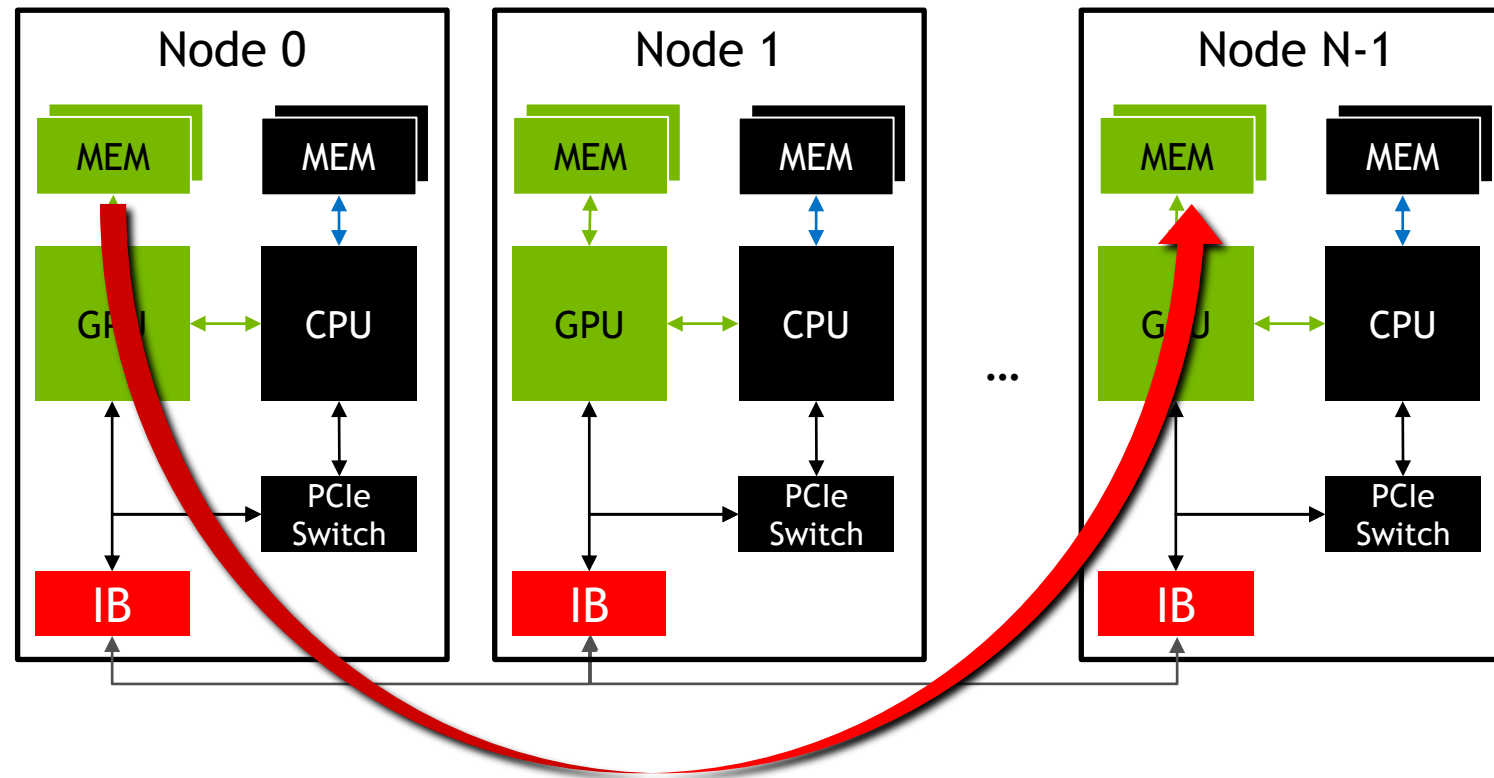


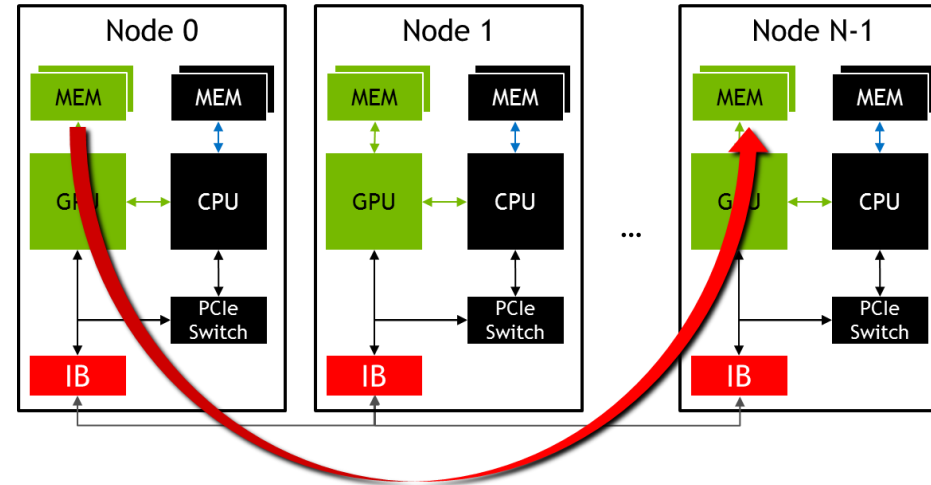
MULTI GPU PROGRAMMING WITH MPI AND OPENACC

28.10.2022 | J.KRAUS (NVIDIA)

MPI+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);
```

WHAT YOU WILL LEARN

- What MPI is
- How to use MPI for inter GPU communication with OpenACC
- How to use pgprof for MPI+OpenACC applications
- 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_Allreduce
- Multiple implementations (open source and commercial)
 - Binding for C/C++, Fortran, Python, ...
 - E.g. MPICH, OpenMPI, Parastation MPI, MVAPICH, IBM Platform MPI, Cray MPT, ...

MPI – A MINIMAL PROGRAM

```
#include <mpi.h>

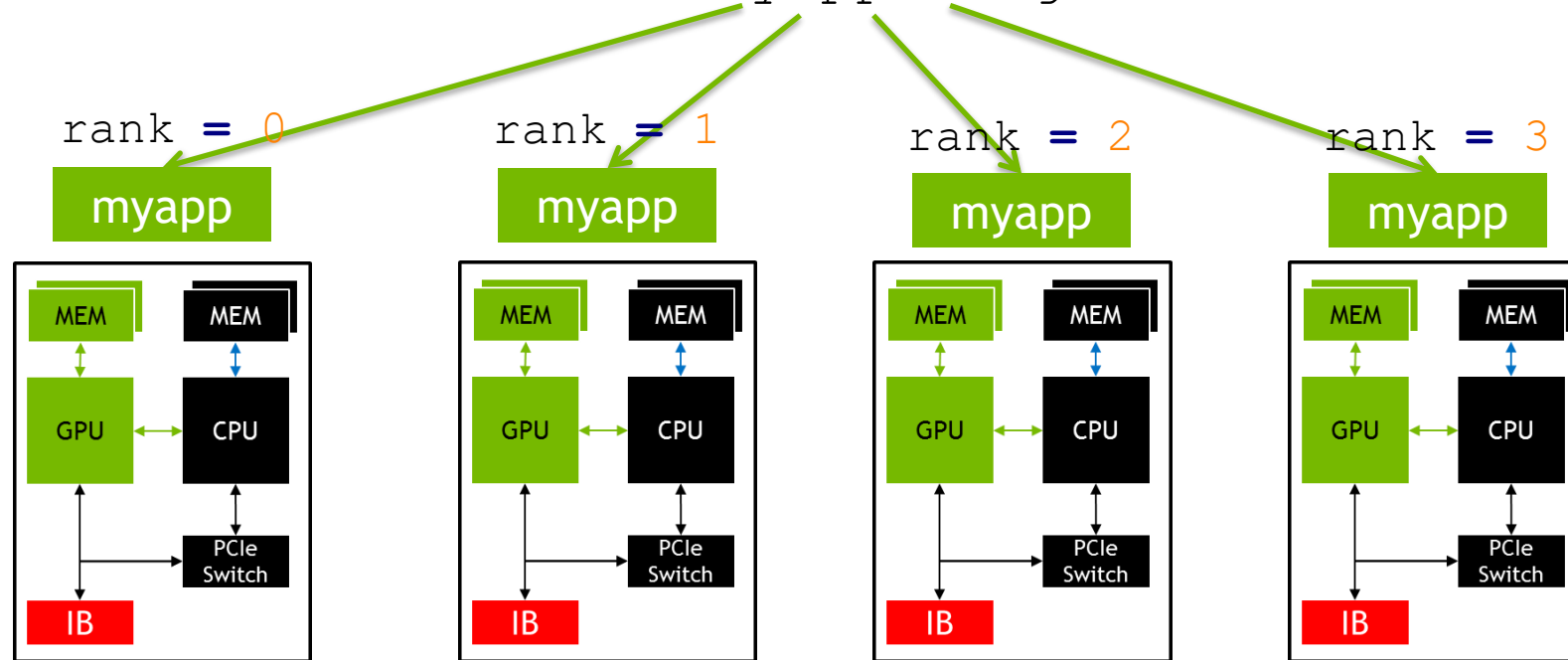
int main(int argc, char *argv[]) {
    int rank, size;
    /* Initialize the MPI library */
    MPI_Init(&argc, &argv);
    /* Determine the calling rank and total number of ranks */
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    /* Call MPI routines like MPI_Send,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

Remark: Almost all MPI routines return an error value which should be checked. The examples and tasks leave that out for brevity.

MPI – COMPILING AND LAUNCHING

```
$ mpicc -o myapp myapp.c
```

```
$ srun -n 4 ./myapp <args>
```



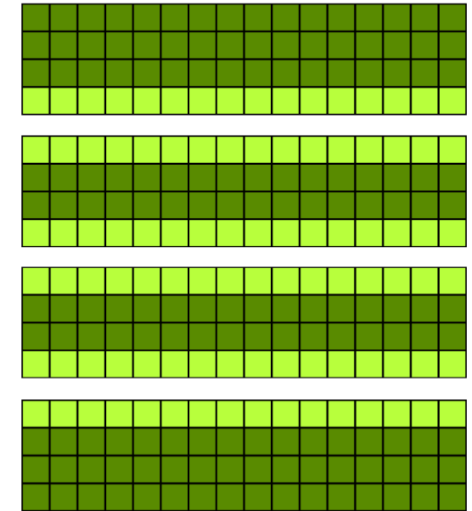
EXAMPLE: JACOBI SOLVER

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:

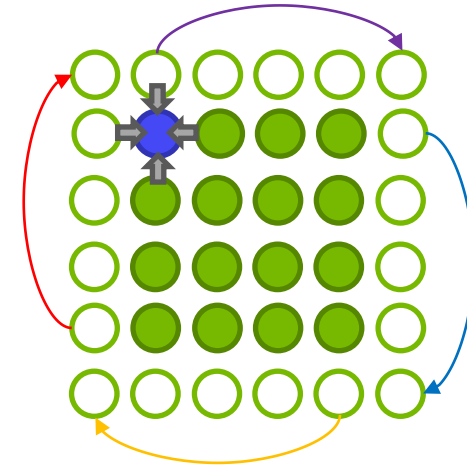
```
for (int iy = 1; iy < ny-1; ++iy)
for (int ix = 1; ix < nx-1; ++ix)

  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

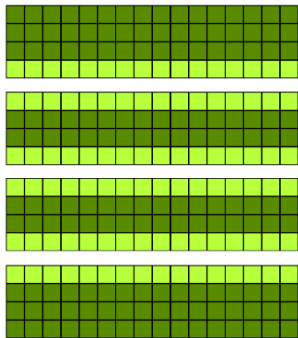


DOMAIN DECOMPOSITION

Different ways to split the work between processes:

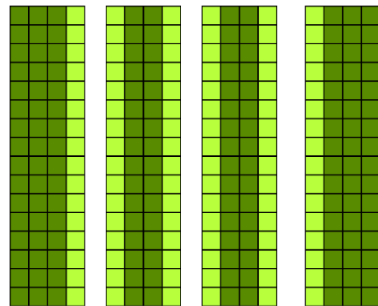
Minimizes number of neighbors:

- Communicate to less neighbors
- Optimal for latency bound communication



Horizontal Stripes

Contiguous if data is row-major

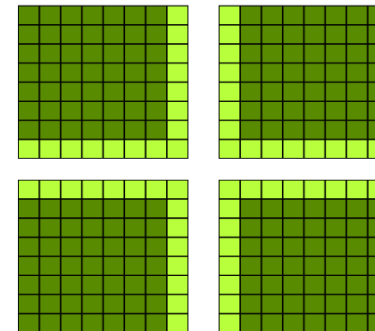


Vertical Stripes

Contiguous if data is column-major

Minimizes surface area/volume ratio:

- Communicate less data
- Optimal for bandwidth bound communication



Tiles

EXAMPLE: JACOBI SOLVER – MULTI GPU

While not converged

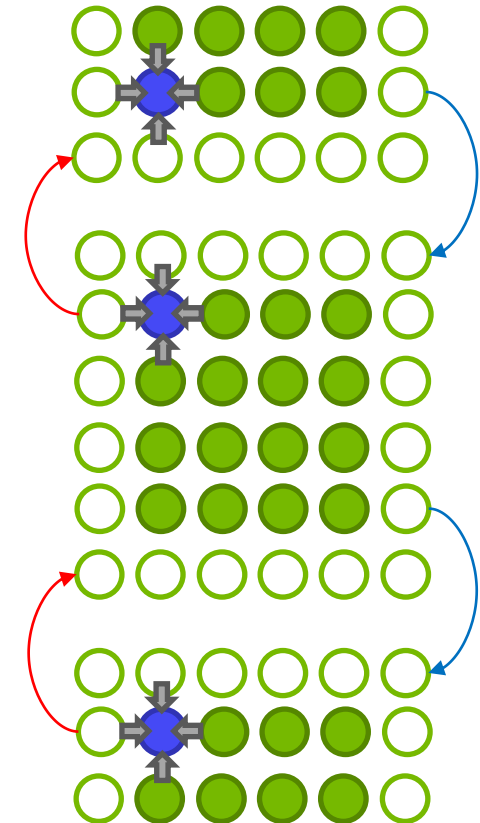
Do Jacobi step:

```
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

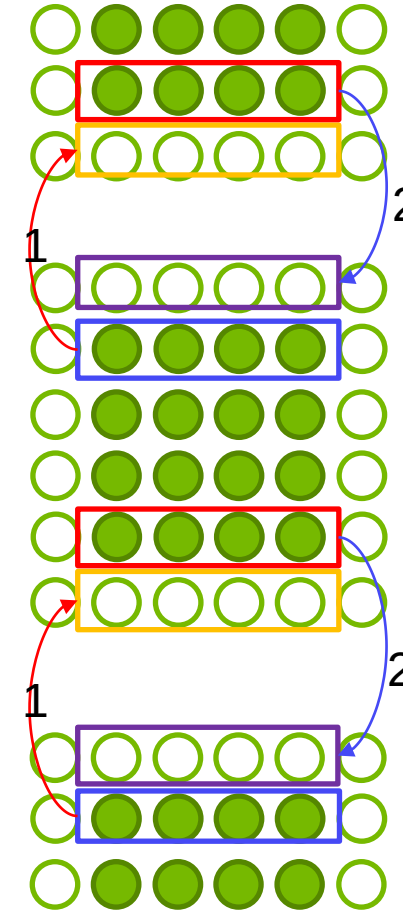
Apply periodic boundary conditions and exchange halo with 2 neighbors

Next iteration

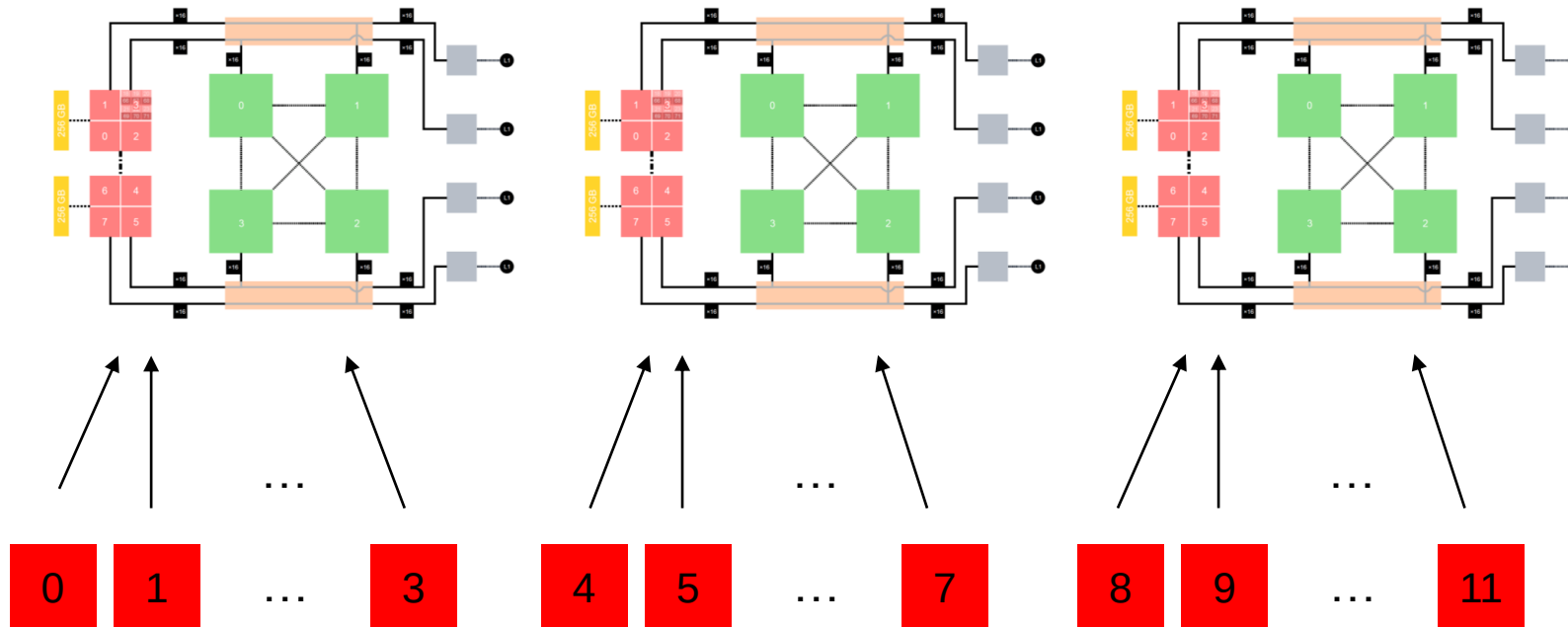


EXAMPLE: JACOBI – TOP/BOTTOM HALO

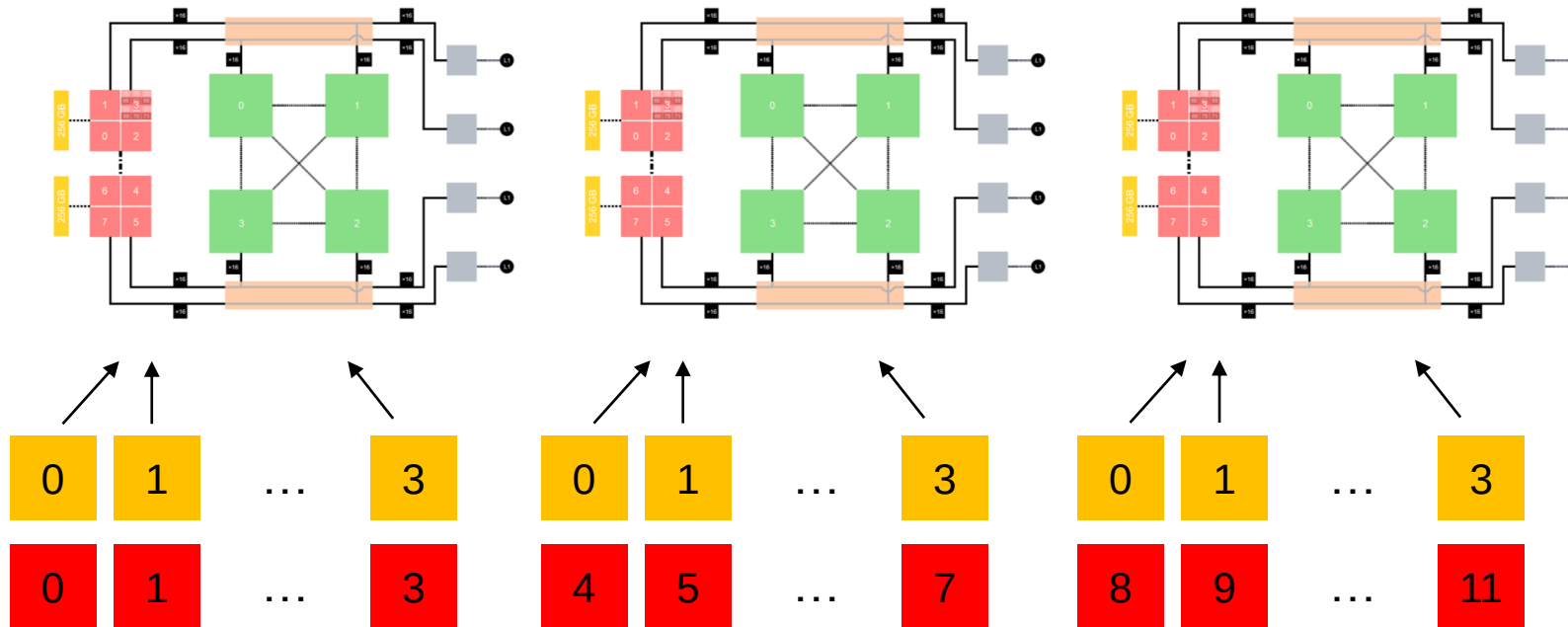
```
#pragma acc host_data use_device ( A ) {  
MPI_Sendrecv(A+iy_start*nx+1, nx-2, MPI_DOUBLE, top, 0,  
             A+iy_end*nx+1, nx-2, MPI_DOUBLE, bottom, 0,  
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
  
MPI_Sendrecv(A+(iy_end-1)*nx+1, nx-2, MPI_DOUBLE, bottom, 1,  
             A+(iy_start-1)*nx+1,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



HANDLING GPU AFFINITY



HANDLING GPU AFFINITY



HANDLING GPU AFFINITY

```
int local_rank = -1;
{
    MPI_Comm local_comm;
    MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, rank,
                        MPI_INFO_NULL, &local_comm);
    MPI_Comm_rank(local_comm, &local_rank);
    MPI_Comm_free(&local_comm);
}
#ifdef _OPENACC
int num_devs = acc_get_num_devices(acc_get_device_type());
#else
int num_devs = 1;
#endif
#pragma acc set device_num( local_rank%num_devs )
```

Needed if resource manager handles GPU affinity.

Handled gracefully on JUWELS-Booster by NVHPC if omitted:
“If the value of *devicenum* is greater than or equal to the value returned by *acc_get_num_devices* for that device type, the behavior is implementation-defined.”

PROFILING MPI+OPENACC APPLICATIONS

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

```
srun nsys profile --trace=mpi,cuda,openacc,nvtx \
                --output profile.%q{PMI_RANK} \
                ./application
```

JURECA-DC: PMI_RANK

OpenMPI: OMPI_COMM_WORLD_RANK

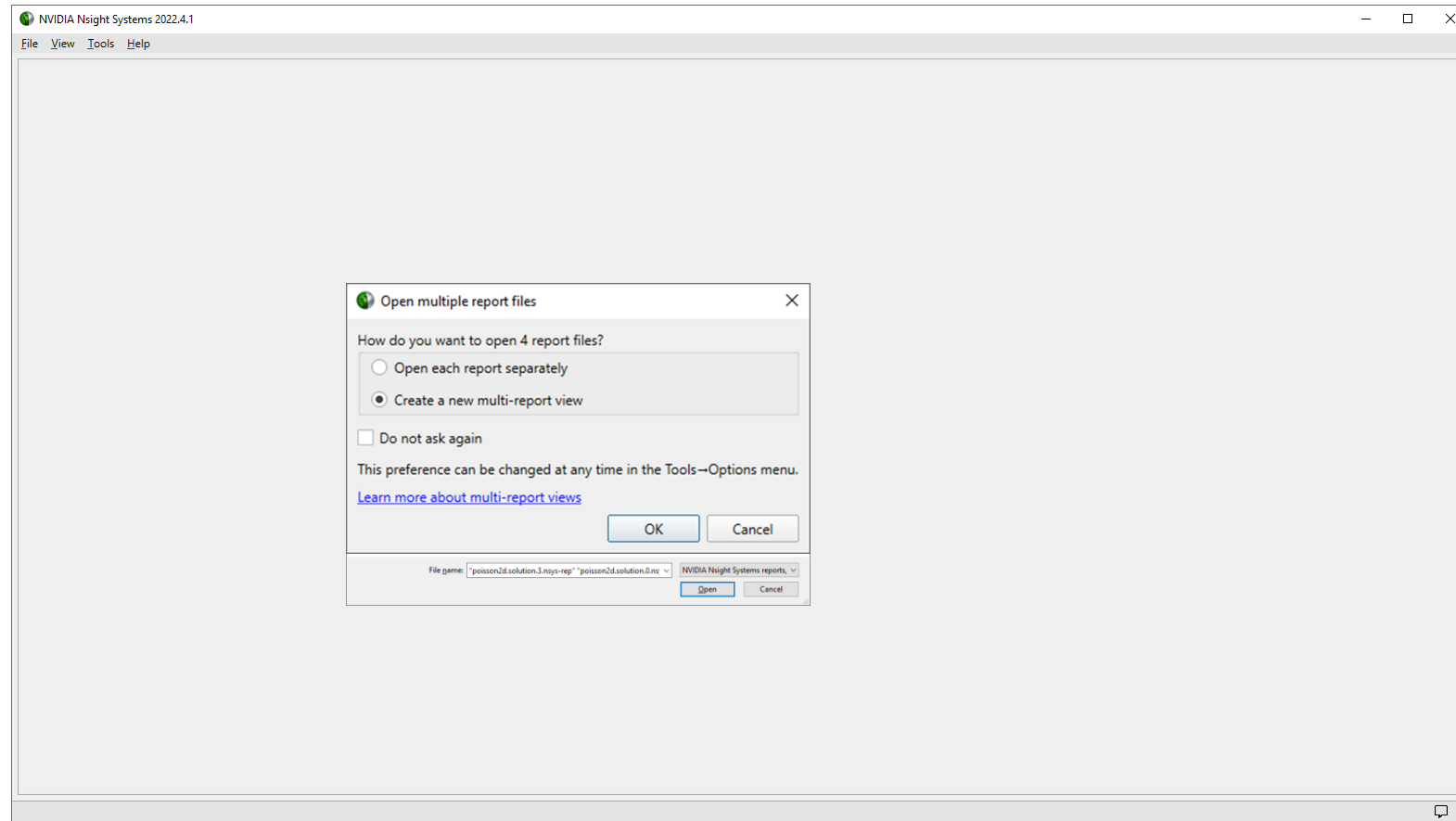
MPICH2: MV2_COMM_WORLD_RANK

PROFILING MPI+OPENACC APPLICATIONS

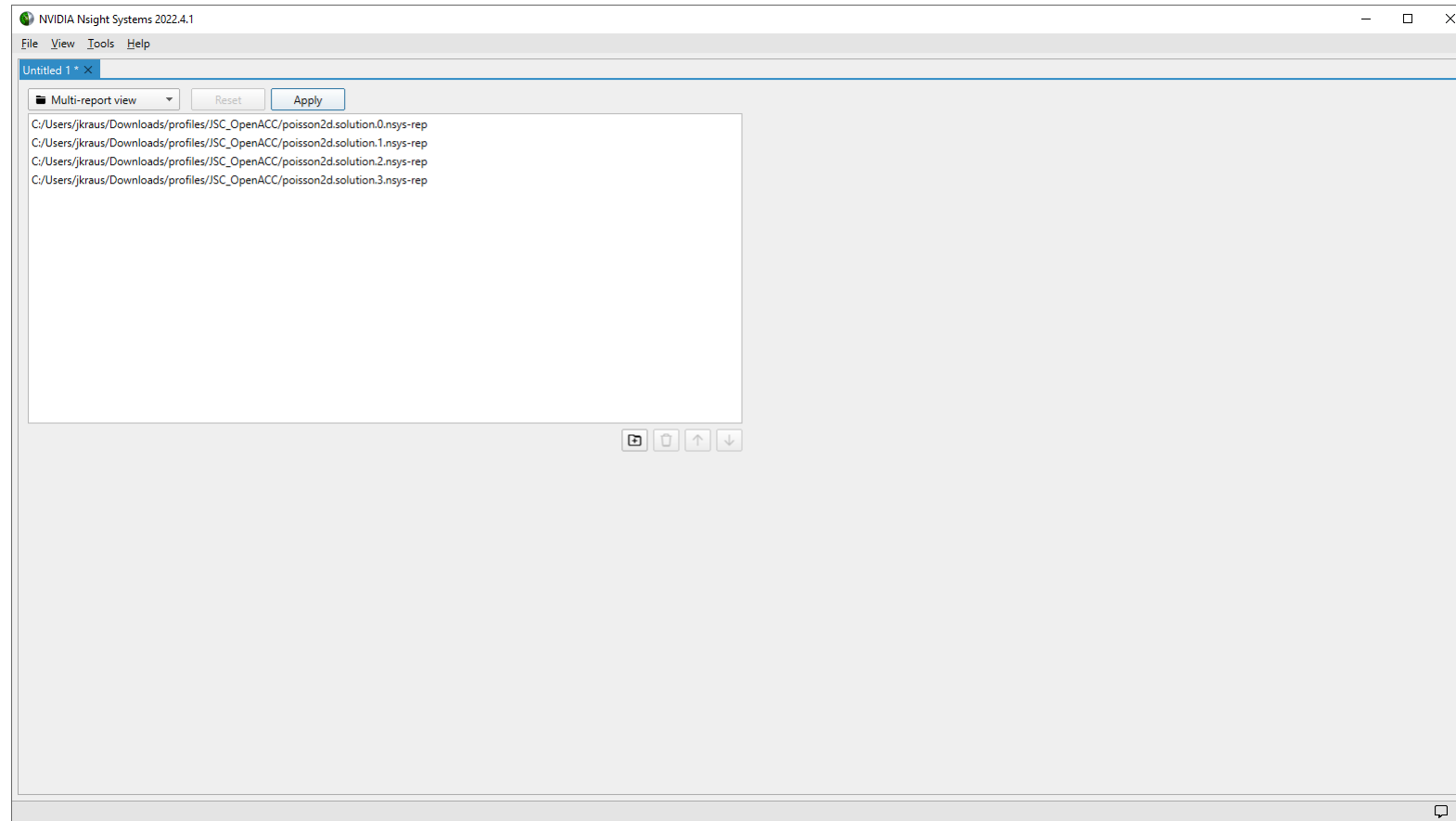
```
kraus1@jrlogin02: /p/home/jus
[kraus1@jrlogin02 task1]$ make profile
srun -A exalab -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 nsys profile --trace=mpi,cuda,openacc,nvtx -o poisson2d.%q{PMI_RANK} ./poisson2d
srun: job 11027030 queued and waiting for resources
srun: job 11027030 has been allocated resources
Warning: LBR backtrace method is not supported on this platform. DWARF backtrace method will be used.
Warning: LBR backtrace method is not supported on this platform. DWARF backtrace method will be used.
Warning: LBR backtrace method is not supported on this platform. DWARF backtrace method will be used.
Warning: LBR backtrace method is not supported on this platform. DWARF backtrace method will be used.
Jacobi relaxation Calculation: 8192 x 8192 mesh
Calculate reference solution and time serial execution.
0, 0.250000
100, 0.249985
200, 0.249970
300, 0.249955
400, 0.249940
500, 0.249925
600, 0.249911
700, 0.249896
800, 0.249881
900, 0.249866
Parallel execution.
0, 0.250000
100, 0.249985
200, 0.249970
300, 0.249955
400, 0.249940
500, 0.249925
600, 0.249911
700, 0.249896
```

```
kraus1@jrlogin02: /p/home/jus
600, 0.249911
700, 0.249896
800, 0.249881
900, 0.249866
Num GPUs: 4.
8192x8192: 1 GPU: 2.4286 s, 4 GPUs: 2.6838 s, speedup: 0.90, efficiency: 22.62%
MPI time: 0.0001 s, inter GPU BW: 2803.63 GiB/s
Generating '/tmp/nsys-report-5220.qdstrm'
Generating '/tmp/nsys-report-04ac.qdstrm'
Generating '/tmp/nsys-report-7c11.qdstrm'
Generating '/tmp/nsys-report-2353.qdstrm'
[1/1] [=====100%] poisson2d.1.nsys-rep
Generated:
/p/home/jusers/kraus1/juwels/workspace/openacc/6-Multi-GPU-Programming-with-MPI_and_OpenACC/exercises/C/task1/poisson2d.1.nsys-rep
[1/1] [=====100%] poisson2d.2.nsys-rep
Generated:
/p/home/jusers/kraus1/juwels/workspace/openacc/6-Multi-GPU-Programming-with-MPI_and_OpenACC/exercises/C/task1/poisson2d.2.nsys-rep
[1/1] [=====100%] poisson2d.3.nsys-rep
Generated:
/p/home/jusers/kraus1/juwels/workspace/openacc/6-Multi-GPU-Programming-with-MPI_and_OpenACC/exercises/C/task1/poisson2d.3.nsys-rep
[1/1] [=====100%] poisson2d.0.nsys-rep
Generated:
/p/home/jusers/kraus1/juwels/workspace/openacc/6-Multi-GPU-Programming-with-MPI_and_OpenACC/exercises/C/task1/poisson2d.0.nsys-rep
[kraus1@jrlogin02 task1]$ ls *.nsys-rep
poisson2d.0.nsys-rep poisson2d.1.nsys-rep poisson2d.2.nsys-rep poisson2d.3.nsys-rep
[kraus1@jrlogin02 task1]$
```

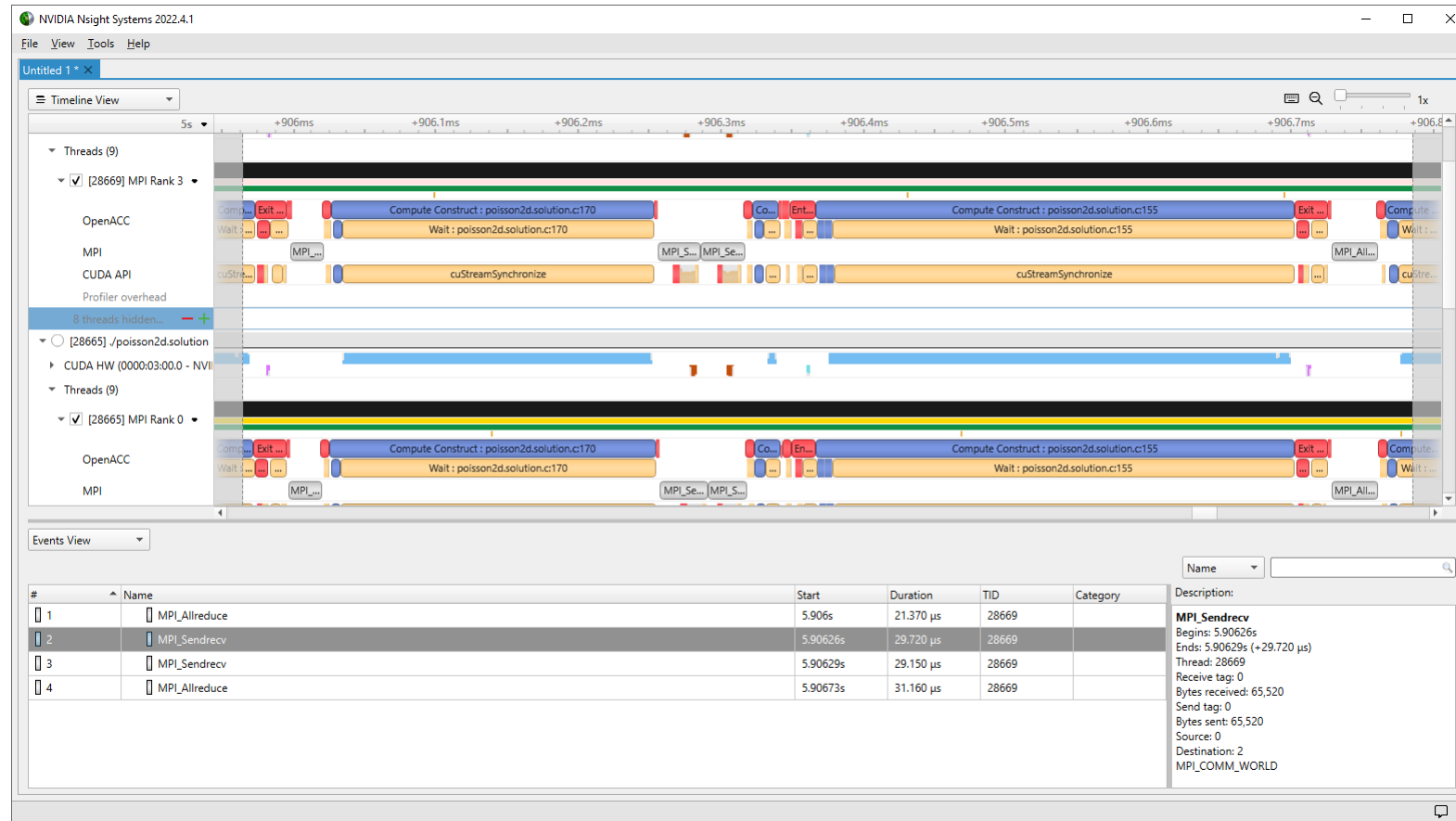
PROFILING MPI+OPENACC APPLICATIONS



PROFILING MPI+OPENACC APPLICATIONS



PROFILING MPI+OPENACC APPLICATIONS

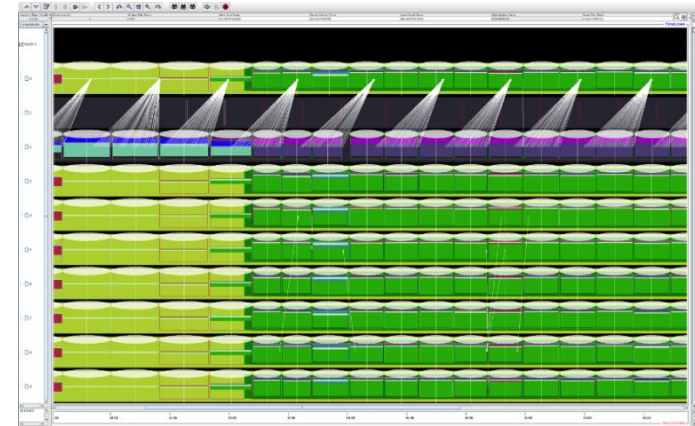
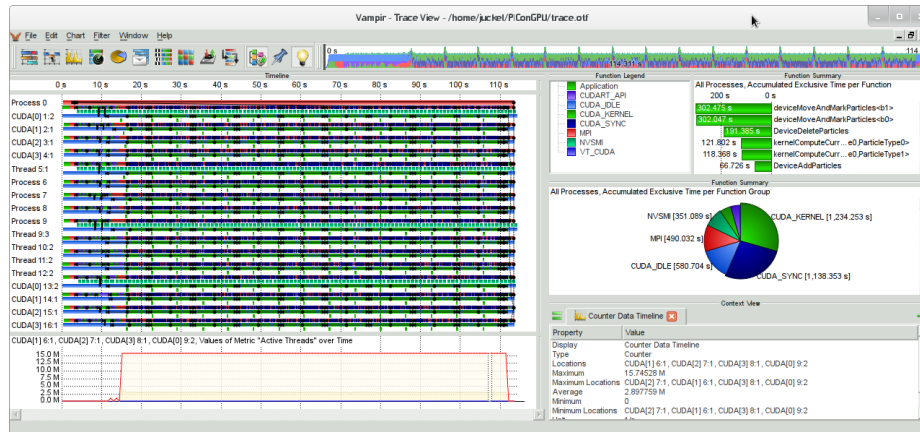


PROFILING MPI+OPENACC APPLICATIONS

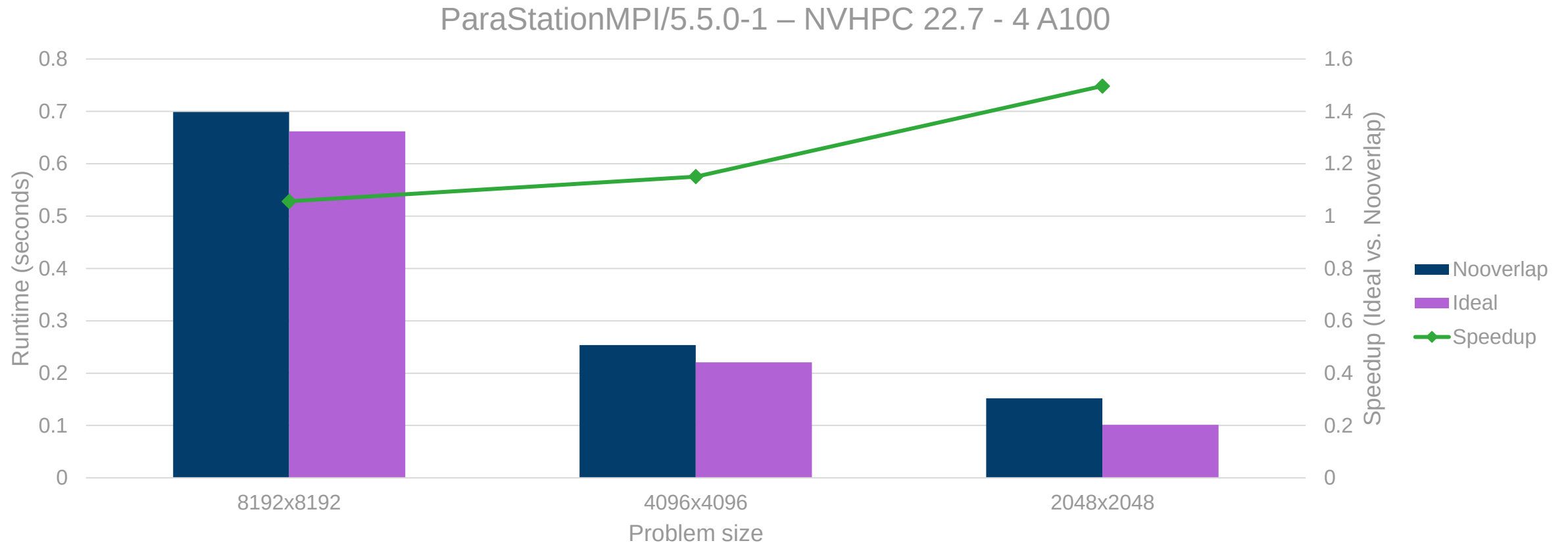
Multiple parallel profiling tools are CUDA-aware

- Score-P
- Vampir
- Tau

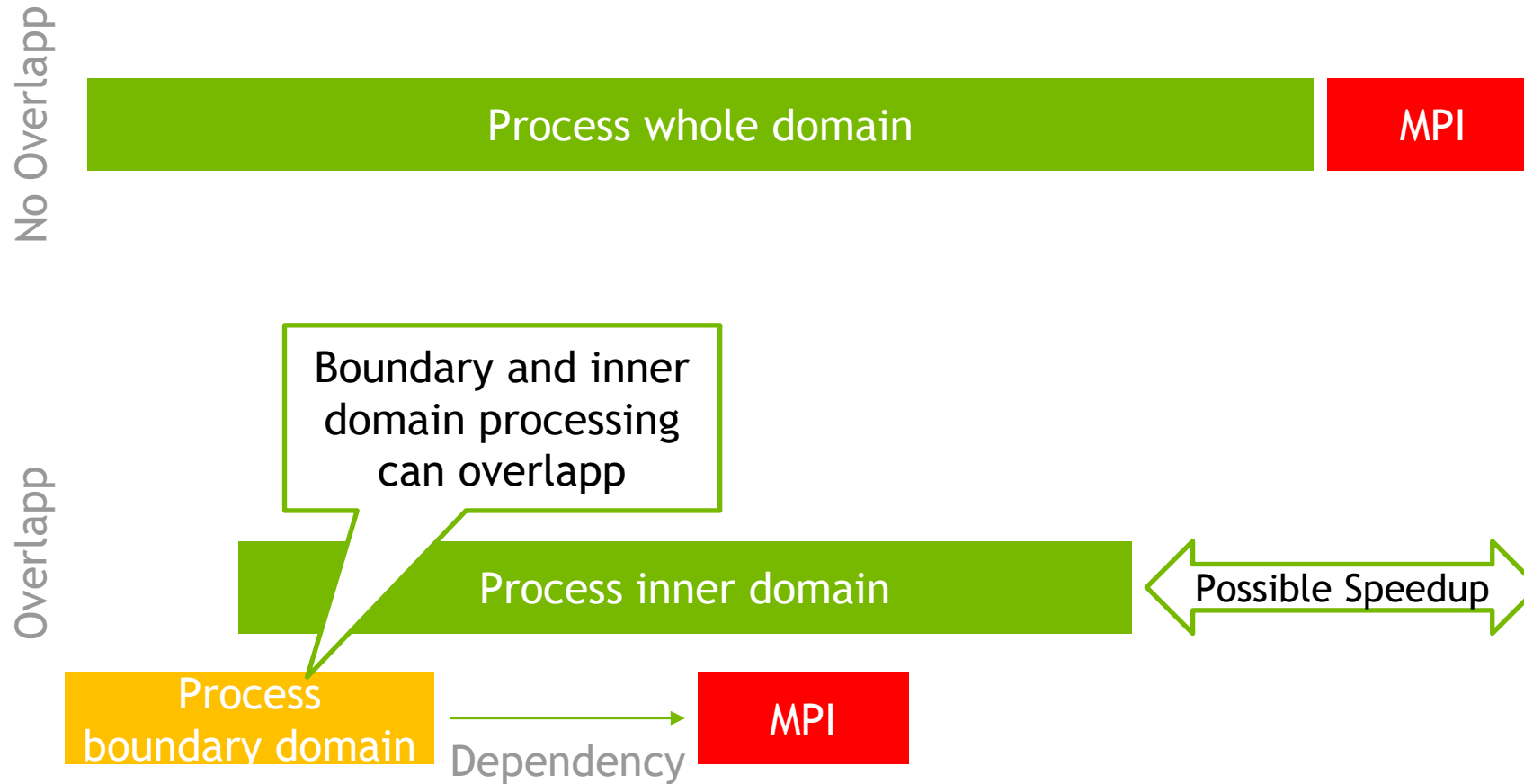
These tools are good for discovering MPI issues as well as basic CUDA performance inhibitors.



COMMUNICATION + COMPUTATION OVERLAP



COMMUNICATION + COMPUTATION OVERLAP



COMMUNICATION + COMPUTATION OVERLAP

```
#pragma acc parallel loop
for ( ... )
    //Process boundary
#pragma acc parallel loop async
for ( ... )
    //Process inner domain

#pragma acc host_data use_device ( A )
{
    //Exchange halo with top and bottom neighbor
    MPI_Sendrecv( A... );
    //...
}
//wait for iteration to finish
#pragma acc wait
```


SCALABILITY METRICS FOR SUCCESS

- Serial Time: T_s :
 - How long it takes to run the problem with a single process
- Parallel Time: T_p
 - How long it takes to run the problem with multiple processes
- Number of Processes: P
 - The number of Processes operating on the task at hand
- Speedup: $S = T_s / T_p$
 - How much faster is the parallel version vs. serial. (optimal is P)
- Efficiency: $E = S / P$
 - How efficient are the processors used (optimal is 1)

TASK 1: APPLY DOMAIN DECOMPOSITION

- Handle GPU affinity
- Halo Exchange

Look for TODOs

```
$ make
mpicc -c -DUSE_DOUBLE -Minfo=accel -fast -acc=gpu -gpu=cc80 poisson2d.c [...]
srun -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d
Jacobi relaxation Calculation: 8192 x 8192 mesh
[...]
Num GPUs: 4.
8192x8192: 1 GPU:    2.3283 s, 4 GPUs:    2.3494 s, speedup:
MPI time:    0.0001 s, inter GPU BW:  4760.23 GiB/s
```

Make Targets:

```
run:          run poisson2d (default)
poisson2d:    build poisson2d binary
profile:      profile with Nsight Systems
*.solution:  same as above with solution
              (poisson2d.solution.*)
```

TASK 2: HIDE MPI COMMUNICATION TIME

- Start copy loop asynchronously
- Wait for async copy loop after MPI comm. is done

Look for TODOs

```
$ make
mpicc -c -DUSE_DOUBLE -Minfo=accel -fast -acc=gpu -gpu=cc80 poisson2d.c [...]
srun -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d
Jacobi relaxation Calculation: 8192 x 8192 mesh
[...]
Num GPUs: 4.
8192x8192: 1 GPU:    2.3289 s, 4 GPUs:    0.6824 s, speedup:
MPI time:    0.0373 s, inter GPU BW:    6.54 GiB/s
```

Make Targets:

```
run:          run poisson2d (default)
poisson2d:    build poisson2d binary
profile:      profile with Nsight Systems
*.solution:   same as above with solution
               (poisson2d.solution.*)
```

TASK 1: INITIAL VERSION

```
kraus1@jrlogin02:~$ make
srun -A exalab -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d
srun: job 11027059 queued and waiting for resources
srun: job 11027059 has been allocated resources
Jacobi relaxation Calculation: 8192 x 8192 mesh
Calculate reference solution and time serial execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Parallel execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Num GPUs: 4.
8192x8192: 1 GPU: 2.3298 s, 4 GPUs: 2.3494 s, speedup: 0.99, efficiency: 24.79%
MPI time: 0.0000 s, inter GPU BW: 6832.03 GiB/s
```

TASK 1: SOLUTION

```
//Initialize MPI and determine rank and size
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

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

#pragma acc set device_num( local_rank )
real* restrict const A = (real*) malloc(nx*ny*sizeof(real));
```

%num_devs omitted see slide 15

TASK 1: SOLUTION

```
// Ensure correctness if ny%size != 0
int chunk_size = ceil( (1.0*ny)/size );
int iy_start = rank * chunk_size;
int iy_end = iy_start + chunk_size;
// Do not process boundaries
iy_start = max( iy_start, 1 );
iy_end = min( iy_end, ny - 1 );
```

TASK 1: SOLUTION

```
int top = (rank == 0) ? (size-1) : rank-1;
int bottom = (rank == (size-1)) ? 0 : rank+1;
#pragma acc host_data use_device( A ) {
    //1. Sent row iy_start (first modified row) to top receive lower boundary (iy_end)
    //from bottom
    MPI_Sendrecv( A+iy_start*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, top, 0,
                  A+iy_end*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, bottom, 0,
                  MPI_COMM_WORLD, MPI_STATUS_IGNORE );
    //2. Sent row (iy_end-1) (last modified row) to bottom
    //receive upper boundary (iy_start-1) from top
    MPI_Sendrecv( A+(iy_end-1)*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, bottom, 0,
                  A+(iy_start-1)*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, top, 0,
                  MPI_COMM_WORLD, MPI_STATUS_IGNORE );
}
```

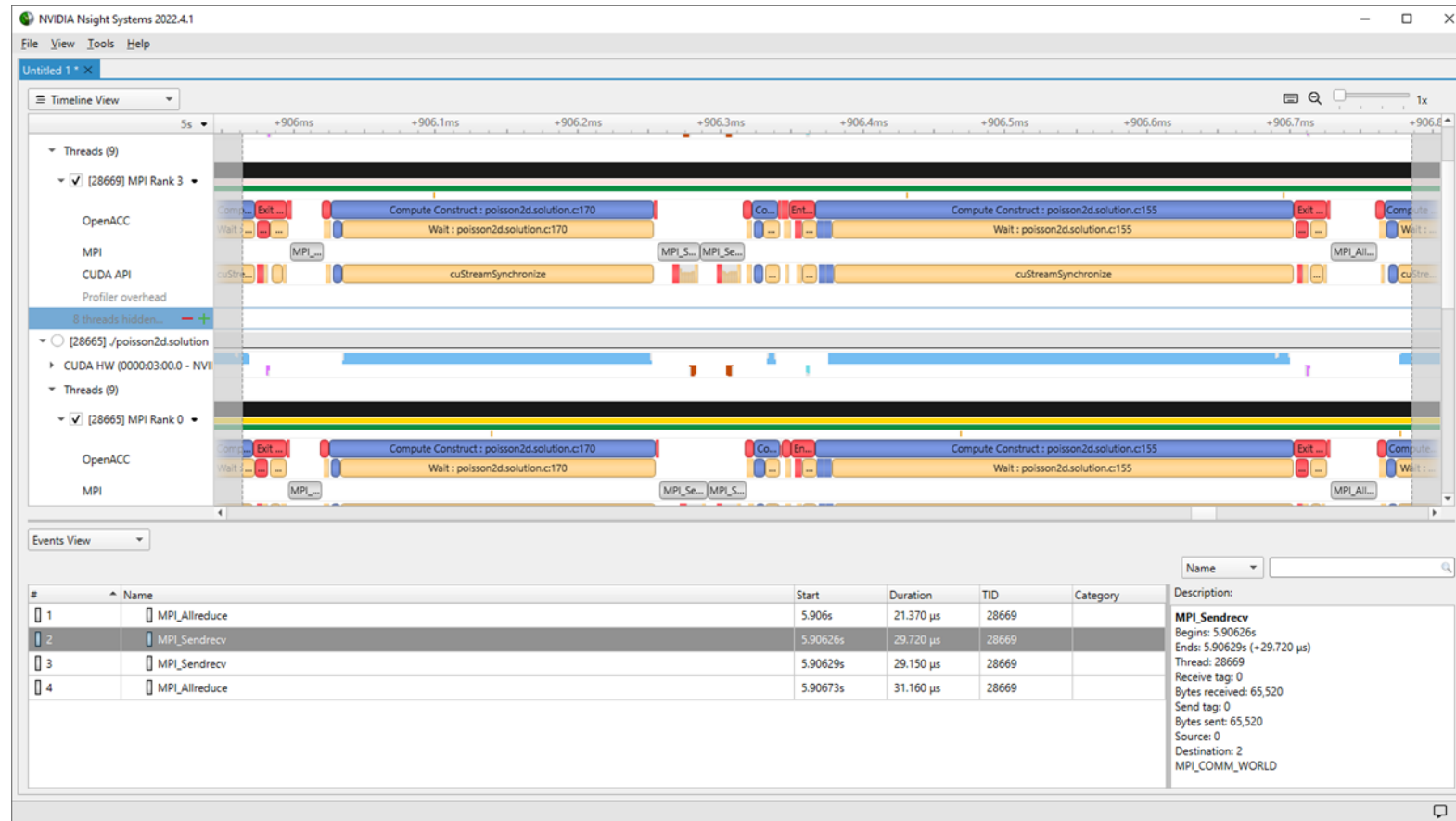

TASK 1: SOLUTION

```
kraus1@jrlogin02:~$ srun -A exalab -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d.solution
srun: job 11027073 queued and waiting for resources
srun: job 11027073 has been allocated resources
Jacobi relaxation Calculation: 8192 x 8192 mesh
Calculate reference solution and time serial execution.
 0, 0.250000
100, 0.249985
200, 0.249970
300, 0.249955
400, 0.249940
500, 0.249925
600, 0.249911
700, 0.249896
800, 0.249881
900, 0.249866
Parallel execution.
 0, 0.250000
100, 0.249985
200, 0.249970
300, 0.249955
400, 0.249940
500, 0.249925
600, 0.249911
700, 0.249896
800, 0.249881
900, 0.249866
Num GPUs: 4.
8192x8192: 1 GPU: 2.3305 s, 4 GPUs: 0.6819 s, speedup: 3.42, efficiency: 85.44%
MPI time: 0.0372 s, inter GPU BW: 6.55 GiB/s
[kraus1@jrlogin02 task1]$
```


TASK 2: INITIAL VERSION

```
kraus1@jrlogin02:~$ srun -A exalab -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d
srun: job 11027080 queued and waiting for resources
srun: job 11027080 has been allocated resources
Jacobi relaxation Calculation: 8192 x 8192 mesh
Calculate reference solution and time serial execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Parallel execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Num GPUs: 4.
8192x8192: 1 GPU: 2.3289 s, 4 GPUs: 0.6826 s, speedup: 3.41, efficiency: 85.29%
MPI time: 0.0378 s, inter GPU BW: 6.45 GiB/s
[kraus1@jrlogin02 task2]$
```

TASK 2: INITIAL VERSION



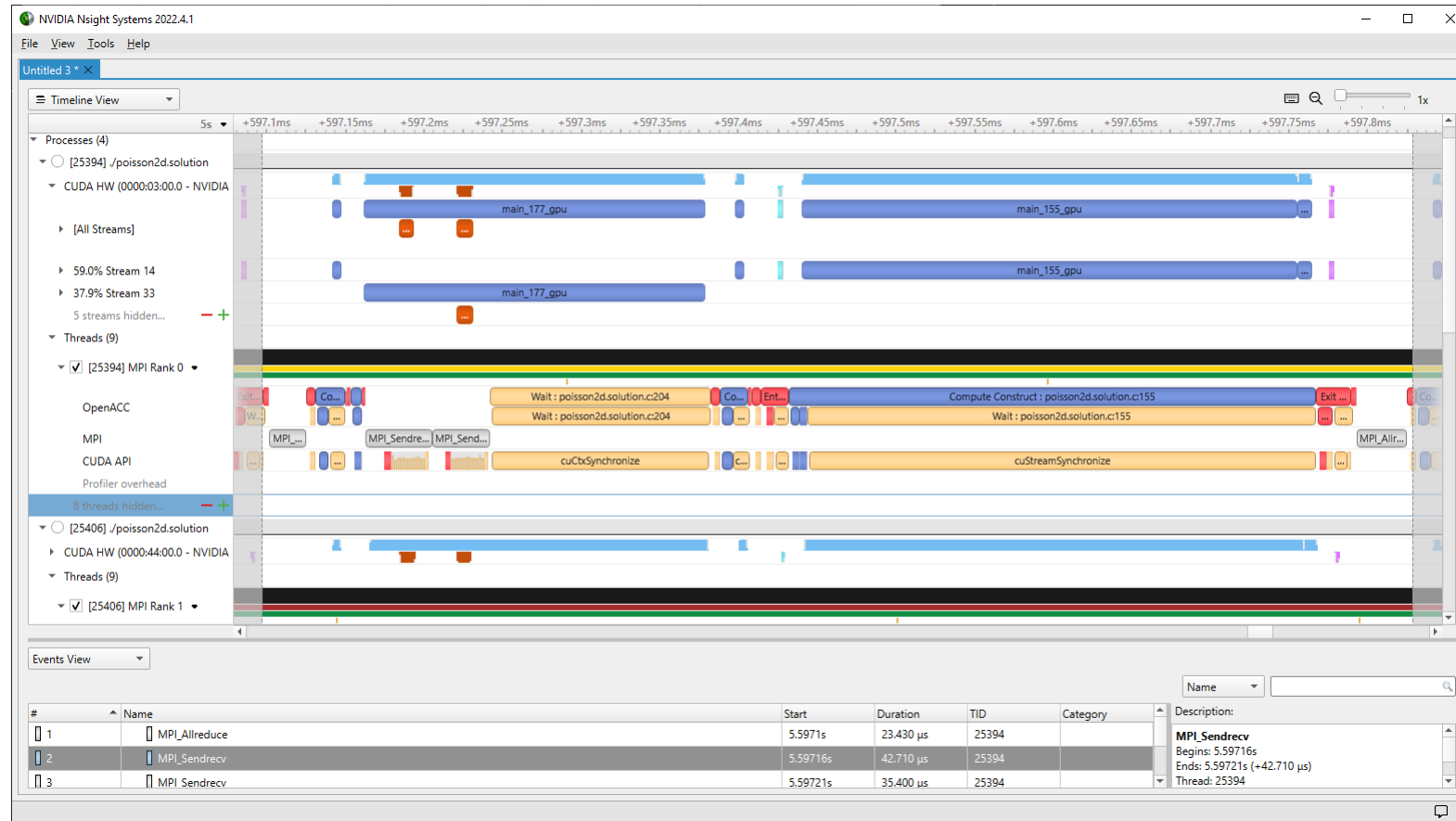
TASK 2: SOLUTION

```
#pragma acc parallel loop present(A,Anew)
for( int ix = ix_start; ix < ix_end; ix++ ) {
    A[(iy_start)*nx+ix] = Anew[(iy_start)*nx+ix];
    A[(iy_end-1)*nx+ix] = Anew[(iy_end-1)*nx+ix];
}
#pragma acc parallel loop present(A,Anew) async
for (int iy = iy_start+1; iy < iy_end-1; iy++) {
for( int ix = ix_start; ix < ix_end; ix++ ) {
    A[iy*nx+ix] = Anew[iy*nx+ix];
} }
int top = (rank == 0) ? (size-1) : rank-1;
int bottom = (rank == (size-1)) ? 0 : rank+1;
#pragma acc host_data use_device( A )
{
    MPI_Sendrecv( A+iy_start*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, top , 0,
                  A+iy_end*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, bottom, 0,
                  MPI_COMM_WORLD, MPI_STATUS_IGNORE );
    MPI_Sendrecv( A+(iy_end-1)*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, bottom, 0,
                  A+(iy_start-1)*nx+ix_start, (ix_end-ix_start), MPI_REAL_TYPE, top , 0,
                  MPI_COMM_WORLD, MPI_STATUS_IGNORE );
}
#pragma acc wait
```

TASK 2: SOLUTION

```
kraus1@jrlogin02:~$ srun -A exalab -p dc-gpu-devel --gres=gpu:4 --time 0:10:00 --pty -n 4 ./poisson2d.solution
srun: job 11027083 queued and waiting for resources
srun: job 11027083 has been allocated resources
Jacobi relaxation Calculation: 8192 x 8192 mesh
Calculate reference solution and time serial execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Parallel execution.
  0, 0.250000
 100, 0.249985
 200, 0.249970
 300, 0.249955
 400, 0.249940
 500, 0.249925
 600, 0.249911
 700, 0.249896
 800, 0.249881
 900, 0.249866
Num GPUs: 4.
8192x8192: 1 GPU:  2.3299 s, 4 GPUs:  0.6602 s, speedup:  3.53, efficiency:  88.23%
MPI time:  0.0522 s, inter GPU BW:  4.68 GiB/s
[kraus1@jrlogin02 task2]$
```

TASK 2: SOLUTION



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