Design and Implementation of MPI-Native GPU-Initiated MPI Partitioned Communication

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Outline

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- MPI Partitioned Point-to-Point Communication was added to the MPI-4.0 in June 2021
  - Better supports hybrid programming models
  - Viable path to obtaining good GPU performance with MPI

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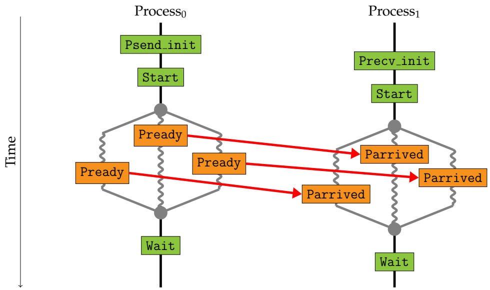
- MPI buffers used for GPU communication are located in GPU Memory

MPI Partitioned Communication

- `MPI_Psend_init`/`MPI_Precv_init` is used to initialize communication between processes



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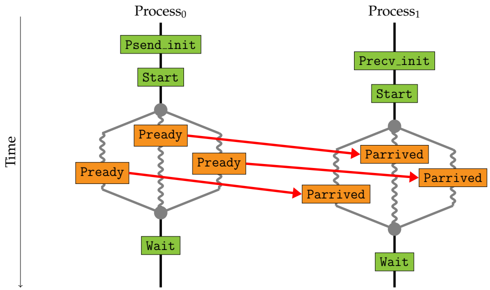

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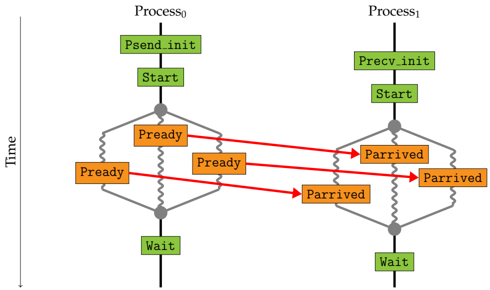

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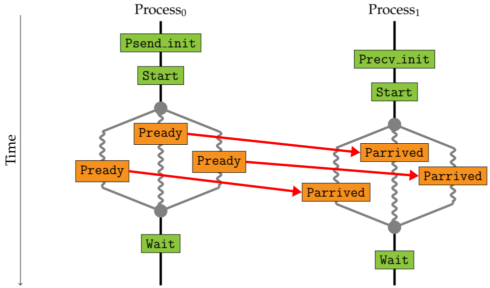

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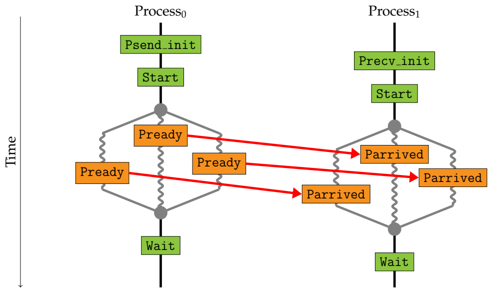

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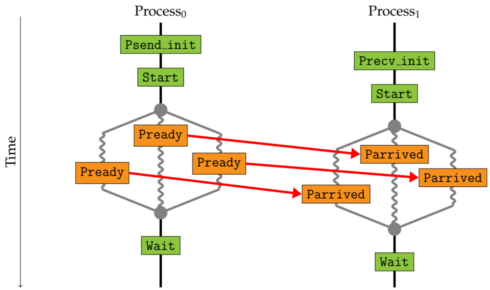

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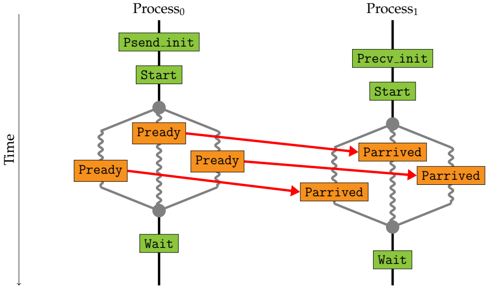

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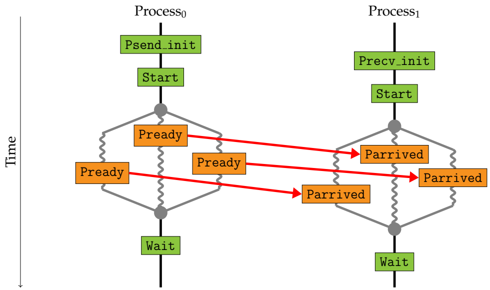
- `MPI_Wait` is called to complete communication



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- How can we avoid `cudaStreamSynchronize`?

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kernel_A<<<stream>>>(sbuf);
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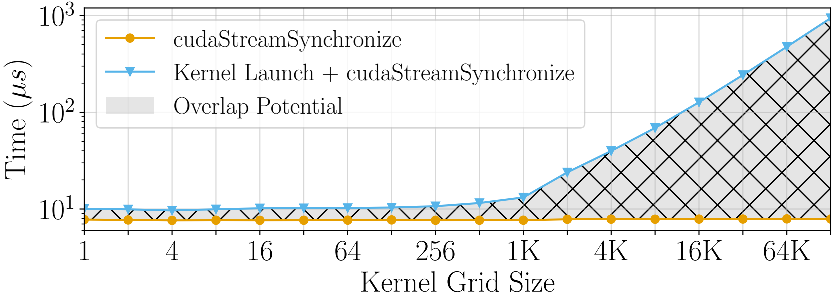
GPU Synchronization Cost

- We evaluate the cost of syncronization for a vector addition ($C = A + B$)



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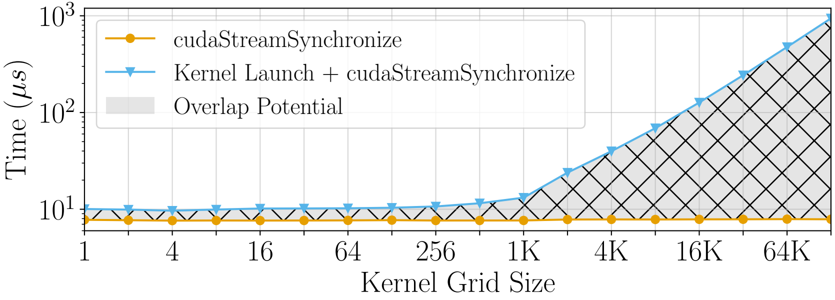

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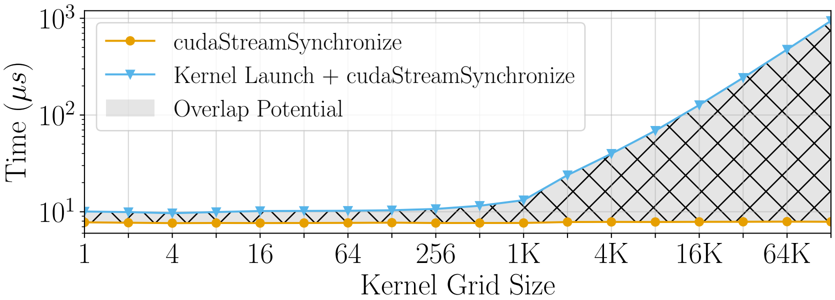

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- How do we use these API calls?

GPU-Support MPI Partitioned Communication

- We start our communication

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__host__ int host_function(MPI_Request req,
                           double *sbuf)
{
  MPI_Start(req)
  MPIX_Pbuf_Prepare(req);
  MPIX_Prequest_create(preq, req);

  kernel_B<<<stream>>>(preq, sbuf);
  /* Do work on host */
  MPI_Wait(req);
}

__global__ int kernel_B(MPIX_Prequest preq,
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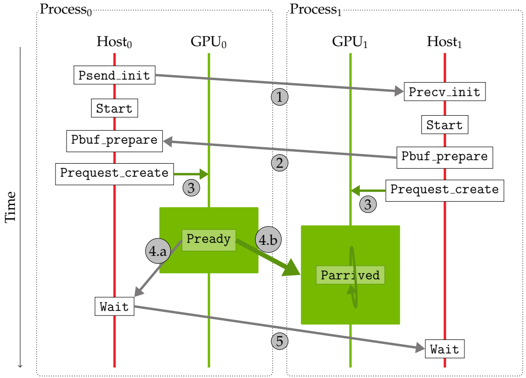

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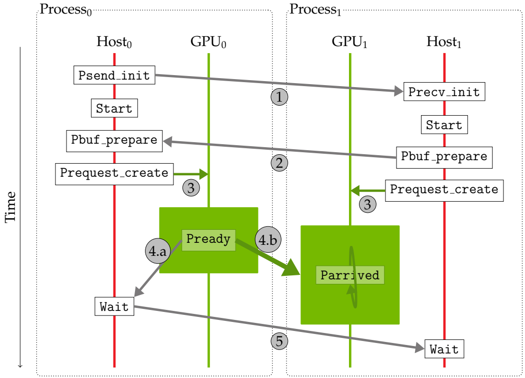

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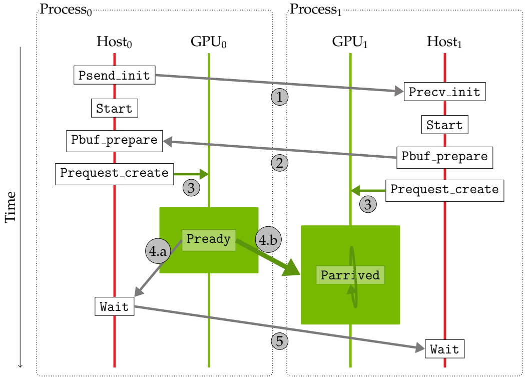

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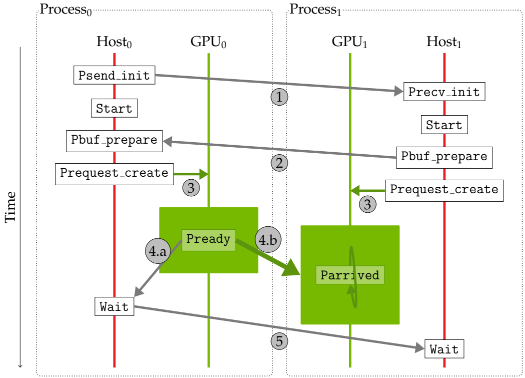

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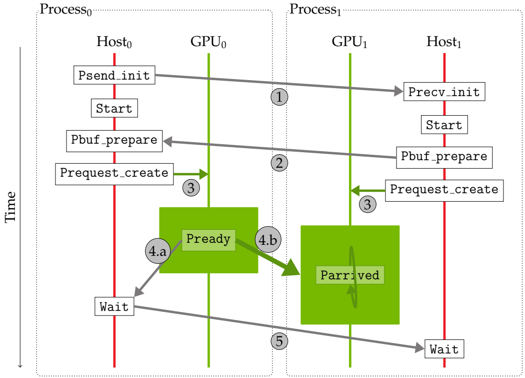

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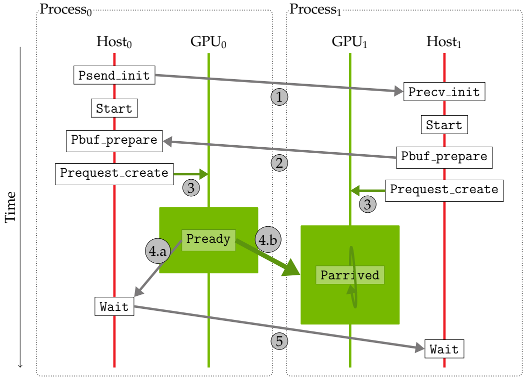

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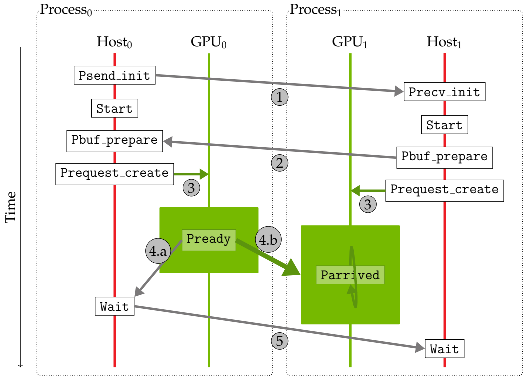

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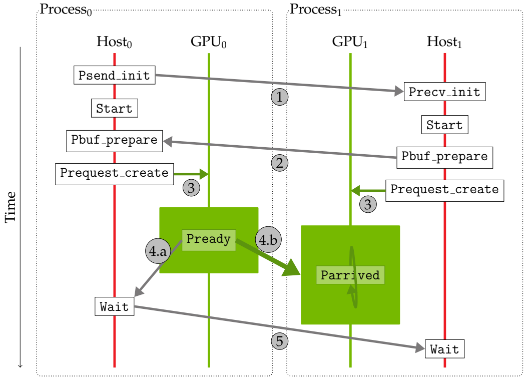

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   - The GPU writes to a flag in host memory
   - The MPI Progression polls the flags and issues a `ucp_put_nbx` when serviced

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- Ideally we could generalize initialization for the 21 proposed MPI Partitioned Collective calls
- `MPI_Pbuf_prepare` now gaurantees readiness for all processes in communicator

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run

---

Algorithm 1: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

---

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
- $I \leftarrow (\text{rank} - 1) \mod P$
- $O \leftarrow (\text{rank} + 1) \mod P$
- $R \leftarrow (\text{rank} + 2P - i) \mod P$
- $A \leftarrow (\text{rank} + 2P - i - 1) \mod P$
- **if** $i < (P-1)$ **then**
  - $\oplus \leftarrow MPI\_Op$
- **else**
  - $\oplus \leftarrow NOP$
- $S_i \leftarrow (I, R, \oplus, O, A)$
- $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
- We list our incomming neighbours (I)

Algorithm 2: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
    $I \leftarrow (\text{rank} - 1) \mod P$
    $O \leftarrow (\text{rank} + 1) \mod P$
    $R \leftarrow (\text{rank} + 2P - i) \mod P$
    $A \leftarrow (\text{rank} + 2P - i - 1) \mod P$
    if $i < (P-1)$ **then**
        $\oplus \leftarrow MPI\_Op$
    else
        $\oplus \leftarrow NOP$
    $S_i \leftarrow (I, R, \oplus, O, A)$
    $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
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- We list our outgoing neighbours (O)

Algorithm 3: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**

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  $O \leftarrow (\text{rank} + 1) \mod P$

  $R \leftarrow (\text{rank} + 2P - i) \mod P$

  $A \leftarrow (\text{rank} + 2P - i - 1) \mod P$

  if $i < (P-1)$ **then**

    $\oplus \leftarrow MPI\_Op$

  else

    $\oplus \leftarrow NOP$

  $S_i \leftarrow (I, R, \oplus, O, A)$

  $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
- We list our incomming neighbours (I)
- We list our outgoing neighbours (O)
- We list our offsets (R, A)

Algorithm 4: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
  $I \leftarrow (\text{rank}-1) \mod P$
  $O \leftarrow (\text{rank}+1) \mod P$
  $R \leftarrow (\text{rank}+2P-i) \mod P$
  $A \leftarrow (\text{rank}+2P-i-1) \mod P$
  if $i < (P-1)$ **then**
    $\oplus \leftarrow MPI\_Op$
  else
    $\oplus \leftarrow NOP$
  $S_i \leftarrow (I, R, \oplus, O, A)$
  $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
- We list our incomming neighbours (I)
- We list our outgoing neighbours (O)
- We list our offsets (R, A)
  - Certain algorithms move data as a part of its execution

Algorithm 5: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
$\quad I \leftarrow (\text{rank} - 1) \mod P$
$\quad O \leftarrow (\text{rank} + 1) \mod P$
$\quad R \leftarrow (\text{rank} + 2P - i) \mod P$
$\quad A \leftarrow (\text{rank} + 2P - i - 1) \mod P$
$\quad$ **if** $i < (P-1)$ **then**
$\quad\quad \oplus \leftarrow MPI\_Op$
$\quad$ **else**
$\quad\quad \oplus \leftarrow NOP$
$\quad S_i \leftarrow (I, R, \oplus, O, A)$
$\quad \mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
- We list our incomming neighbours (I)
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- We list our offsets (R, A)
  - Certain algorithms move data as a part of its execution
- Some collectives a reduce component (allreduce, reducescatter, scan, etc.)

Algorithm 6: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
- $I \leftarrow (\text{rank} - 1) \mod P$
- $O \leftarrow (\text{rank} + 1) \mod P$
- $R \leftarrow (\text{rank} + 2P - i) \mod P$
- $A \leftarrow (\text{rank} + 2P - i - 1) \mod P$
- **if** $i < (P-1)$ **then**
  - $\oplus \leftarrow MPI\_Op$
- **else**
  - $\oplus \leftarrow NOP$
- $S_i \leftarrow (I, R, \oplus, O, A)$
- $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We first create a schedule our partitioned collective will run
- We list our incomming neighbours (I)
- We list our outgoing neighbours (O)
- We list our offsets (R, A)
  - Certain algorithms move data as a part of its execution
- Some collectives a reduce component (allreduce, reducescatter, scan, etc.)
- These parameters populate our schedule $\mathbb{S}$

Algorithm 7: `MPIX_Pallreduce_init` schedule creation for a Ring-Based RSA algorithm

for $i \leftarrow 0$ **to** $2(P-1)$ **do**
    $I \leftarrow (\text{rank} - 1) \mod P$
    $O \leftarrow (\text{rank} + 1) \mod P$
    $R \leftarrow (\text{rank} + 2P - i) \mod P$
    $A \leftarrow (\text{rank} + 2P - i - 1) \mod P$
    if $i < (P-1)$ **then**
        $\oplus \leftarrow MPI\_Op$
    else
        $\oplus \leftarrow NOP$
    $S_i \leftarrow (I, R, \oplus, O, A)$
    $\mathbb{S} \leftarrow S_i$

MPI Partitioned Collectives Design

- We check if all partitions for the algorithm step have completed

Algorithm 8: `MPI_Wait` Progression of a Partitioned Collective Schedule

for *part* $\leftarrow$ 0 **to** num_partitions **do**
    state = states[part]
    $S \leftarrow$ state.step
    if $S > S_k$ **then** continue ;
    if state.parrived_complete $\neq |I|$ **then**
        for $I_x \in I$ **do**
            `MPI_Parrived(flag)`
            if flag = true **then**
                state.parrived_complete++
                if $\oplus \neq$ NOP **then** reduceData() ;
    if state.parrived_complete $= |I|$ **and** state.pready_complete $= |O|$ **then**
        $S \leftarrow S_{(i+1)}$
        state.parrived_complete $\leftarrow 0$
        state.pready_complete $\leftarrow 0$
    if $S \neq S_0$ **and** $S! = S_k$ **and** state.pready_complete $= 0$ **then**
        for $O_x \in O$ **do**
            `MPI_Pready(...)`
            state.pready_complete++

MPI Partitioned Collectives Design

- We check if all partitions for the algorithm step have completed
  - If not, we check with `MPI_Parrived`

Algorithm 9: `MPI_Wait` Progression of a Partitioned Collective Schedule

for *part* $\leftarrow$ 0 **to** num_partitions **do**
    state = states[part]
    $S \leftarrow$ state.step
    if $S > S_k$ **then** continue ;
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        for $O_x \in O$ **do**
            `MPI_Pready(...)`
            state.pready_complete++

MPI Partitioned Collectives Design

- We check if all partitions for the algorithm step have completed
  - If not, we check with `MPI_Parrived`
  - If it has arrived, and there is a reduce operation $\oplus$, we reduce the data.

Algorithm 10: `MPI_Wait` Progression of a Partitioned Collective Schedule

for *part* $\leftarrow$ 0 **to** num_partitions **do**
  state = states[part]
  $S \leftarrow$ state.step
  if $S > S_k$ **then** continue ;
  if state.parrived_complete $\neq |I|$ **then**
    for $I_x \in I$ **do**
      `MPI_Parrived(flag)`
      if flag = true **then**
        state.parrived_complete++
        if $\oplus \neq$ NOP **then** reduceData() ;
  if state.parrived_complete $= |I|$ **and**
    state.pready_complete $= |O|$
  then
    $S \leftarrow S_{(i+1)}$
    state.parrived_complete $\leftarrow 0$
    state.pready_complete $\leftarrow 0$
  if $S \neq S_0$ **and** $S! = S_k$ **and**
    state.pready_complete $= 0$
  then
    for $O_x \in O$ **do**
      `MPI_Pready(...)`
      state.pready_complete++

MPI Partitioned Collectives Design

- We check if all partitions for the algorithm step have completed
  - If not, we check with `MPI_Parrived`
  - If it has arrived, and there is a reduce operation $\oplus$, we reduce the data.
- If all communication is complete, we move to the next step in the schedule

Algorithm 11: `MPI_Wait` Progression of a Partitioned Collective Schedule

```
for part ← 0 to num_partitions do
    state = states[part]
    S ← state.step
    if S > S_k then continue ;
    if state.parrived_complete ≠ |I| then
        for I_x ∈ I do
            MPI_Parrived(flag)
            if flag = true then
                state.parrived_complete++
                if ⊕ ≠ NOP then
                    reduceData() ;
    if state.parrived_complete = |I| and
        state.pready_complete = |O|
    then
        S ← S_(i+1)
        state.parrived_complete ← 0
        state.pready_complete ← 0
    if S ≠ S_0 and S! = S_k and
        state.pready_complete = 0
    then
        for O_x ∈ O do
            MPI_Pready(...)
            state.pready_complete++
```

MPI Partitioned Collectives Design

- We check if all partitions for the algorithm step have completed
  - If not, we check with `MPI_Parrived`
  - If it has arrived, and there is a reduce operation $\oplus$, we reduce the data.
- If all communication is complete, we move to the next step in the schedule
- Then we call `MPI_Pready` for our outgoing neighbors

Algorithm 12: `MPI_Wait` Progression of a Partitioned Collective Schedule

for *part* $\leftarrow 0$ **to** num_partitions **do**
  state = states[part]
  $S \leftarrow$ state.step
  if $S > S_k$ **then** continue ;
  if state.parrived_complete $\neq |I|$ **then**
    for $I_x \in I$ **do**
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    for $O_x \in O$ **do**
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      state.pready_complete++

Experimental Setup

- We used a two-node NVIDIA GH200 Grace Hopper Superchip testbed*

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- Compiled with NVHPC 23.11
- We implemented this with Open MPI v5.0.1rc1 and UCX (master:bc85b70e6)

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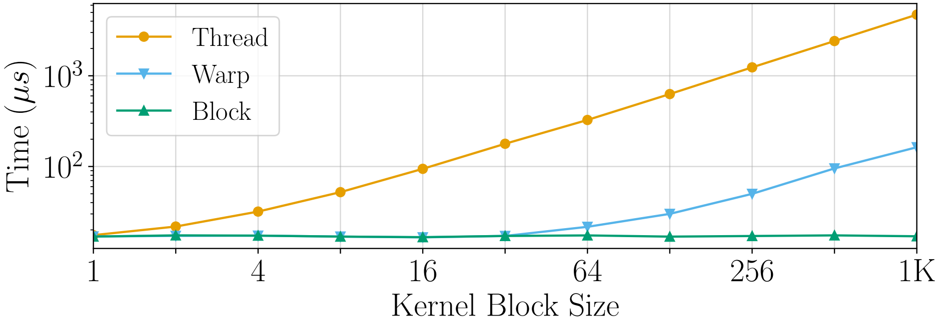
Message Aggregation Results

- The MPI Hybrid Group proposed a few granular bindings for `MPIX_Pready`



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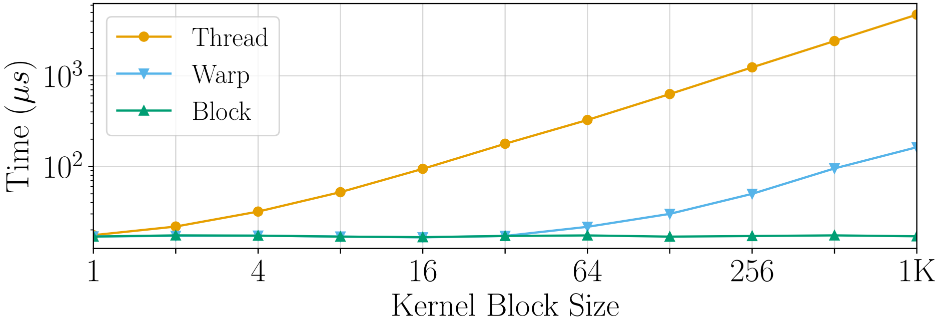

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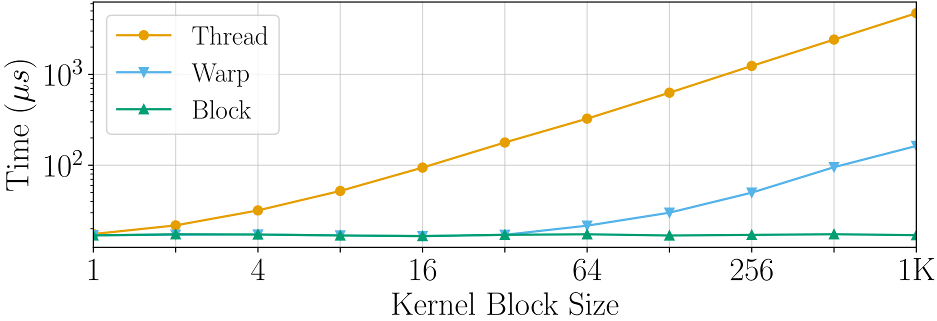
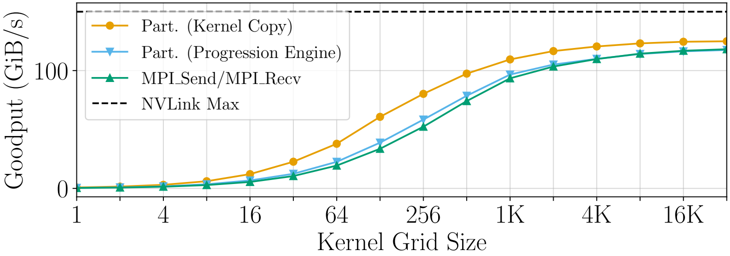
- We found aggregating by blocks performed best



Intra-Node Point-to-Point Results

- We evaluated our intra-node point-to-point performance for our different copy mechanisms:



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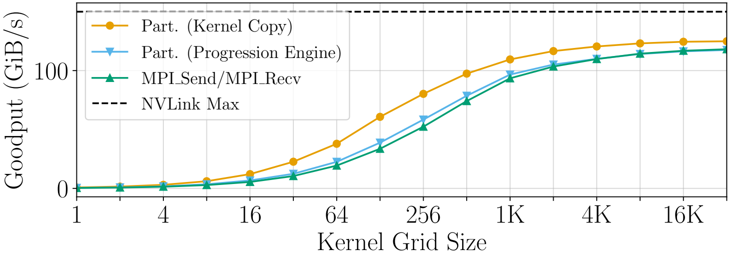

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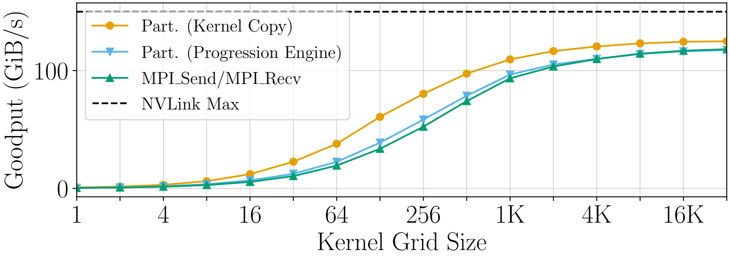
- Generally we see better performance with MPI Partitioned



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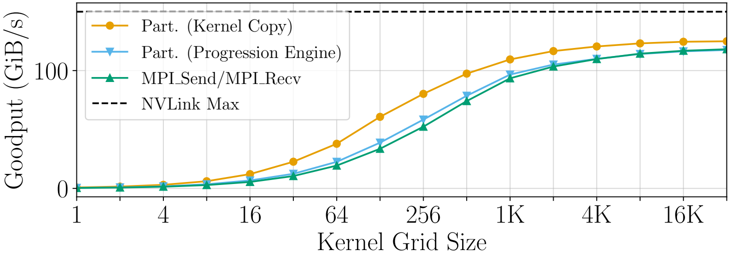

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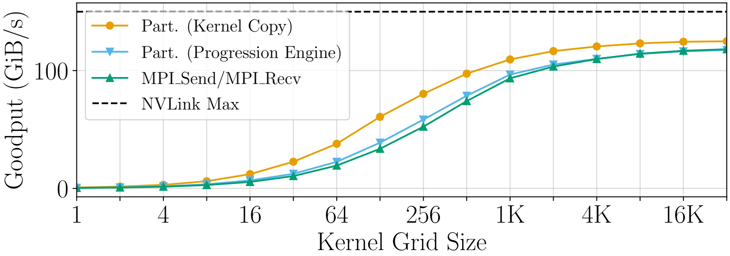
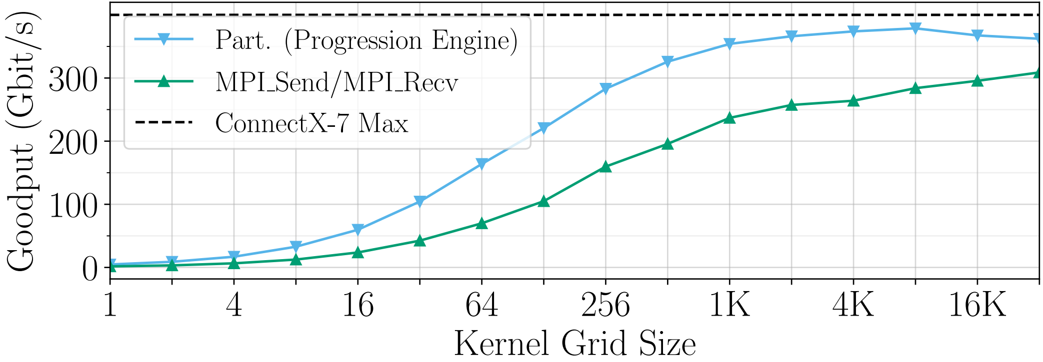
- Generally we see better performance with MPI Partitioned
  - Intra-Node Kernel Copy performs better than Progession Engine Copy
  - The Kernel Copy has the benefit of no host involement



Inter-Node Point-to-Point Results

- We only evaluated the MPI Progression Copy for the inter-node case



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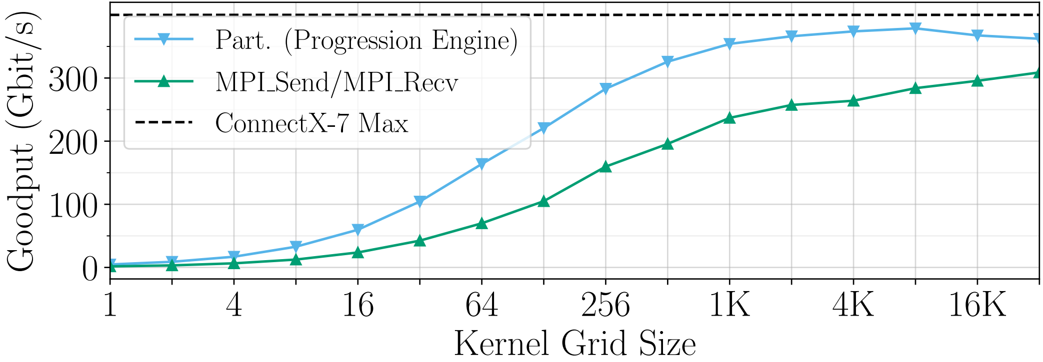

Inter-Node Point-to-Point Results

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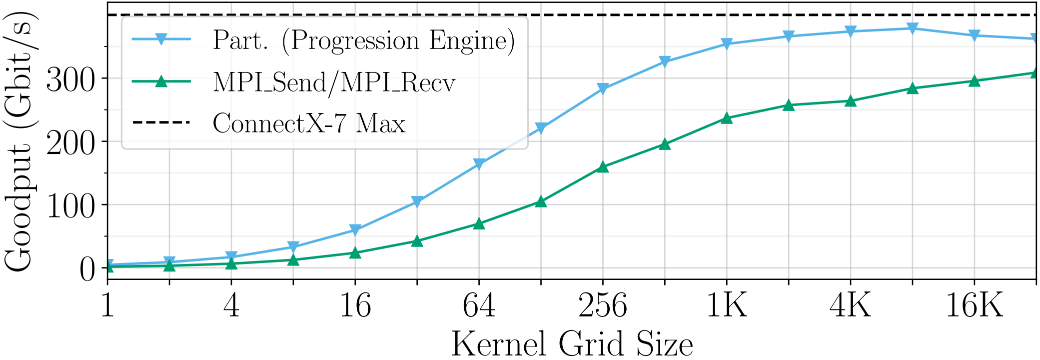

MPI_Pallreduce Results

- Significant improvement compared to `MPI_Allreduce`

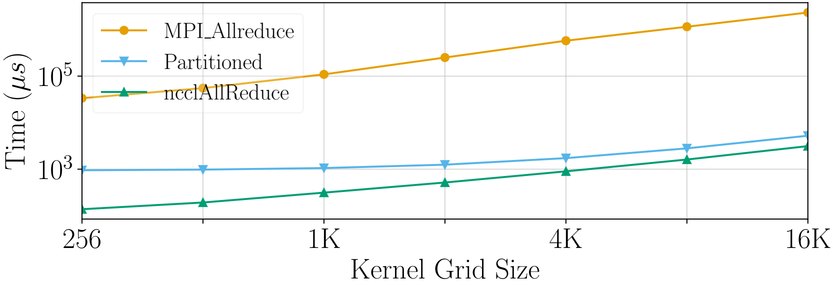

Figure: Eight-Node Allreduce Goodput Performance

MPI_Pallreduce Results

- Significant improvement compared to `MPI_Allreduce`
- Reduces the performance gap between Open MPI and NCCL

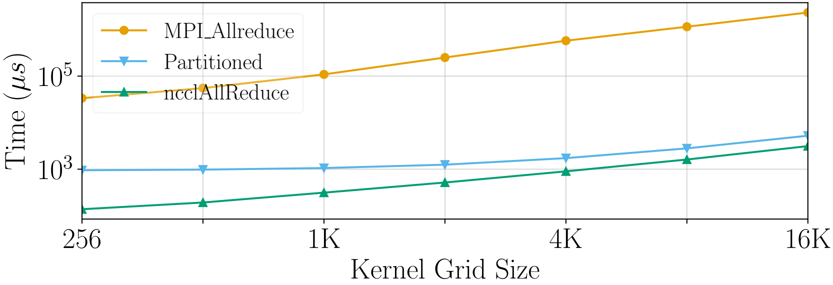

Figure: Eight-Node Allreduce Goodput Performance

Overheads

- The overheads of these new MPI calls must be considered

Table: Overheads for Different MPI Calls

MPI Call	Overhead
`MPI_PSend/Recv_init`	$17.2 \pm 10.2\mu s$
`MPIX_Pallreduce_init`	$62.3 \pm 6.2\mu s$
`MPIX_Prequest_create`	$110.7 \pm 37.8\mu s$
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- Creating `MPIX_Prequest` can have a high overhead so it is important to minimize what must be copied to the device.
- `MPIX_Pbuf_prepare` has a high initial cost as it is required to complete initialization
  - Subsequent calls are low cost

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Jacobi Solver Results

- Evaluated the CUDA-Aware MPI Jacobi Solver

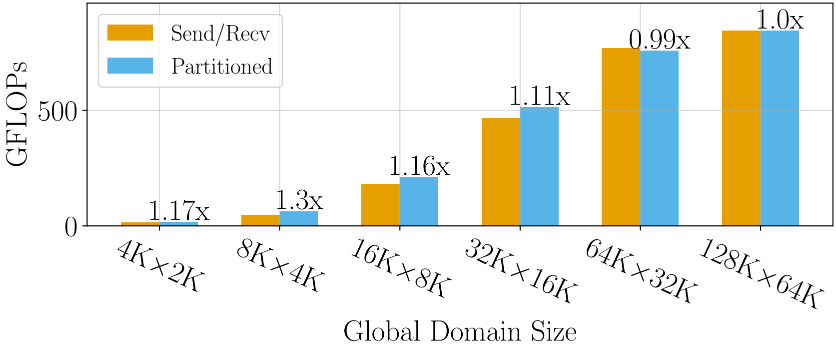

Figure: Eight-Node Jacobi Solver Performance

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- Evaluated the CUDA-Aware MPI Jacobi Solver
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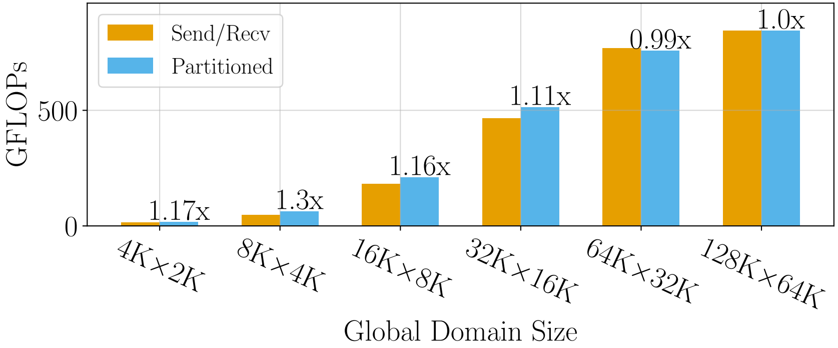

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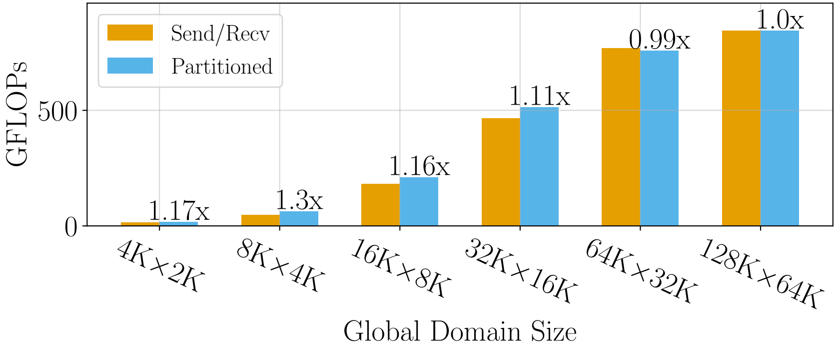
Jacobi Solver Results

- Evaluated the CUDA-Aware MPI Jacobi Solver
  - The solver uses a Point-to-Point Halo Exchange
  - Performs best for smaller kernel



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Deep Learning Kernel Results

- Evaluated a distributed Binary Cross Entropy Loss
  - Depends on Allreduce

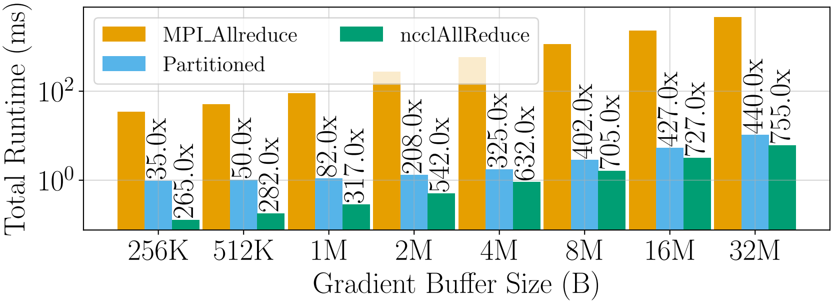

Figure: Eight-Node Deep Learning Kernel Performance

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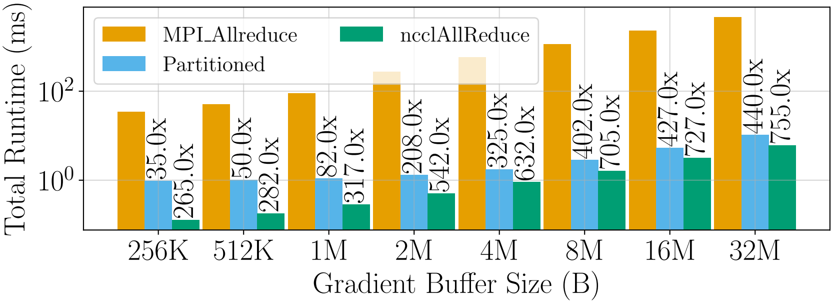

Figure: Eight-Node Deep Learning Kernel Performance

Conclusion

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- Useful optimizations for GPU-Initiated MPI Partition are identified

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  - Partition aggregation at the block-level provides the best performance
  - Intra-node copies can be optimized using a kernel copy
- Application results suggests that this could benefit HPC applications that use smaller kernels
  - Reduces the performance delta between MPI and vendor libaries in AI workloads

Acknowledgements

Questions

Thank You