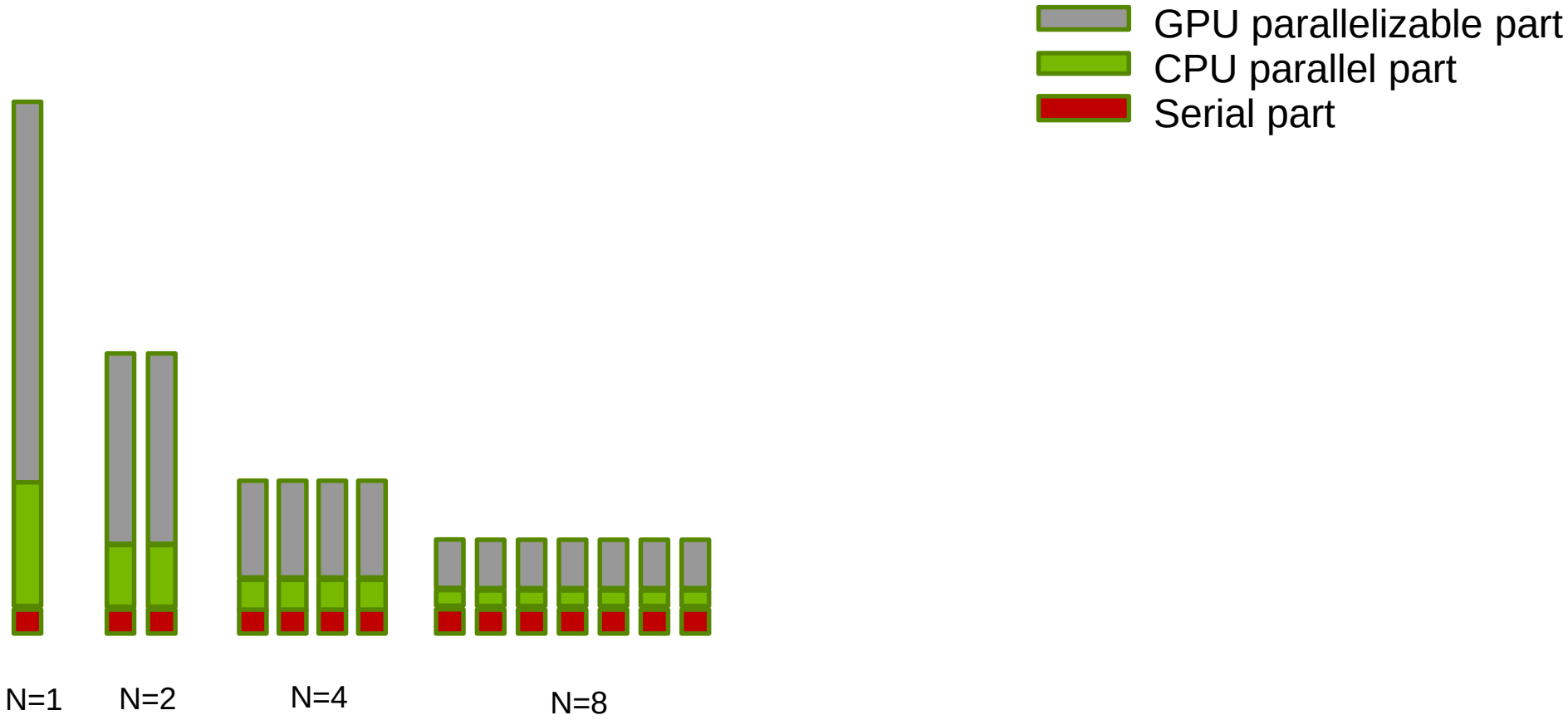
GPU parallelizable part
CPU parallel part
Serial part

Multicore CPU only

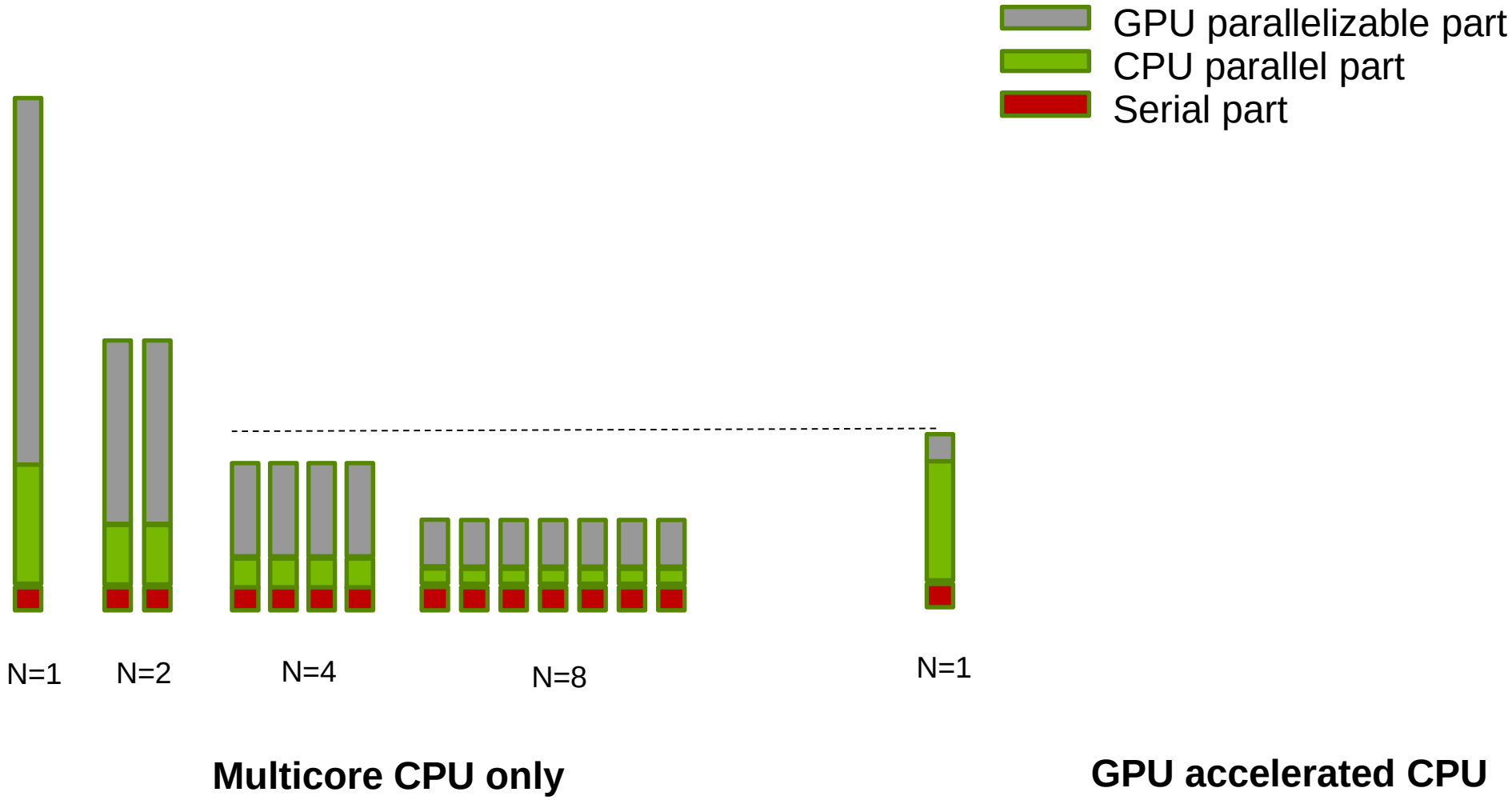


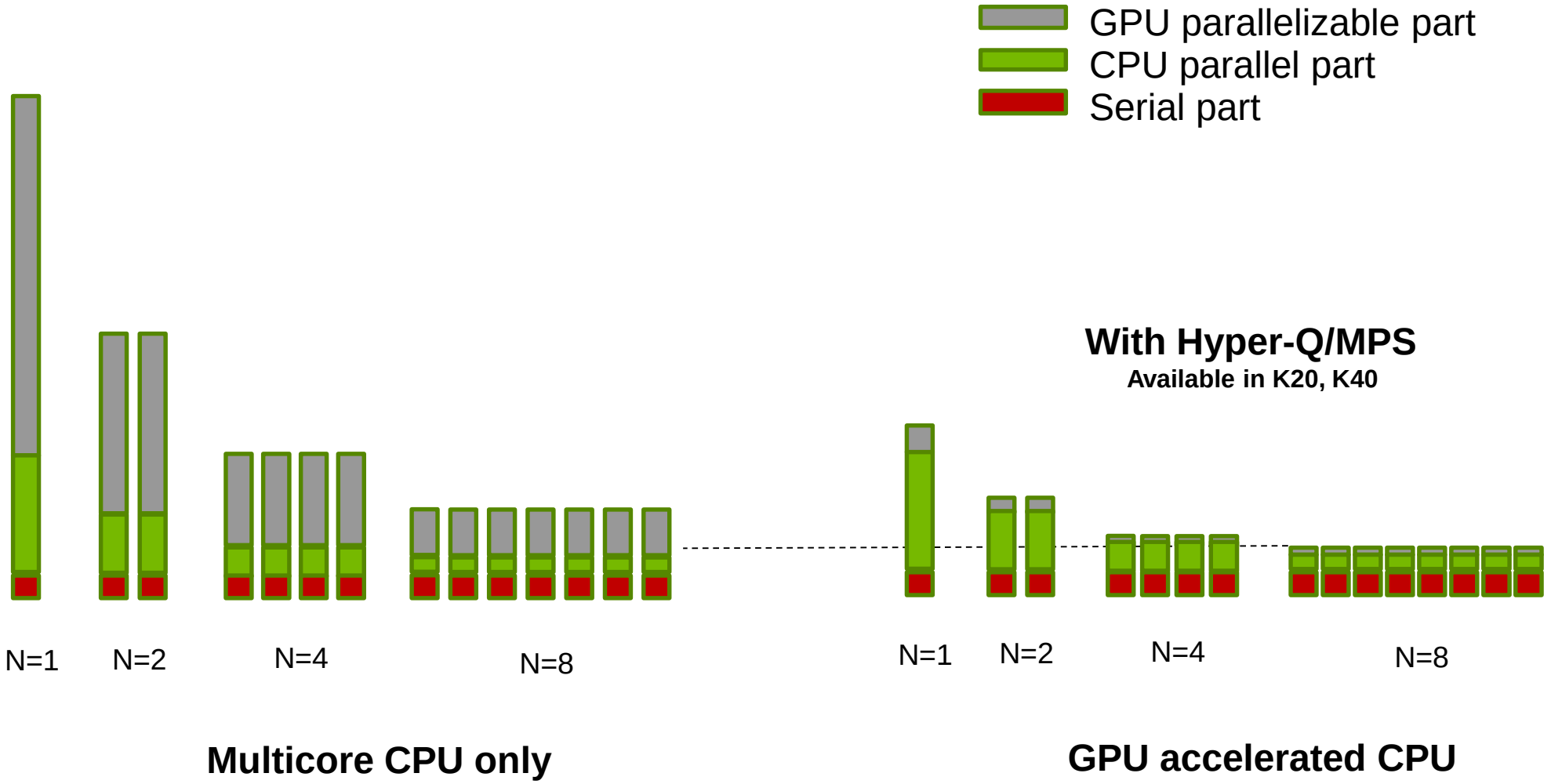
Multicore CPU only

Multicore CPU only

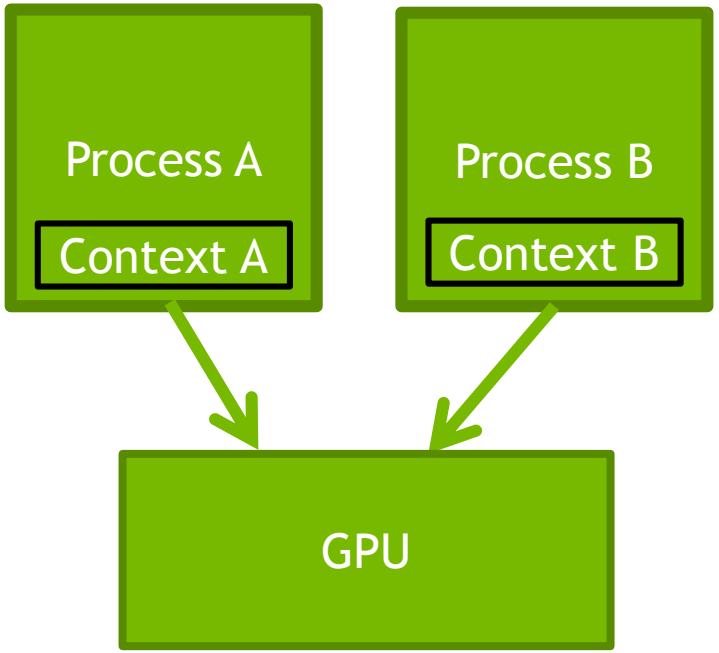


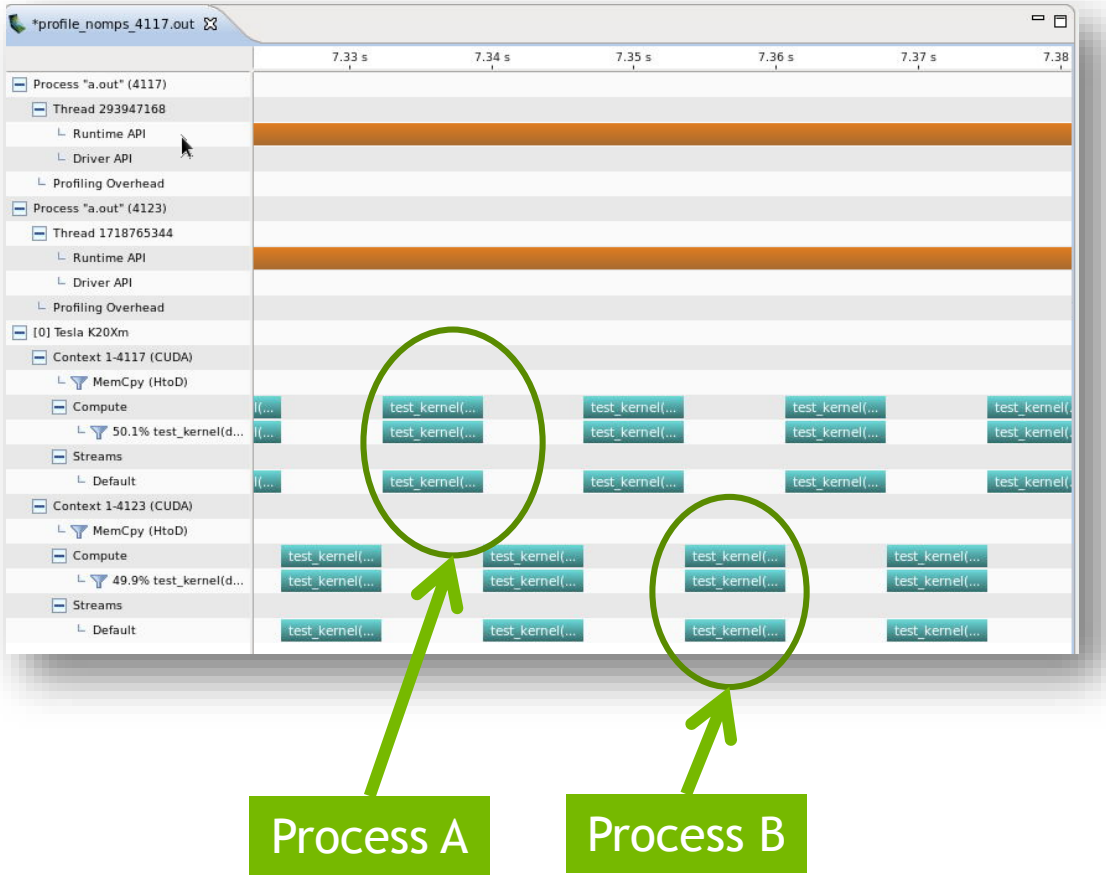
Multicore CPU only



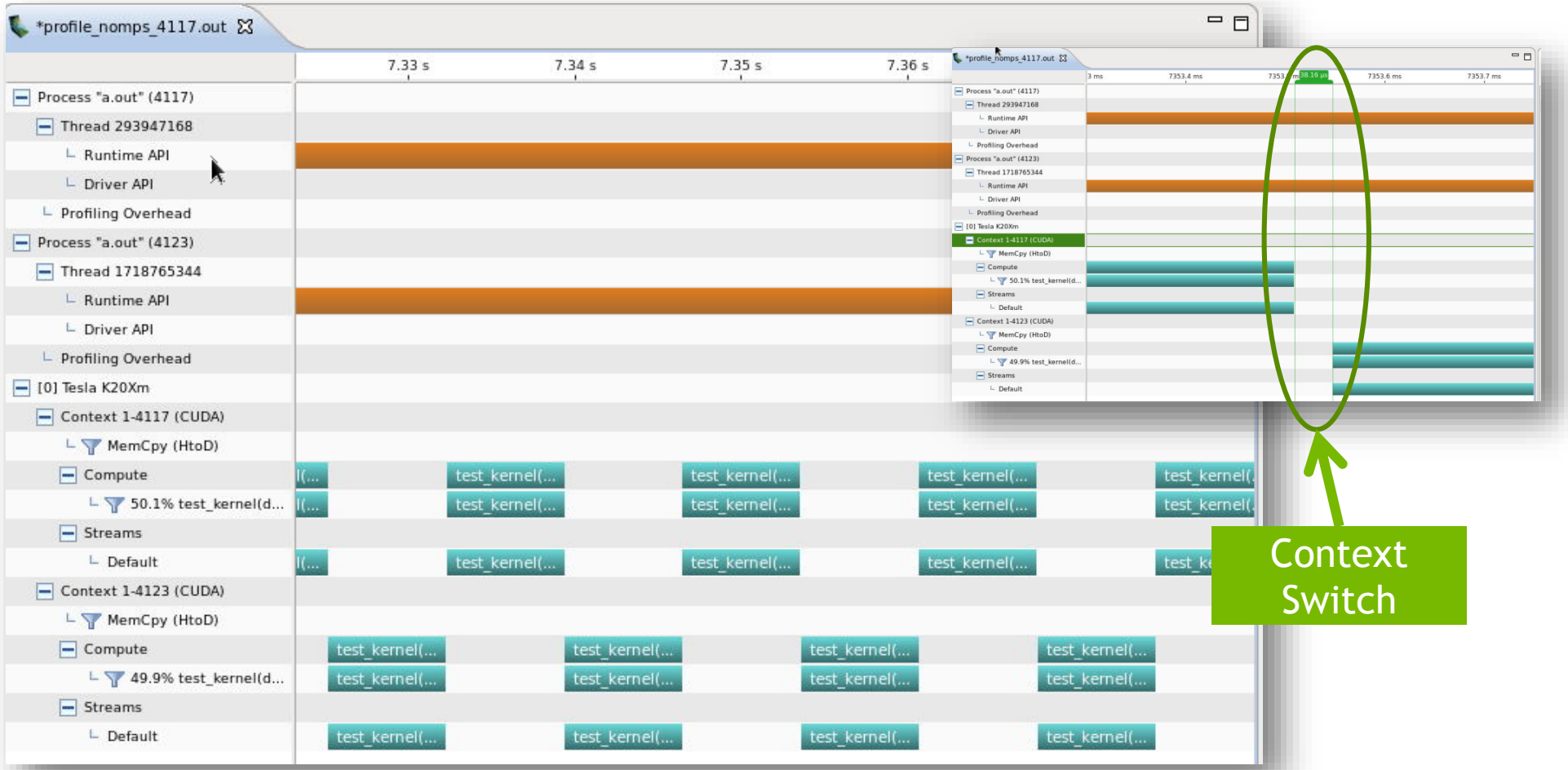


PROCESSES SHARING GPU WITHOUT MPS: NO OVERLAP

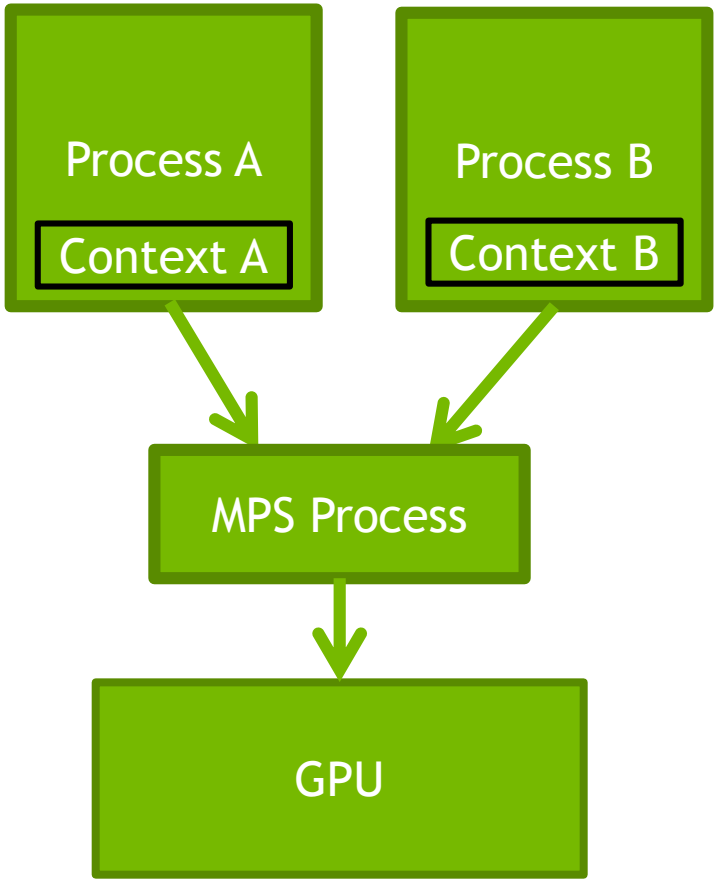


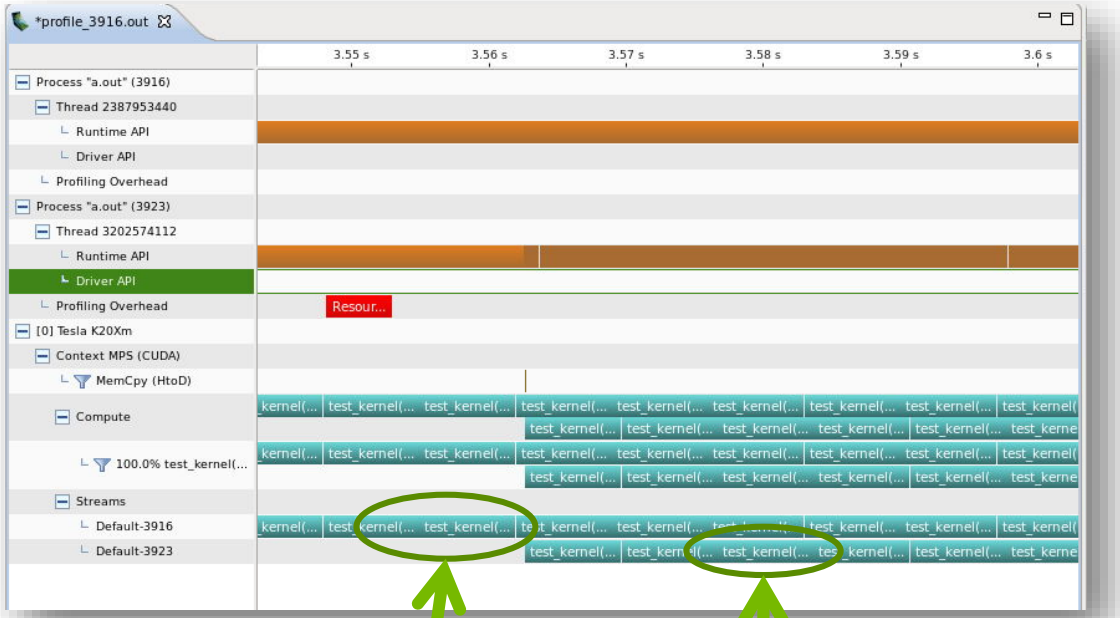


GPU SHARING WITHOUT MPS



PROCESSES SHARING GPU WITH MPS: MAXIMUM OVERLAP

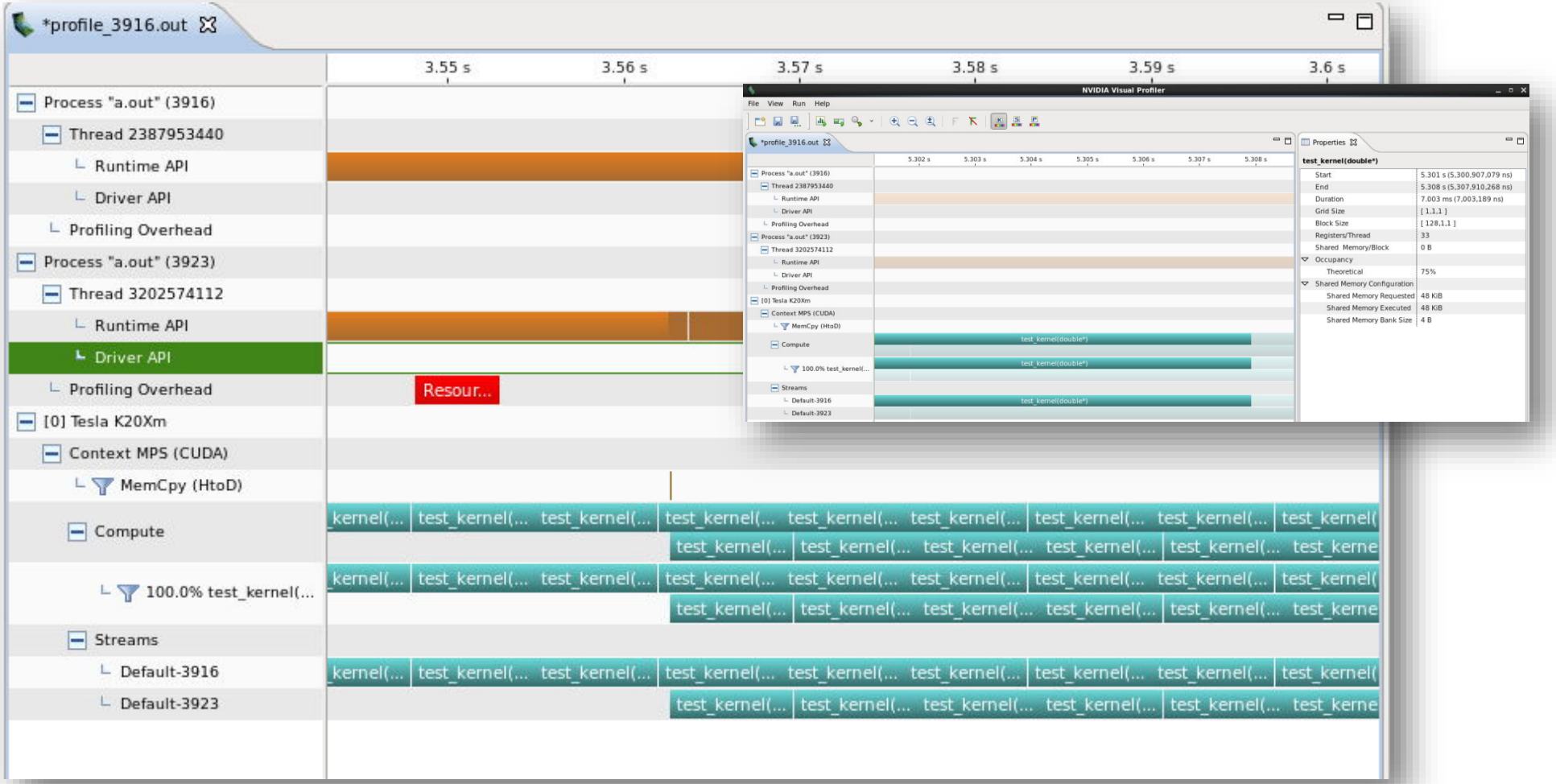




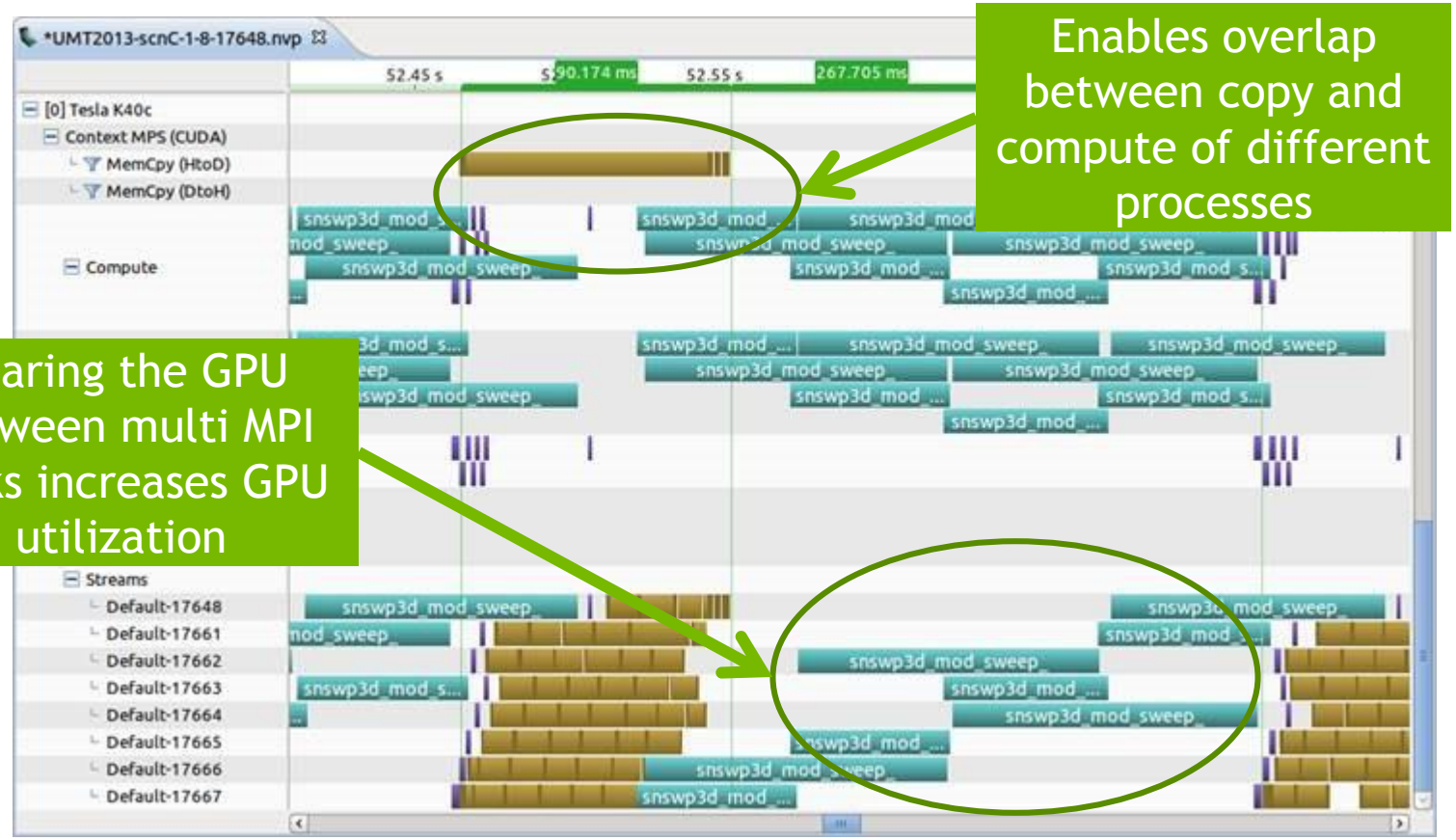
Kernels from Process A

Kernels from Process B

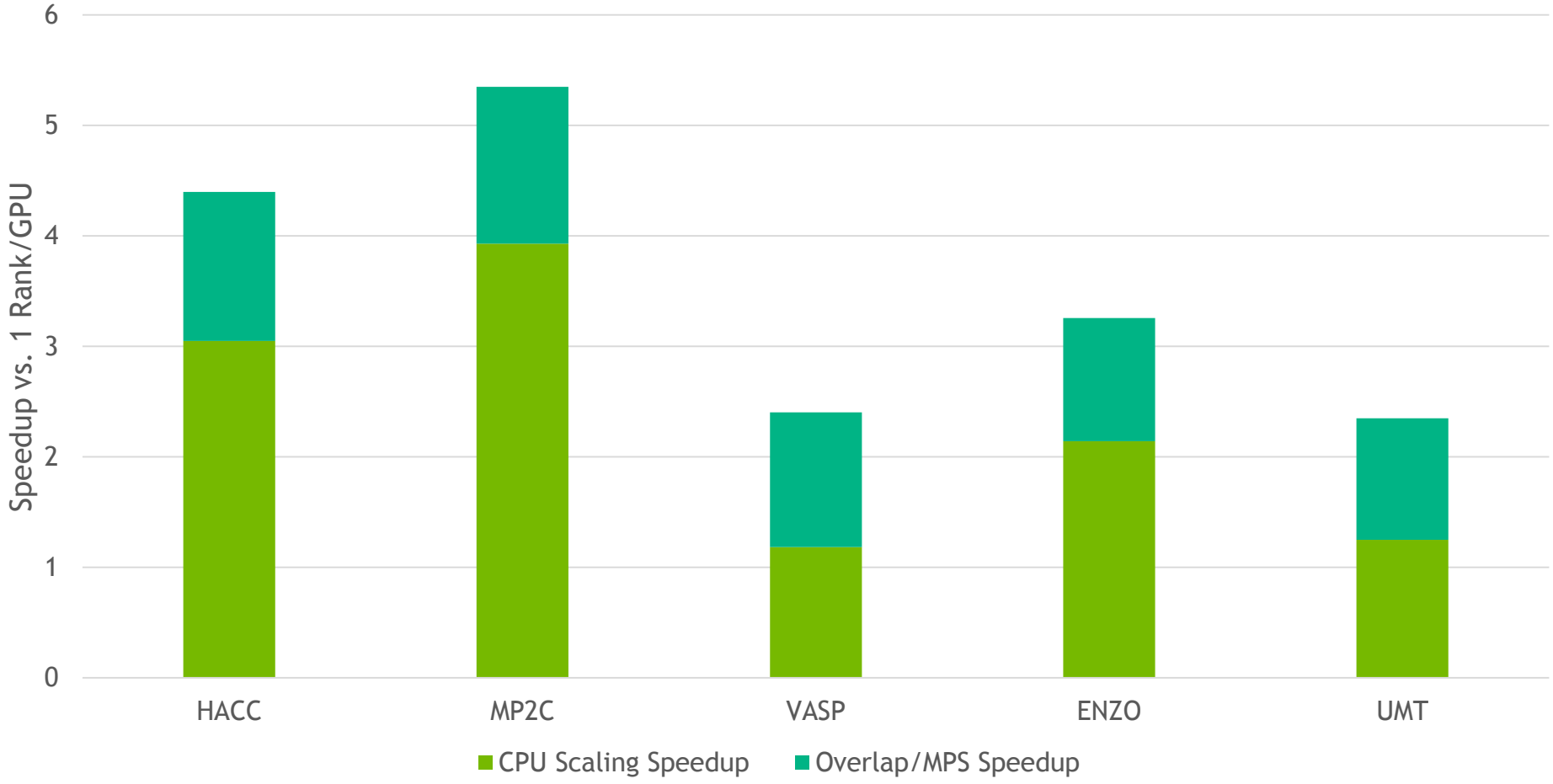
GPU SHARING WITH MPS



CASE STUDY: HYPER-Q/MPS FOR UMT



HYPER-Q/MPS CASE STUDIES



USING MPS

- No application modifications necessary
- Not limited to MPI applications
- MPS control daemon
  - Spawn MPS server upon CUDA application startup

- Typical setup

```
export CUDA_VISIBLE_DEVICES=0
nvidia-smi -i 0 -c EXCLUSIVE_PROCESS
nvidia-cuda-mps-control -d
```

- On Cray XK/XC systems

```
export CRAY_CUDA_MPS=1
```

USING MPS ON MULTI-GPU SYSTEMS

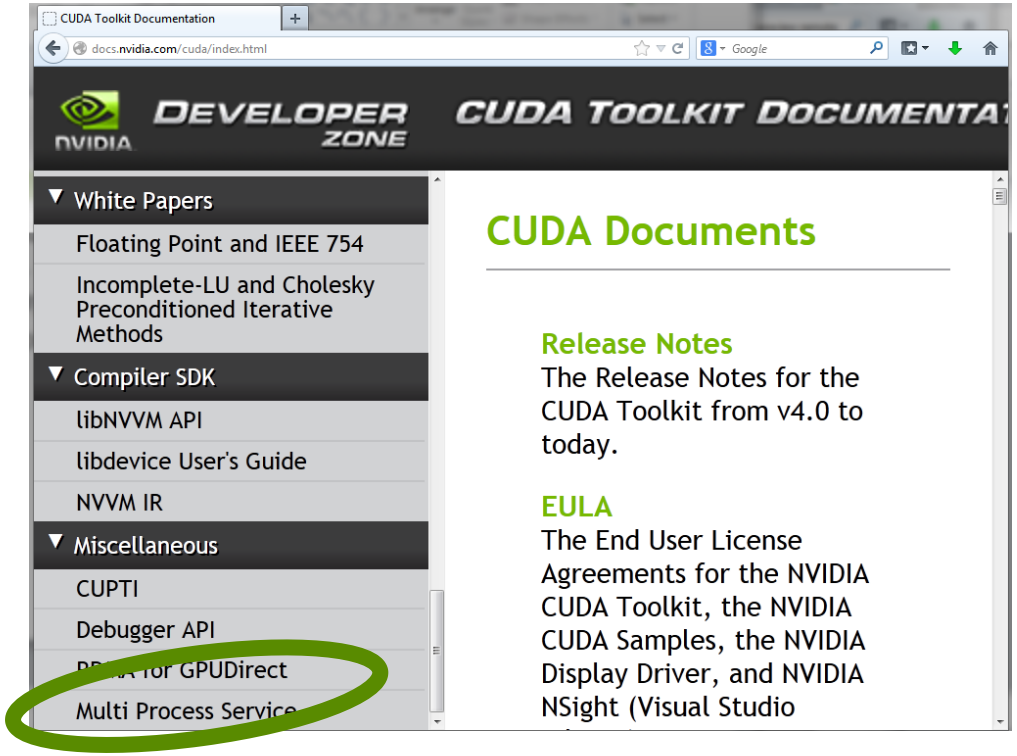
- MPS server only supports a single GPU
  - Use one MPS server per GPU
- Target specific GPU by setting CUDA_VISIBLE_DEVICES
- Adjust pipe/log directory

```
export DEVICE=0
export CUDA_VISIBLE_DEVICES=${DEVICE}
export CUDA_MPS_PIPE_DIRECTORY=${HOME}/mps${DEVICE}/pipe
export CUDA_MPS_LOG_DIRECTORY=${HOME}/mps${DEVICE}/log
cuda_mps_server_control -d
export DEVICE=1    …
```

- More at http://cudamusing.blogspot.de/2013/07/enabling-cuda-multi-process-service-mps.html

MPS SUMMARY

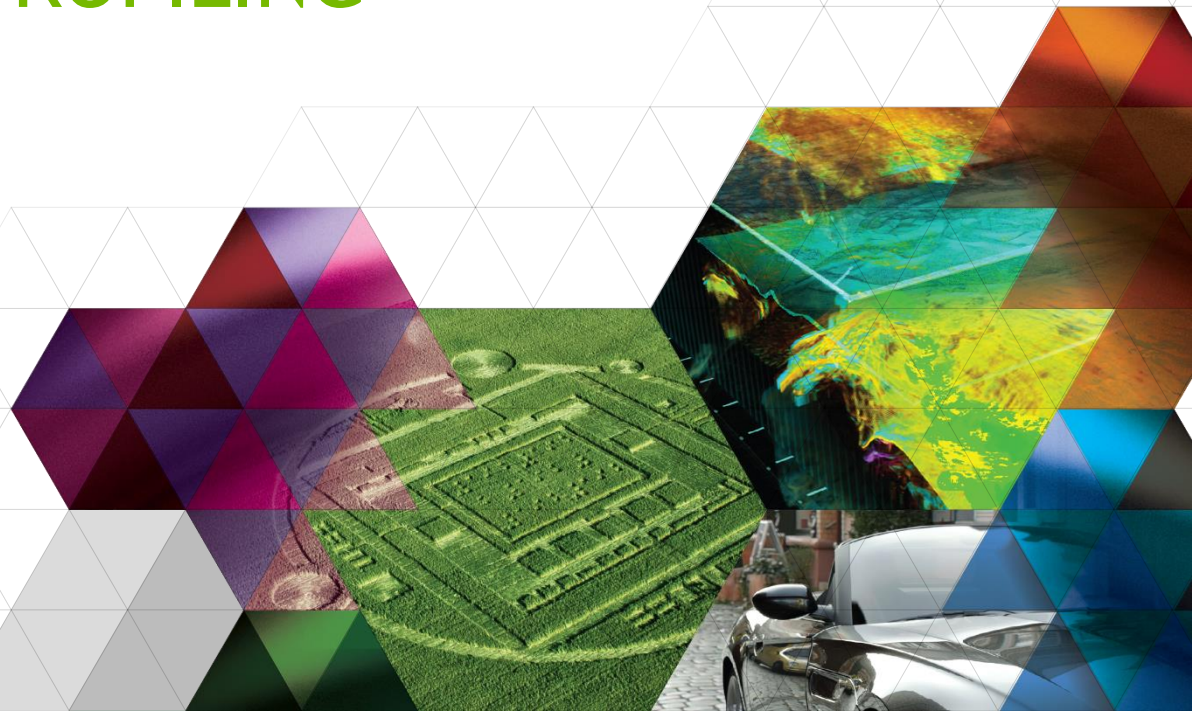
- Easy path to get GPU acceleration for legacy applications
- Enables overlapping of memory copies and compute between different MPI ranks



GPU TECHNOLOGY CONFERENCE

NVIDIA

DEBUGGING AND PROFILING



TOOLS FOR MPI+CUDA APPLICATIONS

- Memory Checking `cuda-memcheck`
- Debugging `cuda-gdb`
- Profiling `nvprof` and NVIDIA Visual Profiler

MEMORY CHECKING WITH CUDA-MEMCHECK

- Cuda-memcheck is a functional correctness checking suite similar to the valgrind memcheck tool
- Can be used in a MPI environment

```
mpiexec -np 2 cuda-memcheck ./myapp <args>
```

- Problem: output of different processes is interleaved
  - Use save, log-file command line options and launcher script

```
#!/bin/bash
LOG=$1.$OMPI_COMM_WORLD_RANK
#LOG=$1.$MV2_COMM_WORLD_RANK
cuda-memcheck --log-file $LOG.log --save $LOG.memcheck $*

mpiexec -np 2 cuda-memcheck-script.sh ./myapp <args>
```

MEMORY CHECKING WITH CUDA-MEMCHECK

jkraus@sb077:~/workspace/Jacobi/main/bin

```
[jkraus@sb077 bin]$ MV2_USE_CUDA=1 mpiexec -np 4 ./cuda-memcheck-script.sh ./jacobi_cuda_aware_m
pi_async -t 2 2 -d 1024 1024 -fs
Topology size: 2 x 2
Local domain size (current node): 1024 x 1024
Global domain size (all nodes): 2048 x 2048
Starting Jacobi run with 4 processes:
Error: CUDA result "unspecified launch failure" for call "cudaDeviceSynchronize()" in file "Host
.c" at line 453. Terminating...

=====================================================================================
=   BAD TERMINATION OF ONE OF YOUR APPLICATION PROCESSES
=   EXIT CODE: 255
=   CLEANING UP REMAINING PROCESSES
=   YOU CAN IGNORE THE BELOW CLEANUP MESSAGES
=====================================================================================
[jkraus@sb077 bin]$ ls *.memcheck
jacobi_cuda_aware_mpi_async.0.memcheck  jacobi_cuda_aware_mpi_async.2.memcheck
jacobi_cuda_aware_mpi_async.1.memcheck  jacobi_cuda_aware_mpi_async.3.memcheck
[jkraus@sb077 bin]$ cuda-memcheck --read jacobi_cuda_aware_mpi_async.0.memcheck
```

MEMORY CHECKING WITH CUDA-MEMCHECK

Read outputfiles with `cuda-memcheck --read`

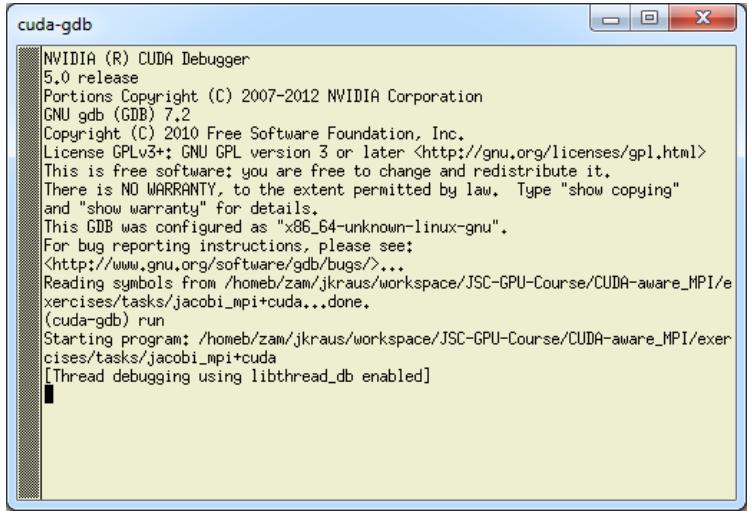
```
jkraus@sb077:~/workspace/Jacobi/main/bin
=========     Saved host backtrace up to driver entry point at kernel launch time
=========     Host Frame:/usr/lib64/libcuda.so.1 (cuLaunchKernel + 0x331) [0x138251]
=========     Host Frame:/shared/apps/cuda/CUDA-v6.0.26/lib64/libcudart.so.6.0 [0xfa98]
=========     Host Frame:/shared/apps/cuda/CUDA-v6.0.26/lib64/libcudart.so.6.0 (cudaLaunch + 0x1
43) [0x2e6a3]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x34bd]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x4067]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x3073]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x1aff]
=========     Host Frame:/lib64/libc.so.6 (__libc_start_main + 0xfd) [0x1ecdd]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x16a5]
=========
========= Invalid __global__ read of size 8
=========     at 0x00000888 in /home-2/jkraus/workspace/Jacobi/main/src/Async/Device.cu:145:Jaco
biComputeKernel(double const *, double*, double*, int2, int, int2, int2)
=========     by thread (1,12,0) in block (4,63,0)
=========     Address 0x2300a04210 is out of bounds
=========     Saved host backtrace up to driver entry point at kernel launch time
=========     Host Frame:/usr/lib64/libcuda.so.1 (cuLaunchKernel + 0x331) [0x138251]
=========     Host Frame:/shared/apps/cuda/CUDA-v6.0.26/lib64/libcudart.so.6.0 [0xfa98]
=========     Host Frame:/shared/apps/cuda/CUDA-v6.0.26/lib64/libcudart.so.6.0 (cudaLaunch + 0x1
43) [0x2e6a3]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x34bd]
=========     Host Frame:./jacobi_cuda_aware_mpi_async [0x4067]
```

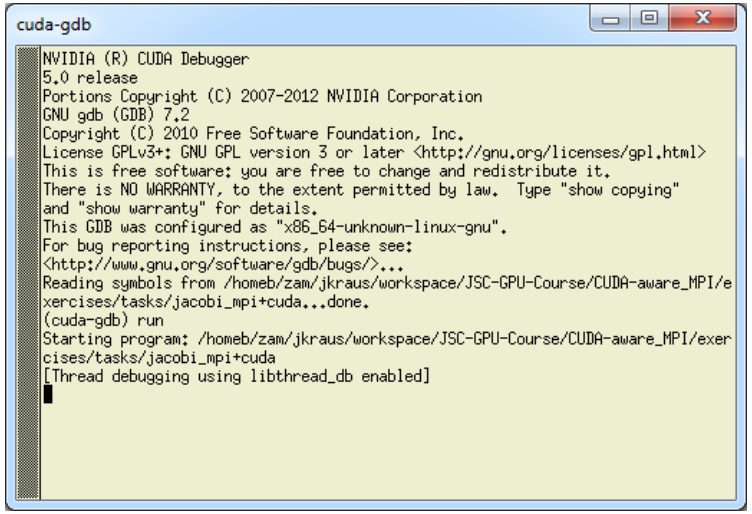
DEBUGGING MPI+CUDA APPLICATIONS

USING CUDA-GDB WITH MPI APPLICATIONS

- You can use cuda-gdb just like gdb with the same tricks
- For smaller applications, just launch xterms and cuda-gdb

```
> mpiexec -x -np 2 xterm -e cuda-gdb ./myapp <args>
```





DEBUGGING MPI+CUDA APPLICATIONS

CUDA-GDB ATTACH

- CUDA 5.0 and forward have the ability to attach to a running process

```
if ( rank == 0 )  {
    int i=0;
    printf("rank %d: pid %d on %s ready for attach\n.", rank, getpid(),name);
    while (0 == i) {
        sleep(5);
    }
}
> mpiexec -np 2 ./jacobi_mpi+cuda
Jacobi relaxation Calculation: 4096 x 4096 mesh with 2 processes and one Tesla
M2070 for each process (2049 rows per process).
rank 0: pid 30034 on judge107 ready for attach
> ssh judge107
jkraus@judge107:~> cuda-gdb --pid 30034
```

DEBUGGING MPI+CUDA APPLICATIONS

CUDA_DEVICE_WAITS_ON_EXCEPTION

jkraus@sb077:~/workspace/Jacobi/main/bin

```
Iteration: 700 - Residue: 0.306564
Iteration: 800 - Residue: 0.306564
Iteration: 900 - Residue: 0.306564
Stopped after 1000 iterations with residue 0.306564
Total Jacobi run time: 0.8700 sec.
Average per-process communication time: 0.2765 sec.
Measured lattice updates: 4.81 GLU/s (total), 1.20 GLU/s (per process)
Measured FLOPS: 24.06 GFLOPS (total), 6.01 GFLOPS (per process)
Measured device bandwidth: 230.95
[jkraus@sb077 bin]$ CUDA_DEVICE_WA
aware_mpi_async -t 2 2 -d 1024 102
Topology size: 2 x 2
Local domain size (current node):
Global domain size (all nodes): 20
Starting Jacobi run with 4 process
sb077: The application encountered
 can now attach a debugger to the
sb077: The application encountered
 can now attach a debugger to the
sb077: The application encountered
 can now attach a debugger to the
sb077: The application encountered
 can now attach a debugger to the
```

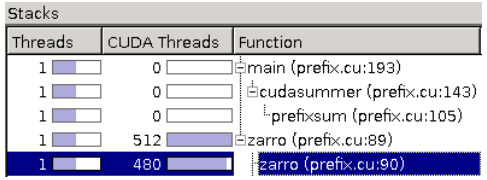
jkraus@sb077:~/workspace/Jacobi/main/bin

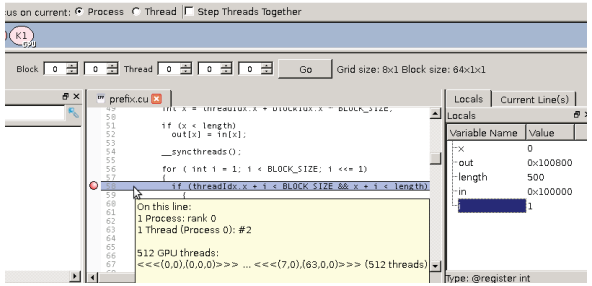
```
Reading symbols from /usr/lib64/libnes-rdmav2.so...(no debugging symbols found)...done.
Loaded symbols for /usr/lib64/libnes-rdmav2.so
Reading symbols from /usr/lib64/libmlx4-rdmav2.so...(no debugging symbols found)...done.
Loaded symbols for /usr/lib64/libmlx4-rdmav2.so
Reading symbols from /usr/lib64/libipathverbs-rdmav2.so...(no debugging symbols found)...done.
Loaded symbols for /usr/lib64/libipathverbs-rdmav2.so
0x00007f5ba011fa01 in clock_gettime ()
$1 = 1

CUDA Exception: Device Illegal Address
The exception was triggered in device 3.

Program received signal CUDA_EXCEPTION_10, Device Illegal Address.
[Switching focus to CUDA kernel 0, grid 8, block (6,36,0), thread (0,6,0), device 3, sm 0, warp
13, lane 0]
0x00000000018e1ce8 in JacobiComputeKernel<<<(64,64,1),(16,16,1)>>> (size=..., startmod=...,
    endmod=..., oldBlock=0x2300200000, newBlock=0x2300b20000, devResidue=0x2301340000,
    stride=1024) at Device.cu:150
150             AtomicMax<real>(devResidue, rabs(newVal - oldBlock[memIdx]));
(cuda-gdb) bt
#0  0x00000000018e1ce8 in JacobiComputeKernel<<<(64,64,1),(16,16,1)>>> (size=...,
    startmod=..., endmod=..., oldBlock=0x2300200000, newBlock=0x2300b20000,
    devResidue=0x2301340000, stride=1024) at Device.cu:150
(cuda-gdb)
```

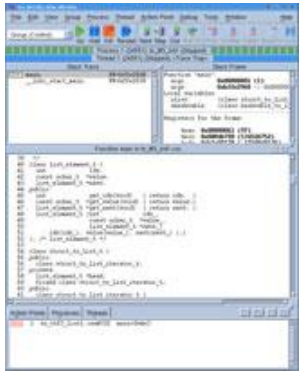
DEBUGGING MPI+CUDA APPLICATIONS

THIRD PARTY TOOLS

- Allinea DDT debugger
- Totalview
- S4284 - Debugging PGI CUDA Fortran and OpenACC on GPUs with Allinea DDT - Tuesday 4pm LL20D







DDT: THREAD LEVEL DEBUGGING

Focus

Breakpoint inside kernel

Launch configuration

Per thread variabless

Allinea DDT 4.2-34071 (on nid00015)

File View Control Search Tools Window Help

Focus on current: Process Thread Step Threads Together Step CUDA threads by: Warp (default)

Threads (1 hidden): 1 K1 GPU

CUDA Threads (gpuTranspose_kernel) Block 0 0 0 Thread 5 2 0 Go Grid size: 32x32x1 Block size: 32x32x1

main.cu

```
42
43    // Stage Matrix tile to Shared memory
44    tile[threadIdx.y][threadIdx.x] = in[j*cols+i];
45
46    __syncthreads();
47
48    i = blockIdx.y * blockDim.y + threadIdx.x;
49    j = blockIdx.x * blockDim.x + threadIdx.y;
51    // Write matrix tile back out, transposed
52    out[j*rows+i] = tile[threadIdx.x][threadIdx.y];
53  }
54  void gpuTranspose(int rows, int cols, float * in, float * out) {
55    gpuTranspose_kernel<<<dim3(rows/32,cols/32),dim3(32,32)>>>(rows,cols,in,out);
56    cudaCheckError();
57  }
58
59
60  int main(int argc, char** argv)
61  {
```

Locals | Current Line(s) | Current Stack | GPU Devices

Current Line(s)

Variable Name	Value
i	5
j	2
out	0xb0060
rows	1024
threadIdx	{x = 5, y = 2, z = 0}
threadIdx.x	5
threadIdx.y	2
tile	

Type: none selected

Inp... Bre... Wat... Stacks Ker... Tra...

Input/Output

```
Process 0: OMP threads: 1
Process 0: CPU+OMP: Kernel bandwidth: 1.106102 gb/sec
Process 0: err = 0
```

Type here ('Enter' to send): More

Evaluate

Expression	Value

Ready

PROFILING MPI+CUDA APPLICATIONS

USING NVPROF+NVVP

3 Usage modes:

- Embed pid in output filename

```
mpirun -np 2 nvprof --output-profile profile.out.%p
```

- Only save the textual output

```
mpirun -np 2 nvprof --log-file profile.out.%p
```

- Collect profile data on all processes that run on a node

```
nvprof --profile-all-processes -o profile.out.%p
```

PROFILING MPI+CUDA APPLICATIONS

USING NVPROF+NVVP

jkraus@sb077:~/workspace/Jacobi/main/bin

```
[jkraus@sb077 bin]$ MV2_USE_CUDA=1 mpiexec -np 4 nvprof -o jacobi_cuda_aware_mpi_async.%p.nvvp
./jacobi_cuda_aware_mpi_async -t 2 2 -d 1024 1024 -fs
==29287== NVPROF is profiling process 29287, command: ./jacobi_cuda_aware_mpi_async -t 2 2 -d 10
24 1024 -fs
==29282== NVPROF is profiling process 29282, command: ./jacobi_cuda_aware_mpi_async -t 2 2 -d 10
24 1024 -fs
==29288== NVPROF is profiling process 29288, command: ./jacobi_cuda_aware_mpi_async -t 2 2 -d 10
24 1024 -fs
==29284== NVPROF is profiling process 29284, command: ./jacobi_cuda_aware_mpi_async -t 2 2 -d 10
24 1024 -fs
```

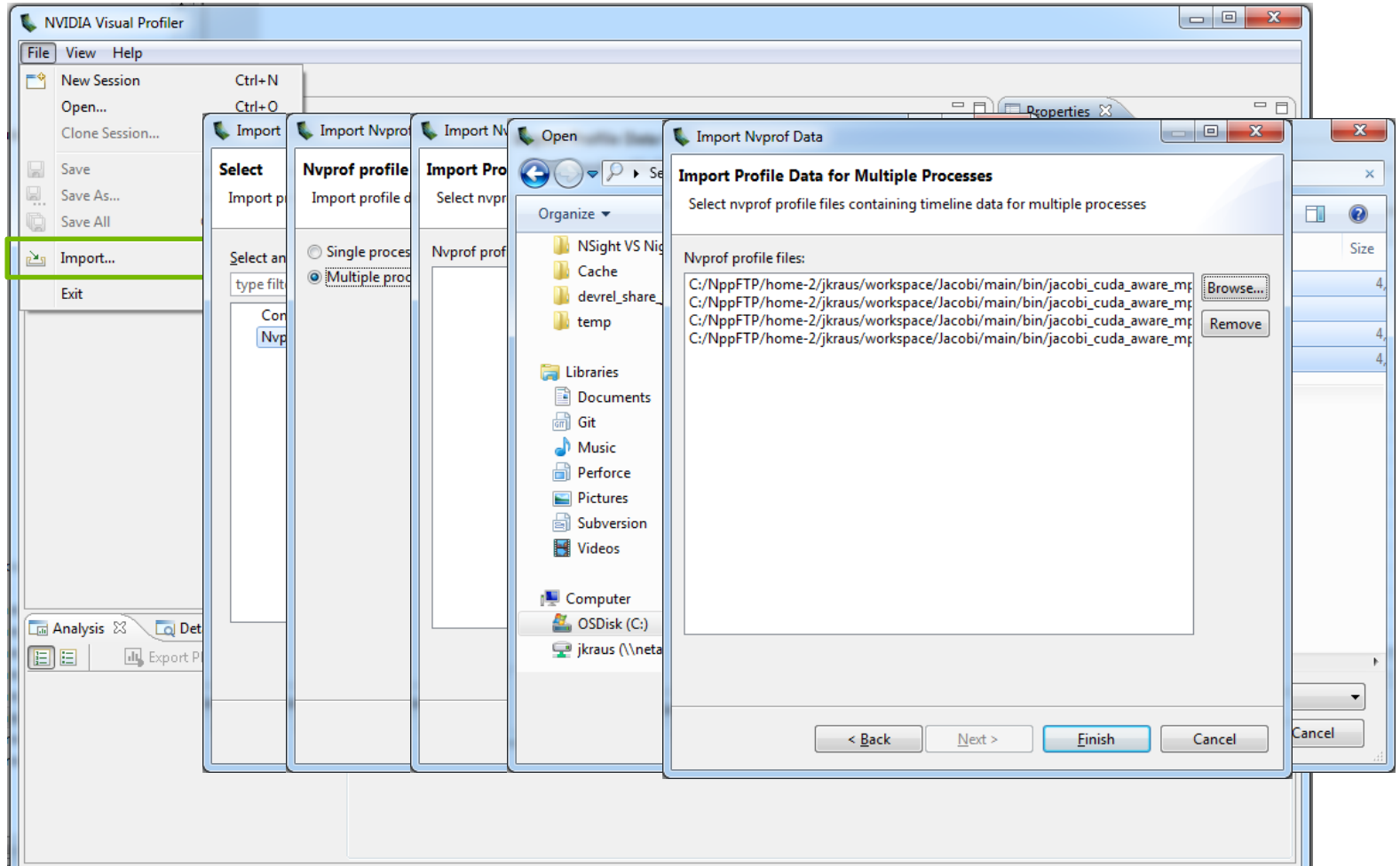
jkraus@sb077:~/workspace/Jacobi/main/bin

```
Iteration: 100 - Residue: 0.002394
Iteration: 200 - Residue: 0.001202
Iteration: 300 - Residue: 0.000801
Iteration: 400 - Residue: 0.000601
Iteration: 500 - Residue: 0.000481
Iteration: 600 - Residue: 0.000400
Iteration: 700 - Residue: 0.000343
Iteration: 800 - Residue: 0.000300
Iteration: 900 - Residue: 0.000266
Stopped after 1000 iterations with residue 0.000240
Total Jacobi run time: 0.4353 sec.
Average per-process communication time: 0.2639 sec.
Measured lattice updates: 9.62 GLU/s (total), 2.40 GLU/s (per process)
Measured FLOPS: 48.08 GFLOPS (total), 12.02 GFLOPS (per process)
Measured device bandwidth: 461.59 GB/s (total), 115.40 GB/s (per process)
==29284== Generated result file: /home-2/jkraus/workspace/Jacobi/main/bin/jacobi_cuda_aware_mpi_
async.29284.nvvp
==29287== Generated result file: /home-2/jkraus/workspace/Jacobi/main/bin/jacobi_cuda_aware_mpi_
async.29287.nvvp
==29288== Generated result file: /home-2/jkraus/workspace/Jacobi/main/bin/jacobi_cuda_aware_mpi_
async.29288.nvvp
==29282== Generated result file: /home-2/jkraus/workspace/Jacobi/main/bin/jacobi_cuda_aware_mpi_
async.29282.nvvp
[jkraus@sb077 bin]$
```

GPU TECHNOLOGY CONFERENCE

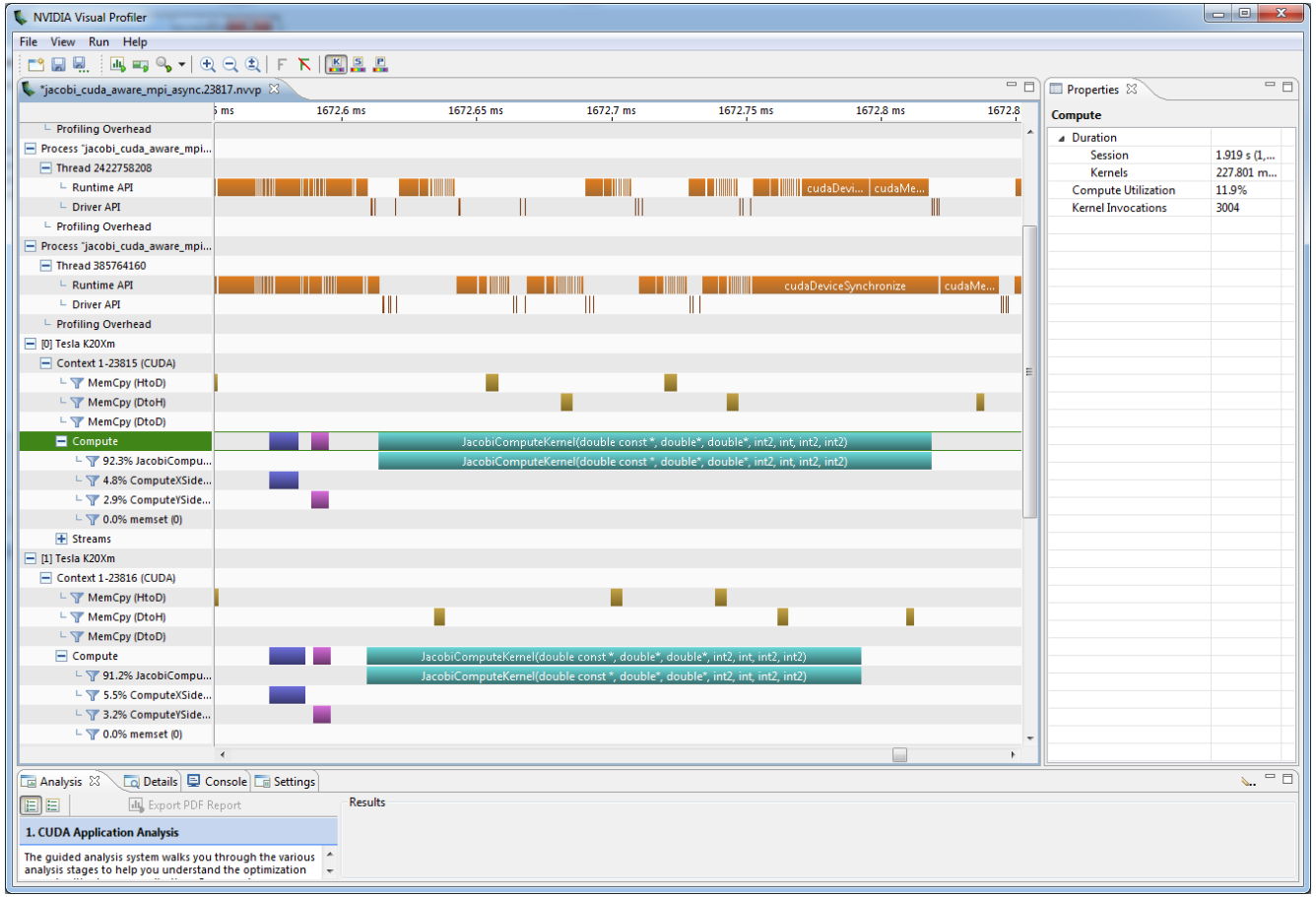
PROFILING MPI+CUDA APPLICATIONS

USING NVPROF+NVVP



PROFILING MPI+CUDA APPLICATIONS

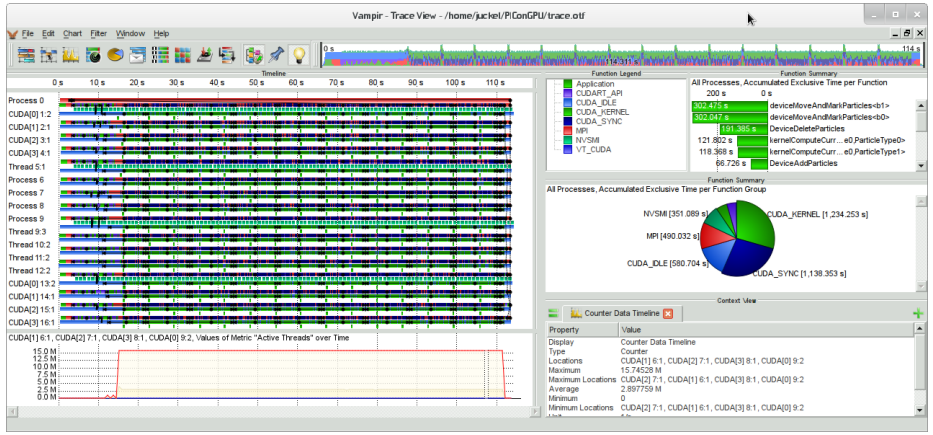
USING NVPROF+NVVP

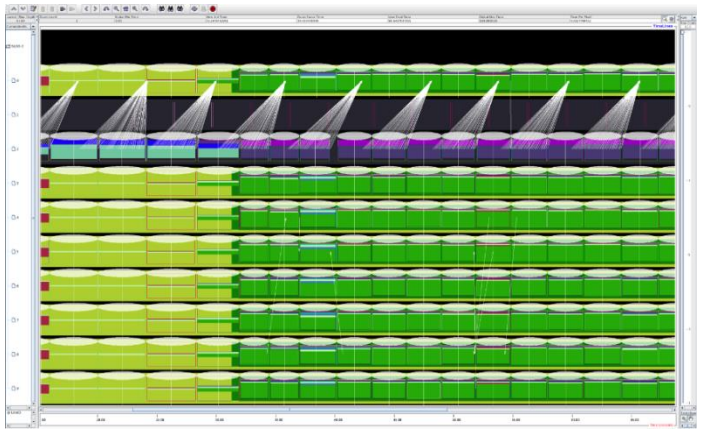


PROFILING MPI+CUDA APPLICATIONS

THIRD PARTY TOOLS

- Multiple parallel profiling tools are CUDA aware
  - Score-P
  - Vampir
  - Tau
- These tools are good for discovering MPI issues as well as basic CUDA performance inhibitors





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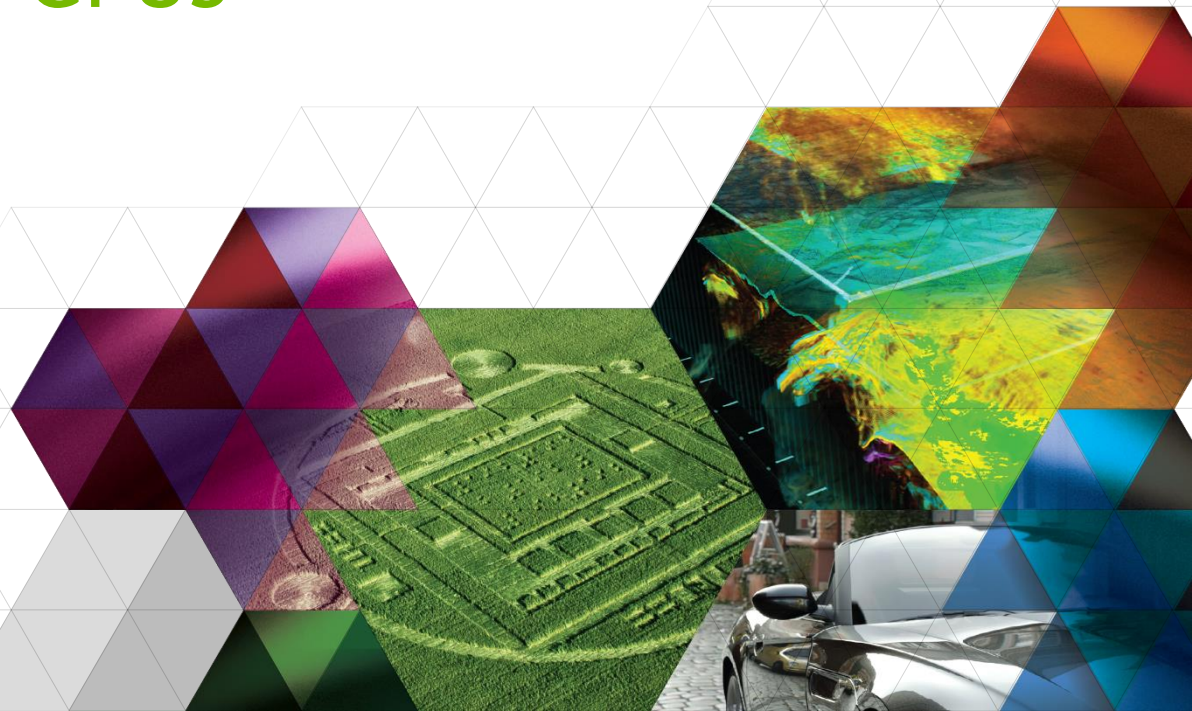
ADVANCED MPI ON GPUS



BEST PRACTICE: USE NONE-BLOCKING MPI

BLOCKING

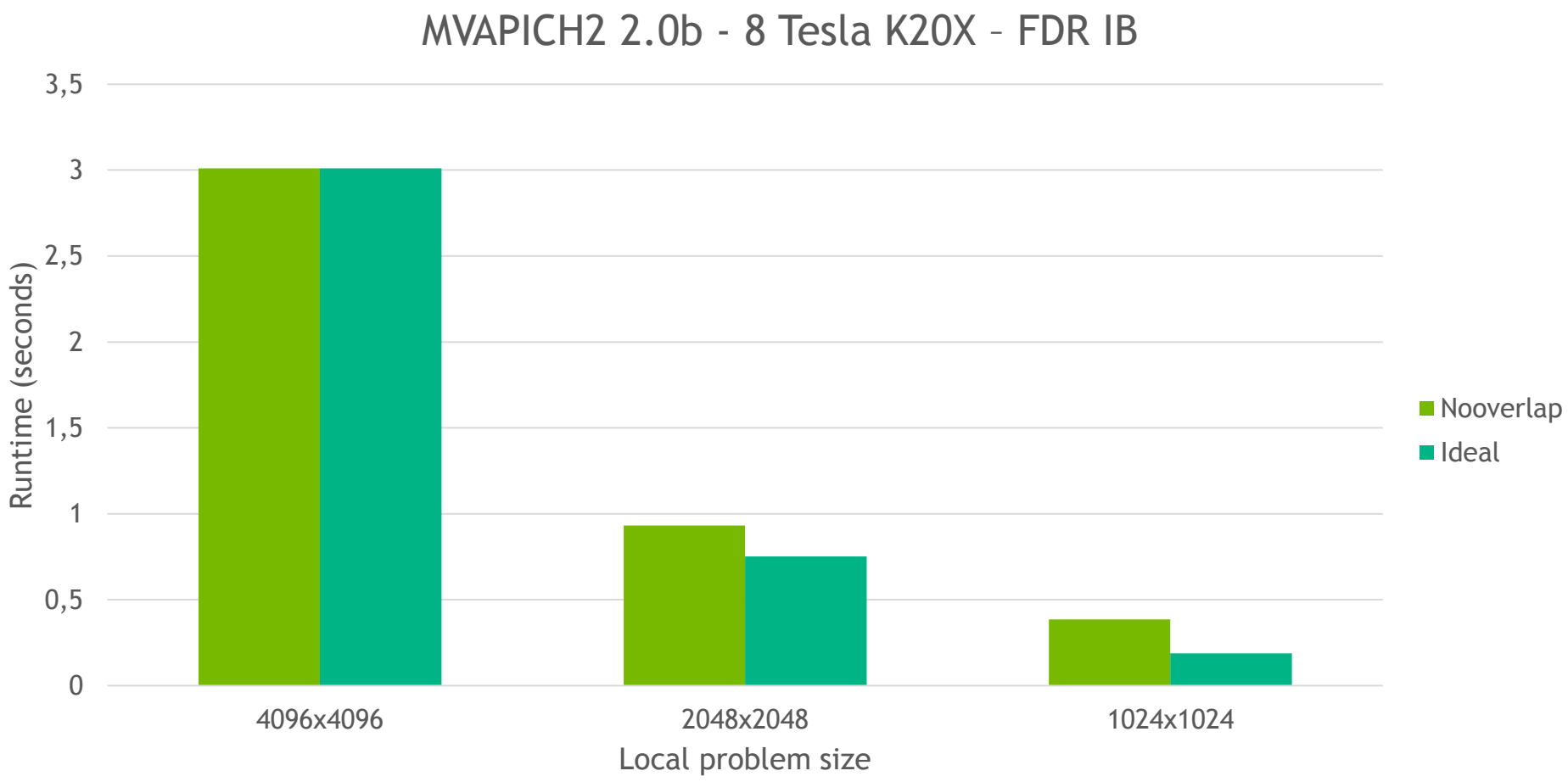
```
#pragma acc host_data use_device ( u_new ) {
MPI_Sendrecv(u_new+offset_first_row, m-2, MPI_DOUBLE, t_nb, 0,
             u_new+offset_bottom_bondary, m-2, MPI_DOUBLE, b_nb, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
MPI_Sendrecv(u_new+offset_last_row, m-2, MPI_DOUBLE, b_nb, 1,
             u_new+offset_top_bondary, m-2, MPI_DOUBLE, t_nb, 1,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

NONE-BLOCKING

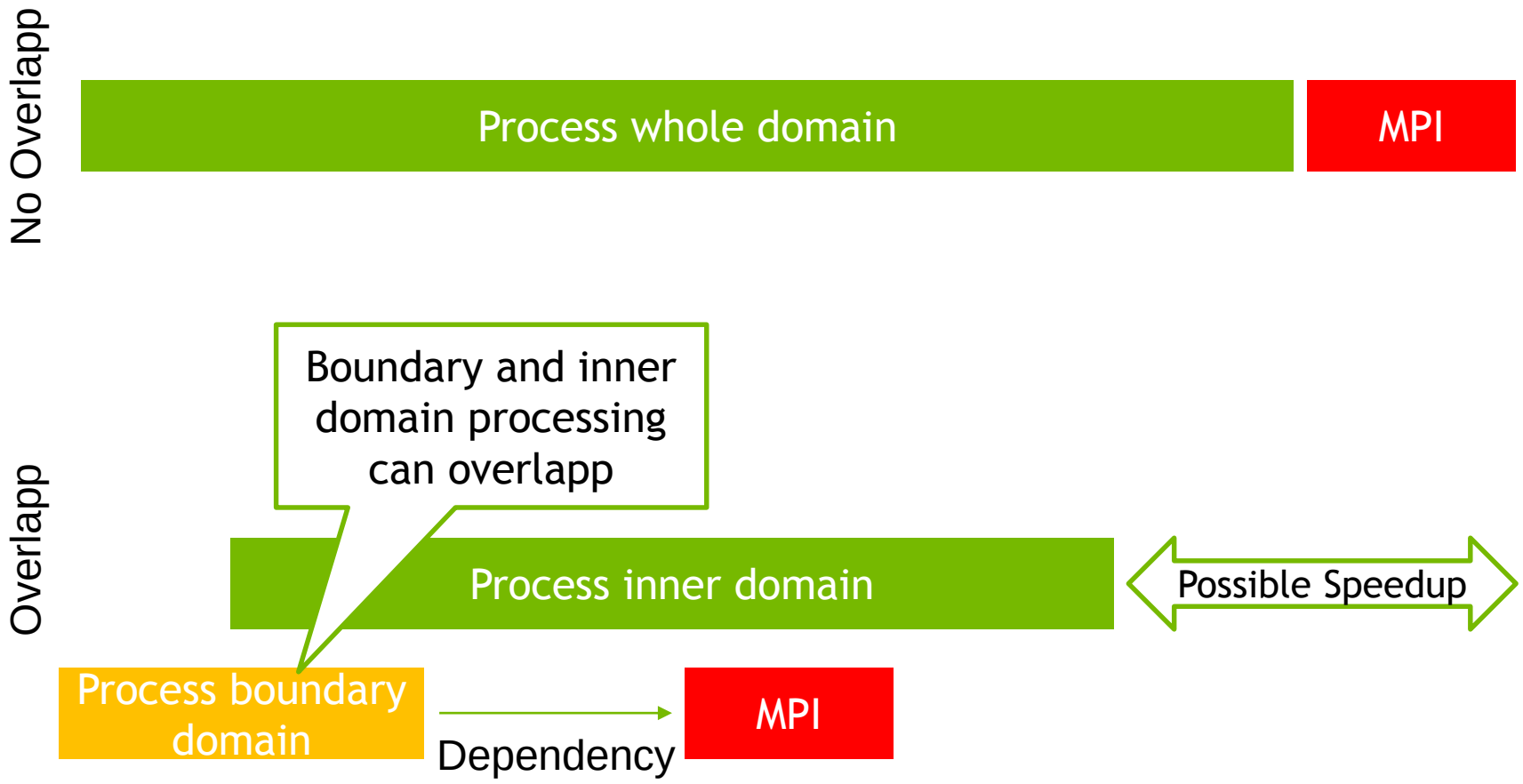
```
MPI_Request t_b_req[4];
#pragma acc host_data use_device ( u_new ) {
  MPI_Irecv(u_new+offset_top_bondary,m-2                                  req);
  MPI_Irecv(u_new+offset_bottom_bondar                                  WORLD,t_b_req+1);
  MPI_Isend(u_new+offset_last_row,m-2,M                                  COMM_WORLD,t_b_req+2);
  MPI_Isend(u_new+offset_first_row,m-2,M                                  nb,1,MPI_COMM_WORLD,t_b_req+3);
}
MPI_Waitall(4, t_b_req, MPI_STATUSES_IGNORE);
```

Gives MPI more opportunities to build efficient piplines

OVELAPPING COMMUNICAITON AND COMPUTATION



OVERLAPPING COMMUNICATION AND COMPUTATION



OVERLAPPING COMMUNICATION AND COMPUTATION

OpenACC

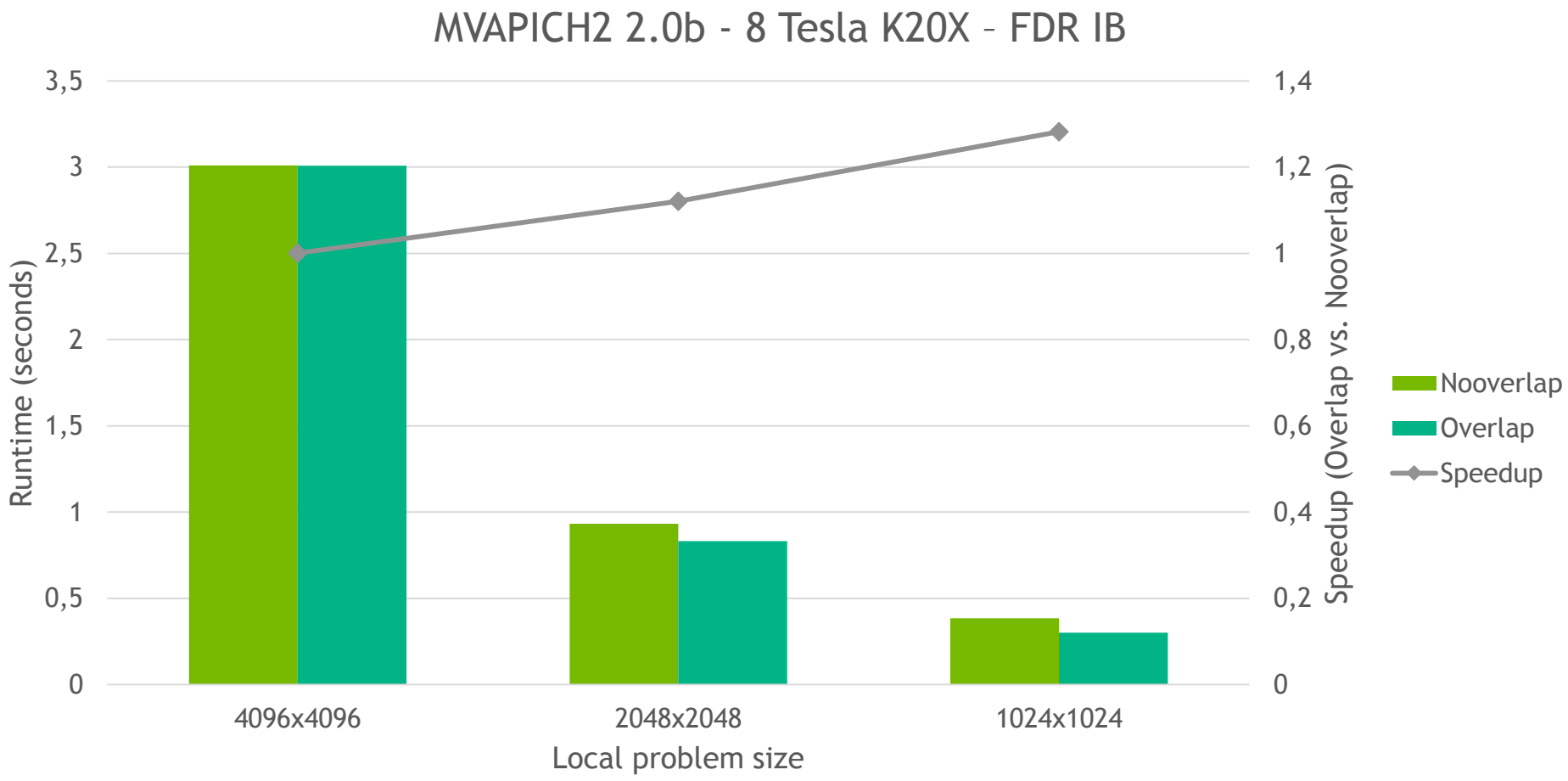
```
#pragma acc parallel loop present ( u_new, u, to_left, to_right ) async(1)
for ( ... )
      //Process boundary and pack to_left and to_right
#pragma acc parallel loop present ( u_new, u ) async(2)
for ( ... )
      //Process inner domain
#pragma acc wait(1)                //wait for boundary
MPI_Request req[8];
#pragma acc host_data use_device ( from_left, to_left, form_right, to_right, u_new ) {
  //Exchange halo with left, right, top and bottom neighbor
}
MPI_Waitall(8, req, MPI_STATUSES_IGNORE);
#pragma acc parallel loop present ( u_new, from_left, from_right )
for ( ... )
      //unpack from_left and from_right
#pragma acc wait                   //wait for iteration to finish
```

OVERLAPPING COMMUNICATION AND COMPUTATION

CUDA

```
process_boundary_and_pack<<<gs_b,bs_b,0,s1>>>(u_new_d,u_d,to_left_d,to_right_d,n,m);



process_inner_domain<<<gs_id,bs_id,0,s2>>>(u_new_d, u_d,to_left_d,to_right_d,n,m);



cudaStreamSynchronize(s1);        //wait for boundary
MPI_Request req[8];

  //Exchange halo with left, right, top and bottom neighbor

MPI_Waitall(8, req, MPI_STATUSES_IGNORE);
unpack<<<gs_s,bs_s>>>(u_new_d, from_left_d, from_right_d, n, m);



cudaDeviceSynchronize();          //wait for iteration to finish
```

OVELAPPING COMMUNICAITON AND COMPUTATION



MPI AND UNIFIED MEMORY

- Unified Memory support for CUDA-aware MPI needs changes to the MPI implementations
  - Check with your MPI implementation of choice for their plans
  - It might work in some situations but it is not supported
- Unified Memory and regular MPI
  - Require unmanaged staging buffers
    - Regular MPI has no knowledge of managed memory
    - CUDA 6 managed memory does not play well with RDMA protocols

HANDLING MULTI GPU NODES

- Multi GPU nodes and GPU-affinity:
  - Use local rank:

```
int local_rank = //determine local rank
int num_devices = 0;
cudaGetDeviceCount(&num_devices);
cudaSetDevice(local_rank % num_devices);
```

  - Use exclusive process mode + `cudaSetDevice(0)`

HANDLING MULTI GPU NODES

- How to determine local rank:
  - Rely on process placement (with one rank per GPU)

```
int rank = 0;
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
int num_devices = 0;
cudaGetDeviceCount(&num_devices); // num_devices == ranks per node
int local_rank = rank % num_devices;
```

  - Use environment variables provided by MPI launcher
    - e.g for OpenMPI

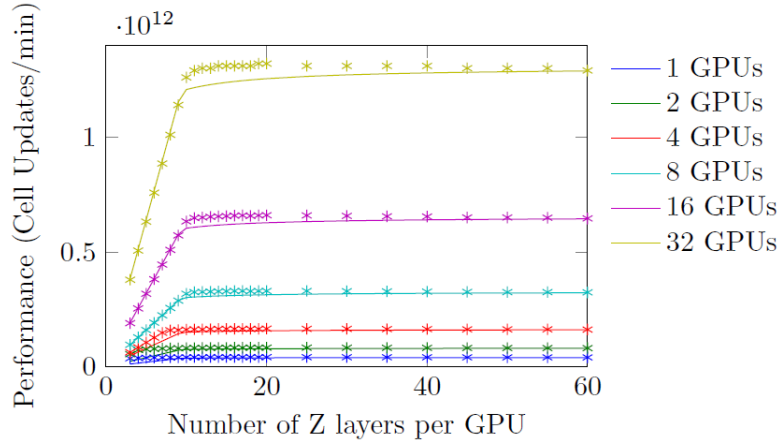
```
int local_rank = atoi(getenv("OMPI_COMM_WORLD_LOCAL_RANK"));
```

    - e.g. For MVPAICH2

```
int local_rank = atoi(getenv("MV2_COMM_WORLD_LOCAL_RANK"));
```

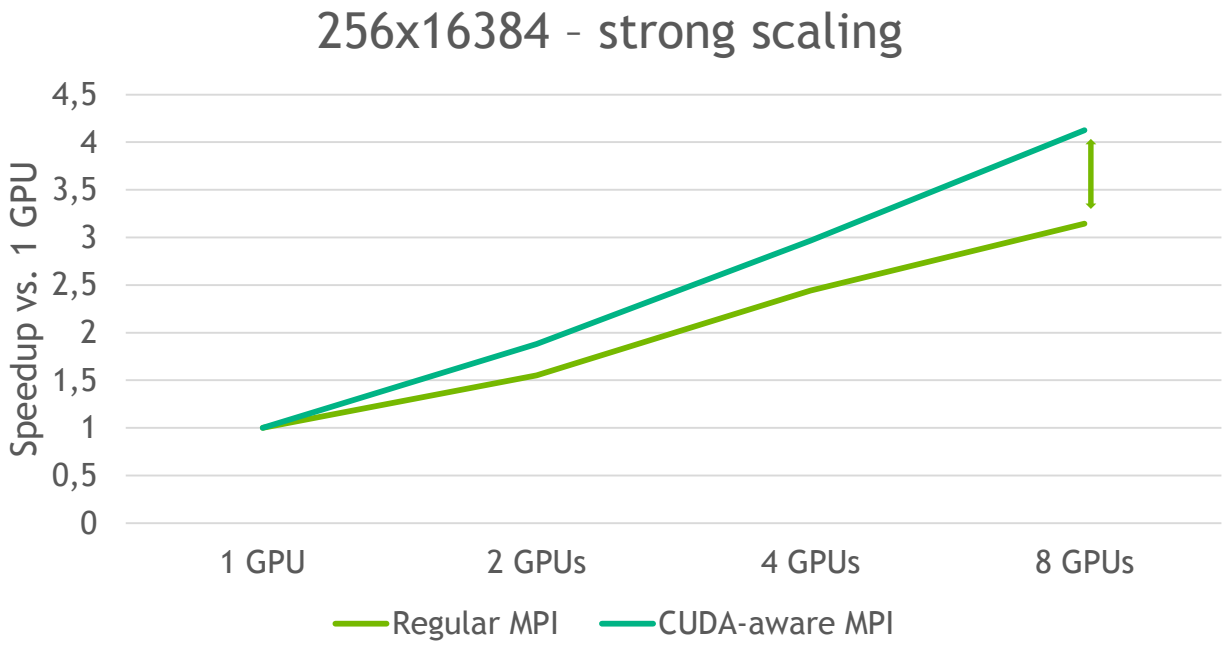
CASE STUDY: B-CALM

- CUDA-aware MPI enabled a easy transition from single node multi GPU to multi node multi GPU
- Multi node multi GPU version allows to solve problems that could not be tackled before
- More info at: S4190 - Finite Difference Simulations on GPU Clusters: How Far Can You Push 1D Domain Decomposition? (Wed. 03/26)



CASE STUDY: LBM D2Q37

- CUDA-aware MPI improves strong scalability and simplifies programming



- More info at: S4186 - Optimizing a LBM code for Compute Clusters with Kepler GPUs (Wed. 03/26)

CONCLUSIONS

- Using MPI as abstraction layer for Multi GPU programming allows multi GPU programs to scale beyond a single node
  - CUDA-aware MPI delivers ease of use, reduced network latency and increased bandwidth
- All NVIDIA tools are usable and third party tools are available
- Multipe CUDA-aware MPI implementations available
  - OpenMPI, MVAPICH2, Cray, IBM Platform MPI
- Other intressting sessions:
  - S4517 - Latest Advances in MVAPICH2 MPI Library for NVIDIA GPU Clusters with InfiniBand – Tuesday 3pm LL21A
  - S4589 - OpenMPI with RDMA Support and CUDA – Thursday 2pm 211B

OVERLAPPING COMMUNICATION AND COMPUTATION – TIPS AND TRICKS

- CUDA-aware MPI might use the default stream
  - Allocate stream with the non-blocking flag (cudaStreamNonBlocking)
  - More info: S4158 - CUDA Streams: Best Practices and Common Pitfalls Tuesday 03/27)
- In case of multiple kernels for boundary handling the kernel processing the inner domain might sneak in
  - Use single stream or events for inter stream dependencies via cudaStreamWaitEvent (#pragma acc wait async) – disables overlapping of boundary and inner domain kernels
  - Use high priority streams for boundary handling kernels – allows overlapping of boundary and inner domain kernels
- As of CUDA 6.0 GPUDirect P2P in multi process can overlap disable it for older releases

HIGH PRIORITY STREAMS

- Improve sclability with high priority streams (cudaStreamCreateWithPriority)
  - S4158 - CUDA Streams: Best Practices and Common Pitfalls (Thu. 03/27)
- Use-case MD Simulations:
  - S4465 - Optimizing CoMD: A Molecular Dynamics Proxy Application Study (Wed. 03/26)