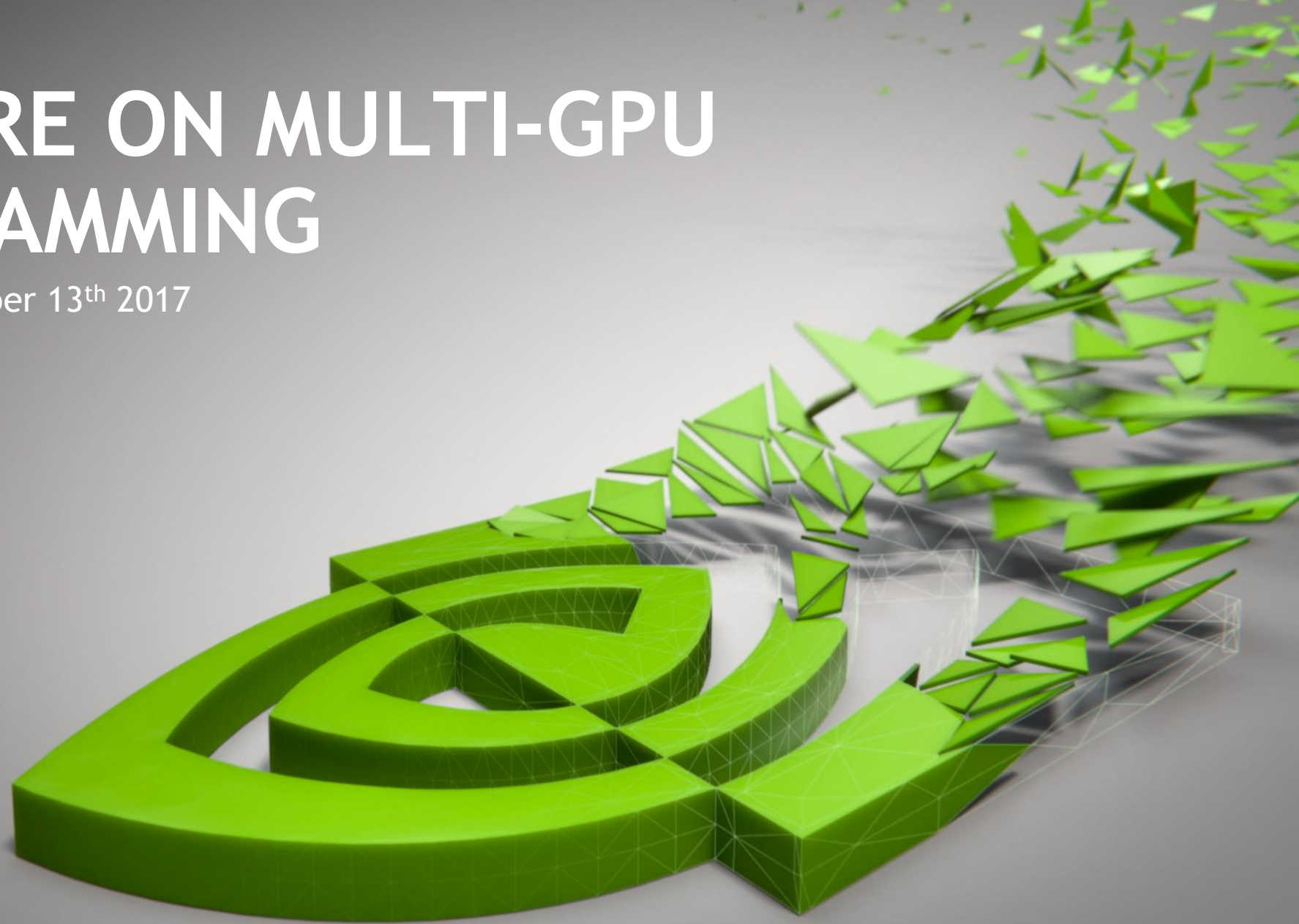


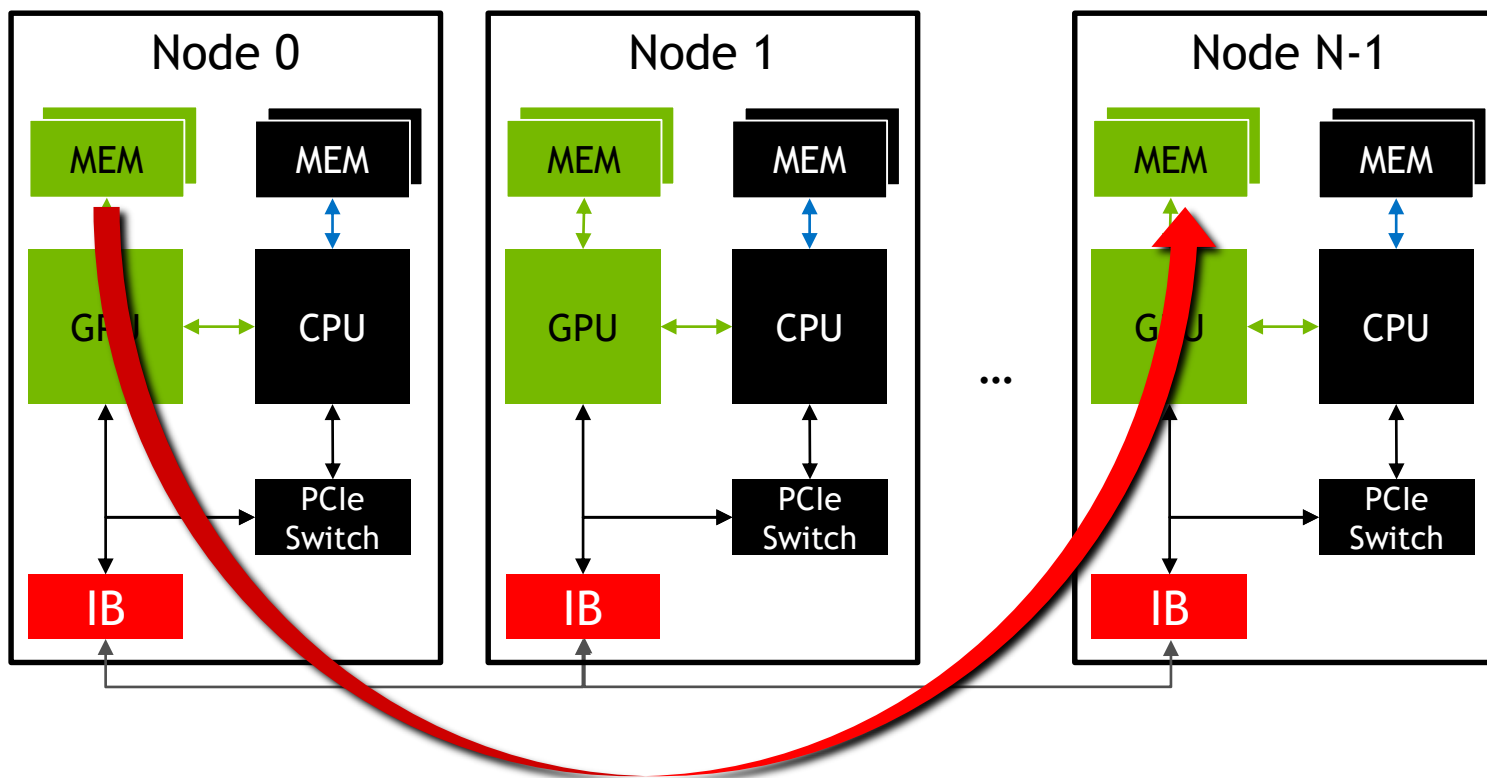
LECTURE ON MULTI-GPU PROGRAMMING

Jiri Kraus, November 13th 2017

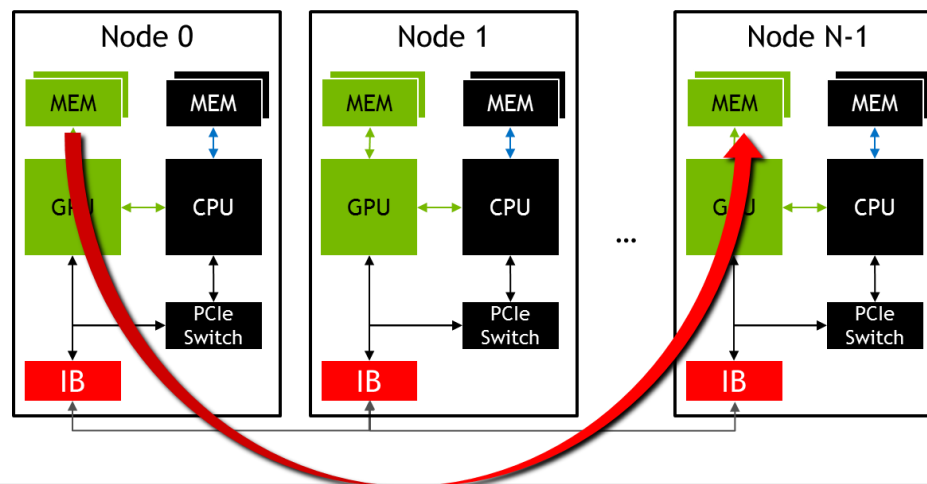


MULTI GPU PROGRAMMING

With MPI and OpenACC



MPI+OPENACC



```
//MPI rank 0
#pragma acc host_data use_device( sbuf )
MPI_Send(sbuf, size, MPI_DOUBLE, n-1, tag, MPI_COMM_WORLD);

//MPI rank n-1
#pragma acc host_data use_device( rbuf )
MPI_Recv(rbuf, size, MPI_DOUBLE, 0, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

USING MPI FOR INTER GPU COMMUNICATION

MESSAGE PASSING INTERFACE - MPI

Standard to exchange data between processes via messages

Defines API to exchanges messages

Point to Point: e.g. `MPI_Send`, `MPI_Recv`

Collectives: e.g. `MPI_Reduce`

Multiple implementations (open source and commercial)

Bindings for C/C++, Fortran, Python, ...

E.g. MPICH, OpenMPI, MVAPICH, IBM Platform MPI, Cray MPT, ...

MPI - SKELETON

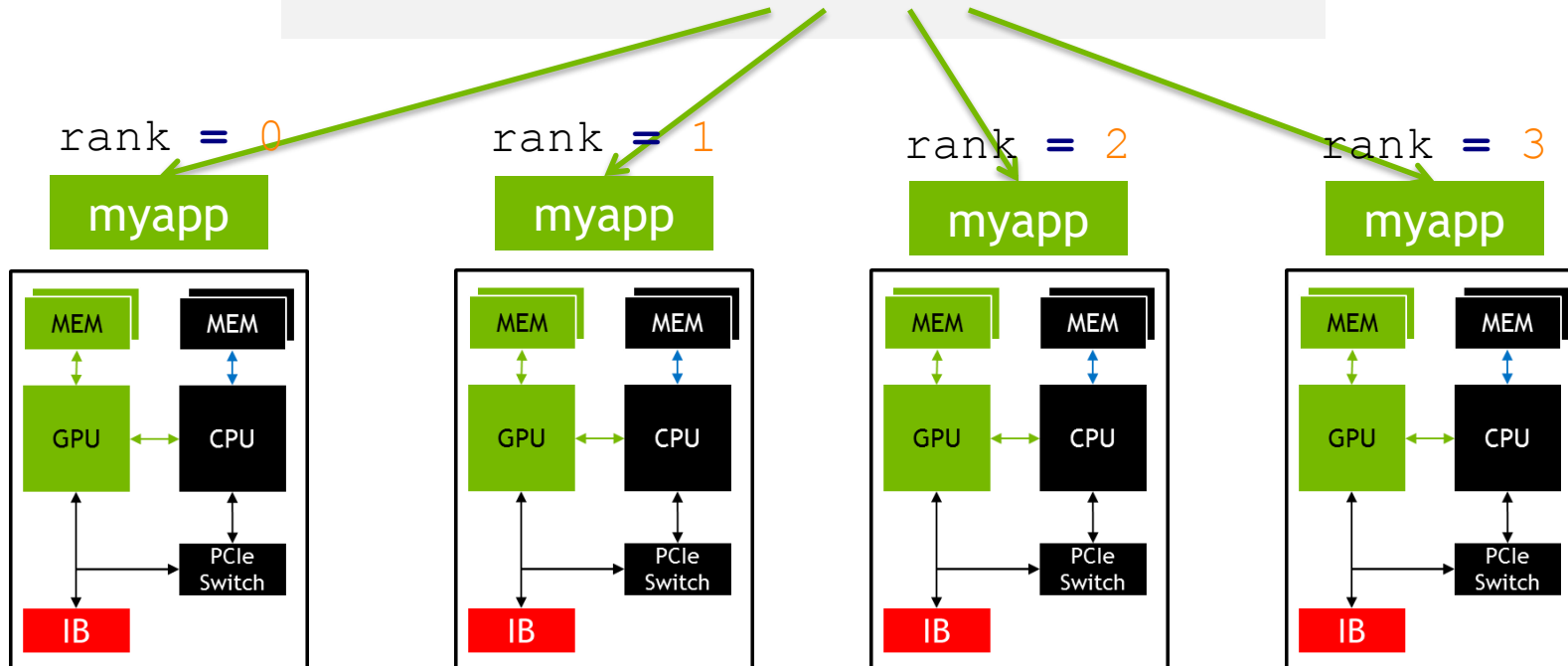
```
#include <mpi.h>

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>
```



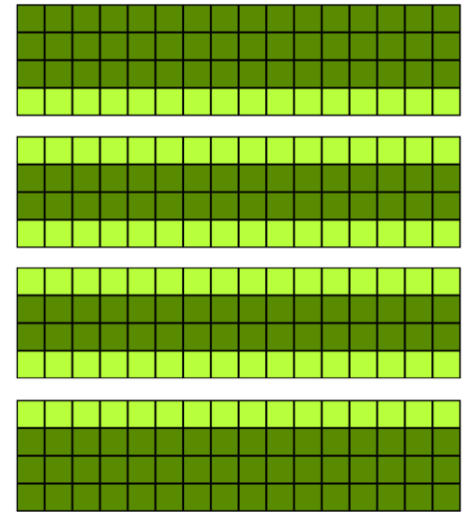
EXAMPLE: JACOBI SOLVER

Solves the 2D-Poisson Equation on a rectangle

$$\Delta u(x, y) = e^{-10*(x^2+y^2)} \quad \forall (x, y) \in \Omega \setminus \delta\Omega$$

Periodic boundary conditions

Domain decomposition with stripes



Horizontal Stripes

EXAMPLE: JACOBI SOLVER

Single GPU

While not converged

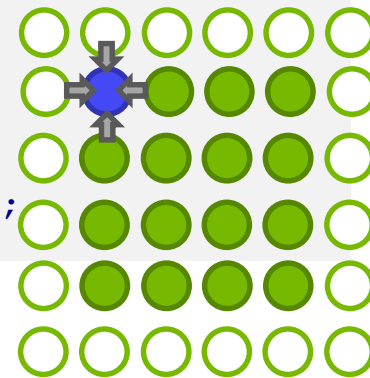
Do Jacobi step:

```
for (int iy = 1; iy < ny-1; ++iy)
for (int ix = 1; ix < nx-1; ++ix)
    Anew[iy*nx+ix]=-0.25f*(rhs[iy*nx+ix]-(A[iy*nx+(ix-1)]+A[iy*nx+(ix+1)]
                                     +A[(iy-1)*nx+ix]+A[(iy+1)*nx+ix]));
```

Copy Anew to A

Apply periodic boundary conditions

Next iteration



EXAMPLE: JACOBI SOLVER

Multi GPU

While not converged

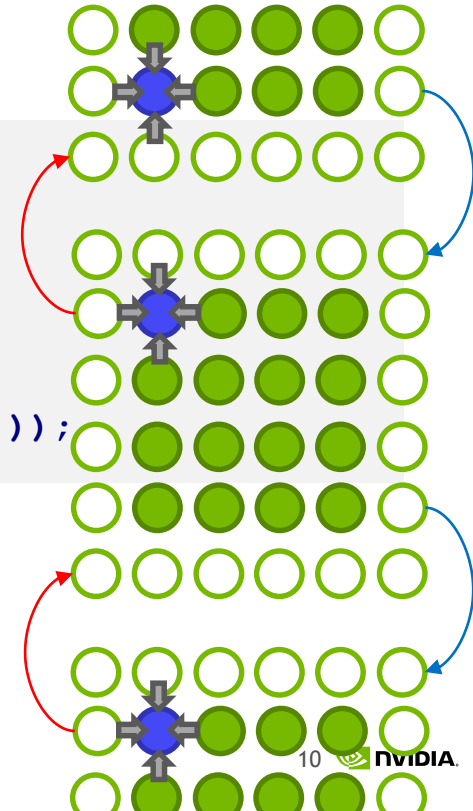
Do Jacobi step:

```
for (int iy = iy_start; iy < iy_end; ++iy)
for (int ix = 1; ix < NX-1; ++ix)
    Anew[iy*nx+ix]=-0.25f*(rhs[iy*nx+ix]-(A[iy*nx+(ix-1)]+A[iy*nx+(ix+1)]
                                         +A[(iy-1)*nx+ix]+A[(iy+1)*nx+ix]));
```

Copy Anew to A

Apply periodic boundary conditions and exchange halo with 2 neighbors

Next iteration

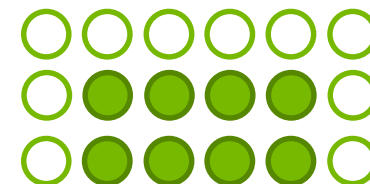
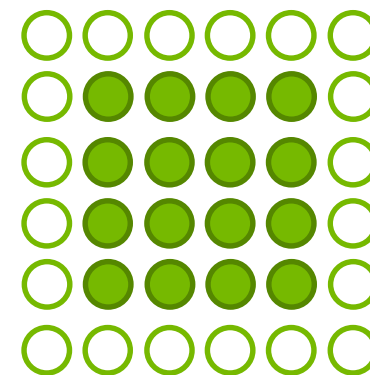
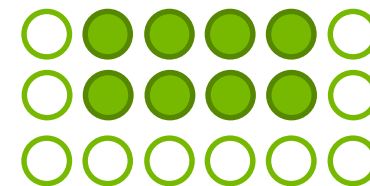


EXAMPLE JACOBI

Top/Bottom Halo

```
#pragma acc host_data use_device ( A )  
{
```

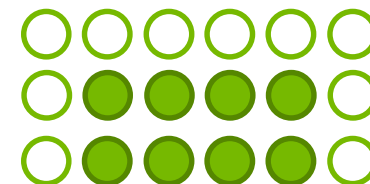
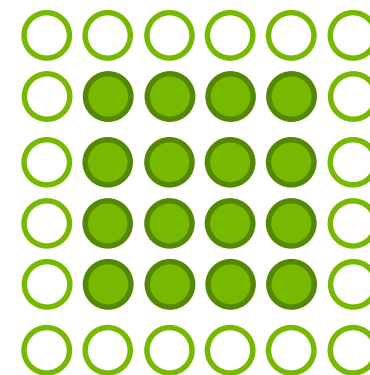
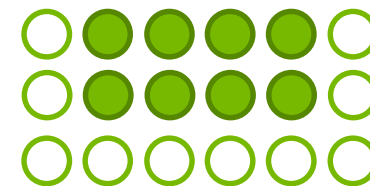
```
}
```



EXAMPLE JACOBI

Top/Bottom Halo

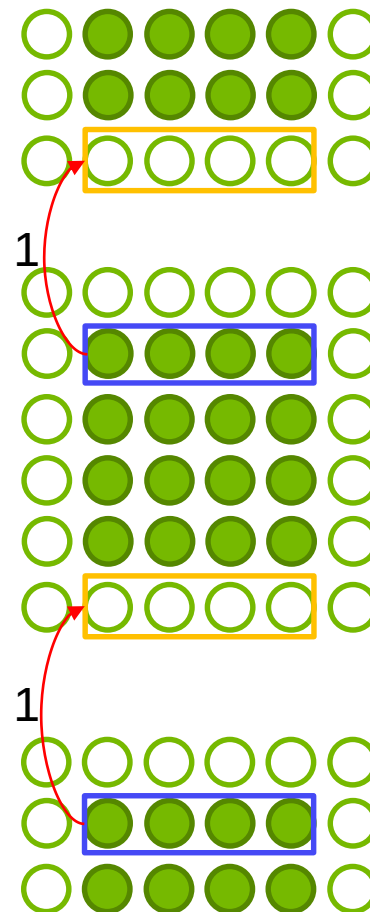
```
#pragma acc host_data use_device ( A )  
{  
  
MPI_Sendrecv(A+iy_start*nx+1, nx-2, MPI_DOUBLE, top, 0,  
             A+iy_end*nx+1, nx-2, MPI_DOUBLE, bottom, 0,  
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
  
}
```



EXAMPLE JACOBI

Top/Bottom Halo

```
#pragma acc host_data use_device ( A )
{
MPI_Sendrecv(A+iy_start*nx+1, nx-2, MPI_DOUBLE, top, 0,
             A+iy_end*nx+1, nx-2, MPI_DOUBLE, bottom, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

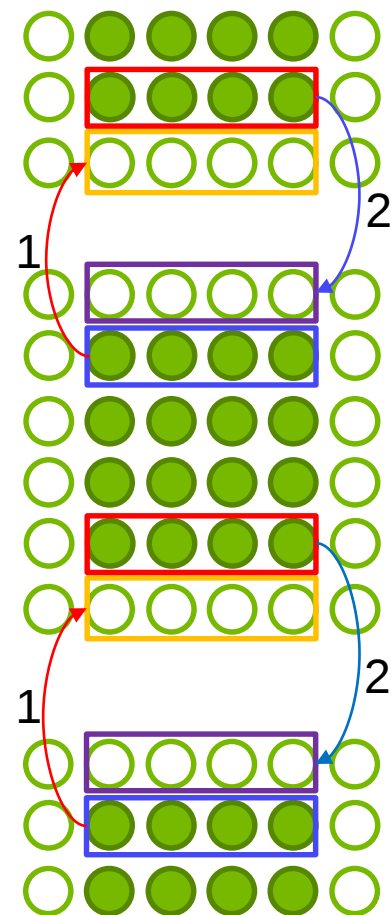


EXAMPLE JACOBI

Top/Bottom Halo

```
#pragma acc host_data use_device ( A )
{
    MPI_Sendrecv(A+iy_start*nx+1, nx-2, MPI_DOUBLE, top, 0,
                 A+iy_end*nx+1, nx-2, MPI_DOUBLE, bottom, 0,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);

    MPI_Sendrecv(A+(iy_end-1)*nx+1, nx-2, MPI_DOUBLE, bottom, 1,
                 A+(iy_start-1)*nx+1, nx-2, MPI_DOUBLE, top, 1,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```



HANDLING MULTI GPU NODES

GPU-affinity

```
#pragma acc set device_num( devicenum )

// Or using the API:

#if _OPENACC

acc_device_t device_type = acc_get_device_type();

int ngpus=acc_get_num_devices(device_type);

int devicenum=rank%ngpus;

acc_set_device_num(devicenum,device_type);

#endif /*_OPENACC*/
```

Alternative (OpenMPI):

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

Alternative (MVAPICH2):

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

PROFILING OF MPI+OPENACC APPS

PROFILING MPI+OPENACC APPLICATIONS

Using pgprof

Embed MPI rank in output filename, process name, and context name

```
mpirun -np $np pgprof --output-profile profile.%q{OMPI_COMM_WORLD_RANK}
```

OpenMPI: OMPI_COMM_WORLD_RANK

MVAPICH2: MV2_COMM_WORLD_RANK

PROFILING MPI+OPENACC APPLICATIONS

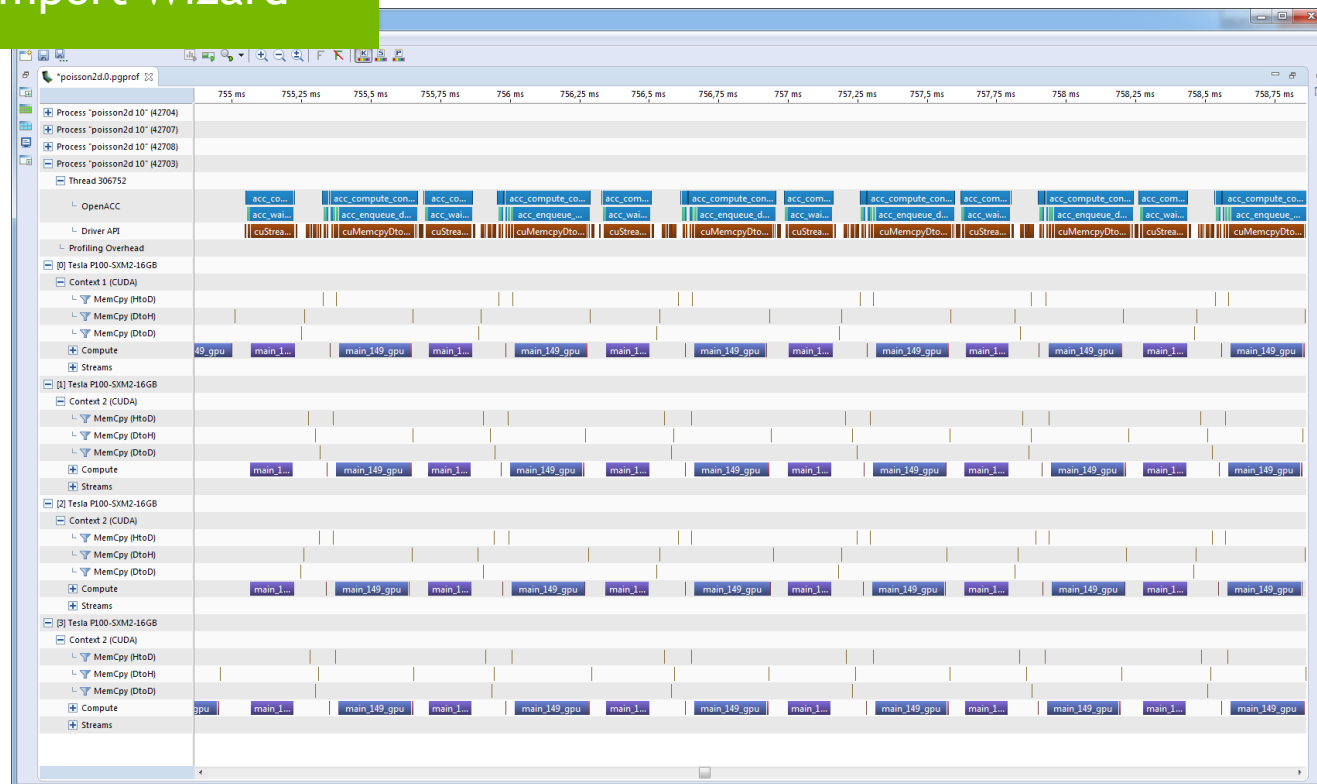
Using pgprof

```
pcp0032@juronb1:~/workspace/sc16-tutorial-openpower/5-Multi_GPU/Tasks/C/task2
[pcp0032@juronb1 task2]$ make profile
bsub -env "all, TMPDIR=/tmp" -n 4 -I -R "rusage[ngpus_share]
ocket 2 -bind-to core -np 4 pgprof --cpu-profiling off -
_WORLD_RANK}.pgprof ./poisson2d 10
Job <4707> is submitted to default queue <interactive>.
<<Waiting for dispatch ...>>
<<Starting on juronc04>>
==42703== PGPROF is profiling process 42703, command: ./
==42704== PGPROF is profiling process 42704, command: ./
==42707== PGPROF is profiling process 42707, command: ./
==42708== PGPROF is profiling process 42708, command: ./
Jacobi relaxation Calculation: 4096 x 4096 mesh
Calculate reference solution and time serial execution.
0, 0.250000
Parallel execution.
0, 0.250000
Num GPUs: 4.
4096x4096: 1 GPU: 0.0305 s, 4 GPUs: 0.0206 s, speedup:
36.98%
MPI time: 0.0037 s, inter GPU BW: 0.33 GiB/s
==42704== Generated result file: /gpfs/homeb/pcp0/pcp0032/workspace/sc16-tutoria
l-openpower/5-Multi_GPU/Tasks/C/task2/poisson2d.0.pgprof
==42708== Generated result file: /gpfs/homeb/pcp0/pcp0032/workspace/sc16-tutoria
l-openpower/5-Multi_GPU/Tasks/C/task2/poisson2d.3.pgprof
==42707== Generated result file: /gpfs/homeb/pcp0/pcp0032/workspace/sc16-tutoria
l-openpower/5-Multi_GPU/Tasks/C/task2/poisson2d.2.pgprof
==42703== Generated result file: /gpfs/homeb/pcp0/pcp0032/workspace/sc16-tutoria
l-openpower/5-Multi_GPU/Tasks/C/task2/poisson2d.1.pgprof
[pcp0032@juronb1 task2]$
```

PROFILING MPI+OPENACC APPLICATIONS

Using pgprof

Use the import Wizard



PROFILING MPI+OPENACC APPLICATIONS

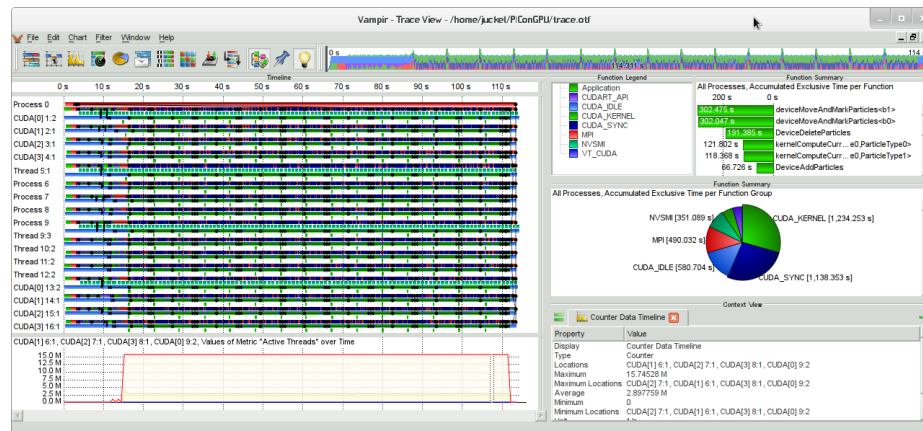
Third Party Tools

Multiple parallel profiling tools are
OpenACC-aware

Score-P

Vampir

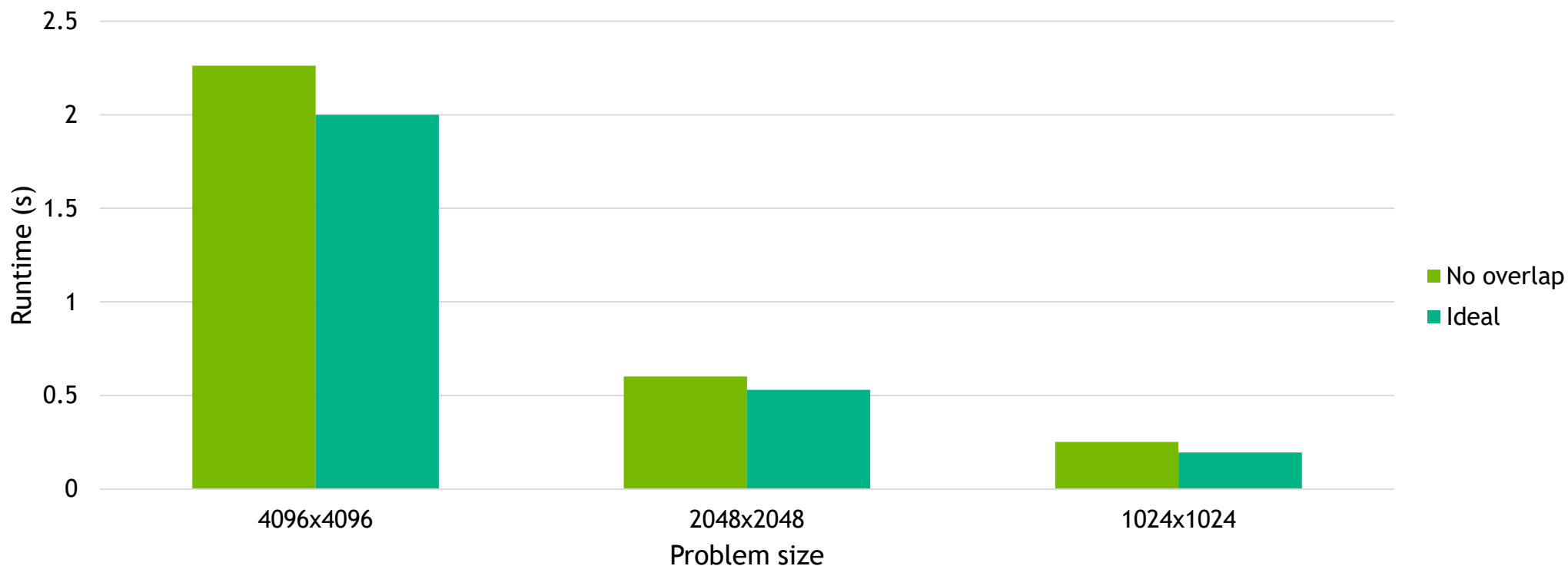
These tools are good for discovering MPI
issues as well as basic OpenACC performance
inhibitors.



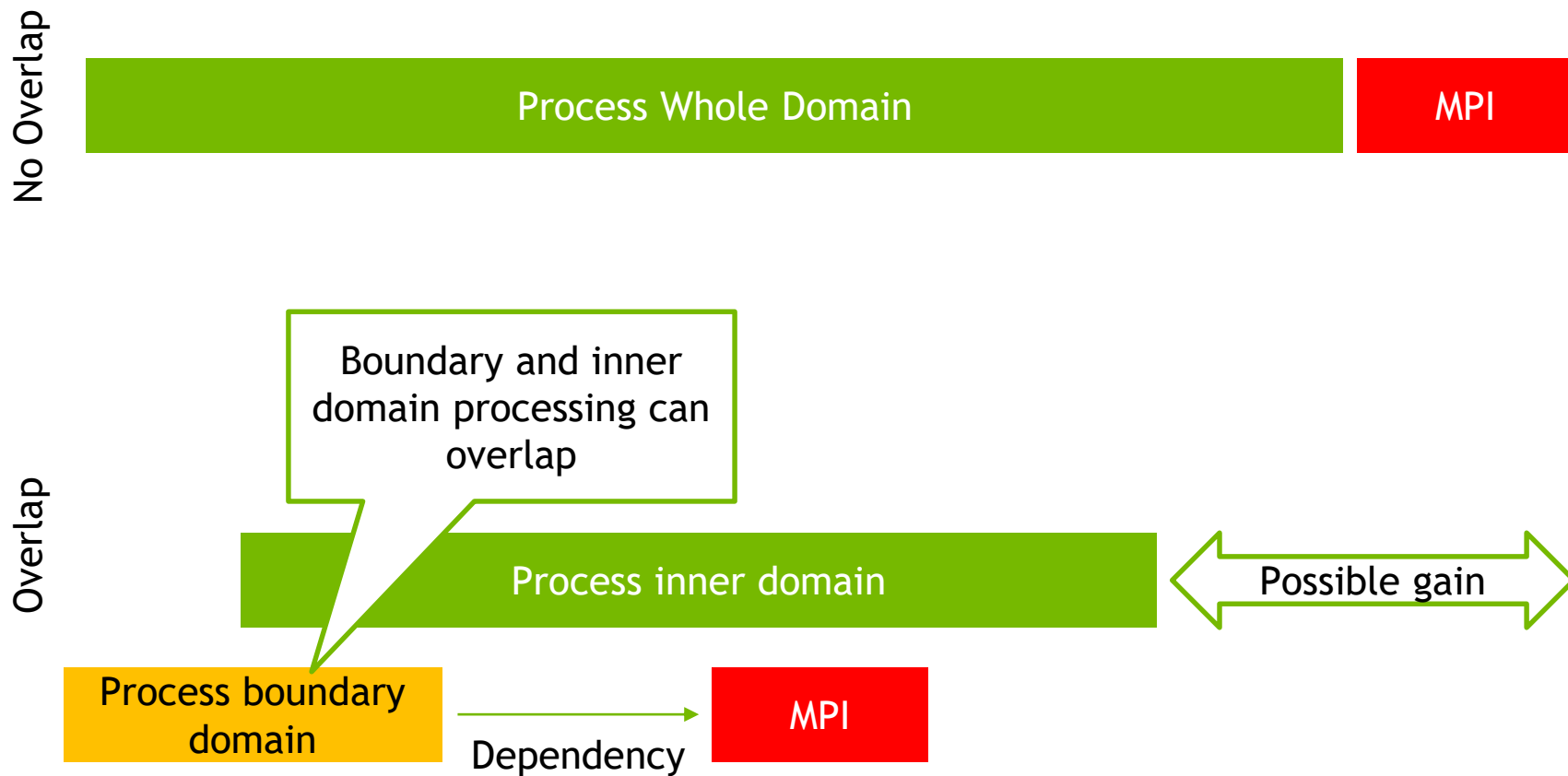
OVERLAPPING COMMUNICATION AND COMPUTATION

COMMUNICATION + COMPUTATION OVERLAP

OpenMPI 1.10.2 - 2 Tesla K40



COMMUNICATION + COMPUTATION OVERLAP



COMMUNICATION + COMPUTATION OVERLAP

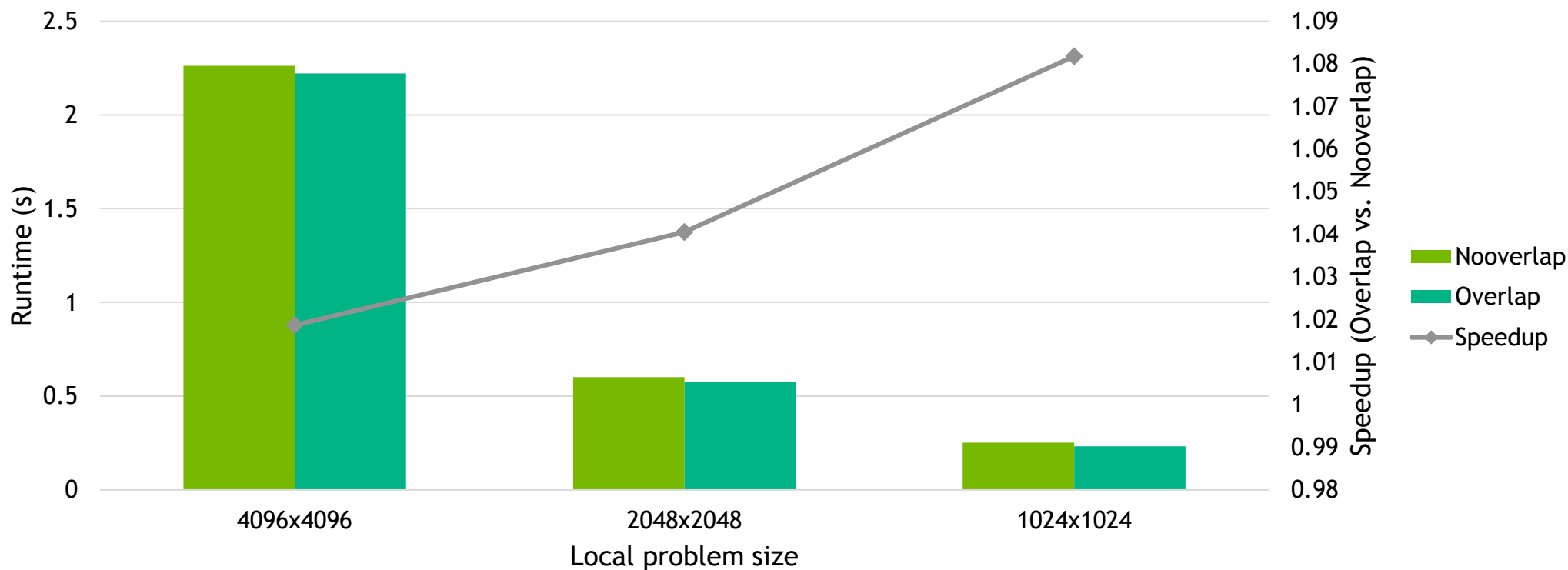
OpenACC with Async Queues

```
#pragma acc parallel loop present(A,Anew)
for ( ... ) //Process boundary

#pragma acc parallel loop present(A,Anew) async
for ( ... ) //Process inner domain
#pragma acc host_data use_device ( A ) {
    MPI_Sendrecv(A+iy_start*nx+1, nx-2, MPI_DOUBLE, top, 0,
                 A+iy_end*nx+1, nx-2, MPI_DOUBLE, bottom, 0,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    MPI_Sendrecv(A+(iy_end-1)*nx+1, nx-2, MPI_DOUBLE, bottom, 1,
                 A+(iy_start-1)*nx+1, nx-2, MPI_DOUBLE, top, 1,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
#pragma acc wait //wait for iteration to finish
```

COMMUNICATION + COMPUTATION OVERLAP

OpenMPI 1.10.2 - 2 Tesla K40



MPI AND UNIFIED MEMORY

MPI AND UNIFIED MEMORY

CAVEAT

Using Unified Memory with a non Unified Memory-aware MPI might break in some cases, e.g. when registering memory for RDMA, or even worse silently produce wrong results.



Use a Unified Memory-aware MPI with Unified Memory and MPI

Unified Memory-aware: CUDA-aware MPI with support for Unified Memory

MPI AND UNIFIED MEMORY

Current Status

Available Unified Memory-aware MPI implementations

- OpenMPI (since 1.8.5)
- MVAPICH2-GDR (since 2.2b)
 - Performance improvements with 2.2RC1 for Intranode GPU to GPU communication

Currently both treat all Unified Memory as Device Memory



Good performance if all buffers used in MPI are touched mainly on the GPU.

MPI AND UNIFIED MEMORY

Without Unified Memory-aware MPI

Only use non Unified Memory Buffers for MPI: cudaMalloc, cudaMallocHost or malloc

Application managed non Unified Memory Buffers also allow to work around current missing cases in Unified Memory-aware MPI Implementations.