Sandia National Laboratories

Optimization Techniques for Multi-GPU Applications

Simon Garcia de Gonzalo, Sandia National Laboratories

(slides from Jiri Kraus, NVIDIA Principal Devtech Compute)

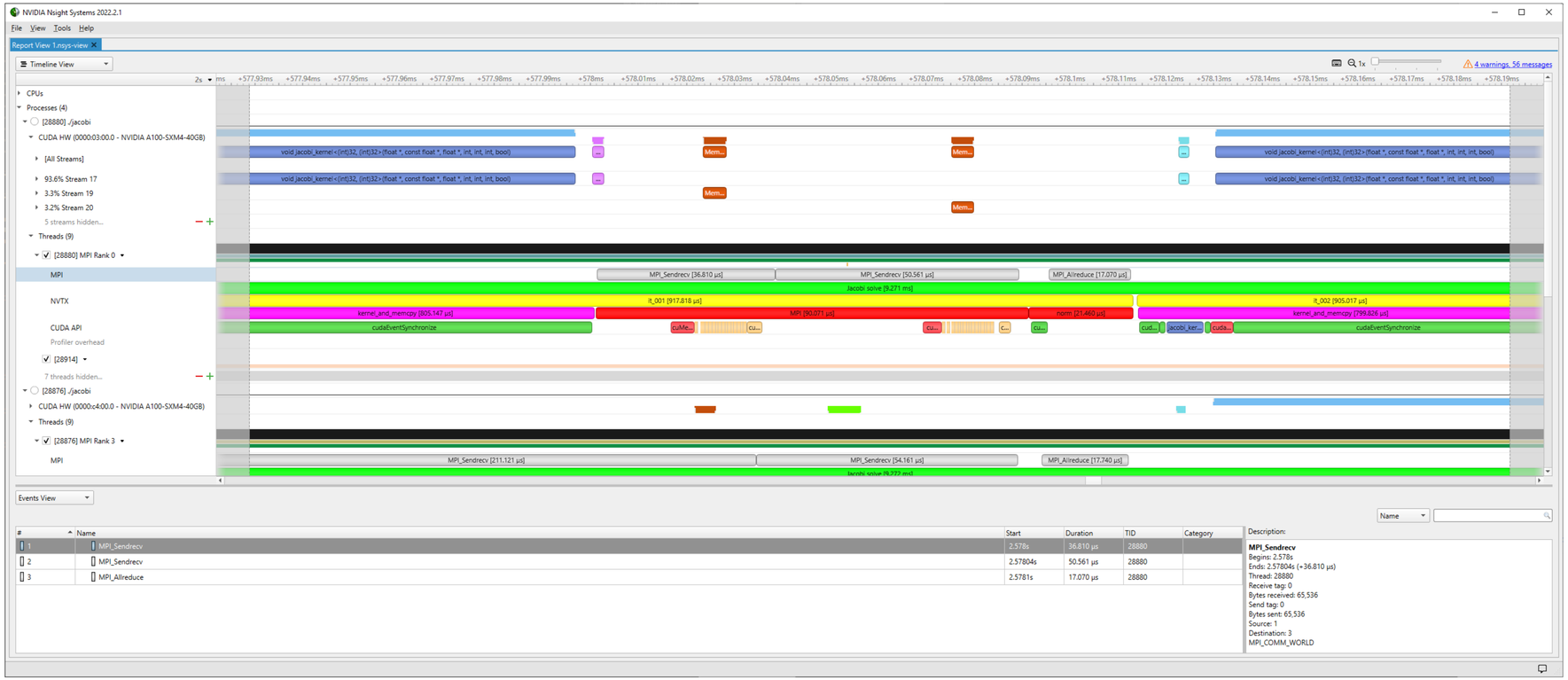
SC25 St. Louis, MO hpc ignites.

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

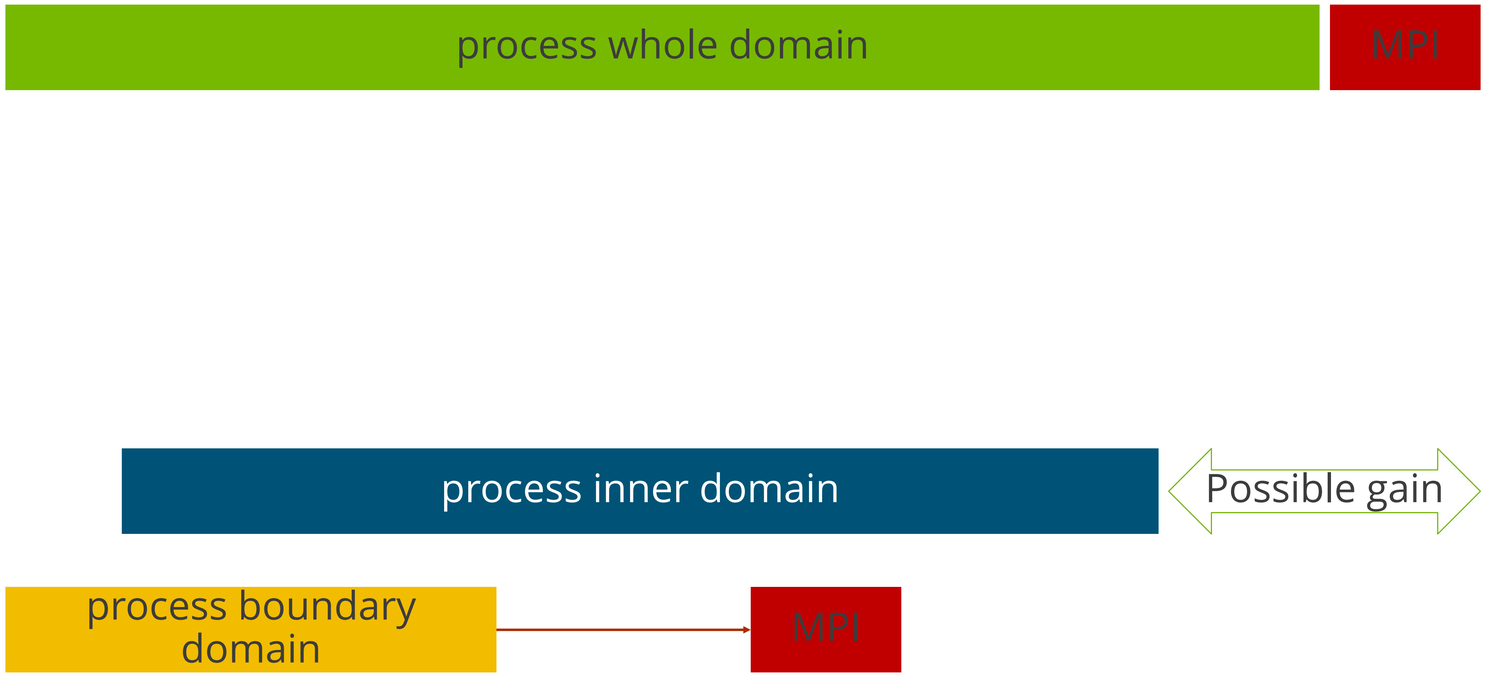
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Multi GPU Jacobi Nsight Systems Timeline

MPI 8 NVIDIA A100 40GB on JUWELS Booster

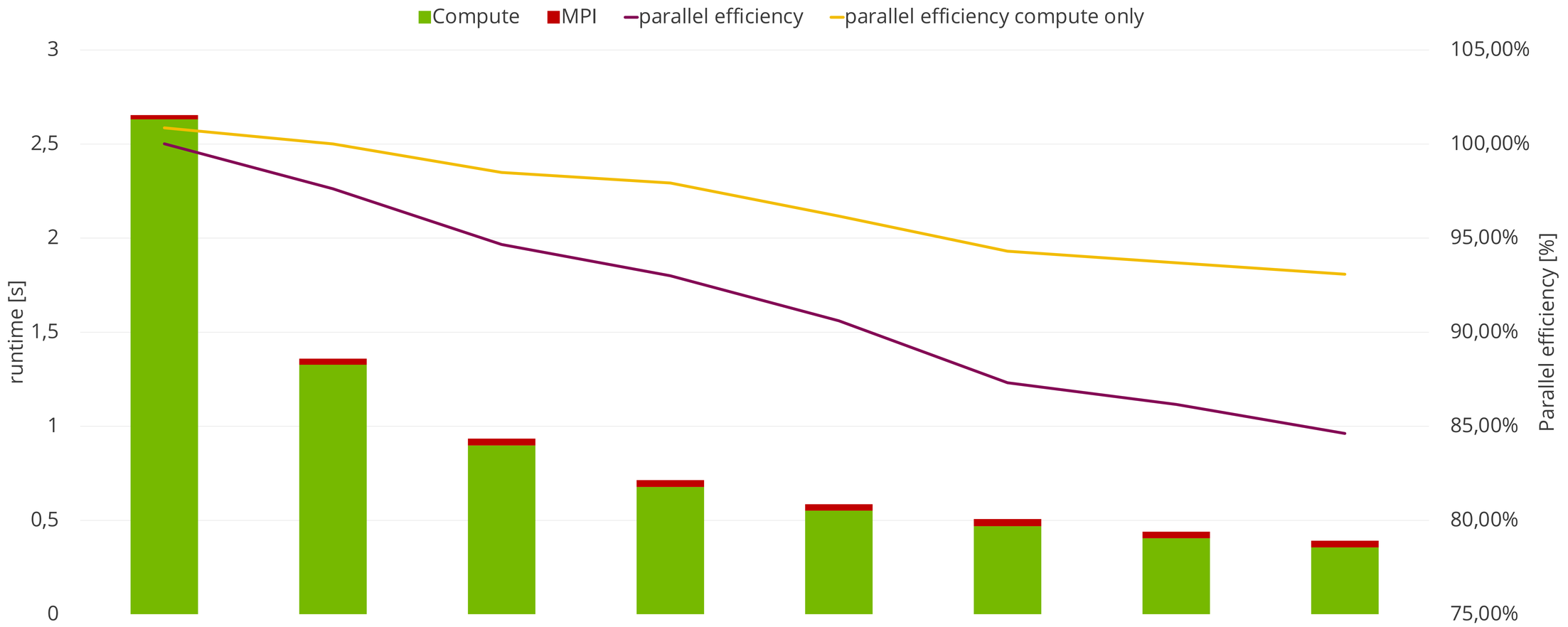


Communication + Computation Overlap



Communication + Computation Overlap

ParaStationMPI 5.4.10-1 – JUWELS Booster – NVIDIA A100 40 GB – Jacobi on 17408x17408



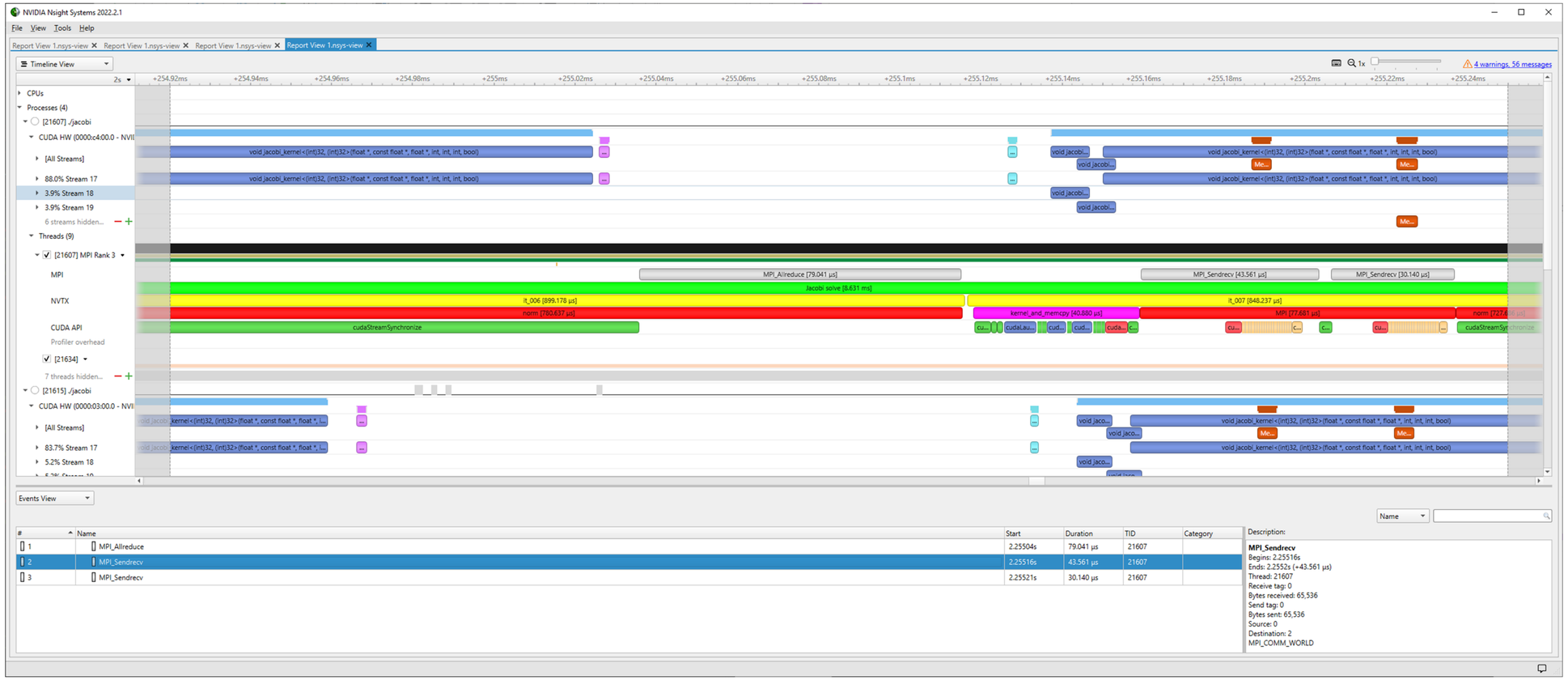
Source: https://github.com/NVIDIA/multi-gpu-programming-models
JUWELS Booster: https://apps.fz-juelich.de/jsc/hps/juwels/booster-overview.html

MPI Communication + Computation Overlap

```
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start, (iy_start + 1), nx, push_top_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_end - 1), iy_end, nx, push_bottom_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_start + 1), (iy_end - 1), nx, compute_stream);


const int top = rank > 0 ? rank - 1 : (size - 1);
const int bottom = (rank + 1) % size;

CUDA_RT_CALL(cudaStreamSynchronize(push_top_stream));
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));
CUDA_RT_CALL(cudaStreamSynchronize(push_bottom_stream));
MPI_CALL(MPI_Sendrecv(a_new + (iy_end - 1) * nx, nx, MPI_REAL_TYPE, bottom, 0,
                      a_new,                     nx, MPI_REAL_TYPE, top, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE));
```

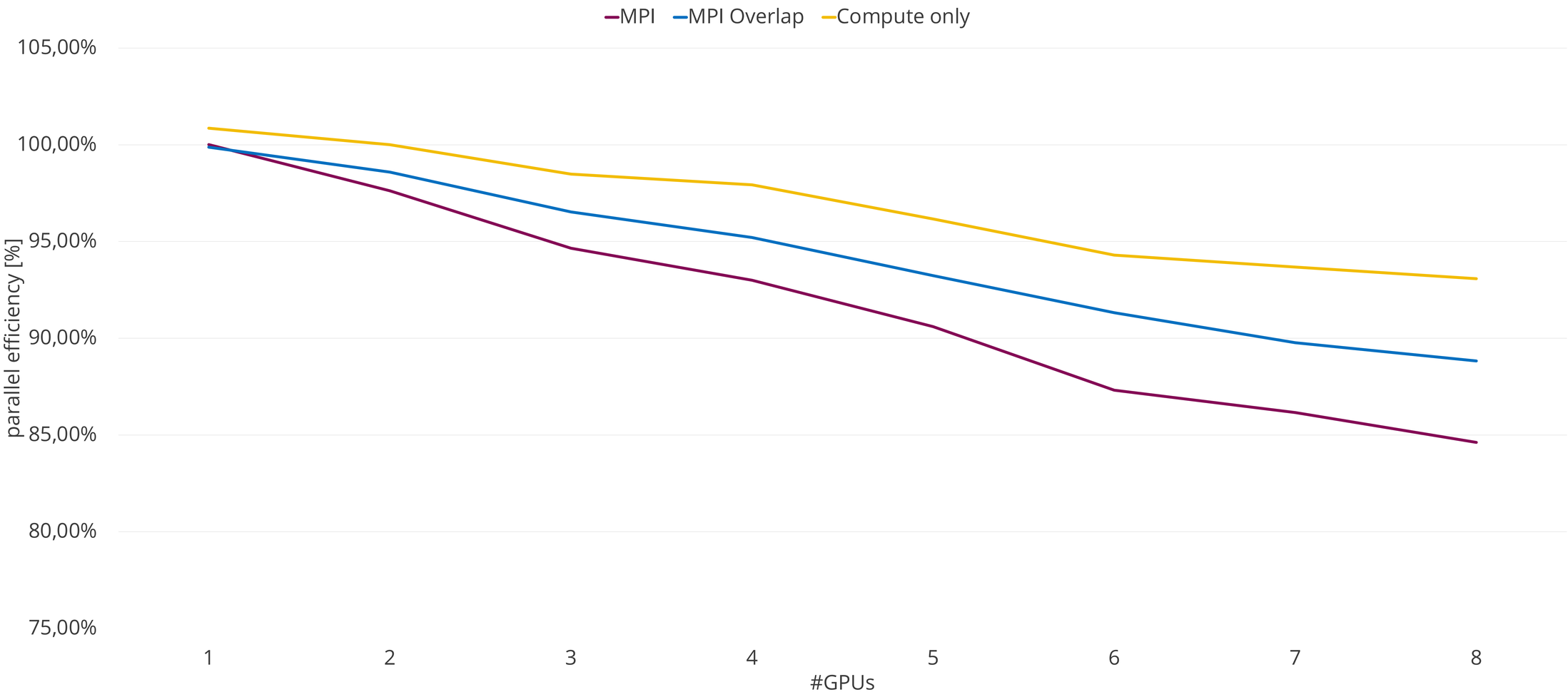
Multi GPU Jacobi Nsight Systems Timeline

MPI Overlap 8 NVIDIA A100 40GB on JUWELS Booster



Communication + Computation Overlap

ParaStationMPI 5.4.10-1 – JUWELS Booster – NVIDIA A100 40 GB – Jacobi on 17408x17408



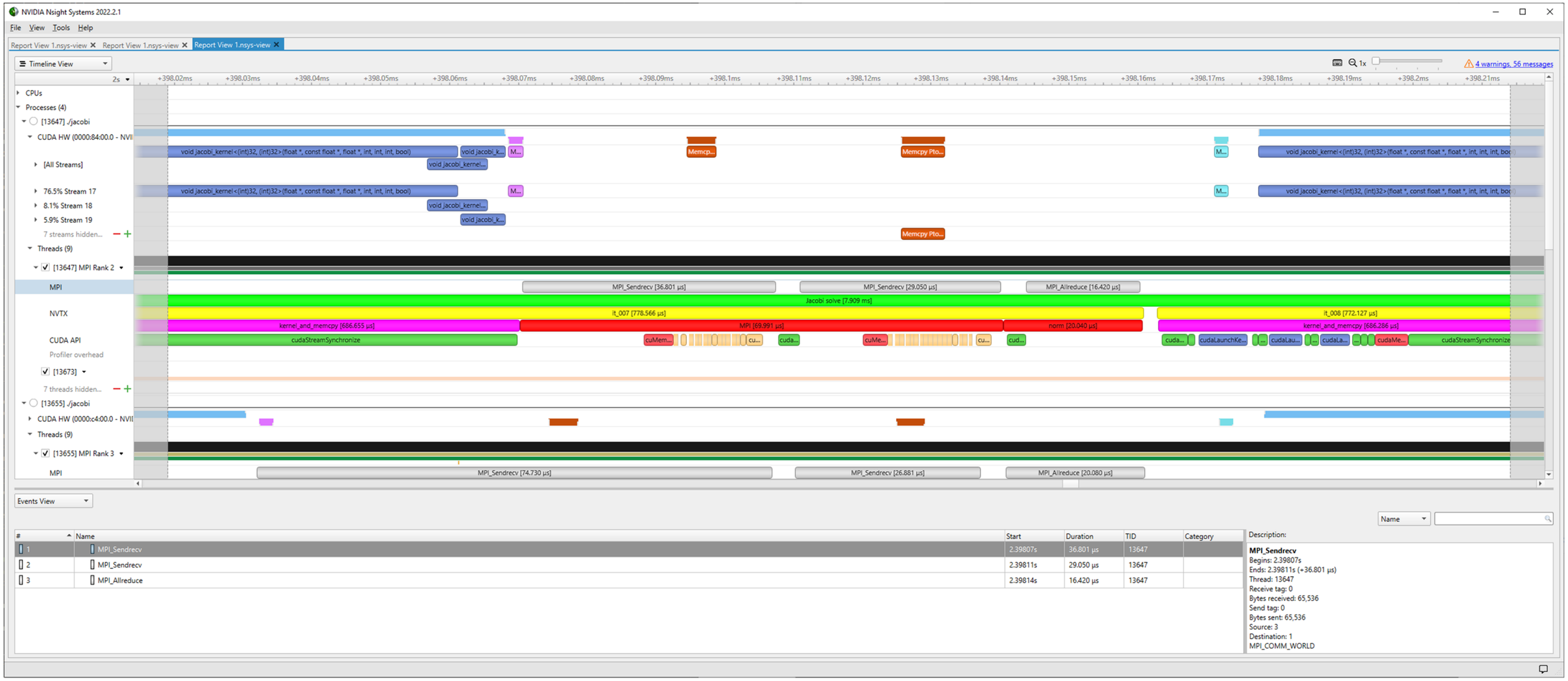
Source: https://github.com/NVIDIA/multi-gpu-programming-models
JUWELS Booster: https://apps.fz-juelich.de/jsc/hps/juwels/booster-overview.html

MPI Communication + Computation Overlap

```
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_start + 1), (iy_end - 1), nx, compute_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, iy_start, (iy_start + 1), nx, push_top_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_end - 1), iy_end, nx, push_bottom_stream);
launch_jacobi_kernel(a_new, a, l2_norm_d, (iy_start + 1), (iy_end - 1), nx, compute_stream);

const int top = rank > 0 ? rank - 1 : (size - 1);
const int bottom = (rank + 1) % size;


CUDA_RT_CALL(cudaStreamSynchronize(push_top_stream));
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));
CUDA_RT_CALL(cudaStreamSynchronize(push_bottom_stream));
MPI_CALL(MPI_Sendrecv(a_new + (iy_end - 1) * nx, nx, MPI_REAL_TYPE, bottom, 0,
                      a_new, nx, MPI_REAL_TYPE, top, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE));
```

Multi GPU Jacobi Nsight Systems Timeline

MPI Overlap 8 NVIDIA A100 40GB on JUWELS Booster

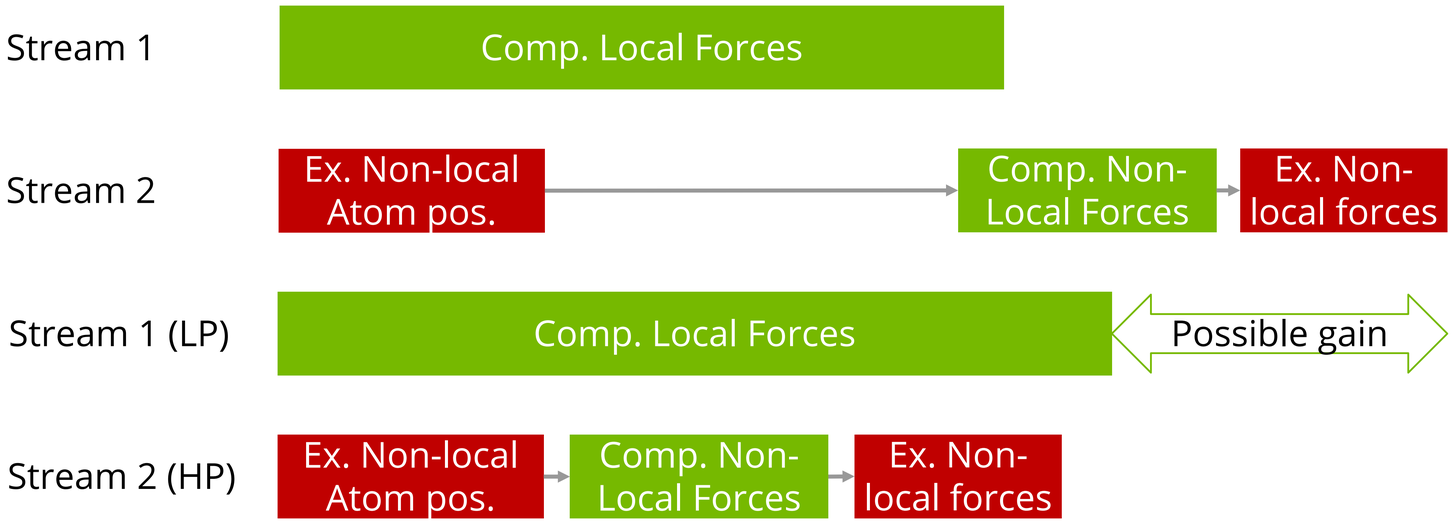


High Priority Streams

Improve scalability with high priority streams (available on CC 3.5+)

```
cudaStreamCreateWithPriority ( cudaStream_t* pStream, unsigned int  flags, int  priority )
```

Use-case MD-Simulations



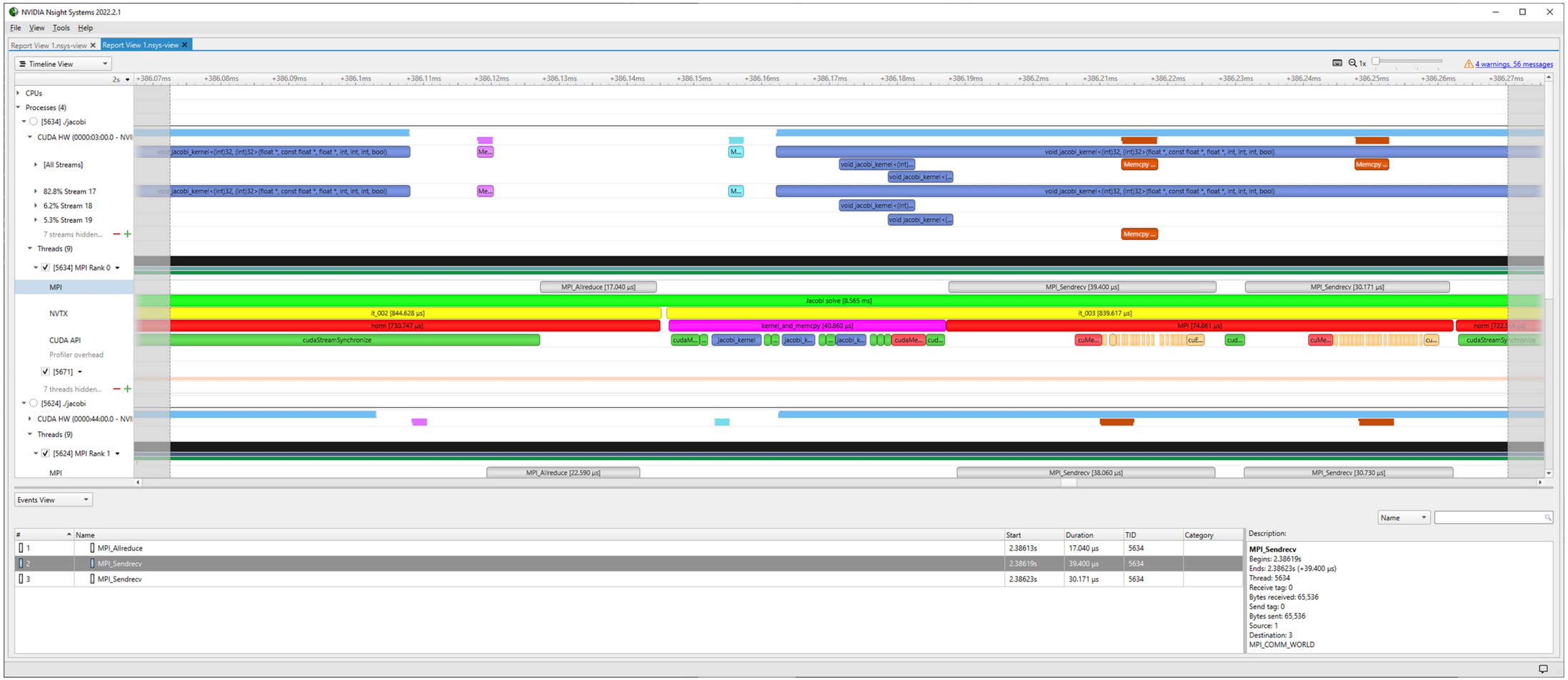
MPI Communication + Computation Overlap

with high priority streams

```
int leastPriority = 0;
int greatestPriority = leastPriority;
CUDA_RT_CALL(cudaDeviceGetStreamPriorityRange(&leastPriority, &greatestPriority));

cudaStream_t compute_stream;
cudaStream_t push_top_stream;
cudaStream_t push_bottom_stream;

CUDA_RT_CALL(cudaStreamCreateWithPriority(&compute_stream, cudaStreamDefault, leastPriority));
CUDA_RT_CALL(cudaStreamCreateWithPriority(&push_top_stream, cudaStreamDefault, greatestPriority));
CUDA_RT_CALL(cudaStreamCreateWithPriority(&push_bottom_stream, cudaStreamDefault, greatestPriority));
```

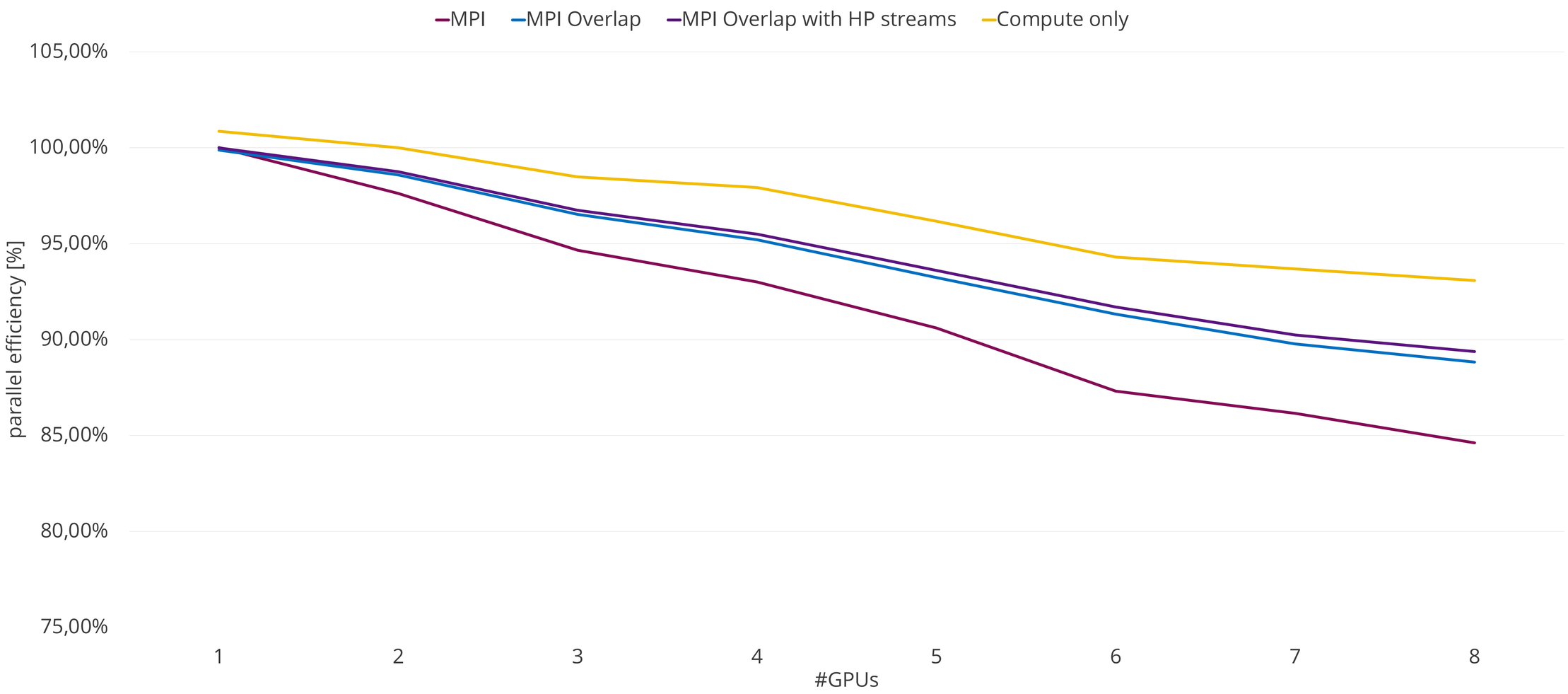
Multi GPU Jacobi Nsight Systems Timeline

MPI Overlap 8 NVIDIA A100 40GB on JUWELS Booster



Communication + Computation Overlap

ParaStationMPI 5.4.10-1 – JUWELS Booster – NVIDIA A100 40 GB – Jacobi on 17408x17408



Source: https://github.com/NVIDIA/multi-gpu-programming-models
JUWELS Booster: https://apps.fz-juelich.de/jsc/hps/juwels/booster-overview.html

CUDA-aware MPI

Example:

MPI Rank 0 `MPI_Send` from GPU Buffer

MPI Rank 1 `MPI_Recv` to GPU Buffer

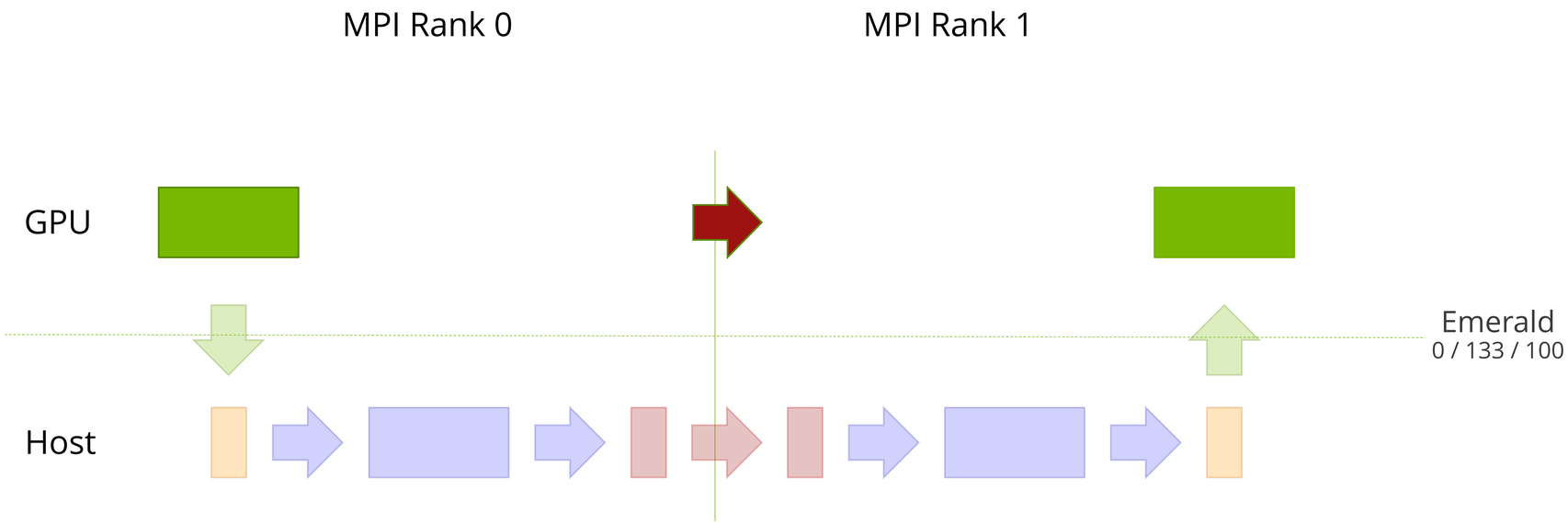
Show how CUDA+MPI works in principle

- Depending on the MPI implementation, message size, system setup, … situation might be different

Two GPUs in two nodes

GPU to remote GPU

CUDA-aware MPI with support for GPUDirect RDMA

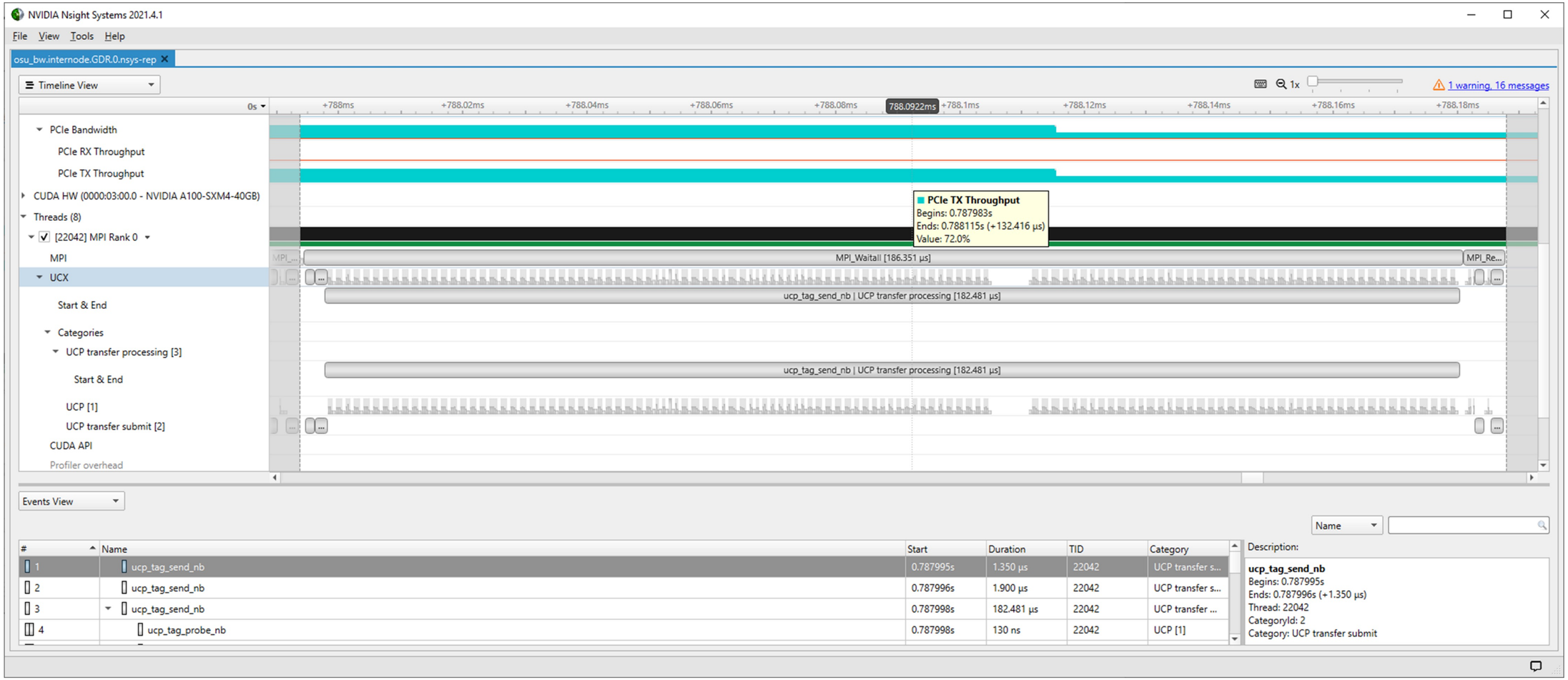



```
MPI_Send(s_buf_d, size, MPI_BYTE, 1, tag, MPI_COMM_WORLD);

MPI_Recv(r_buf_d, size, MPI_BYTE, 0, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

osu_bw Nsight Systems Timeline

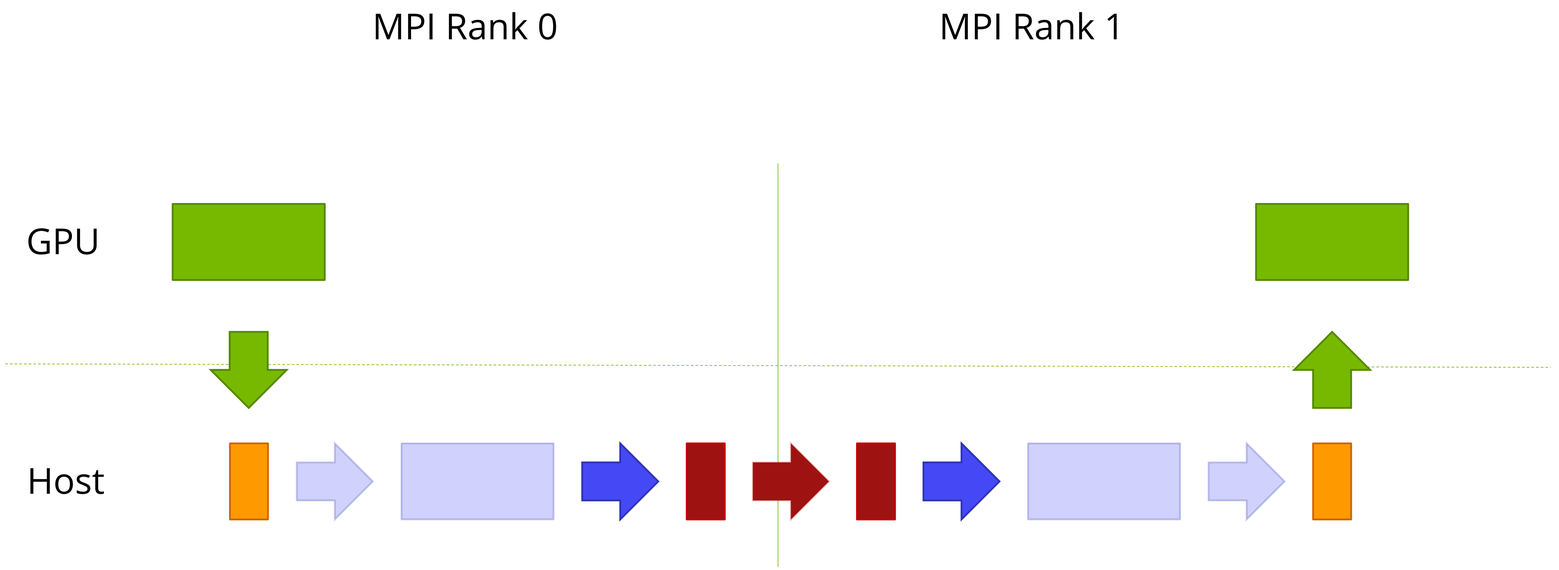
Internode with GPUDirect RDMA on JUWELS Booster

```
nsys profile --gpu-metrics-device=0 --trace=mpi,ucx,cuda -o osu_bw.internode.GDR.%q{SLURM_PROCID}
```



GPU to remote GPU

CUDA-aware MPI without support for GPUDirect

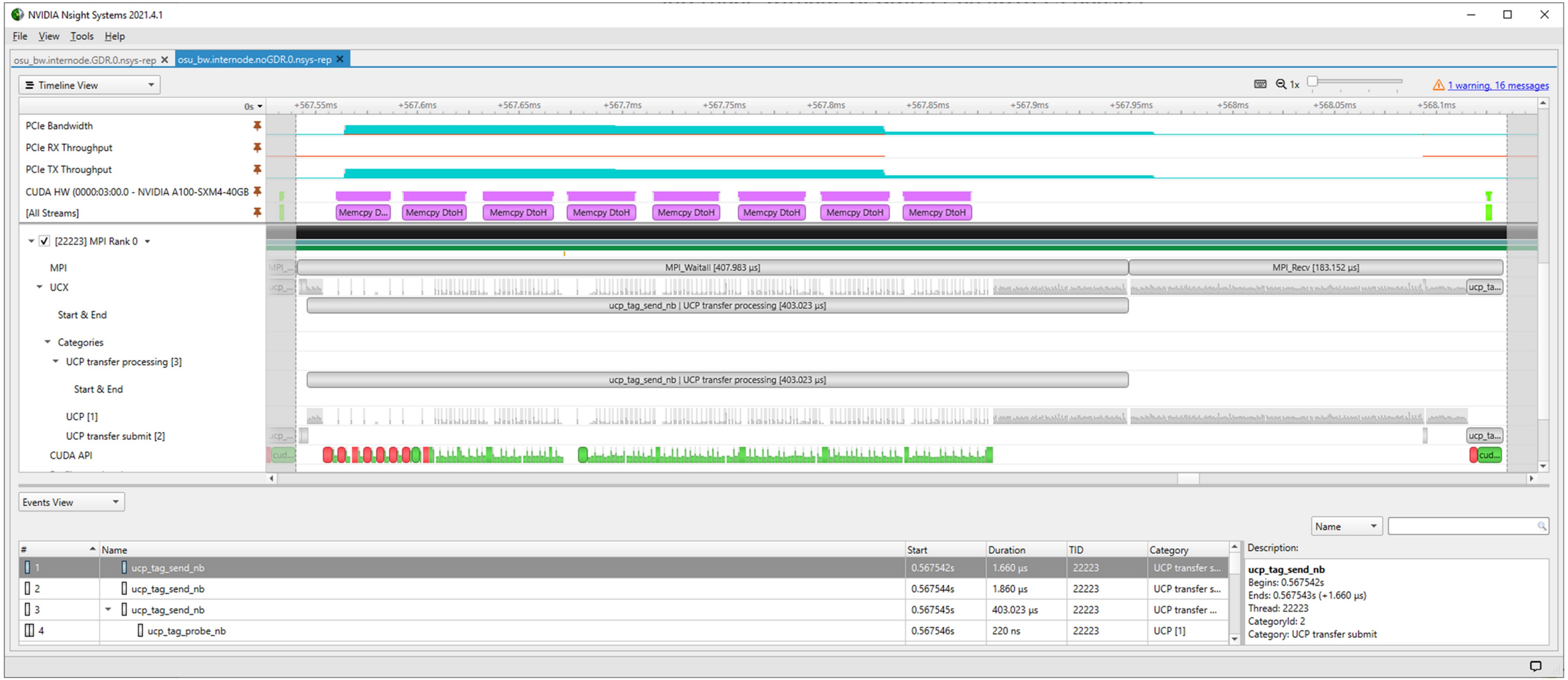



```
MPI_Send(s_buf_d, size, MPI_BYTE, 1, tag, MPI_COMM_WORLD);

MPI_Recv(r_buf_d, size, MPI_BYTE, 0, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

osu_bw Nsight Systems Timeline

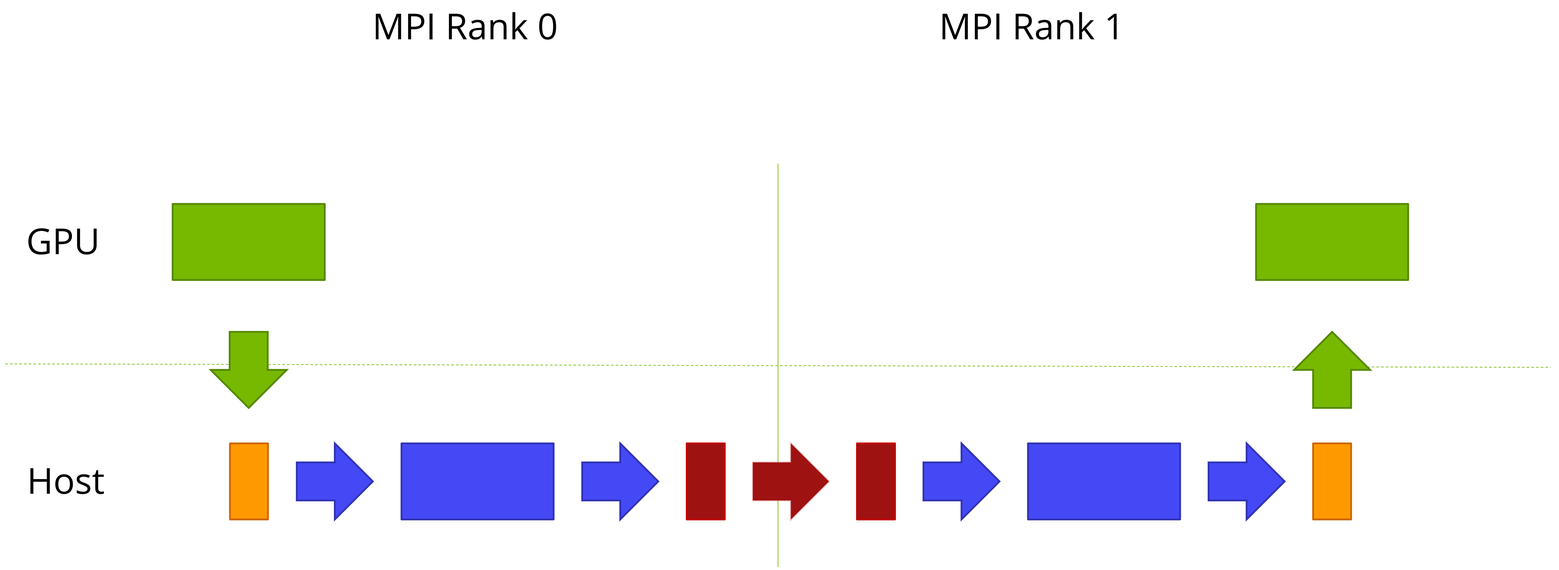
Internode without GPUDirect RDMA on JUWELS Booster

```
nsys profile --gpu-metrics-device=0 --trace=mpi,ucx,cuda -o osu_bw.internode.GDR.%q{SLURM_PROCID}
```



GPU to remote GPU

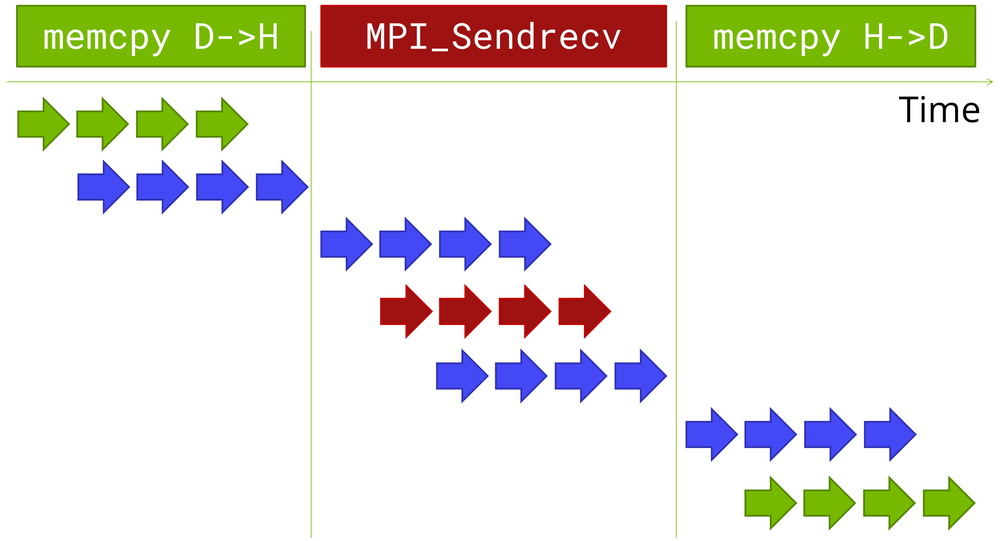
MPI without CUDA support




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

MPI_Recv(r_buf_d, size, MPI_BYTE, 0, tag, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
cudaMemcpy(r_buf_d, r_buf_h, size, cudaMemcpyHostToDevice);
```

GPU to remote GPU

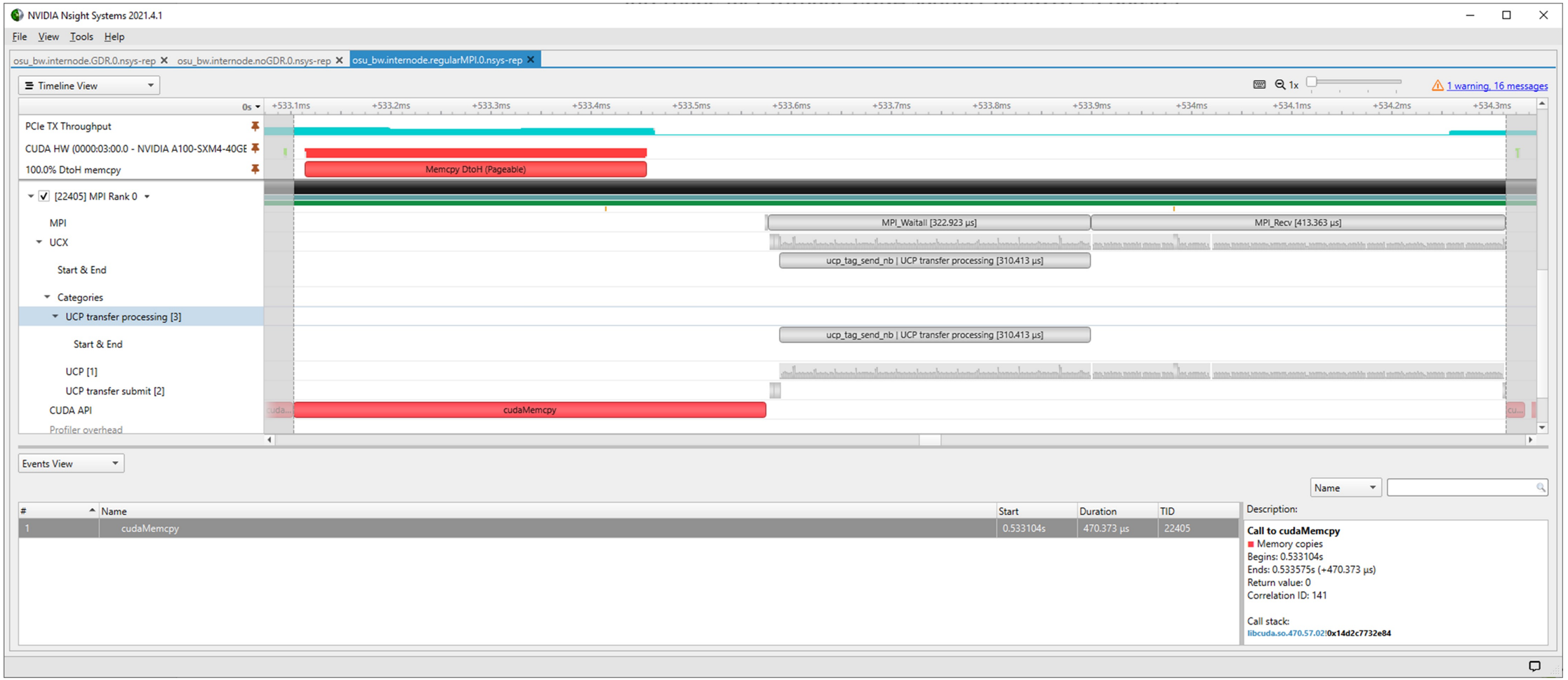
MPI without CUDA support



osu_bw Nsight Systems Timeline

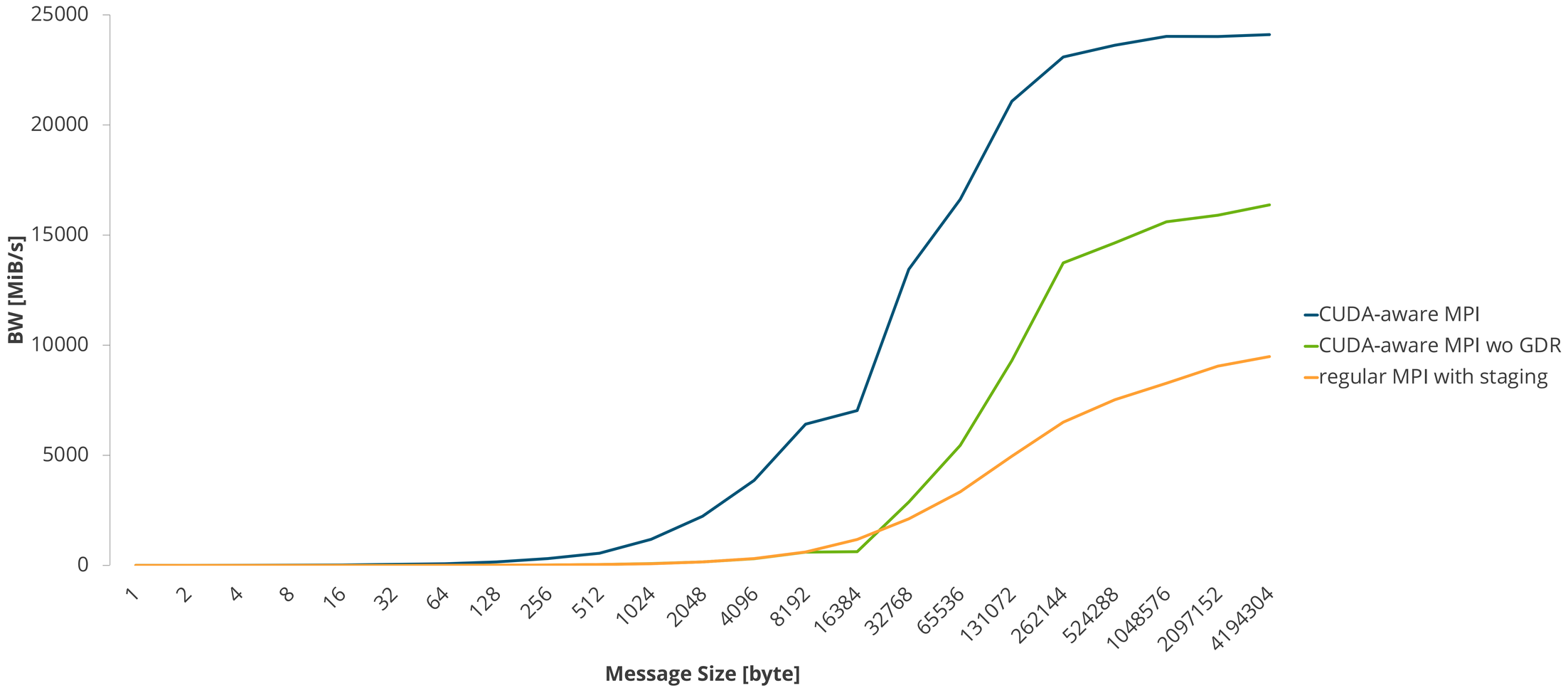
Internode MPI without CUDA support on JUWELS Booster

```
nsys profile --gpu-metrics-device=0 --trace=mpi,ucx,cuda -o osu_bw.internode.GDR.%q{SLURM_PROCID}
```



Performance Results GPUDirect RDMA

Open MPI 4.1.0RC1 + UCX 1.9.0 on JUWELS Booster

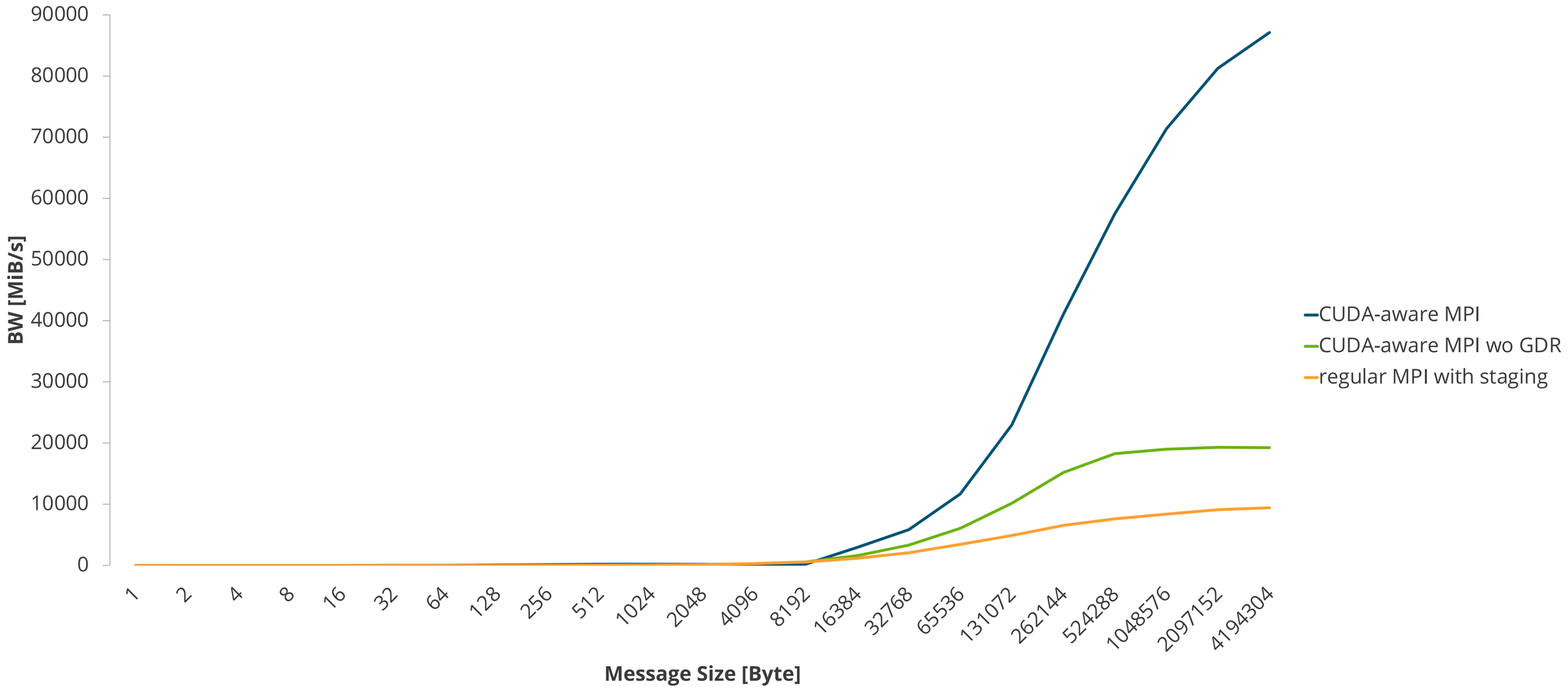


Latency (1 byte) 4.27 us 24.56 us 25.64 us

JUWELS Booster: https://apps.fz-juelich.de/jsc/hps/juwels/booster-overview.html

Performance Results GPUDirect P2P

Open MPI 4.1.0RC1 + UCX 1.9.0 on JUWELS Booster



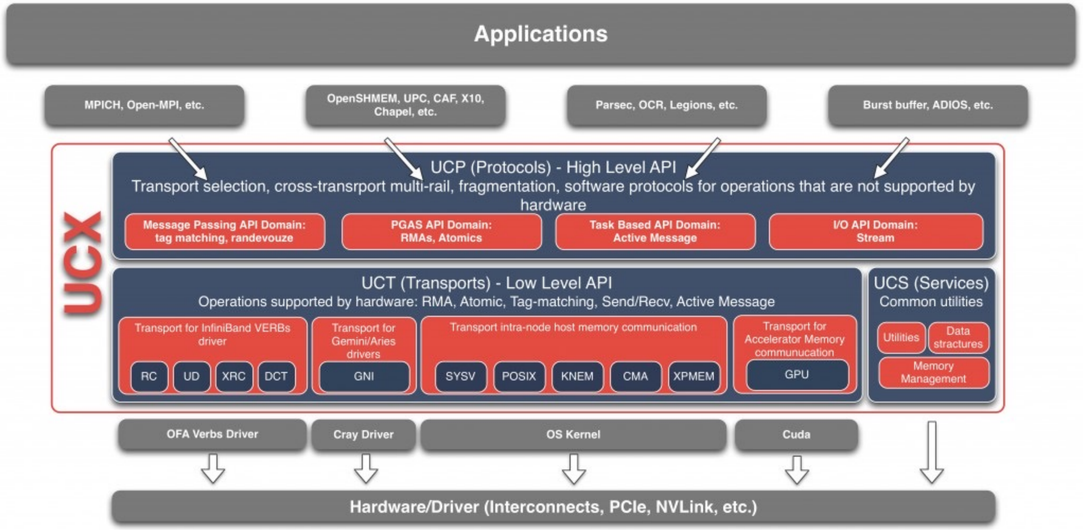
Latency (1 byte) 2.45 us 22.01 us 23.50 us

JUWELS Booster: https://apps.fz-juelich.de/jsc/hps/juwels/booster-overview.html

UCX Tips and Tricks

Check setting and knobs with ucx_info

```
$ ucx_info -caf | grep -B9 UCX_RNDV_SCHEME

#

# Communication scheme in RNDV protocol.

#  get_zcopy - use get_zcopy scheme in RNDV protocol.

#  put_zcopy - use put_zcopy scheme in RNDV protocol.

#  auto      - runtime automatically chooses optimal scheme
to use.

#

# syntax:    [get_zcopy|put_zcopy|auto]

#

UCX_RNDV_SCHEME=auto
```



UCX Tips and Tricks

Enable logging to see what is going on

`UCX_LOG_LEVEL=data UCX_LOG_FILE=log-%h-%p` helpful to check for used protocols and selected HCAs:

```
[1605706306.970537] [jwb1238:7263 :0]      ucp_worker.c:1627 UCX
INFO  ep_cfg[0]: tag(cuda_copy/cuda); rma(gdr_copy/cuda);

[1605706306.972721] [jwb1238:7263 :0]      ucp_worker.c:1627 UCX
INFO  ep_cfg[1]: tag(self/memory rc_mlx5/mlx5_1:1 cma/memory
cuda_copy/cuda);

[1605706306.997849] [jwb1238:7263 :1]      ucp_worker.c:1627 UCX
INFO  ep_cfg[2]: tag(rc_mlx5/mlx5_1:1);
```

UCX Tips and Tricks

https://github.com/openucx/ucx/wiki/UCX-environment-parameters

UCX_NET_DEVICES: To select HCA for optimal GPU-HCA affinity, should not be necessary with UCX 1.9 or newer

UCX_TLS: Select transports to use, default: all

cuda is an alias for: `cuda_copy, cuda_ipc, gdr_copy`

To run without any GPUDirect flavor set `UCX_TLS` to only include `cuda_copy` from the CUDA related transports, e.g. `UCX_TLS=rc,sm,cuda_copy` and `UCX_IB_GPU_DIRECT_RDMA=no` (`rc` transport uses GPUDirect RDMA otherwise).

Parastation MPI also has `PSP_CUDA_ENFORCE_STAGING=1`.

UCX_MEMTYPE_CACHE: Set to n to disable mem type cache. Sometimes necessary if the CUDA runtime is linked statically!

Summary

Asynchronously computing on the GPU while MPI communication allows to hide MPI communication times

Using high priority streams some CUDA API overheads can be also hidden

GPUDirect can provide significant performance improvements both inter and intra node

Knowing UCX performance tuning knobs is important when working with CUDA-aware MPI implementations like OpenMPI and Parastation MPI built on UCX.