HPC.NRW

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MPI in Small Bites

PPCES 2025

HPC.NRW Competence Network

Blocking Collective Communication

HPC.NRW Competence Network

MPI in Small Bites

Collective Operations

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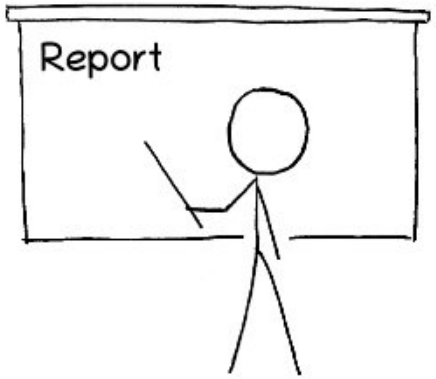
- Involve all ranks in a given communicator
  - Create a smaller communicator for collective communication in a subgroup
- All ranks must call the same MPI operation to succeed
  - There should be only one call per MPI rank (i.e., not per thread)
- Process synchronization behaviour is implementation 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

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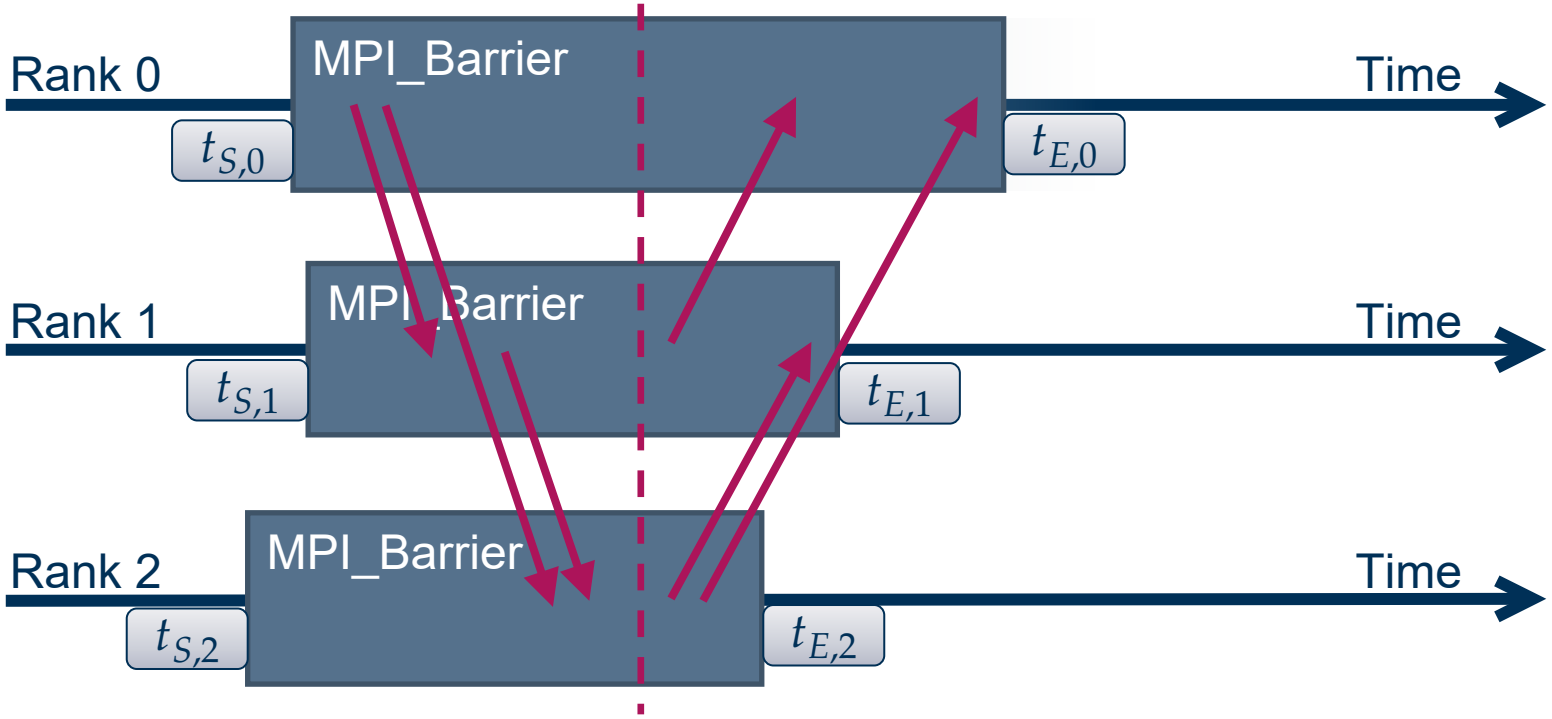
– The only explicit synchronisation operation in MPI:

```
MPI_Barrier (MPI_Comm comm)
```



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

Barrier Synchronisation

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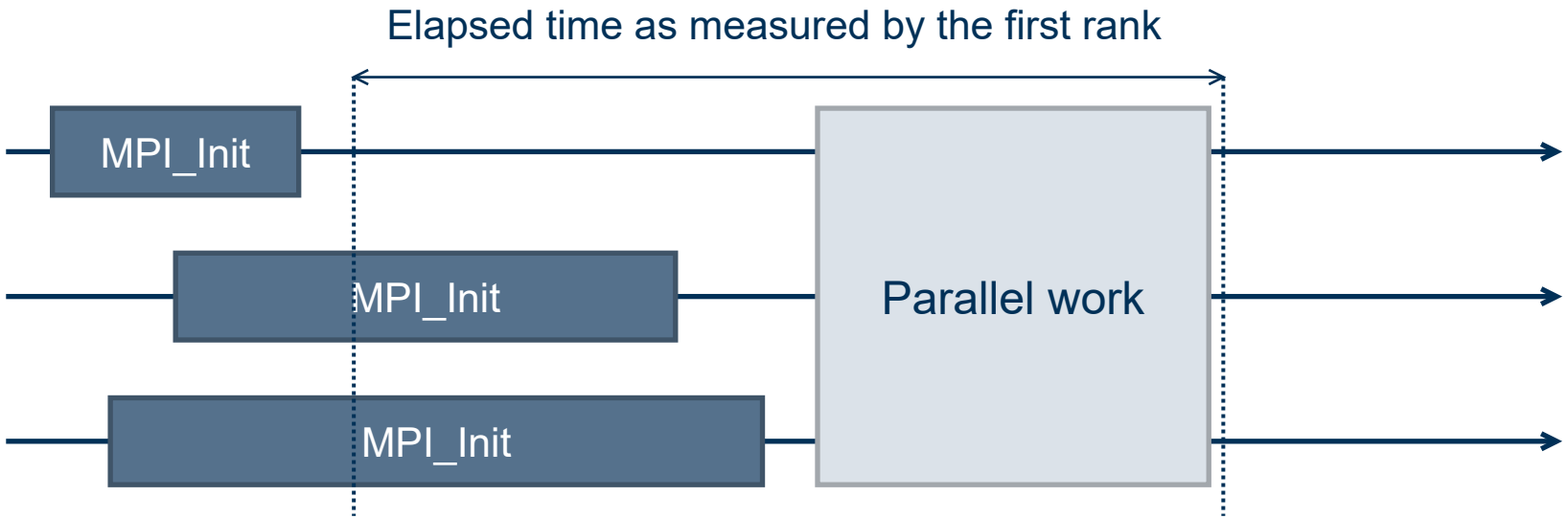
- Useful for benchmarking
  - Always synchronise before taking time measurements



  - Huge discrepancy between the actual work time and the measurement

Barrier Synchronisation

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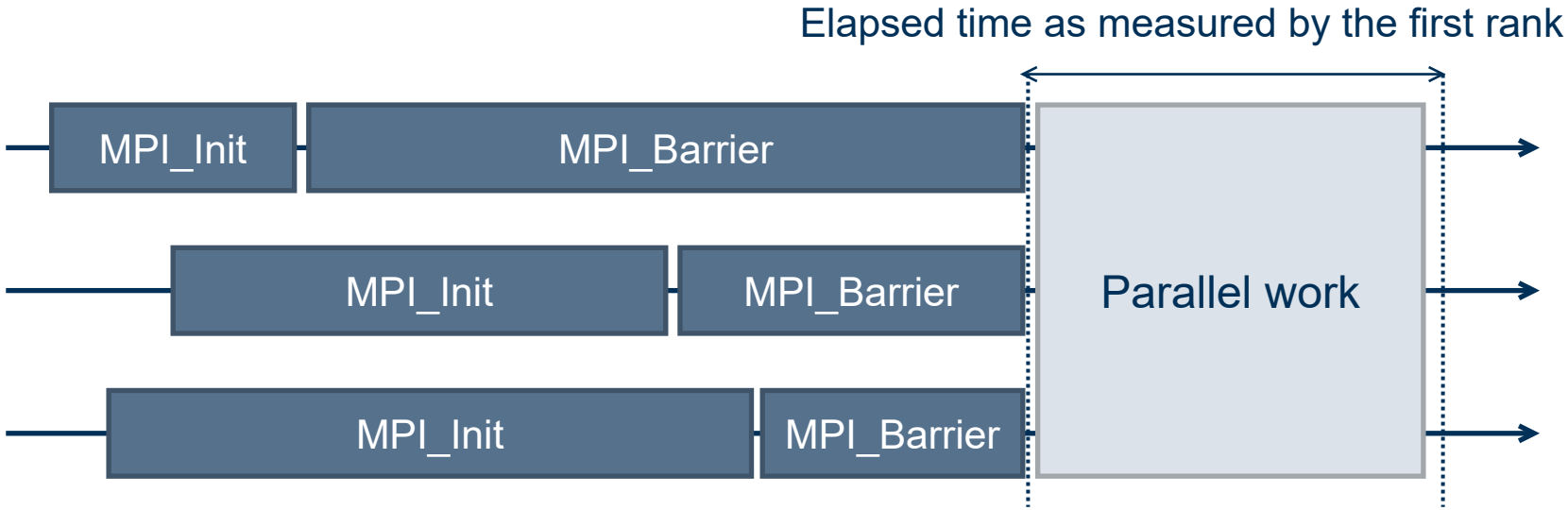

  - Huge discrepancy between the actual work time and the measurement

Broadcast (one-to-many data replication)

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– 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)

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– 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

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– 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

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```
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)

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– 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)

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– 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)

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

```
MPI_Scatter (void *sendbuf, int sendcount, MPI_Datatype sendtype,
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```

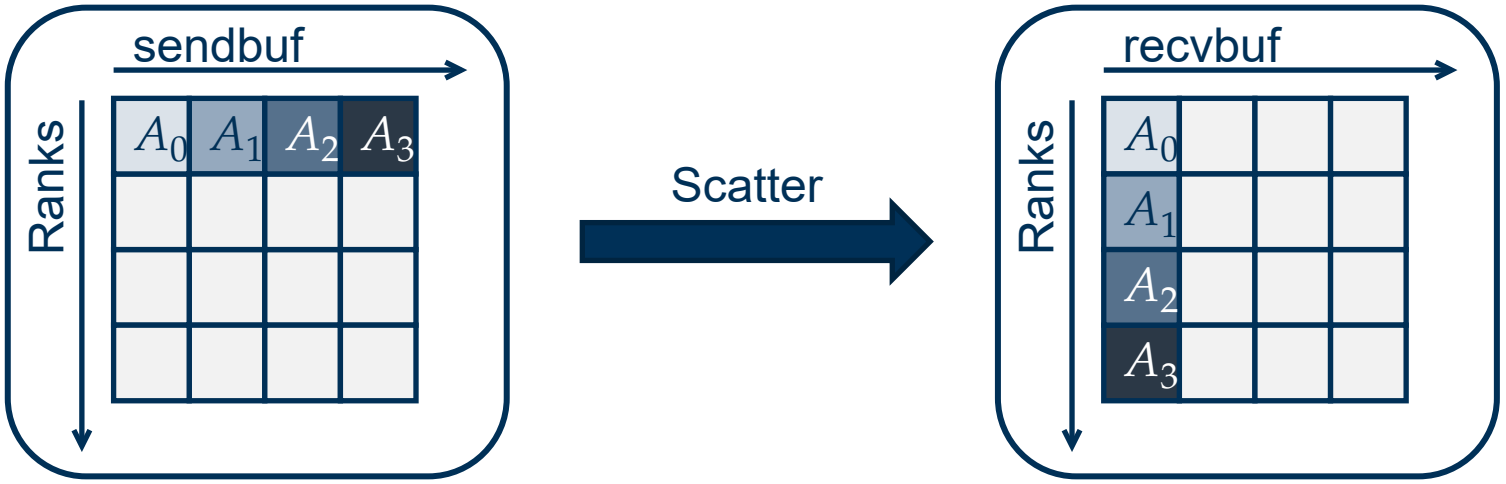

Scatter (one-to-many data distribution) – Example

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– 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)

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- 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)
```

Significant at root rank only

- 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`**

Gather (many-to-one data distribution)

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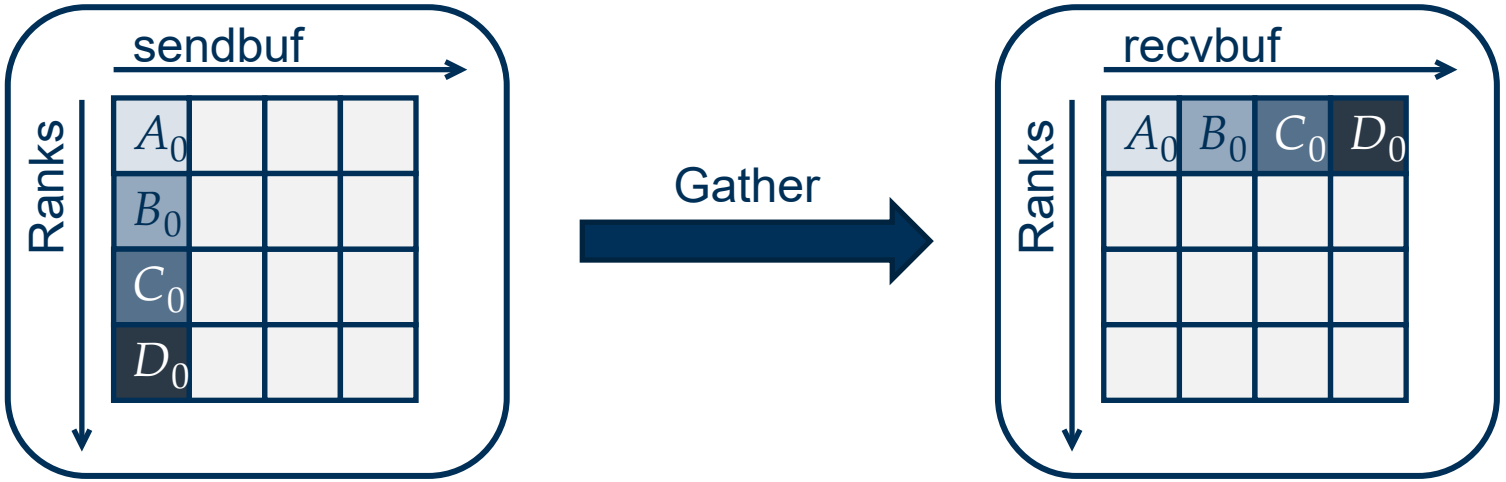
– Collect chunks of data from all ranks in one place:

```
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)

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– 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)
```

– 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)

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– 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)
```

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

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– 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)

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– Combined scatter and gather operation:

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

Reduce (many-to-one data reduction)

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- 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

Reduction Operators

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– 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

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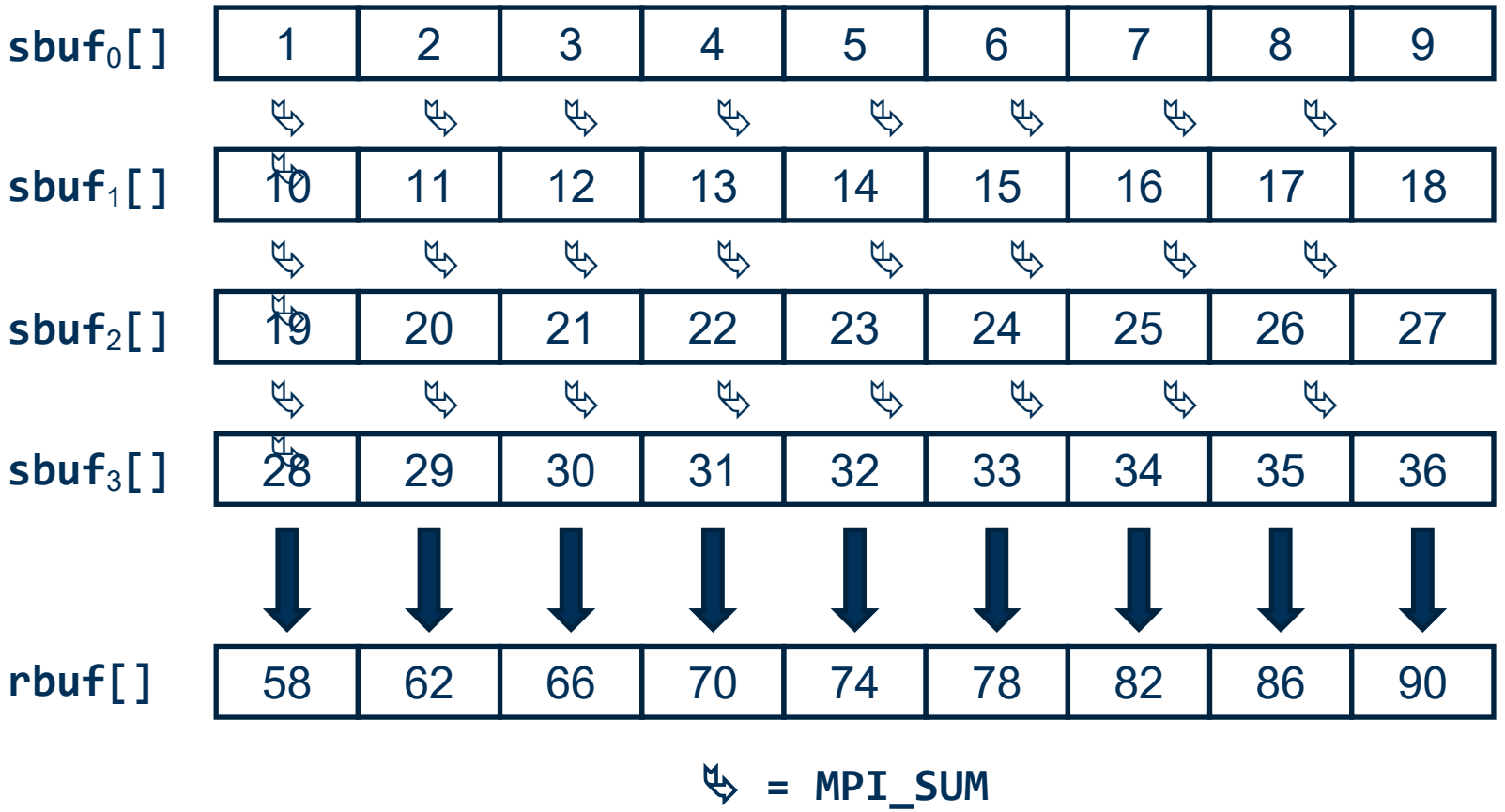
- Element-wise and cross-rank operation
  - **`rbuf[i] = sbuf`$_0$`[i] op sbuf`$_1$`[i] op sbuf`$_2$`[i] op … sbuf`$_{nranks-1}$`[i]`**



Allreduce (many-to-many data reduction)

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– 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

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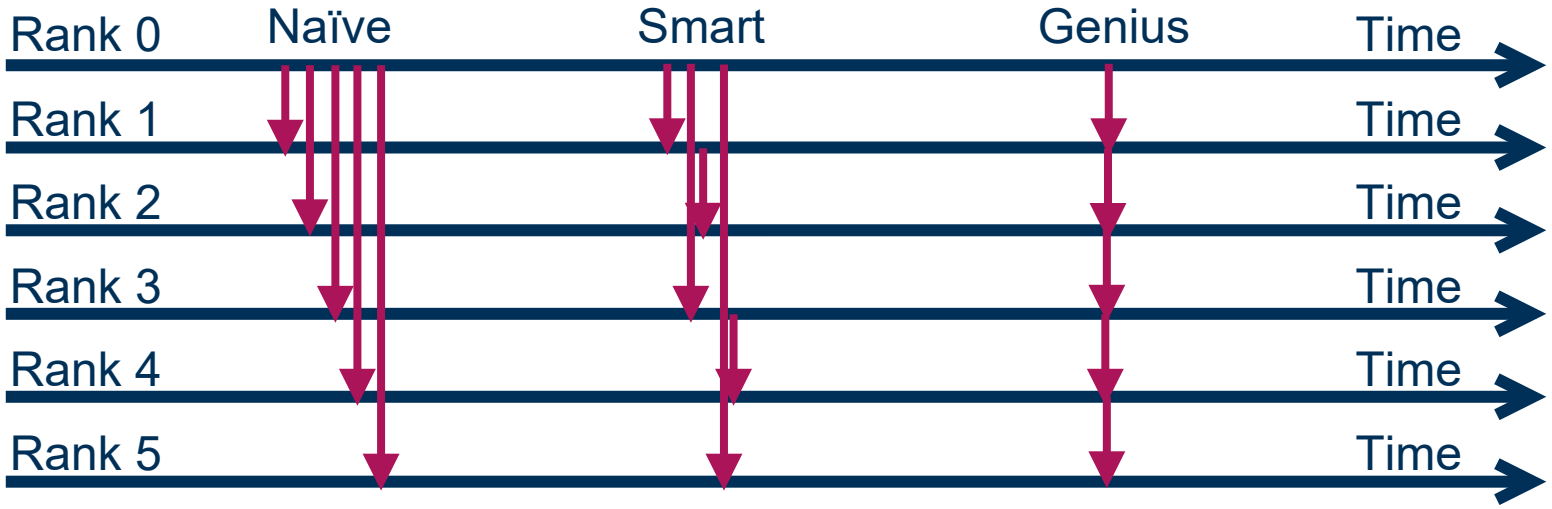
- Collective operations implement common SPMD patterns portably
- Platform/Vendor-specific implementation, but standard behaviour
- Example: Broadcast
  - Naïve: root sends separate message to every other rank, O(#ranks)
  - Smart: tree-based hierarchical communication, O(log(#ranks))
  - Genius: pipelined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



Summary: Collective Operations

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- 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