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\* NCCL and MPI

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\* \* \*

# NCCL and MPI¶

## ## API¶

The NCCL API and usage is similar to MPI but there are many minor differences.

The following list summarizes these differences:

### ### Using multiple devices per process¶

Similarly to the concept of MPI endpoints, NCCL does not require ranks to be mapped 1:1 to processes. A NCCL communicator may have many ranks (and, thus, multiple devices) associated to a single process. Hence, if used with MPI, a single MPI rank (a NCCL process) may have multiple devices associated with it.

### ### ReduceScatter operation¶

The `ncclReduceScatter` operation is similar to the `MPI_Reduce_scatter_block` operation, not the `MPI_Reduce_scatter` operation. The `MPI_Reduce_scatter` function is intrinsically a “vector” function, while `MPI_Reduce_scatter_block` (defined later to fill the missing semantics) provides regular counts similarly to the mirror function `MPI_Allgather`. This is an oddity of MPI which has not been fixed for legitimate retro-compatibility reasons and that NCCL does not follow.

### ### Send and Receive counts¶

In many collective operations, MPI allows for different send and receive counts and types, as long as `sendcount*sizeof(sendtype) == rcvcount*sizeof(rcvtype)`. NCCL does not allow that, defining a single count

and a single data-type.

For AllGather and ReduceScatter operations, the count is equal to the per-rank size, which is the smallest size; the other count being equal to  $n_{\text{ranks}} \times \text{count}$ .

The function prototype clearly shows which count is provided. `ncclAllGather` has a `sendcount` as argument, while `ncclReduceScatter` has a `recvcount` as argument.

Note: When performing or comparing AllReduce operations using a combination of ReduceScatter and AllGather, define the `sendcount` and `recvcount` as the total count divided by the number of ranks, with the correct count rounding-up, if it is not a perfect multiple of the number of ranks.

### ### Other collectives and point-to-point operations¶

NCCL does not define specific verbs for `sendrecv`, `gather`, `gatherv`, `scatter`, `scatterv`, `alltoall`, `alltoallv`, `alltoallw`, nor neighbor collectives. All those operations can be simply expressed using a combination of `ncclSend`, `ncclRecv`, and `ncclGroupStart/ncclGroupEnd`, similarly to how they can be expressed with `MPI_Isend`, `MPI_Irecv` and `MPI_Waitall`.

`ncclRecv` does not support the equivalent of `MPI_ANY_SOURCE`; a specific source rank must always be provided. Similarly, the provided receive count must match the send count. Further, there is no concept of message tags.

### ### In-place operations¶

For more information, see [In-place Operations](usage/inplace.html#in-place-operations).

## ## Using NCCL within an MPI Program¶

NCCL can be easily used in conjunction with MPI. NCCL collectives are similar to MPI collectives, therefore, creating a NCCL communicator out of an MPI communicator is straightforward. It is therefore easy to use MPI for CPU-to-CPU communication and NCCL for GPU-to-GPU communication.

However, some implementation details in MPI can lead to issues when using NCCL inside an MPI program.

## ### MPI Progress¶

MPI defines a notion of progress which means that MPI operations need the program to call MPI functions (potentially multiple times) to make progress and eventually complete.

In some implementations, progress on one rank may need MPI to be called on another rank. While this is usually bad for performance, it can be argued that this is a valid MPI implementation.

As a result, blocking on a NCCL collective operation, for example calling `cudaStreamSynchronize`, may create a deadlock in some cases because not calling MPI on one rank could block other ranks, preventing them from reaching the NCCL call that would unblock the NCCL collective on the first rank.



In that case, the `cudaStreamSynchronize` call should be replaced by a loop like the following:

```
cudaError_t err = cudaErrorNotReady;

int flag;

while (err == cudaErrorNotReady) {
    err = cudaStreamQuery(args->streams[i]);

    MPI_Iprobe(MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &flag,
MPI_STATUS_IGNORE);
}
```

### ### Inter-GPU Communication with CUDA-aware MPI¶

Using NCCL to perform inter-GPU communication concurrently with CUDA-aware MPI may create deadlocks.

NCCL creates inter-device dependencies, meaning that after it has been launched, a NCCL kernel will wait (and potentially block the CUDA device) until all ranks in the communicator launch their NCCL kernel. CUDA-aware MPI may also create such dependencies between devices depending on the MPI implementation.

Using both MPI and NCCL to perform transfers between the same sets of CUDA

devices concurrently is therefore not guaranteed to be safe.

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\* \* \*

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