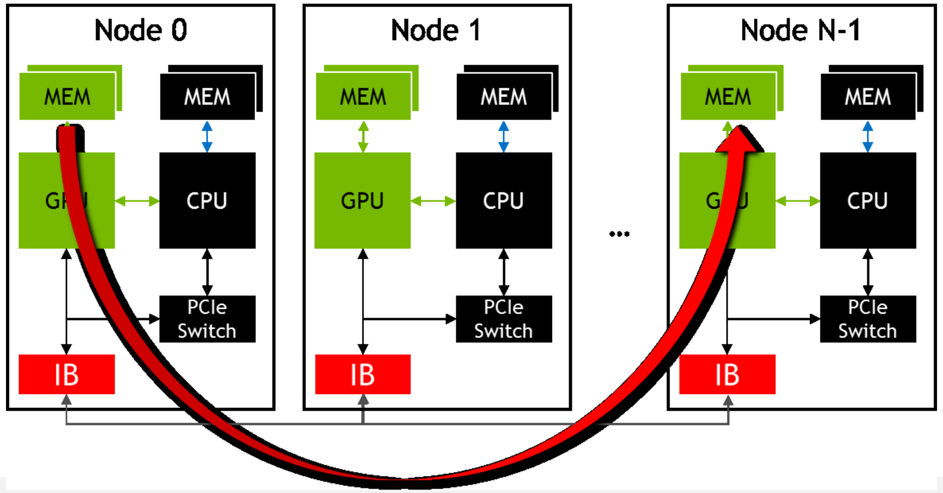
MULTI GPU PROGRAMMING WITH CUDA AND MPI

Jiri Kraus, Senior Devtech Compute, April 24th 2018

NVIDIA.

MPI+CUDA



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

//MPI rank n-1
MPI_Recv(rbuf_d, 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, …

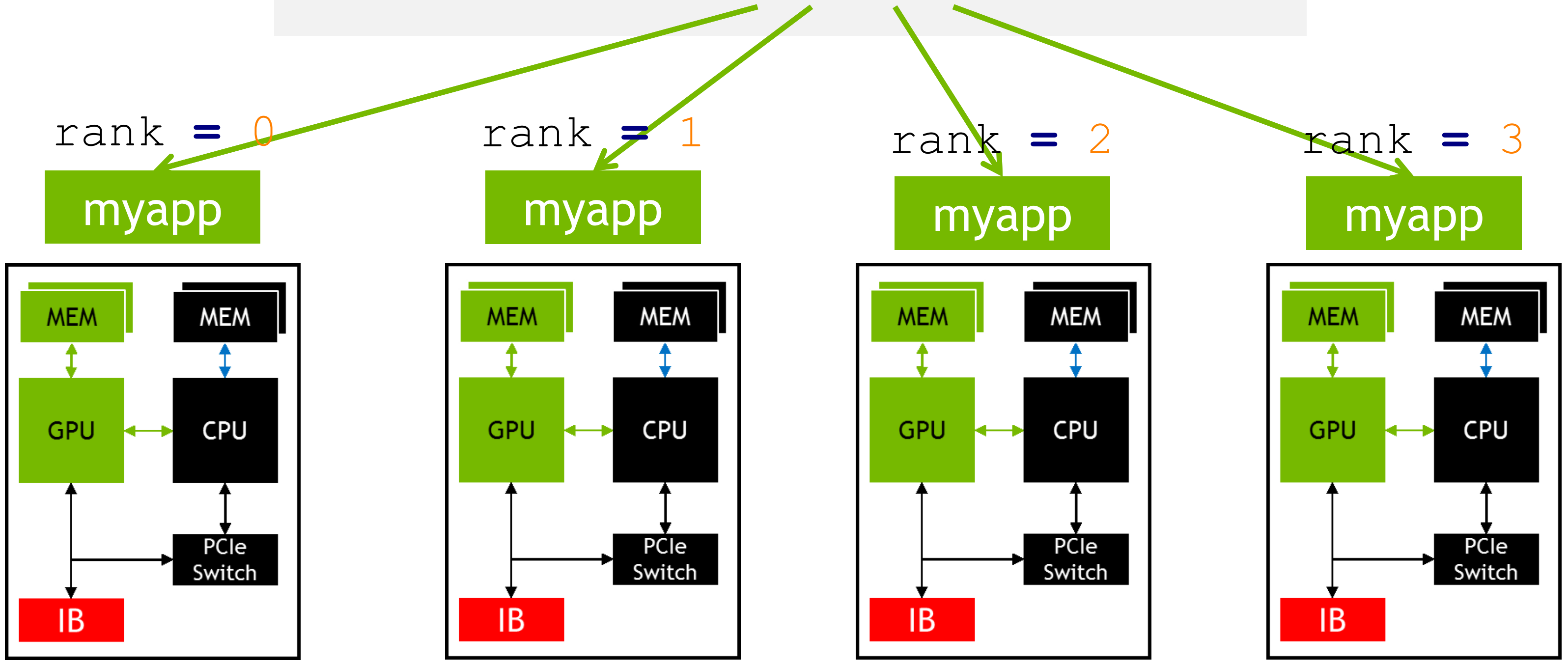
MPI - SKELETON

```
#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

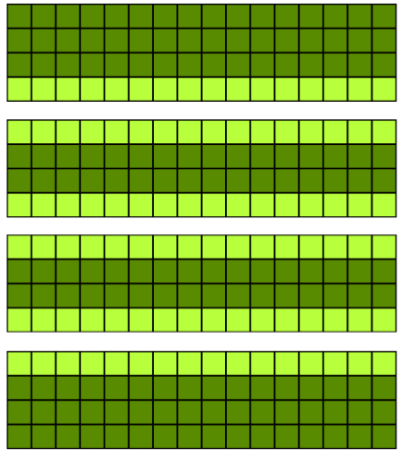
Solves the 2D-Laplace Equation on a rectangle

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

Dirichlet boundary conditions (constant values on boundaries) on left and right boundary

Periodic boundary conditions on top and bottom boundary

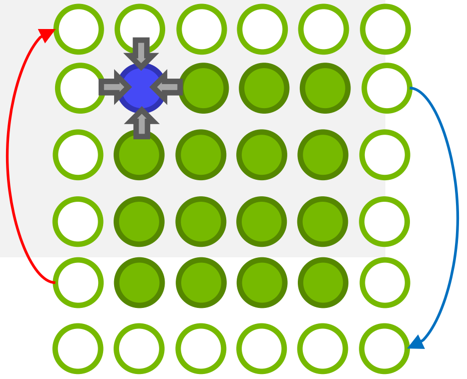
Domain decomposition with stripes


Horizontal Stripes

EXAMPLE: JACOBI SOLVER

Single GPU

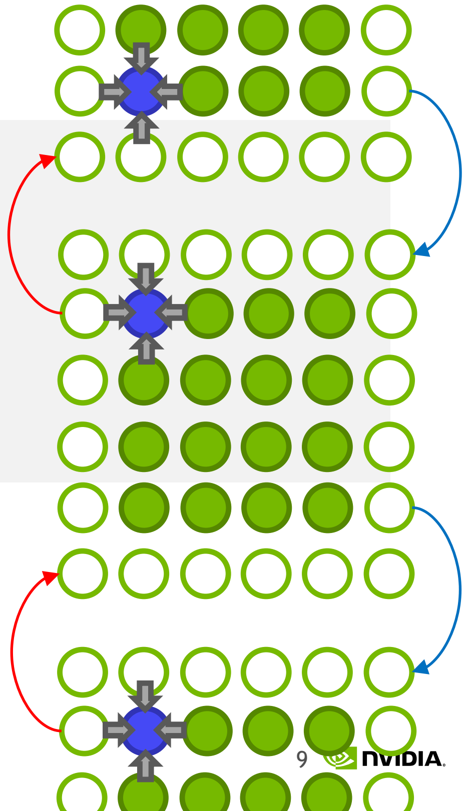
```
While not converged
    Do Jacobi step:
        for (int iy = 1; iy < (ny-1); ++iy)
        for (int ix = 1; ix < (nx-1); ++ix)
          a_new[iy*nx+ix] = 0.25f*((a[ iy   *nx + ix+1]+a[ iy   *nx + ix-1]
                                 +a[(iy+1)*nx + ix]  +a[(iy-1)*nx + ix]));
    Apply periodic boundary conditions
    swap a_new and a
    Next iteration
```



EXAMPLE: JACOBI SOLVER

Multi GPU

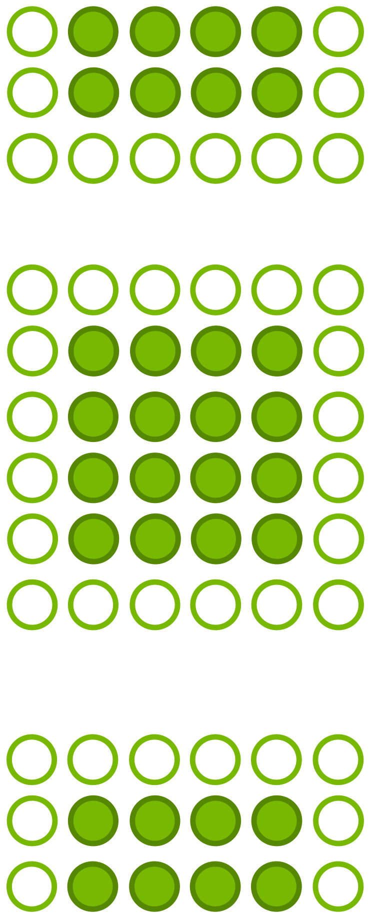
```
While not converged
    Do Jacobi step:
        for (int iy = iy_start; iy < iy_end; ++iy)
        for (int ix = 1; ix < (nx-1); ++ix)
          a_new[iy*nx+ix] = 0.25f*((a[ iy   *nx + ix+1]+a[ iy   *nx + ix-1]
                                   +a[(iy+1)*nx + ix]  +a[(iy-1)*nx + ix]));
    Apply periodic boundary conditions and exchange halo with 2 neighbors
    swap a_new and a
    Next iteration
```



EXAMPLE JACOBI

Top/Bottom Halo

```
MPI_Sendrecv(a_new+iy_start*nx, nx, MPI_DOUBLE, top, 0,
             a_new+iy_end*nx,   nx, MPI_DOUBLE, bottom, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```



EXAMPLE JACOBI

Top/Bottom Halo

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MPI_Sendrecv(a_new+iy_start*nx, nx, MPI_DOUBLE, top, 0,
             a_new+iy_end*nx,   nx, MPI_DOUBLE, bottom, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);
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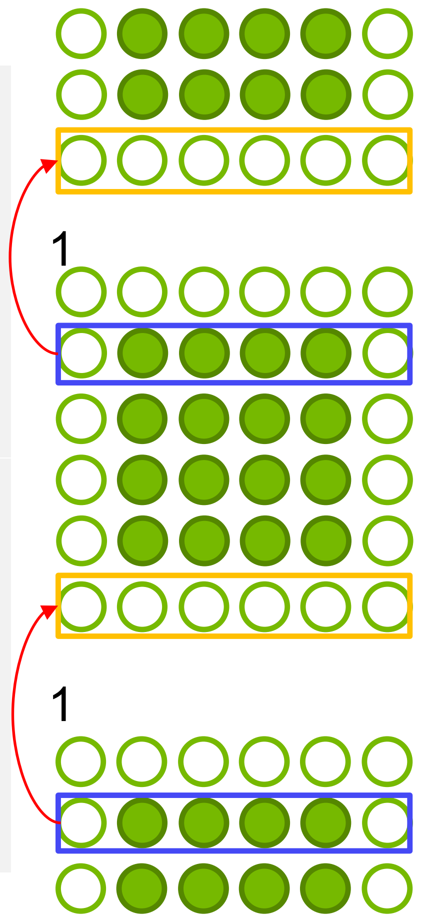
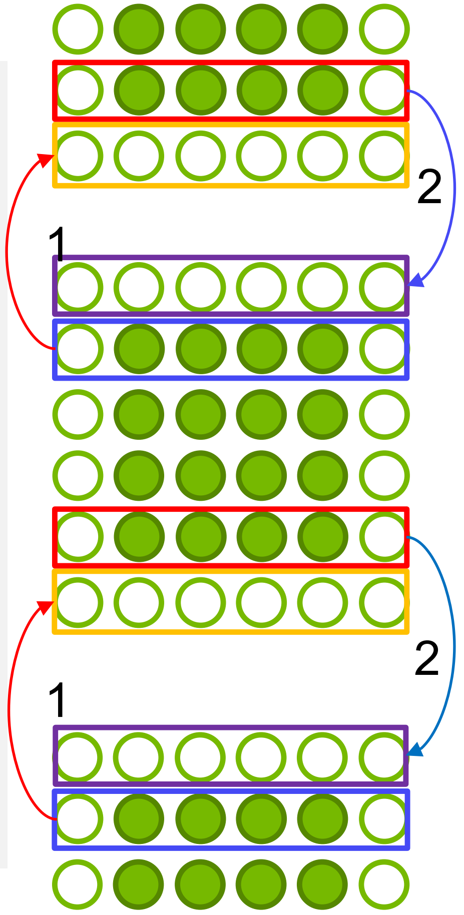


EXAMPLE JACOBI

Top/Bottom Halo

```
MPI_Sendrecv(a_new+iy_start*nx,  nx, MPI_DOUBLE, top, 0,
             a_new+iy_end*nx,    nx, MPI_DOUBLE, bottom, 0,
             MPI_COMM_WORLD, MPI_STATUS_IGNORE);


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



HANDLING MULTI GPU NODES

GPU-affinity

Use local rank:

```
int local_rank = //determine local rank

cudaSetDevice(local_rank);
```

HANDLING MULTI GPU NODES

How to determine the local rank? – MPI-3

```
MPI_Comm local_comm;

MPI_Info info;

MPI_Info_create(&info);

MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, rank, info, &local_comm);

int local_rank = -1;

MPI_Comm_rank(local_comm,&local_rank);

MPI_Comm_free(&local_comm);

MPI_Info_free(&info);
cudaSetDevice(local_rank);
```

PROFILING OF MPI+CUDA APPS

PROFILING MPI+CUDA APPLICATIONS

Using `nvprof`+NVVP

New since CUDA 9

Embed MPI rank in output filename, process name, and context name (OpenMPI)

```
mpirun -np $np nvprof --output-profile profile.%q{OMPI_COMM_WORLD_RANK}    \
                      --process-name "rank %q{OMPI_COMM_WORLD_RANK}"      \
                      --context-name "rank %q{OMPI_COMM_WORLD_RANK}"      \
                      --annotate-mpi openmpi
```

Alternatives:

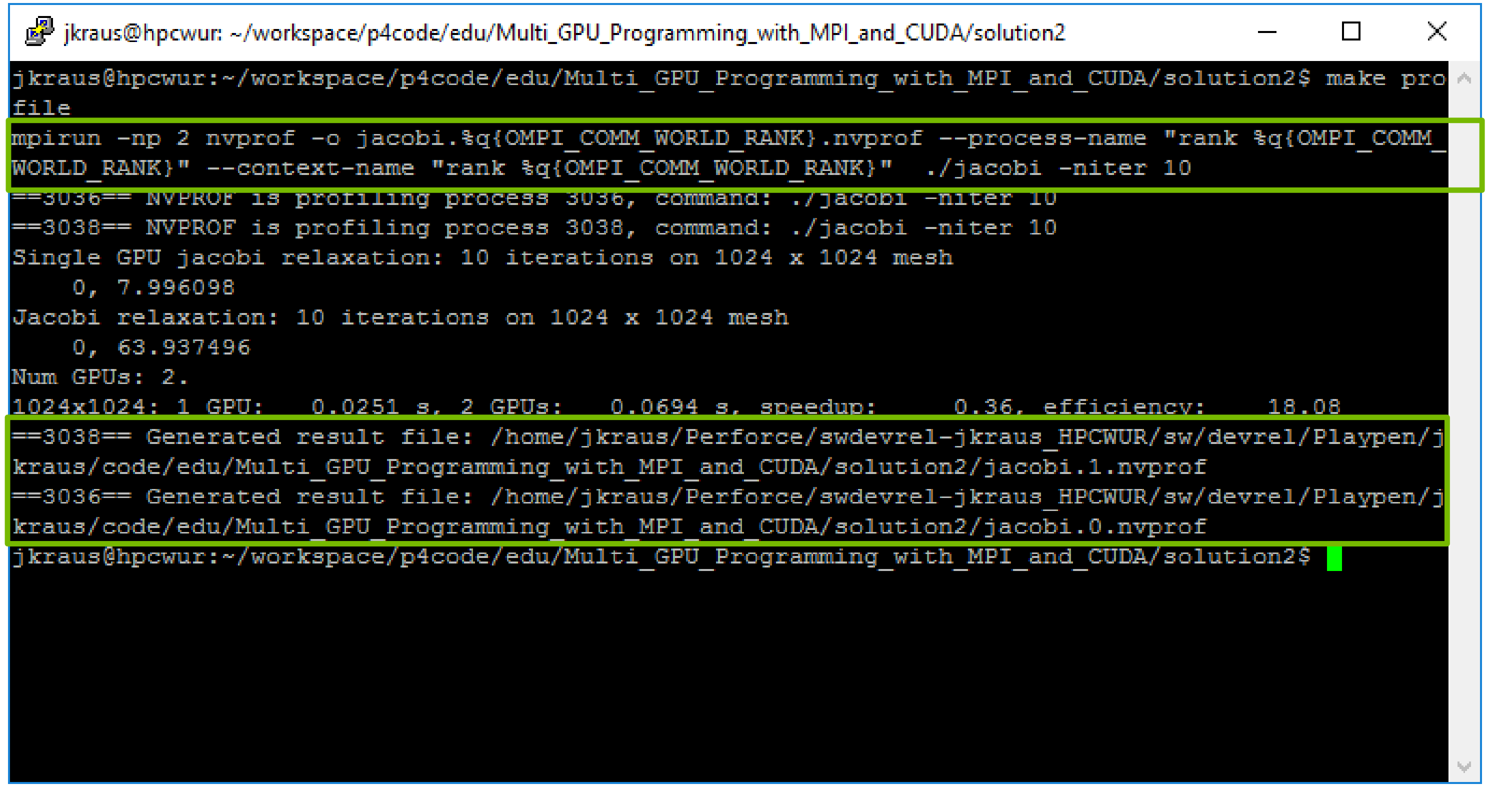
Only save the textual output (`--log-file`)

MVAPICH2: `MV2_COMM_WORLD_RANK`

```
--annotate-mpi mpich
```

PROFILING MPI+CUDA APPLICATIONS

Using `nvprof`+NVVP



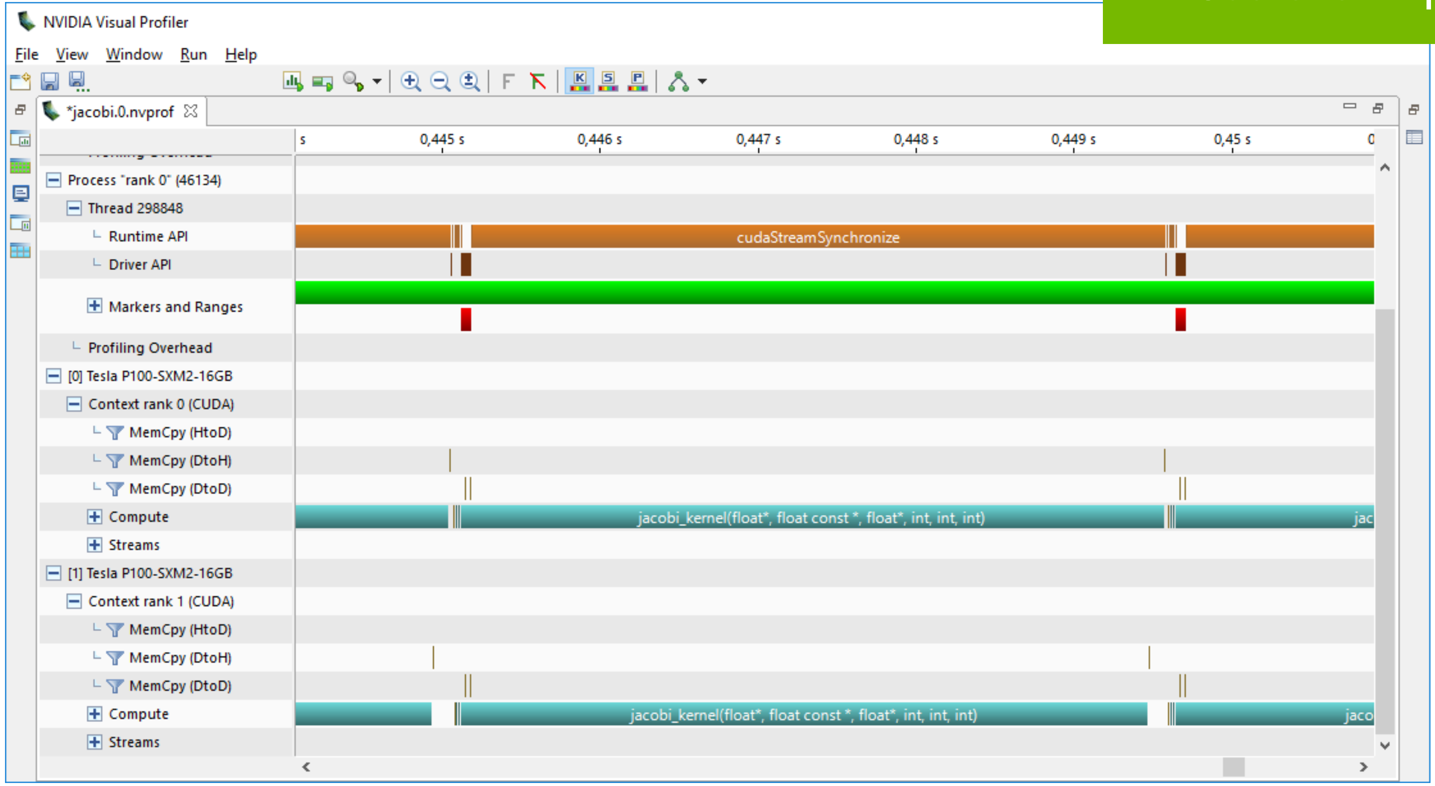
jkraus@hpcwur: ~/workspace/p4code/edu/Multi_GPU_Programming_with_MPI_and_CUDA/solution2

```
jkraus@hpcwur:~/workspace/p4code/edu/Multi_GPU_Programming_with_MPI_and_CUDA/solution2$ make pro
file
mpirun -np 2 nvprof -o jacobi.%q{OMPI_COMM_WORLD_RANK}.nvprof --process-name "rank %q{OMPI_COMM_
WORLD_RANK}" --context-name "rank %q{OMPI_COMM_WORLD_RANK}"  ./jacobi -niter 10
==3036== NVPROF is profiling process 3036, command: ./jacobi -niter 10
==3038== NVPROF is profiling process 3038, command: ./jacobi -niter 10
Single GPU jacobi relaxation: 10 iterations on 1024 x 1024 mesh
    0, 7.996098
Jacobi relaxation: 10 iterations on 1024 x 1024 mesh
    0, 63.937496
Num GPUs: 2.
1024x1024: 1 GPU:   0.0251 s, 2 GPUs:   0.0694 s, speedup:     0.36, efficiency:    18.08
==3038== Generated result file: /home/jkraus/Perforce/swdevrel-jkraus_HPCWUR/sw/devrel/Playpen/j
kraus/code/edu/Multi_GPU_Programming_with_MPI_and_CUDA/solution2/jacobi.1.nvprof
==3036== Generated result file: /home/jkraus/Perforce/swdevrel-jkraus_HPCWUR/sw/devrel/Playpen/j
kraus/code/edu/Multi_GPU_Programming_with_MPI_and_CUDA/solution2/jacobi.0.nvprof
jkraus@hpcwur:~/workspace/p4code/edu/Multi_GPU_Programming_with_MPI_and_CUDA/solution2$
```

PROFILING MPI+CUDA APPLICATIONS

Using `nvprof`+NVVP

Use the import Wizard



https://devblogs.nvidia.com/parallelforall/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx

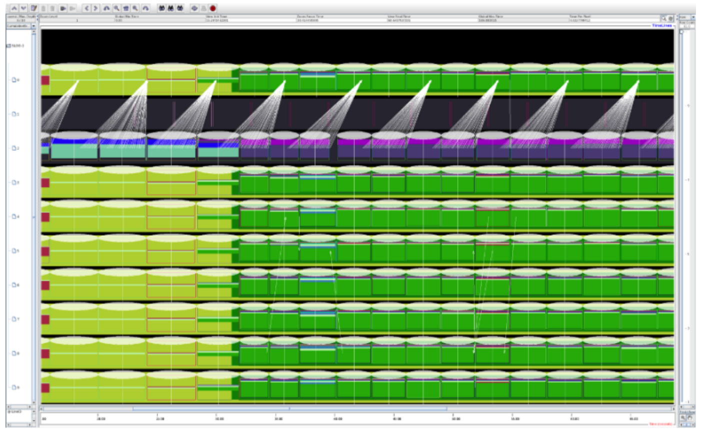
PROFILING MPI+CUDA APPLICATIONS

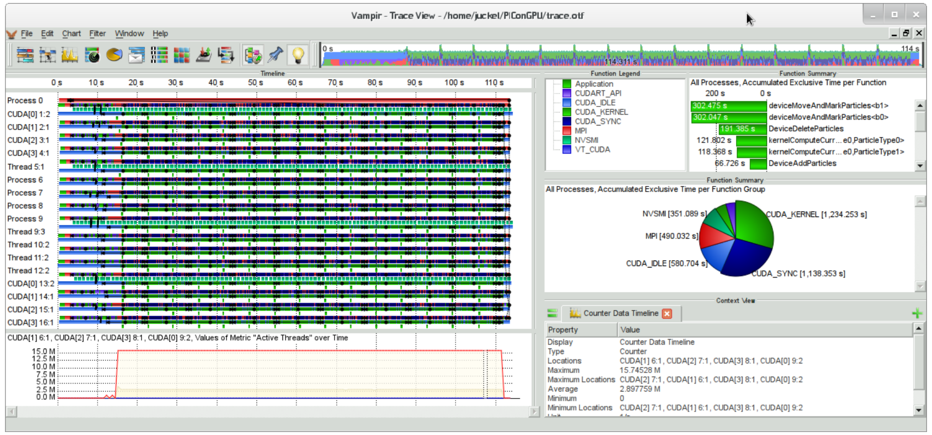
Third Party Tools

Multiple parallel profiling tools are CUDA-aware

- Score-P
- Vampir
- Tau

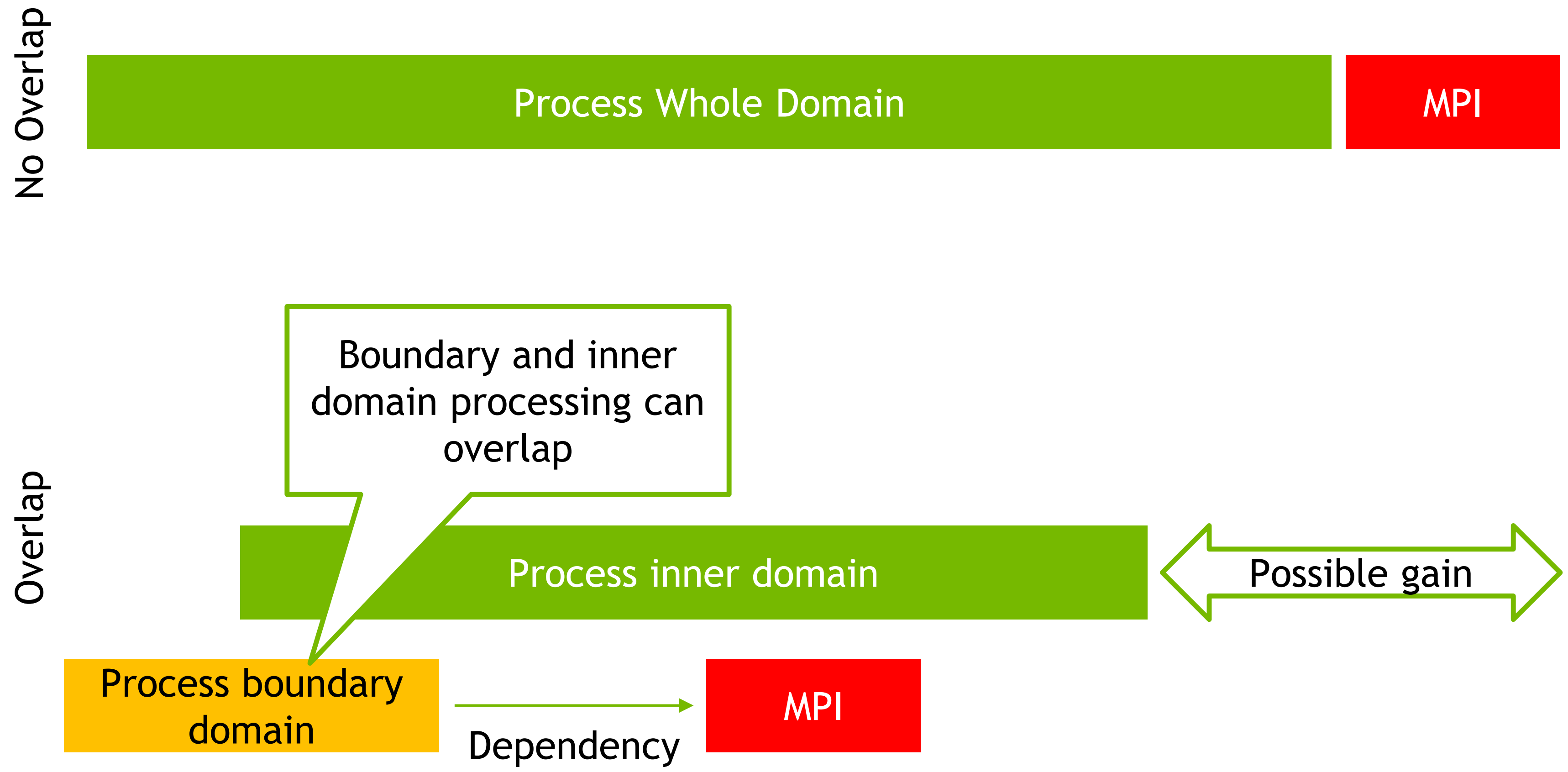
These tools are good for discovering MPI issues as well as basic CUDA performance inhibitors.





OVERLAPPING MPI AND COMPUTATION

COMMUNICATION + COMPUTATION OVERLAP



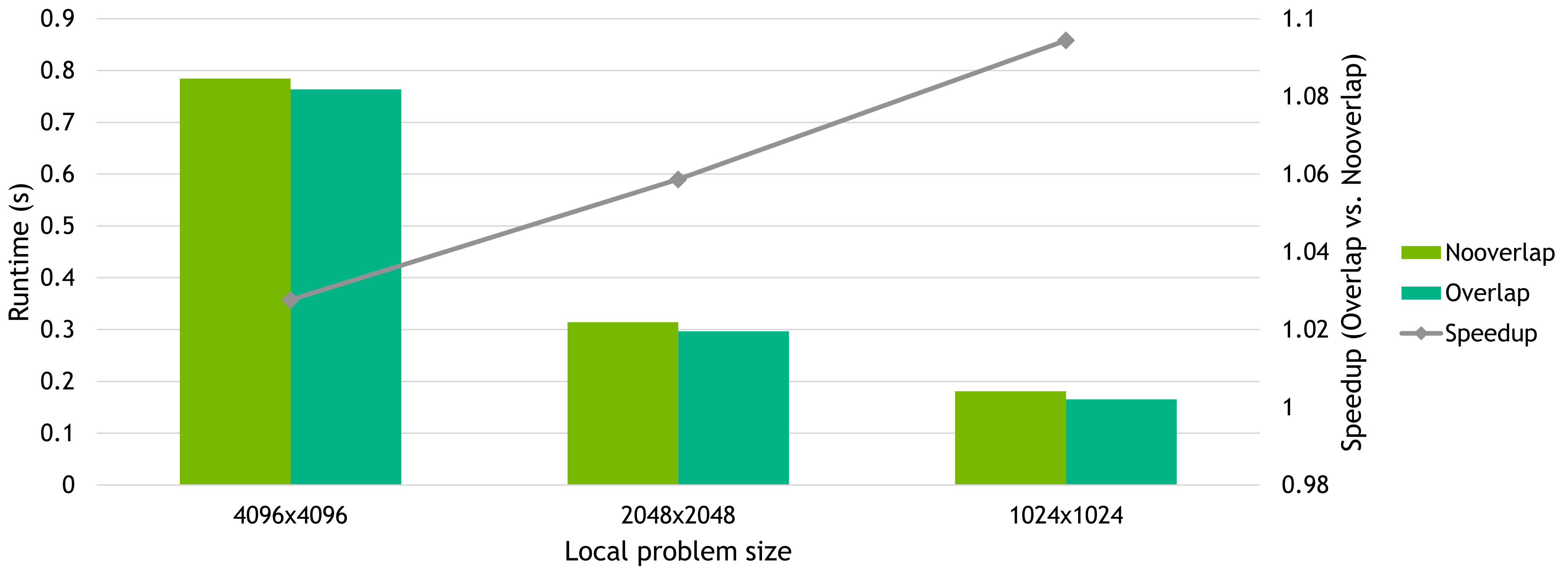
COMMUNICATION + COMPUTATION OVERLAP

Asynchronous execution with CUDA streams

```
launch_jacobi_kernel( a_new, a, l2_norm_m, iy_start, (iy_start+1), nx, halo_stream );
launch_jacobi_kernel( a_new, a, l2_norm_m, (iy_end-1), iy_end, nx, halo_stream );
launch_jacobi_kernel( a_new, a, l2_norm_m, (iy_start+1), (iy_end-1), nx, compute_stream );
int top = rank > 0 ? rank - 1 : (size-1); int bottom = (rank+1)%size;
//Apply periodic boundary conditions
cudaStreamSynchronize( halo_stream );
MPI_Sendrecv( a_new+iy_start*nx, nx, MPI_REAL_TYPE, top , 0,
              a_new+(iy_end*nx), nx, MPI_REAL_TYPE, bottom, 0,
              MPI_COMM_WORLD, MPI_STATUS_IGNORE ));
MPI_Sendrecv( a_new+(iy_end-1)*nx, nx, MPI_REAL_TYPE, bottom, 0,
              a_new+(iy_start-1)*nx, nx, MPI_REAL_TYPE, top, 0,
              MPI_COMM_WORLD, MPI_STATUS_IGNORE ));
cudaStreamSynchronize( compute_stream );
```

COMMUNICATION + COMPUTATION OVERLAP

OpenMPI 3.0.0 - 2 Tesla P100



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.

HANDS-ON

HANDS-ON MENU

4 tasks to choose from

Task 0: Using MPI

Task 1: Handle GPU Affinity

Task 2: Apply Domain Decomposition

Task 3: Overlap MPI and Compute

TASK 0: USING MPI

`task0`

Determine rank (`MPI_Comm_rank`) and size (`MPI_Comm_size`)

Add `MPI_Barrier` to ensure correct timing

Look for TODOs

```
Num GPUs: 1.
Num GPUs: 1.
2048x2048: 1 GPU:   1.0288 s, 1 GPUs:   0.9059 s, speedup:
2048x2048: 1 GPU:   1.0369 s, 1 GPUs:   0.9039 s
```

Make Targets:

`run:`	run `jacobi` with `$NP` procs.
`jacobi:`	build `jacobi` bin (default)
`memcheck:`	profile with `cuda-memcheck`
`profile:`	profile with `nvprof`

Solution is in `solution0`

https://www.open-mpi.org/doc/current/

TASK 1: HANDLING GPU AFFINITY

task1

Handle GPU affinity with `MPI_COMM_TYPE_SHARED`

Run and report the performance

Look for TODOs

```
   900, 0.061312
Num GPUs: 2.
2048x2048: 1 GPU:   1.0267 s, 2 GPUs:   0.9096 s, speedup: 1.13
```

Make Targets:

`run:`	run `jacobi` with `$NP` procs.
`jacobi:`	build `jacobi` bin (default)
`memcheck:`	profile with `cuda-memcheck`
`profile:`	profile with `nvprof`

Solution is in `solution1`

https://www.open-mpi.org/doc/current/

TASK 2: APPLY DOMAIN DECOMPOSITION

`task2`

Calculate first (`iy_start`) and last (`iy_end`) row to be processed by each rank

Use `MPI_Sendrecv` to handle halo updates and periodic boundary conditions

Use `MPI_Allreduce` to calculate global L2 norm

Look for TODOs

```
 900, 0.061312
Num GPUs: 2.
2048x2048: 1 GPU:   0.4304 s, 2 GPUs:   0.4188 s, speedup: 1.03
```

Make Targets:

`run:`	run `jacobi` with `$NP` procs.
`jacobi:`	build `jacobi` bin (default)
`memcheck:`	profile with `cuda-memcheck`
`profile:`	profile with `nvprof`

Solution is in `solution2`

https://www.open-mpi.org/doc/current/

TASK 3: OVERLAP MPI AND COMPUTE

`task3`

Use `cudaStreamCreate` to create halo processing stream

Split jacobi step in top boundary, bottom boundary and bulk part

Launch top and bottom boundary part in halo processing stream

Look for TODOs

```
 900, 0.061312
Num GPUs: 2.
2048x2048: 1 GPU:   0.4351 s, 2 GPUs:   0.3133 s, speedup: 1.39
```

Make Targets:

`run:`	run `jacobi` with `$NP` procs.
`jacobi:`	build `jacobi` bin (default)
`memcheck:`	profile with `cuda-memcheck`
`profile:`	profile with `nvprof`

Solution is in `solution3`

https://www.open-mpi.org/doc/current/

SOLUTIONS

TASK 0: USING MPI

Solution

```
int main(int argc, char * argv[]) {
    int rank = 0;
    int size = 1;
    MPI_CALL( MPI_Init(&argc,&argv) );
    MPI_CALL( MPI_Comm_rank(MPI_COMM_WORLD,&rank) );
    MPI_CALL( MPI_Comm_size(MPI_COMM_WORLD,&size) );
    //…
    MPI_CALL( MPI_Barrier(MPI_COMM_WORLD) );
    double start = MPI_Wtime();
    while ( l2_norm > tol && iter < iter_max )
    //…
    MPI_CALL( MPI_Finalize() );
    return result_correct == 1 ? 0 : 1; }
```

TASK 1: HANDLING GPU AFFINITY

Solution

```
int dev_id = -1;
{
    MPI_Comm local_comm;
    MPI_Info info;
    MPI_CALL( MPI_Info_create(&info) );
    MPI_CALL( MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED,
                                  rank, info, &local_comm) );
    MPI_CALL( MPI_Comm_rank(local_comm,&dev_id) );
    MPI_CALL( MPI_Comm_free(&local_comm) );
    MPI_CALL( MPI_Info_free(&info) );
}

CUDA_RT_CALL( cudaSetDevice( dev_id ) );
```

TASK 2: APPLY DOMAIN DECOMPOSITION

Solution I

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

TASK 2: APPLY DOMAIN DECOMPOSITION

Solution II

```
//Apply periodic boundary conditions
CUDA_RT_CALL( cudaStreamSynchronize( compute_stream ) );
PUSH_RANGE("MPI",5)
MPI_CALL( MPI_Sendrecv( a_new+iy_start*nx, nx, MPI_REAL_TYPE, top , 0,
                        a_new+(iy_end*nx), nx, MPI_REAL_TYPE, bottom, 0,
                        MPI_COMM_WORLD, MPI_STATUS_IGNORE ));
MPI_CALL( MPI_Sendrecv( a_new+(iy_end-1)*nx, nx, MPI_REAL_TYPE, bottom, 0,
                        a_new+(iy_start-1)*nx, nx, MPI_REAL_TYPE, top, 0,
                        MPI_COMM_WORLD, MPI_STATUS_IGNORE ));
POP_RANGE
```

TASK 2: APPLY DOMAIN DECOMPOSITION

Solution III

```
CUDA_RT_CALL( cudaStreamSynchronize( compute_stream ) );
MPI_CALL( MPI_Allreduce( l2_norm_m, &l2_norm, 1, MPI_REAL_TYPE,
                         MPI_SUM, MPI_COMM_WORLD ) );
l2_norm = std::sqrt( l2_norm );
```

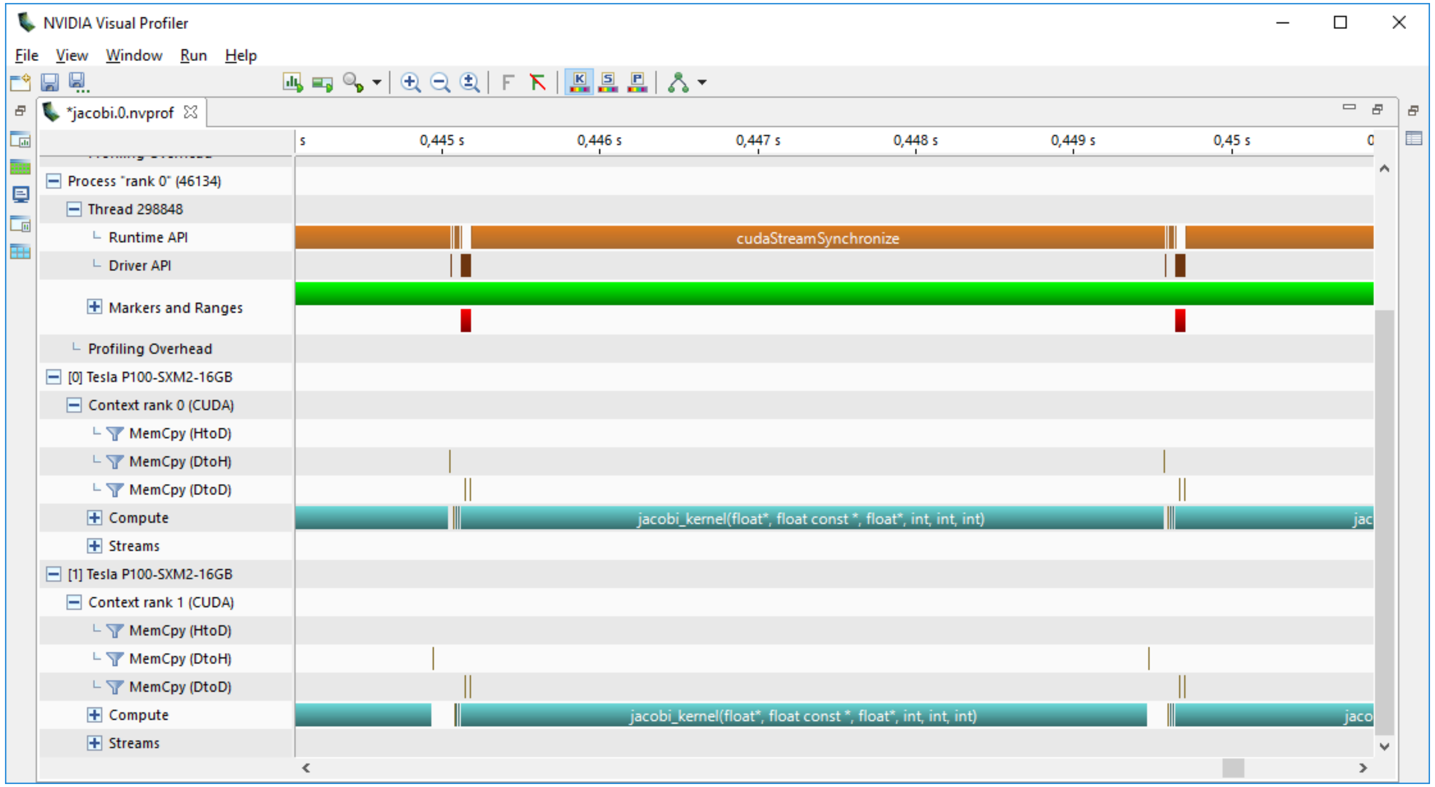
TASK 3: OVERLAP MPI AND COMPUTE

Solution

```
launch_jacobi_kernel( a_new, a, l2_norm_d,
                      iy_start, (iy_start+1), nx, halo_stream );
launch_jacobi_kernel( a_new, a, l2_norm_d,
                      (iy_end-1), iy_end, nx, halo_stream );
launch_jacobi_kernel( a_new, a, l2_norm_d, (iy_start+1),
                      (iy_end-1), nx, compute_stream );
int top = rank > 0 ? rank - 1 : (size-1); int bottom = (rank+1)%size;
//Apply periodic boundary conditions
CUDA_RT_CALL( cudaStreamSynchronize( halo_stream ) );
PUSH_RANGE("MPI",5)
MPI_CALL( MPI_Sendrecv( a_new+iy_start*nx, …
```

TASK 3: OVERLAP MPI AND COMPUTE

Solution



https://devblogs.nvidia.com/parallelforall/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx