OPTIMIZATION TECHNIQUES FOR MULTI-GPU APPLICATIONS

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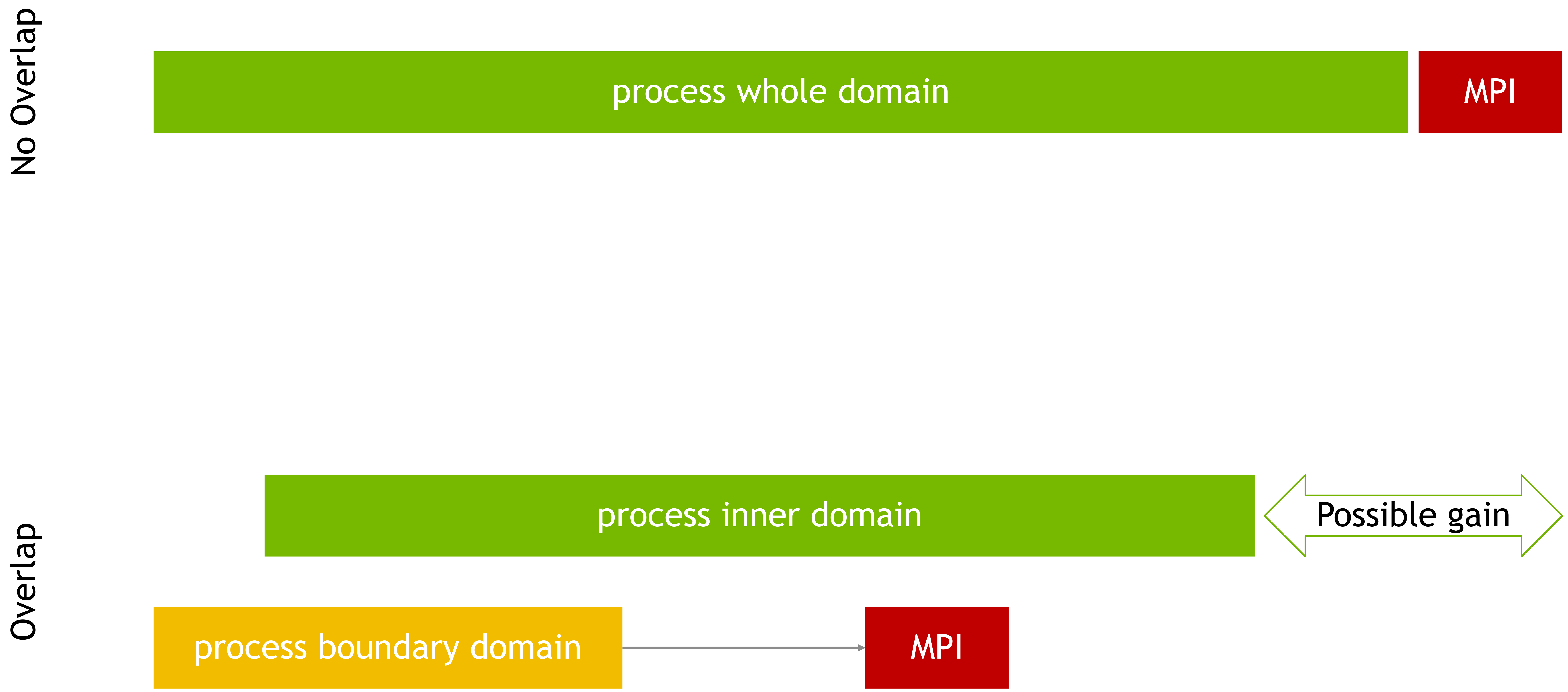
MULTI GPU JACOBI NSIGHT SYSTEMS TIMELINE

MPI 8 NVIDIA A100 40GB on JUWELS Booster

#	Name	Start	Duration	TID
1	MPI_Sendrecv	2.12489s	32.270 µs	27013
2	MPI_Sendrecv	2.12492s	28.850 µs	27013
3	MPI_Allreduce	2.12495s	25.930 µs	27013

Description:

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));
```

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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);

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                      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

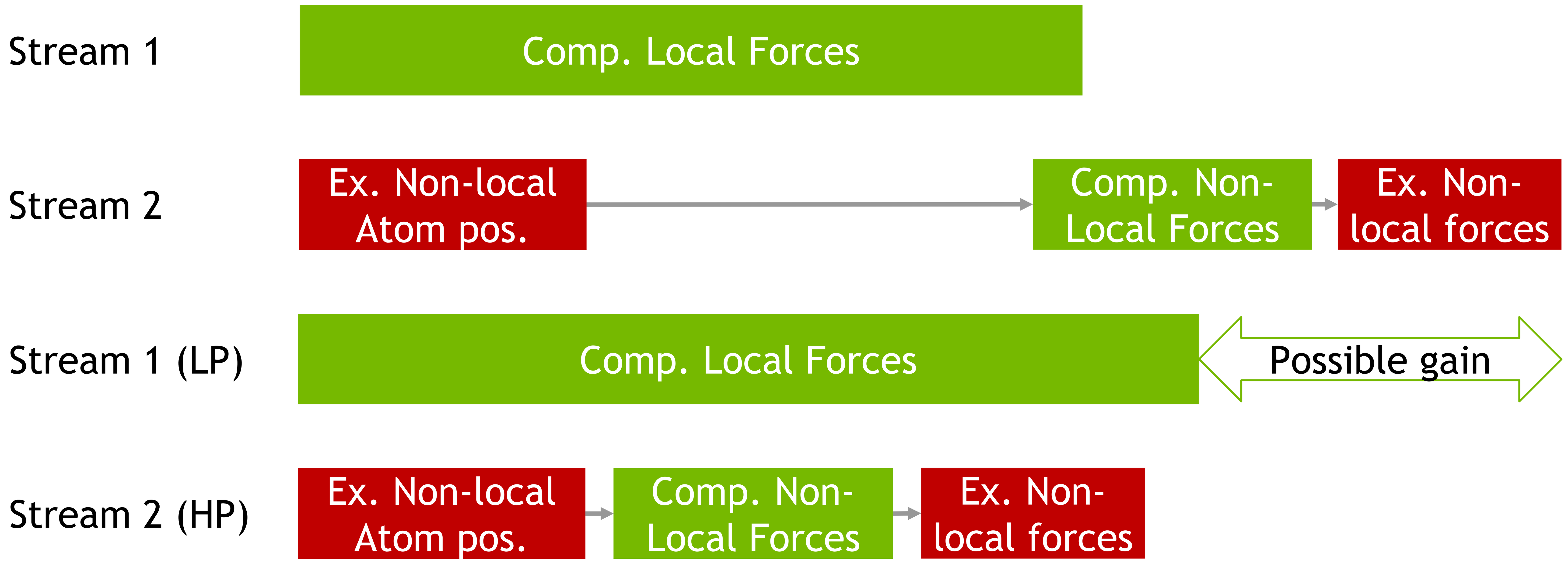
MPI Overlap 8 NVIDIA A100 40GB on JUWELS Booster

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

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COMMUNICATION + COMPUTATION OVERLAP

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CUDA-AWARE MPI

Example:

MPI Rank 0 `MPI_Send` from GPU Buffer

MPI Rank 1 `MPI_Recv` to GPU Buffer

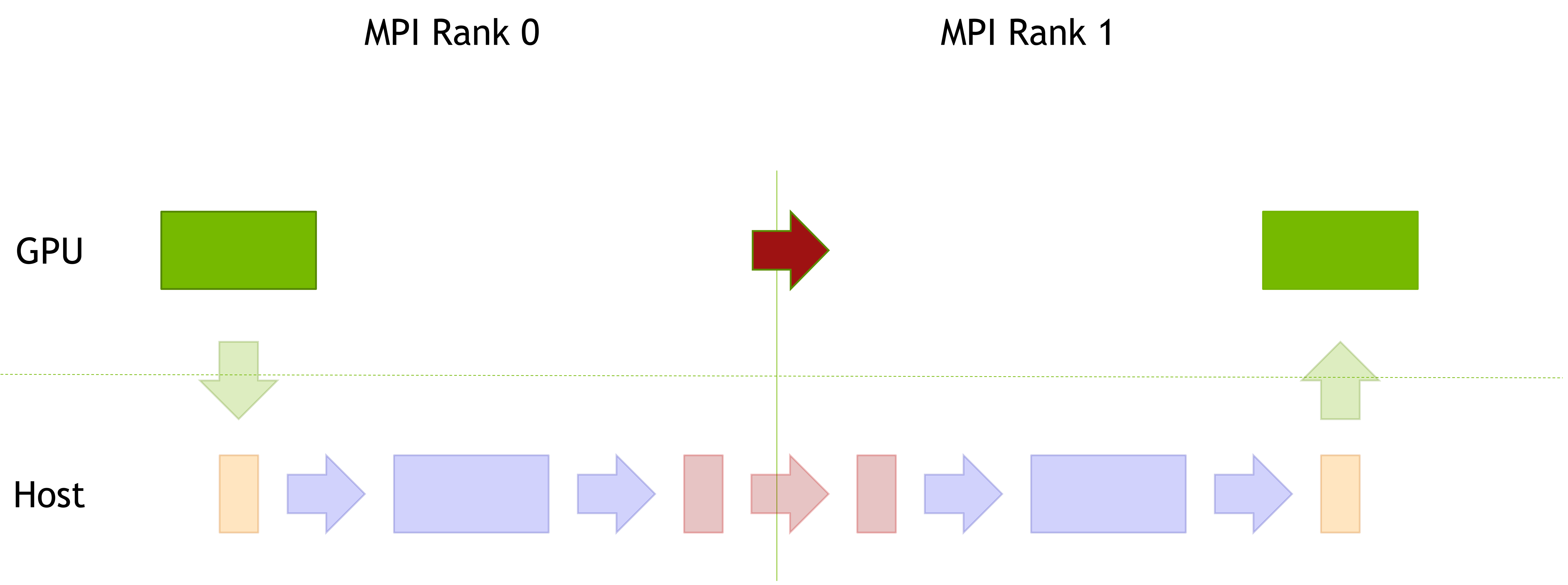
Show how CUDA+MPI works in principle

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);
```

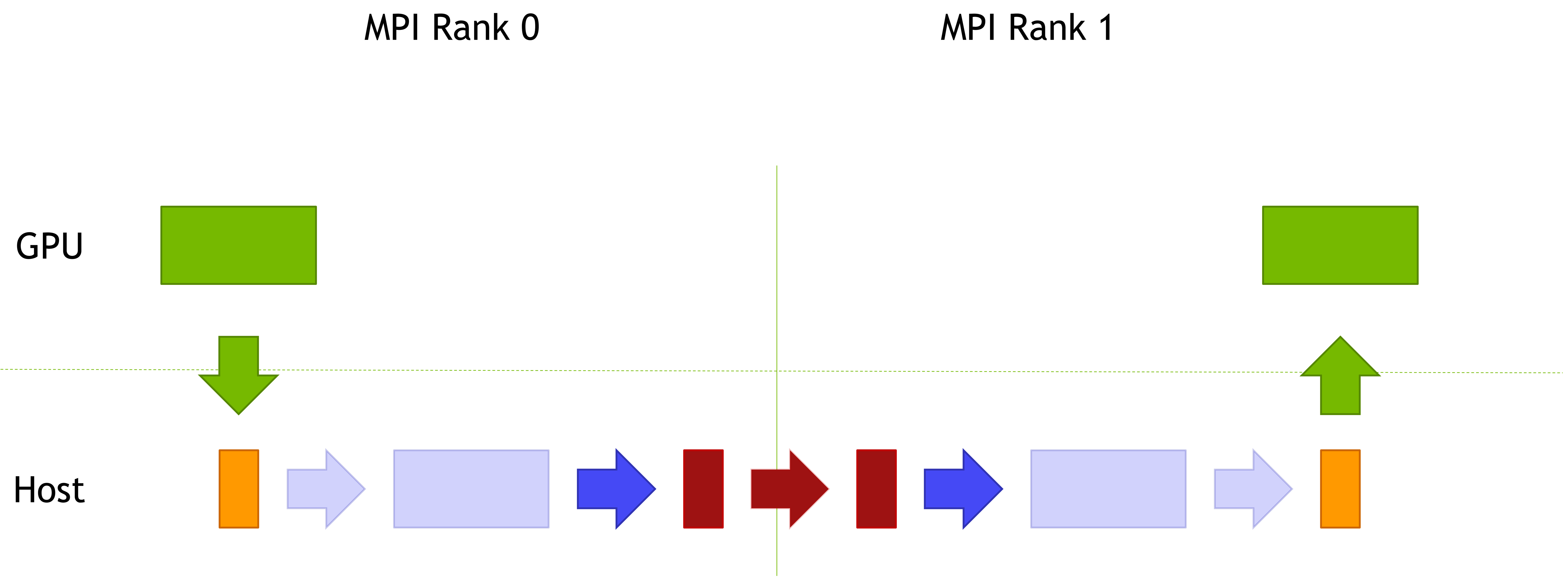
OSU_BW NSIGHT SYSTEMS TIMELINE

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

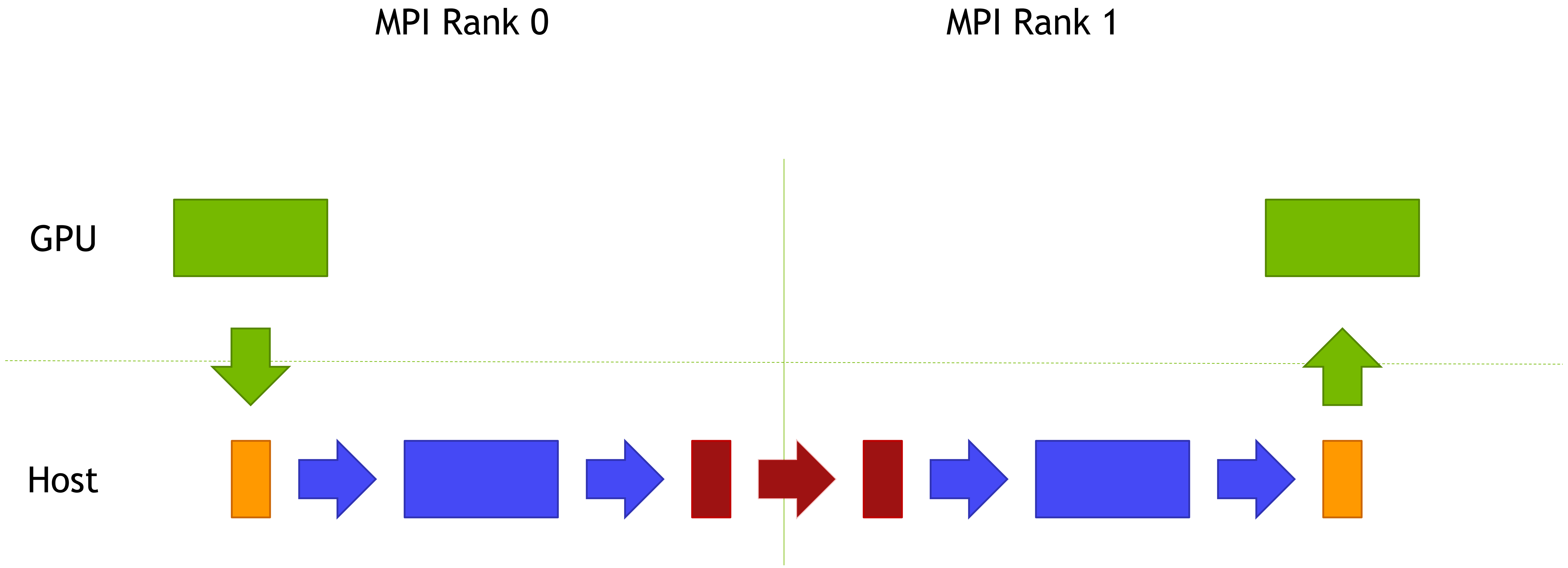
Internode without GPUDirect on JUWELS Booster

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

#	Name	Start	Duration	TID	Category
1	ucp_tag_send_nb	0.567542s	1.660 µs	22223	UCP transfer s...
2	ucp_tag_send_nb	0.567544s	1.860 µs	22223	UCP transfer s...
3	ucp_tag_send_nb	0.567545s	403.023 µs	22223	UCP transfer ...
4	ucp_tag_probe_nb	0.567546s	220 ns	22223	UCP [1]

GPU TO REMOTE GPU

MPI without CUDA support

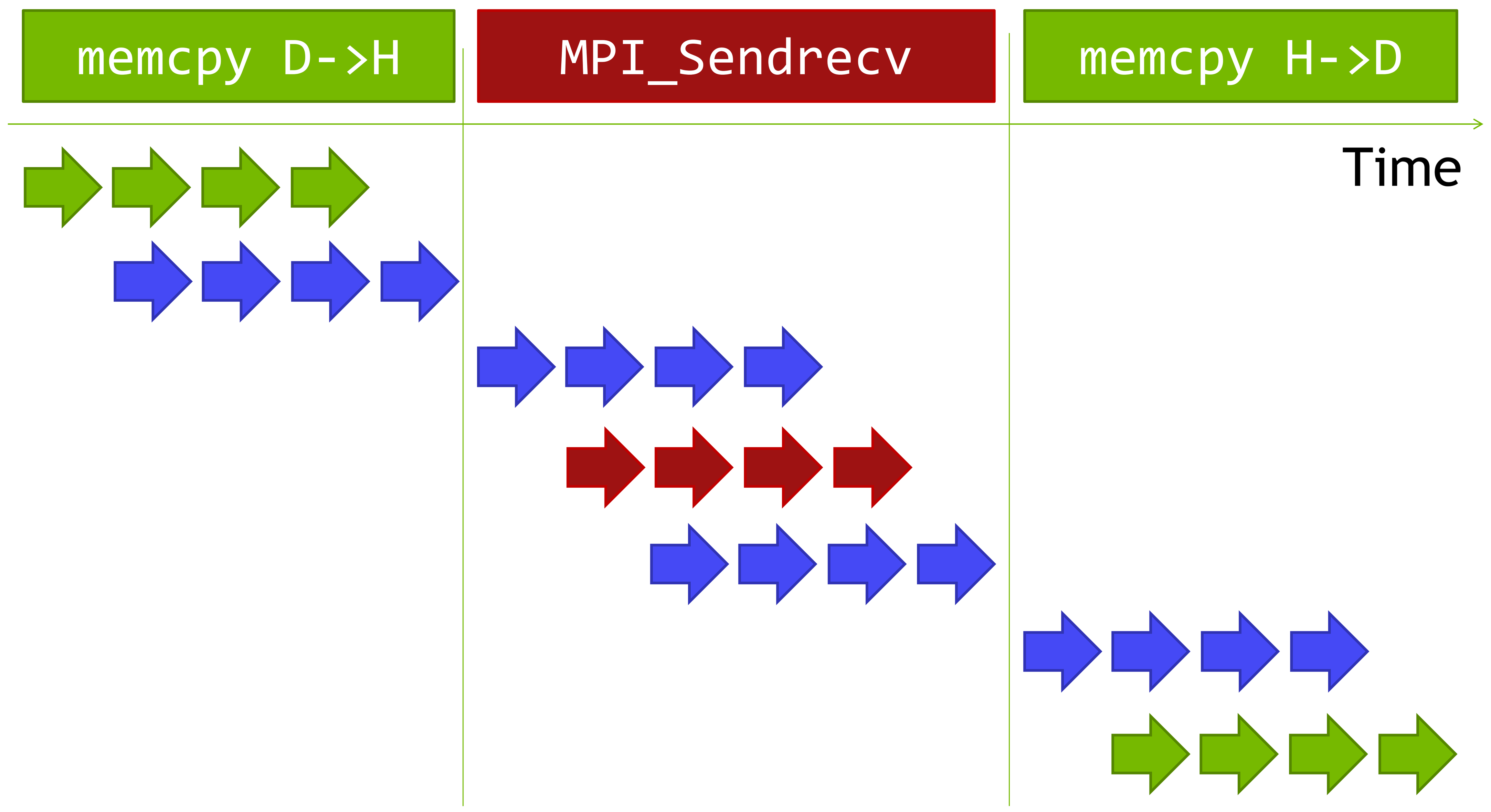



```
cudaMemcpy(s_buf_h, s_buf_d, size, cudaMemcpyDeviceToHost);
MPI_Send(s_buf_d, size, MPI_BYTE, 1, tag, MPI_COMM_WORLD);

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.noCUDAMPI.%q{SLURM_PROCID}`

PERFORMANCE RESULTS GPUDIRECT RDMA

OpenMPI 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

OpenMPI 4.1.0RC1 + UCX 1.9.0 on JUWELS Booster

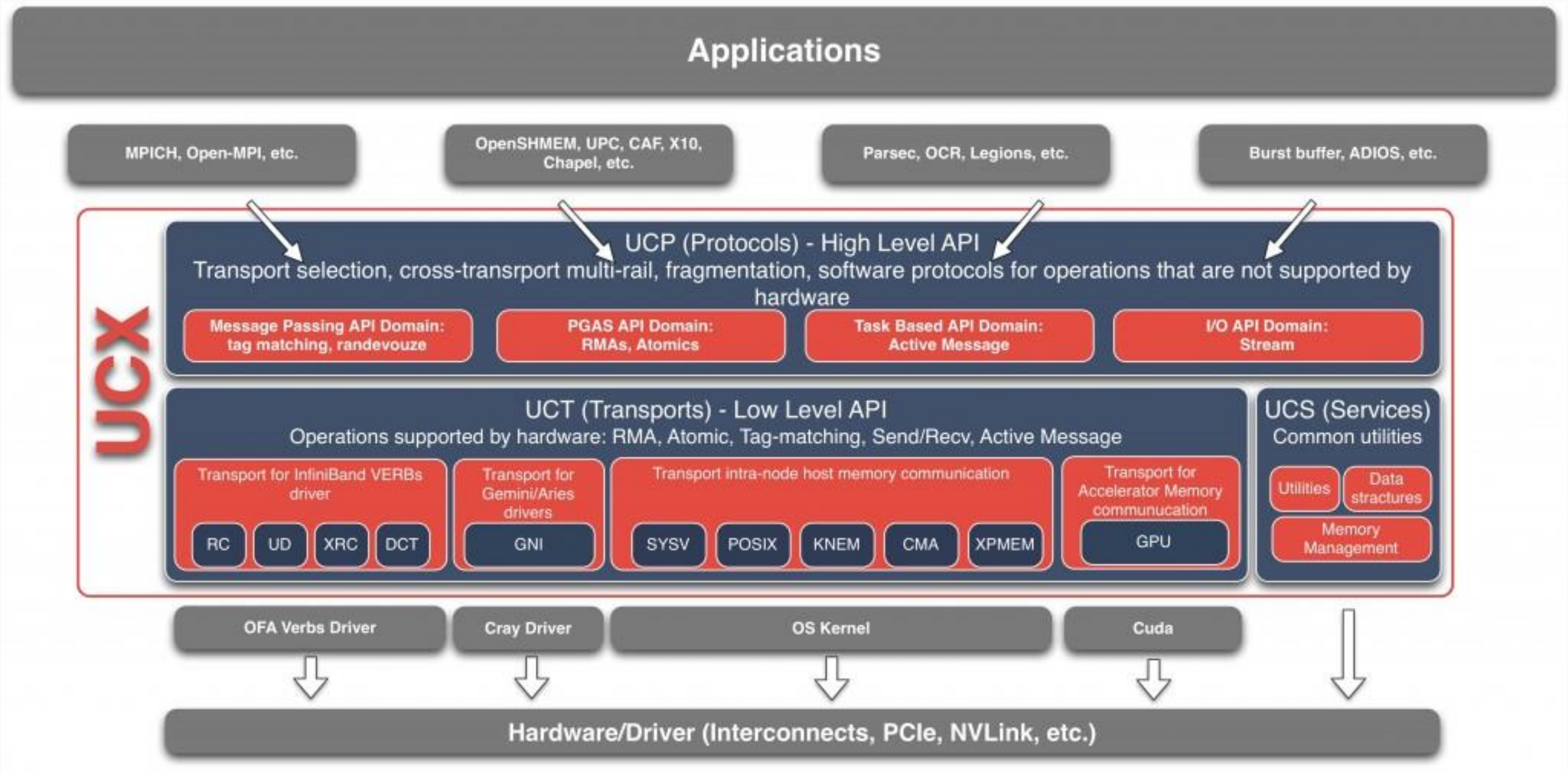
Latency (1 byte) 2.45 us 22.01 us 23.50 us

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`, 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.