



MPI in Small Bites

PPCES 2025

HPC.NRW Competence Network



THE COMPETENCE NETWORK FOR HIGH PERFORMANCE COMPUTING IN NRW.

Blocking Collective Communication

HPC.NRW Competence Network

MPI in Small Bites

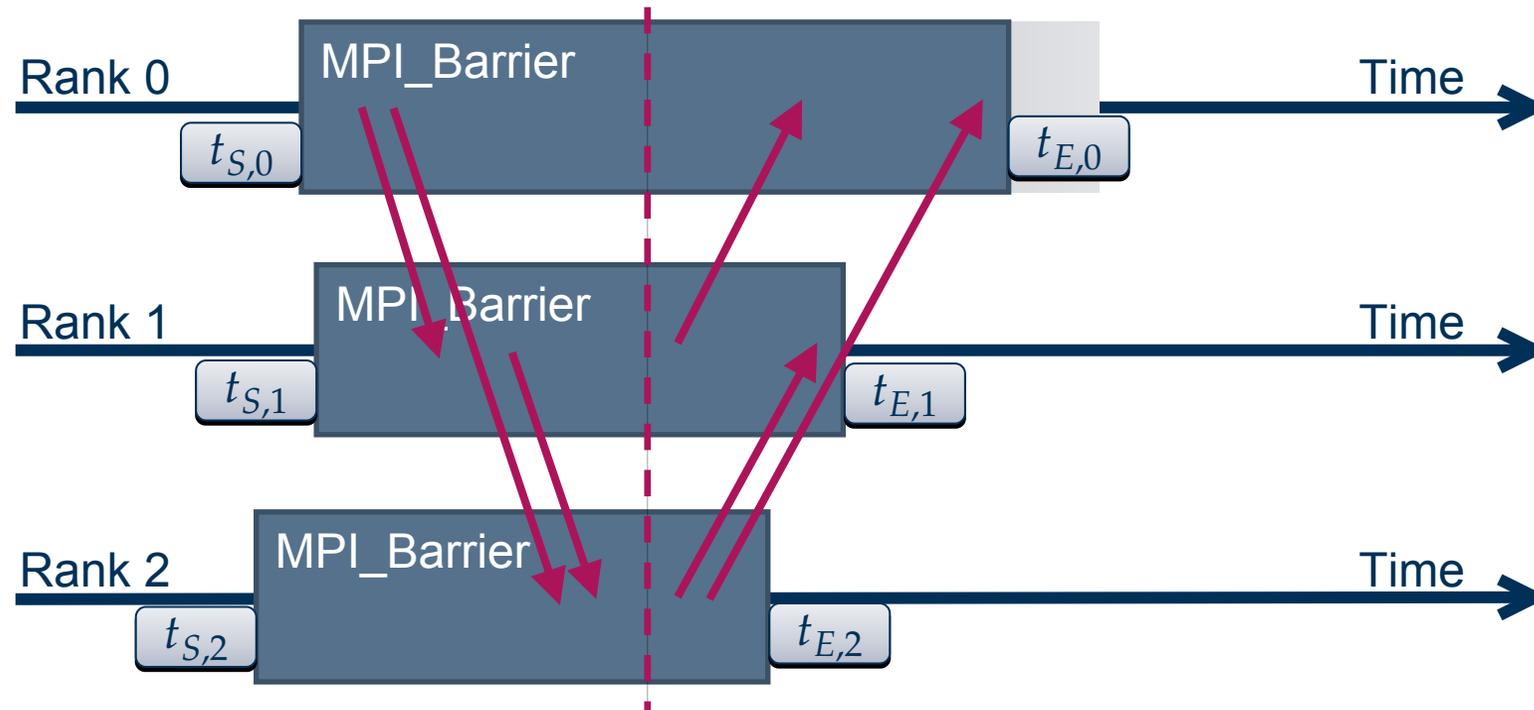
- Involve all ranks in a given communicator
 - Create a smaller communicator for collective communication in a subgroup
- All ranks must call the same MPI operation to succeed
 - There should be only one call per MPI rank (i.e., not per thread)
- Process synchronization behaviour is implementation specific
 - The MPI standard may allow for early return on some ranks
- Implement common group-communication patterns
 - Usually tuned to deliver the best system performance
 - **Do not reinvent the wheel!**



Barrier Synchronisation

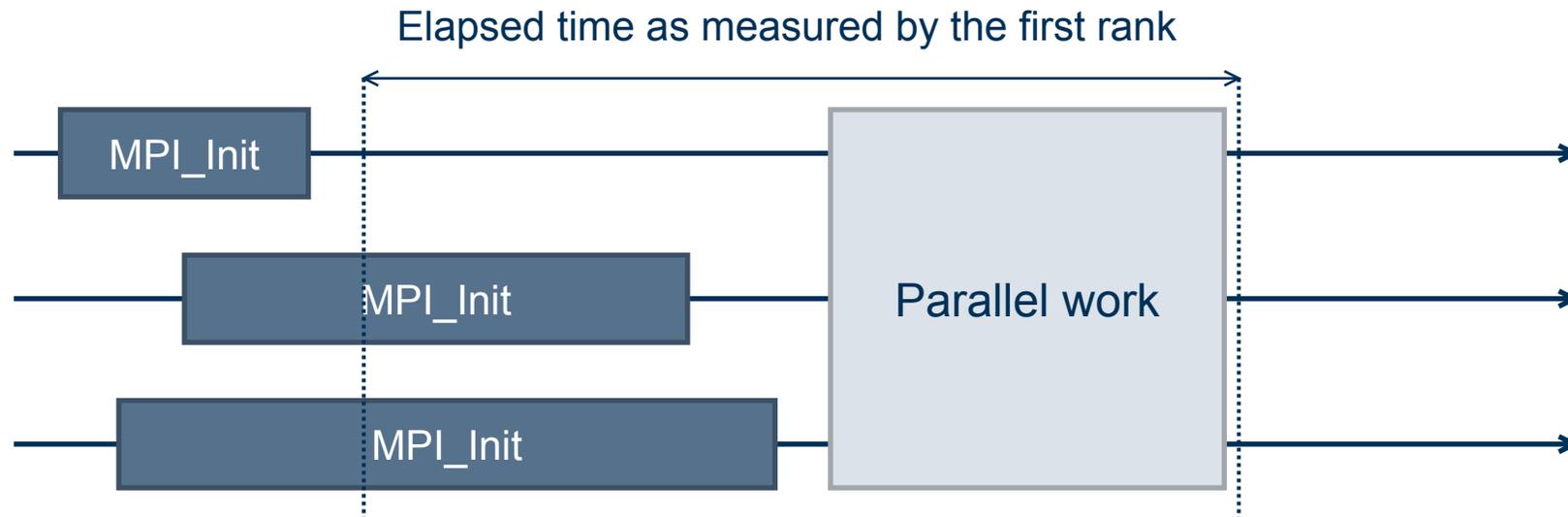
- The only explicit synchronisation operation in MPI:

`MPI_Barrier (MPI_Comm comm)`



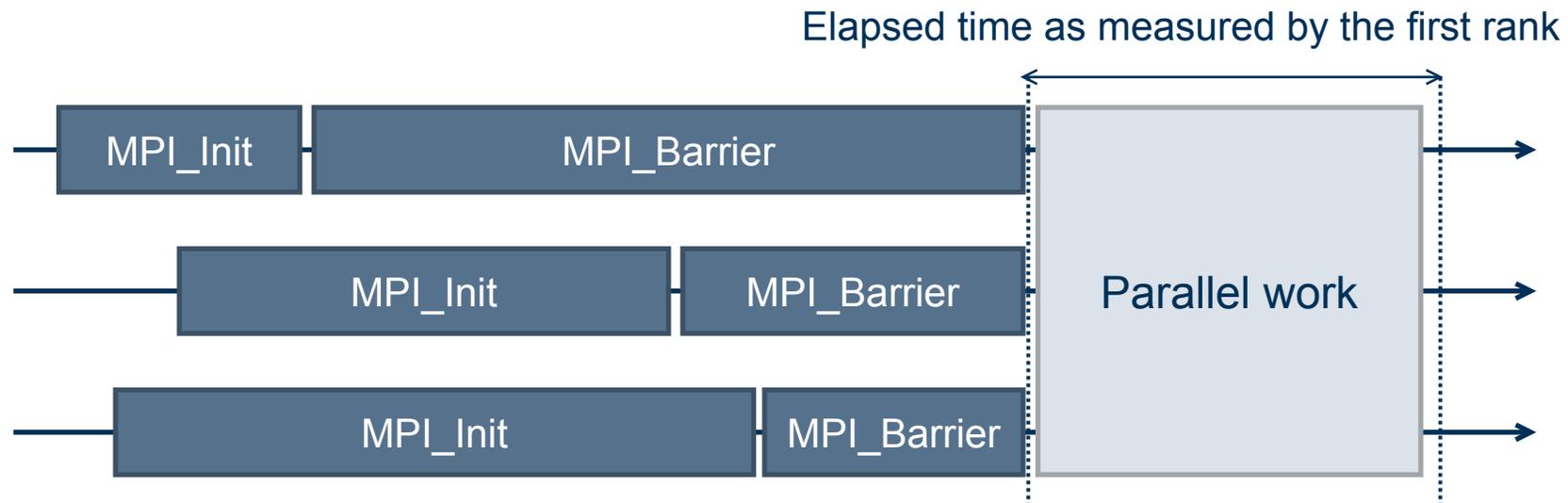
$$\max(t_{S,0}, t_{S,1}, t_{S,2}) < \min(t_{E,0}, t_{E,1}, t_{E,2})$$

- Useful for benchmarking
 - Always synchronise before taking time measurements



- Huge discrepancy between the actual work time and the measurement

- Useful for benchmarking
 - Always synchronise before taking time measurements



- Huge discrepancy between the actual work time and the measurement

Broadcast (one-to-many data replication)

- Replicate data from one rank to all other ranks:

```
MPI_Bcast (void *data, int count, MPI_Datatype datatype,  
          int root, MPI_Comm comm)
```

What?

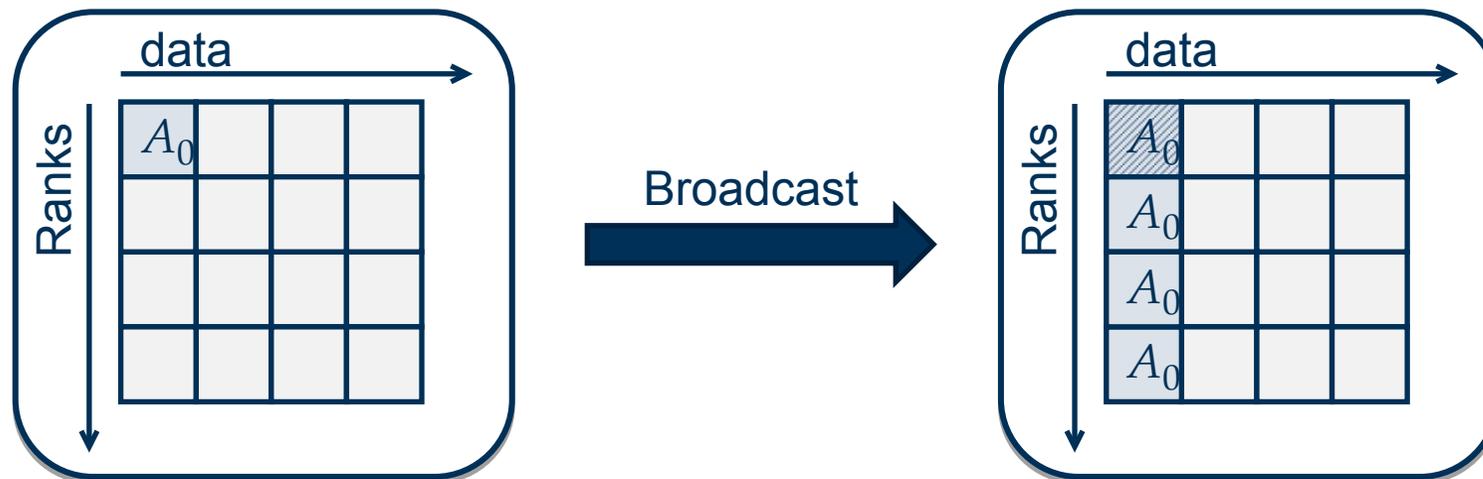
From whom?

- **data:** send buffer at **root** rank; receive buffer on all other ranks
 - **count:** number of data elements
 - **datatype:** elements' datatype
 - **root:** source rank; all ranks must specify the same value
 - **comm:** communicator
-
- On all ranks but **root**, **data** is an output argument
 - On rank **root**, **data** is an input argument
 - Type signatures must match across all ranks ( Datatypes)

Broadcast (one-to-many data replication)

- Replicate data from one rank to all other ranks:

```
MPI_Bcast (void *data, int count, MPI_Datatype dtype,  
          int root, MPI_Comm comm)
```



Broadcast (one-to-many data replication) – Wrong usage

- Replicate data from one rank to all other ranks:

```
MPI_Bcast (void *data, int count, MPI_Datatype dtype,  
          int root, MPI_Comm comm)
```

- Example:

```
int ival;  
  
if (rank == 0)  
    ival = read_int_from_user();  
  
MPI_Bcast(&ival, 1, MPI_INT, 0, MPI_COMM_WORLD);  
  
// WRONG USAGE!  
if (rank == 0) {  
    ival = read_int_from_user();  
    MPI_Bcast(&ival, 1, MPI_INT, 0, MPI_COMM_WORLD);  
}  
// The other ranks do not call MPI_Bcast ☹ Deadlock
```

Broadcast (one-to-many data replication) – Naïve Implementation

```
void broadcast (void *data, int count, MPI_Type dtype,
               int root, MPI_Comm comm)
{
    int rank, nprocs, i;

    MPI_Comm_rank(comm, &rank);
    MPI_Comm_size(comm, &nprocs);
    if (rank == root) {
        for (i = 0; i < nprocs; i++)
            if (i != root)
                MPI_Send(data, count, dtype, i, TAG_BCAST, comm);
    }
    else
        MPI_Recv(data, count, dtype, root, TAG_BCAST, comm,
                MPI_STATUS_IGNORE);
}
```

Scatter (one-to-many data distribution)

- Distribute **chunks** of data from one rank to all ranks:

```
MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
            void *recvbuf, int recvcount, MPI_Datatype recvtype,  
            int root, MPI_Comm comm)
```

Significant at root
rank only



Scatter (one-to-many data distribution)

- Distribute **chunks** of data from one rank to all ranks:

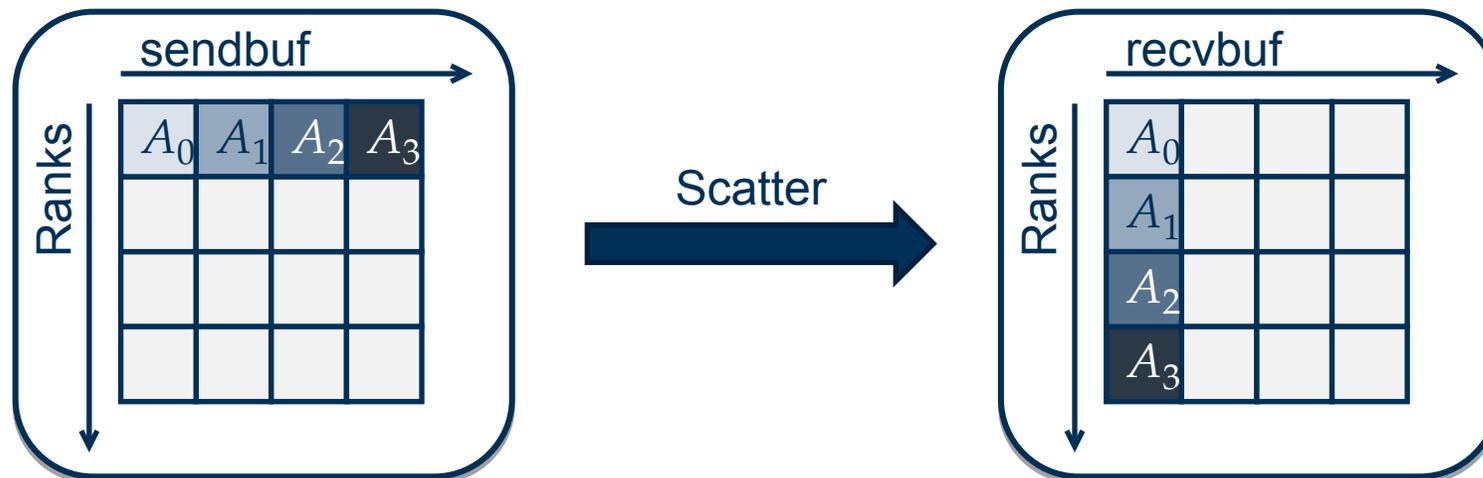
```
MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
            void *recvbuf, int recvcount, MPI_Datatype recvtype,  
            int root, MPI_Comm comm)
```

- **sendbuf** must be large enough in order to supply **sendcount** elements of data to **each** rank in the communicator
- Data chunks are taken in **increasing rank order** following
- **root** also sends one data chunk to itself
- **Type signatures** of must match across all ranks (☾ Datatypes)

Scatter (one-to-many data distribution)

- Distribute chunks of data from one rank to all ranks:

```
MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
            void *recvbuf, int recvcount, MPI_Datatype recvtype,  
            int root, MPI_Comm comm)
```



Scatter (one-to-many data distribution) – Example

- Distribute chunks of data from one rank to all ranks:

```
MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
            void *recvbuf, int recvcount, MPI_Datatype recvtype,  
            int root, MPI_Comm comm)
```

- **sendbuf** is only accessed on the root rank
- **recvbuf** is written into in all ranks

- Example:

```
int bigdata[100];           // 10x10 elements  
int localdata[10];  
  
MPI_Scatter(bigdata, 10, MPI_INT,           // send buffer, root only  
            localdata, 10, MPI_INT,       // receive buffer  
            0, MPI_COMM_WORLD);
```

Gather (many-to-one data distribution)

- Collect chunks of data from all ranks in one place:

```
MPI_Gather (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
           void *recvbuf, int recvcount, MPI_Datatype recvtype,  
           int root, MPI_Comm comm)
```

- The inverse operation to MPI_Scatter
- **recvbuf** must be large enough to hold **recvcount** elements from each rank
- **root** also receives one data chunk from itself
- Data chunks are stored in **increasing order** of the sender's rank
- Type signature of **sendcount** and **sendtype** must match **recvcount** and **recvtype**

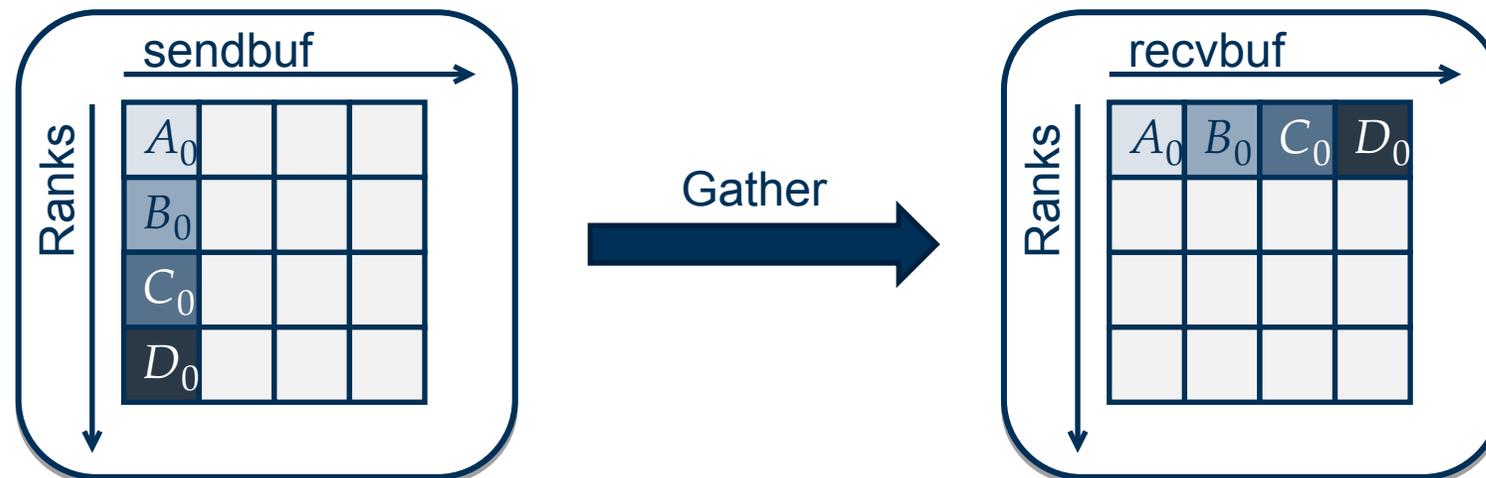
Significant at root rank only



Gather (many-to-one data distribution)

- Collect chunks of data from all ranks in one place:

```
MPI_Gather (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
           void *recvbuf, int recvcount, MPI_Datatype recvtype,  
           int root, MPI_Comm comm)
```



Allgather (many-to-many data distribution)

- Collect chunks of data from all ranks in all ranks:

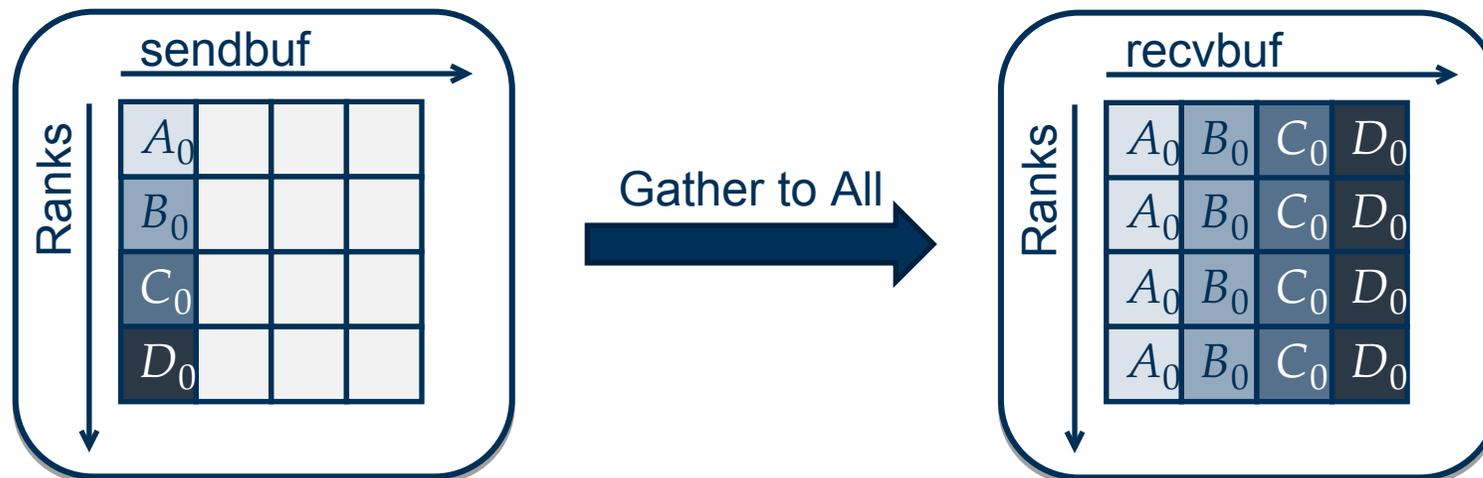
```
MPI_Allgather (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
              void *recvbuf, int recvcount, MPI_Datatype recvtpe,  
              MPI_Comm comm)
```

- No **root** rank – all ranks receive a copy of the gathered data
- Each rank also receives one data chunk from itself
- Data chunks are stored in **increasing order** of sender's rank
- **Type signatures of must match across all ranks** (☾ Datatypes)
- Logically equivalent to **MPI_Gather + MPI_Bcast**, but potentially more efficient

Allgather (many-to-many data distribution)

- Collect chunks of data from all ranks in all ranks:

```
MPI_Allgather (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
              void *recvbuf, int recvcount, MPI_Datatype recvtype,  
              MPI_Comm comm)
```



- Combined scatter and gather operation:

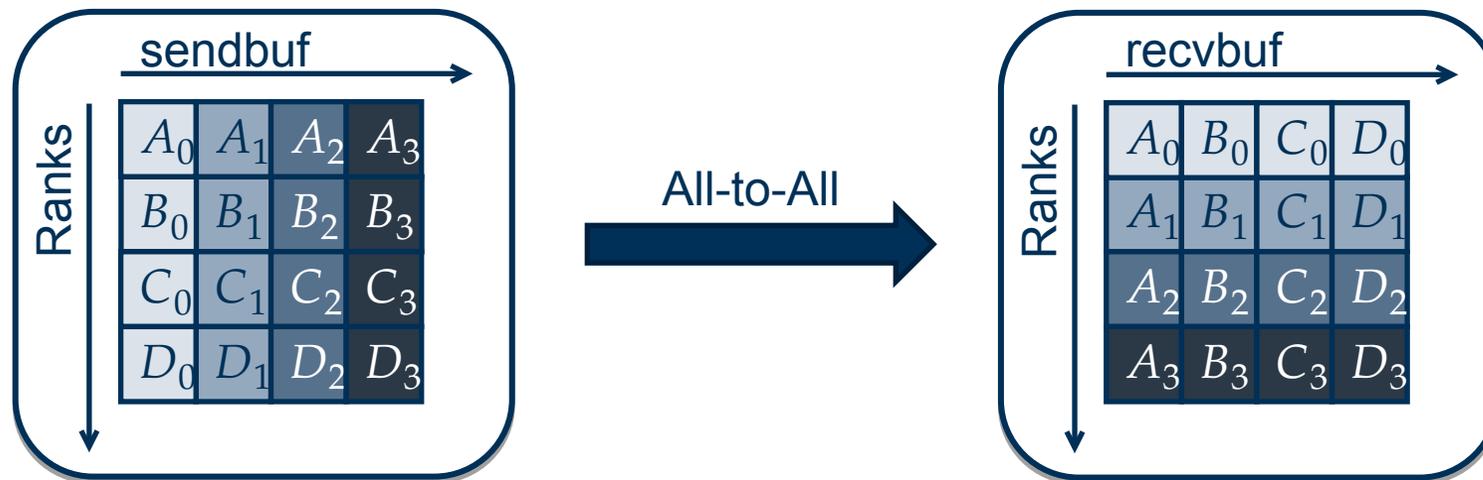
```
MPI_Alltoall (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
             void *recvbuf, int recvcount, MPI_Datatype recvtype,  
             MPI_Comm comm)
```

- Each rank distributes its **sendbuf** to every rank in the communicator (including itself)
- Data chunks are **read** in increasing order of the receiver's rank
- Data chunks are **stored** in increasing order of the sender's rank
- Almost equivalent to multiple **MPI_Scatter + MPI_Gather**

All-to-All (many-to-many data distribution)

- Combined scatter and gather operation:

```
MPI_Alltoall (void *sendbuf, int sendcount, MPI_Datatype sendtype,  
             void *recvbuf, int recvcount, MPI_Datatype recvtype,  
             MPI_Comm comm)
```



- Perform an arithmetic reduction operation while gathering data

```
MPI_Reduce (void *sendbuf, void *recvbuf, int count,  
            MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)
```

- **sendbuf:** data to be reduced
- **recvbuf:** location for the result(s) (significant at root only)
- **count/datatype:** type signature of data
- **op:** reduction operation handle
- **root:** destination rank
- **comm:** communicator
- Result is computed in- or out-of-order depending on the operation:
 - All predefined operations are *associative* and *commutative*
 - Beware of non-commutative effects on floats

- Some predefined operation handles:

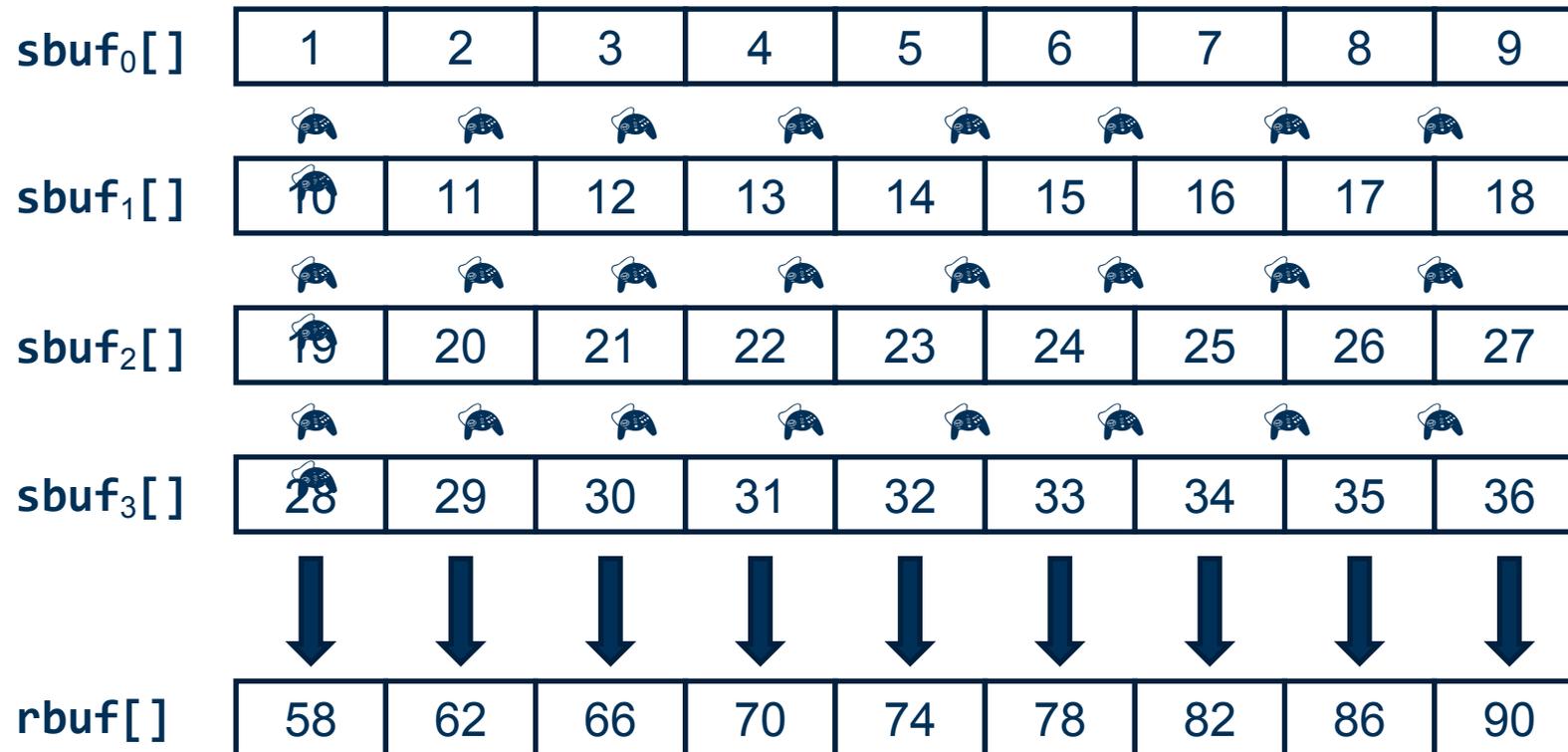
| MPI_Op | Result value |
|----------|----------------------------|
| MPI_MAX | Maximum value |
| MPI_MIN | Minimum value |
| MPI_SUM | Sum of all values |
| MPI_PROD | Product of all values |
| MPI_LAND | Logical AND of all values |
| MPI_BAND | Bit-wise AND of all values |
| MPI_LOR | Logical OR of all values |
| ... | ... |

- User-define operators possible (not covered here)

Reduce (many-to-one data reduction) – Example

– Element-wise and cross-rank operation

$$- \text{rbuf}[i] = \text{sbuf}_0[i] \text{ op } \text{sbuf}_1[i] \text{ op } \text{sbuf}_2[i] \text{ op } \dots \text{sbuf}_{\text{nranks}-1}[i]$$



 = MPI_SUM

Allreduce (many-to-many data reduction)

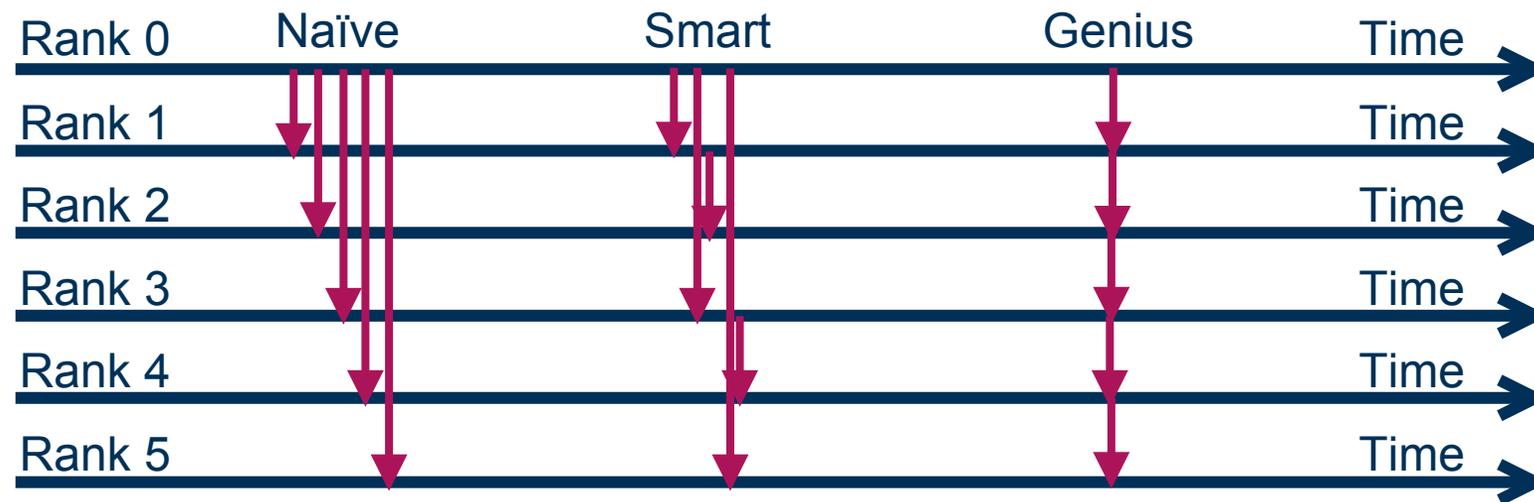
- Reduction result available on all ranks:

```
MPI_Allreduce (void *sendbuf, void *recvbuf, int count,  
              MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)
```

- Logically equivalent to **MPI_Reduce + MPI_Bcast** with the same root

Advantages of Collective Operations

- Collective operations implement common SPMD patterns portably
- Platform/Vendor-specific implementation, but standard behaviour
- Example: Broadcast
 - Naïve: root sends separate message to every other rank, $O(\#\text{ranks})$
 - Smart: tree-based hierarchical communication, $O(\log(\#\text{ranks}))$
 - Genius: pipelined segmented transport, $O(1)$



- All ranks in the communicator must call the MPI collective operation
 - Both, data sources and data receivers have to make the same call and supply the same value for the root rank where needed
 - Observe the significance of each argument
- The sequence of collective calls must be the same on all ranks
- MPI_Barrier is the only explicitly synchronising MPI collective
 - Some may synchronize implicitly (e.g., Allgather, Allreduce)
- Communication paradigms are independent of each other
 - Collective communication does not interfere with point-to-point communication on the same communicator