MPI in Small Bites

HPC.NRW Competence Network

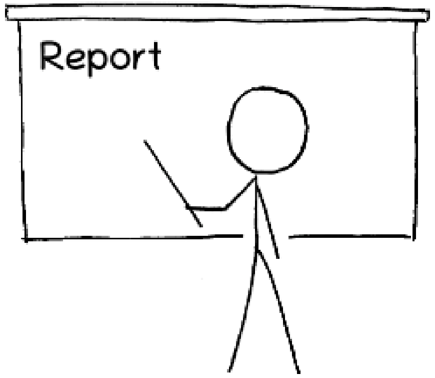
Blocking Collective Communication

HPC.NRW Competence Network

MPI in Small Bites

Collective Operations

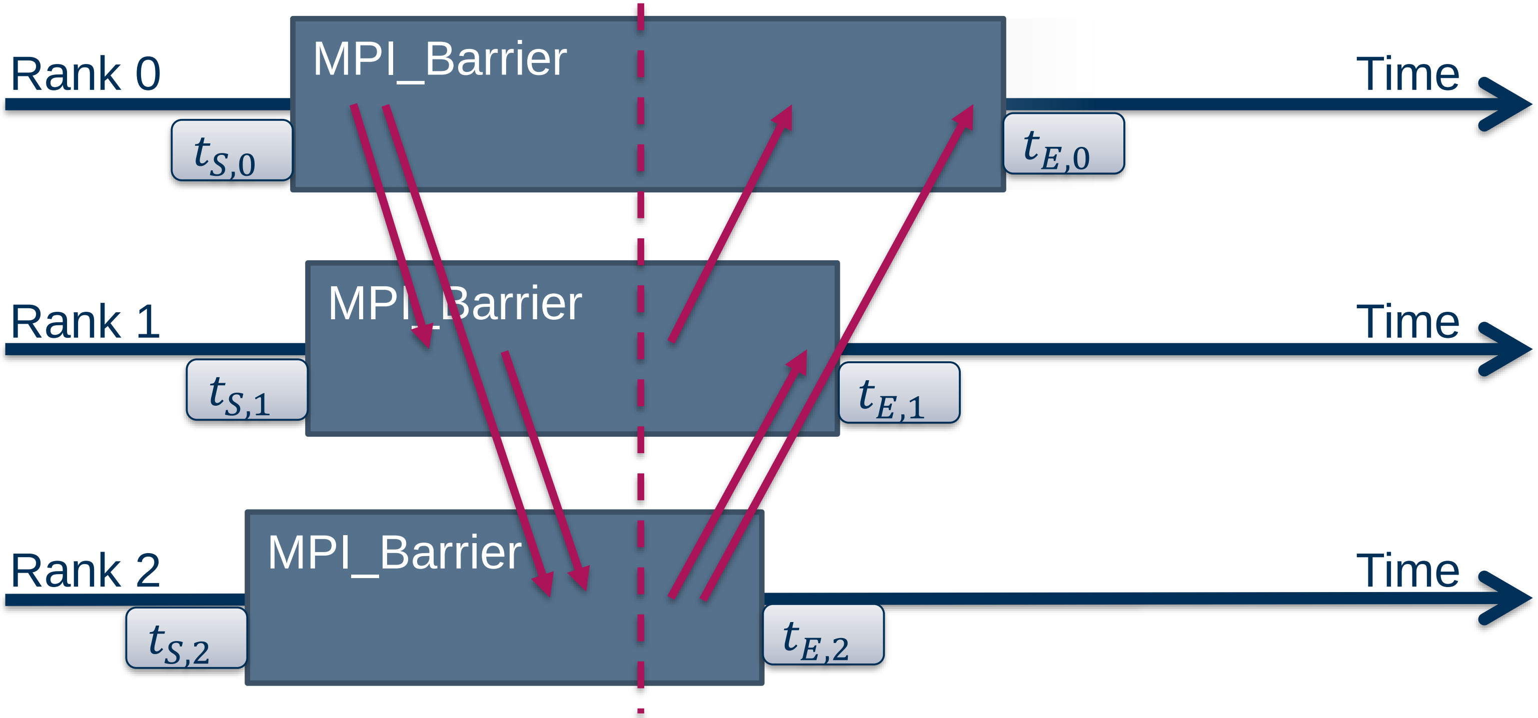
- Involve all ranks in a given communicator
  - Create a smaller communicator for collective communication in a subgroup
- All ranks must call the same MPI operation to succeed
  - There should be only one call per MPI rank (i.e., not per thread)
- Process synchronization behaviour is implementation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

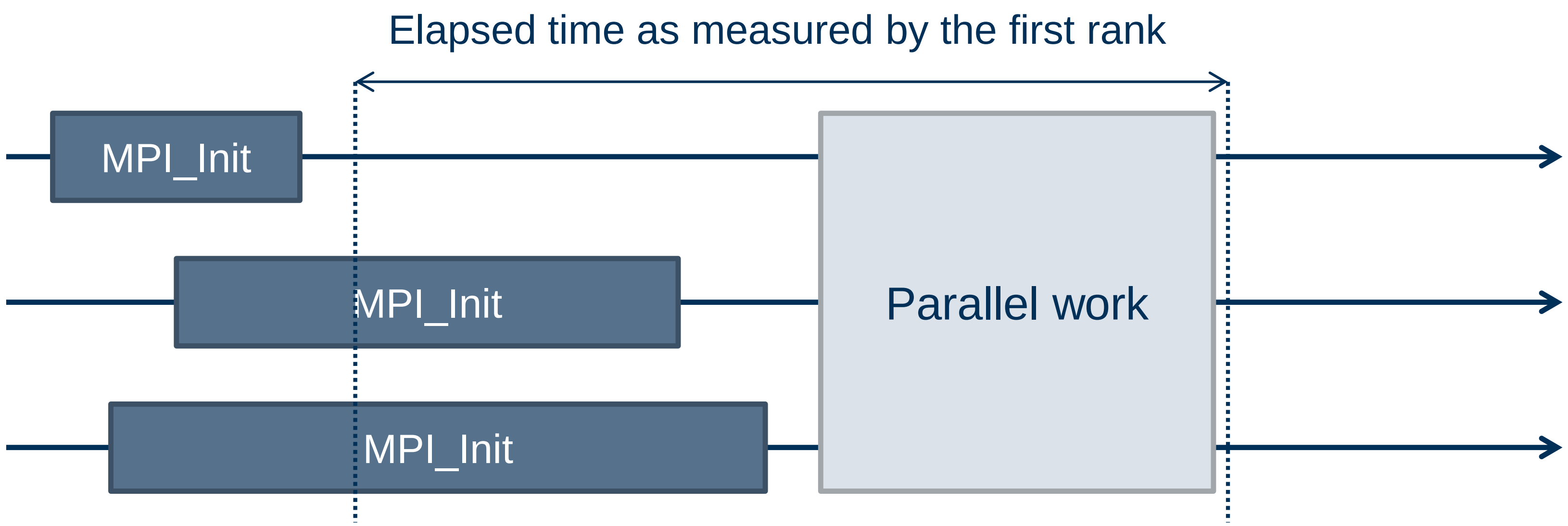
```
MPI_Barrier (MPI_Comm comm)
```



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

Barrier Synchronisation

- Useful for benchmarking
  - Always synchronise before taking time measurements



  - Huge discrepancy between the actual work time and the measurement

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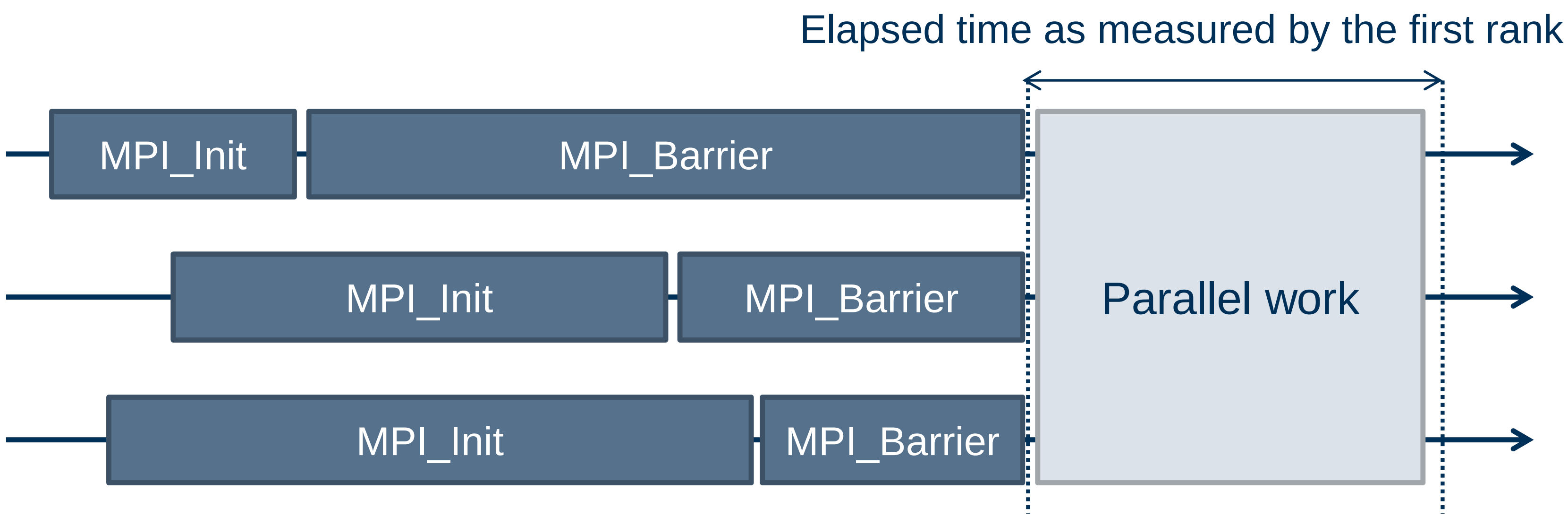

  - Huge discrepancy between the actual work time and the measurement

Broadcast (one-to-many data replication)

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– Replicate data from one rank to all other ranks:

What?

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

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:

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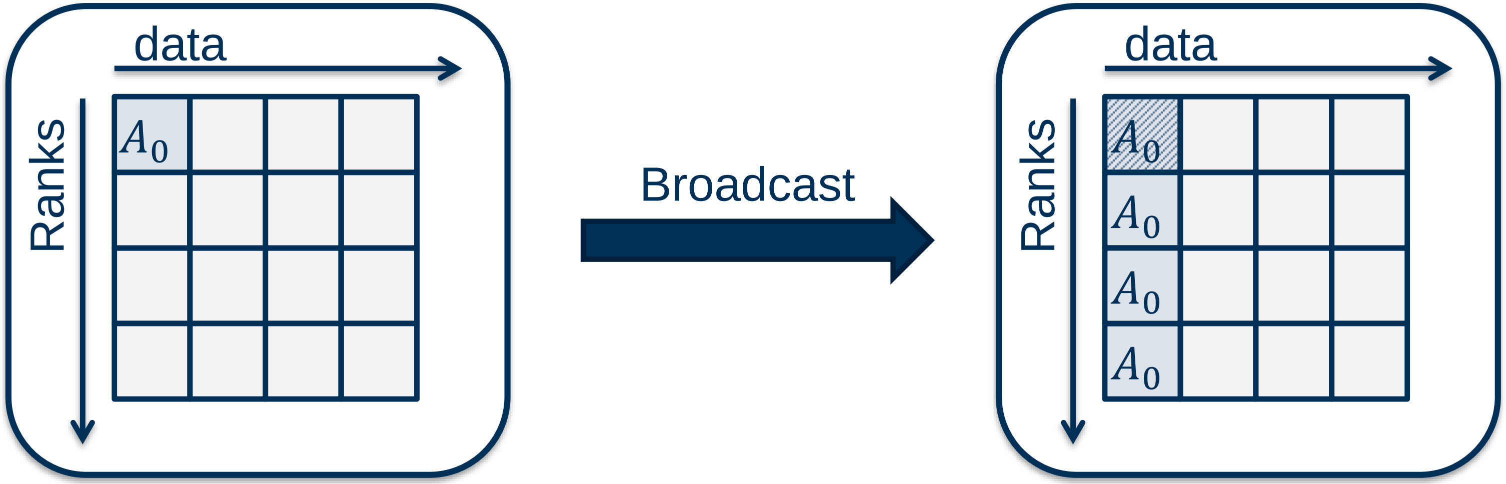
MPI_Bcast (void *data, int count, MPI_Datatype dtype,
           int root, MPI_Comm comm)
```



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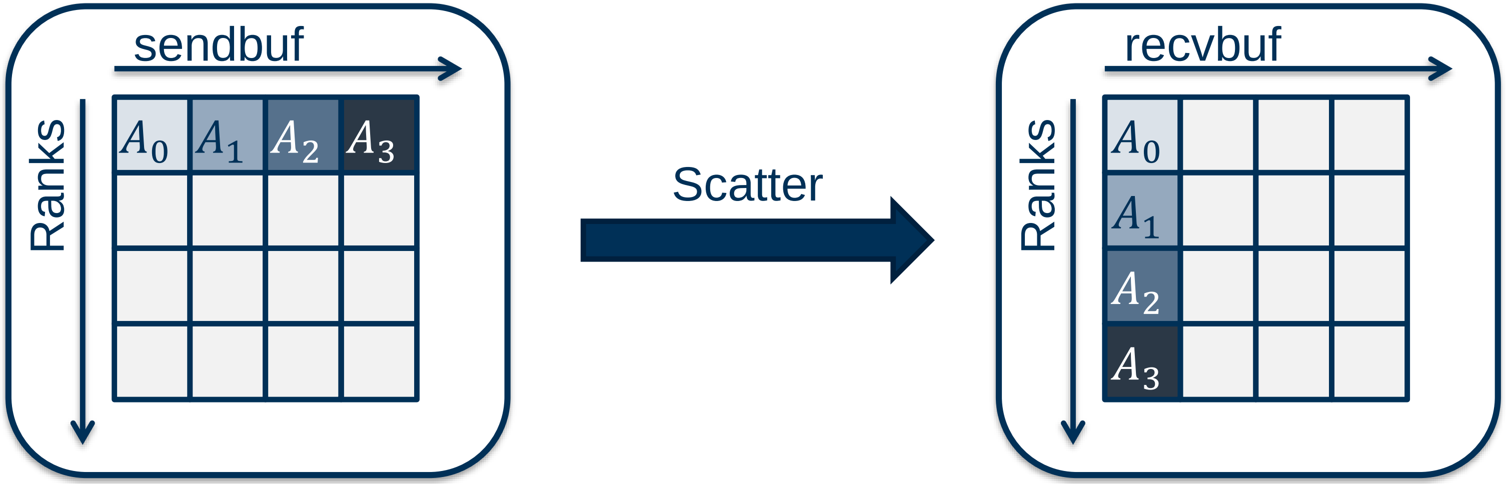
– Distribute chunks of data from one rank to all ranks:

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



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)
```

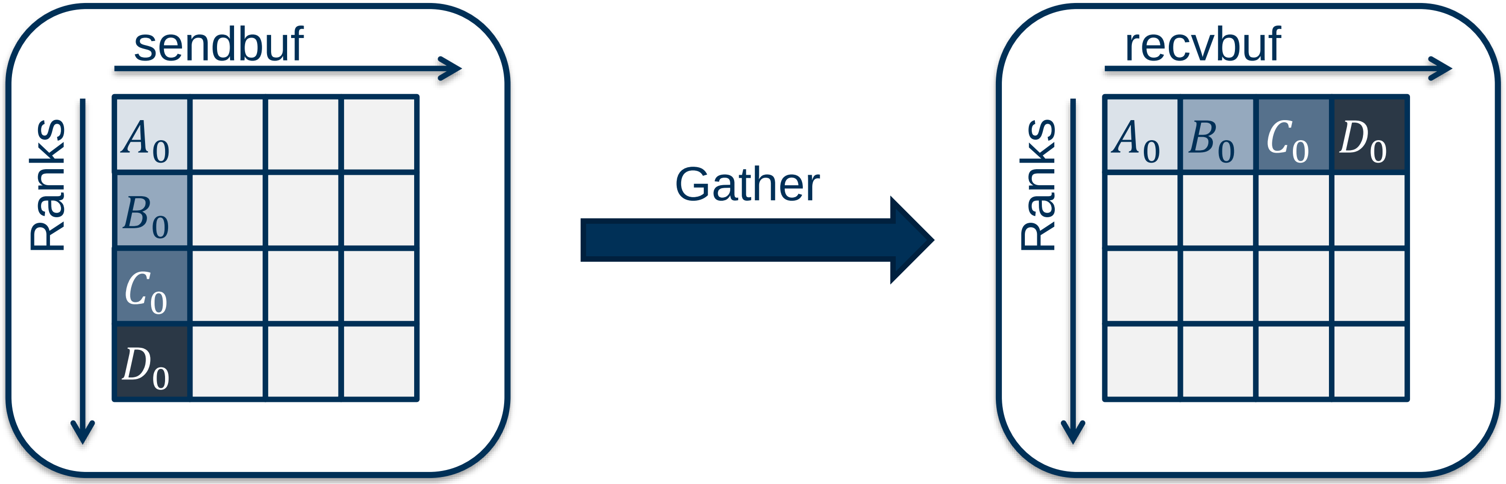
Significant at root rank only

– 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)

– 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)

- 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)
```

Reduce (many-to-one data reduction)

– 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]`

`sbuf`$_0$`[]`	1	2	3	4	5	6	7	8	9
	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗
`sbuf`$_1$`[]`	10	11	12	13	14	15	16	17	18
	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗
`sbuf`$_2$`[]`	19	20	21	22	23	24	25	26	27
	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗	⊗
`sbuf`$_3$`[]`	28	29	30	31	32	33	34	35	36
`rbuf[]`	58	62	66	70	74	78	82	86	90

⊗ = `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

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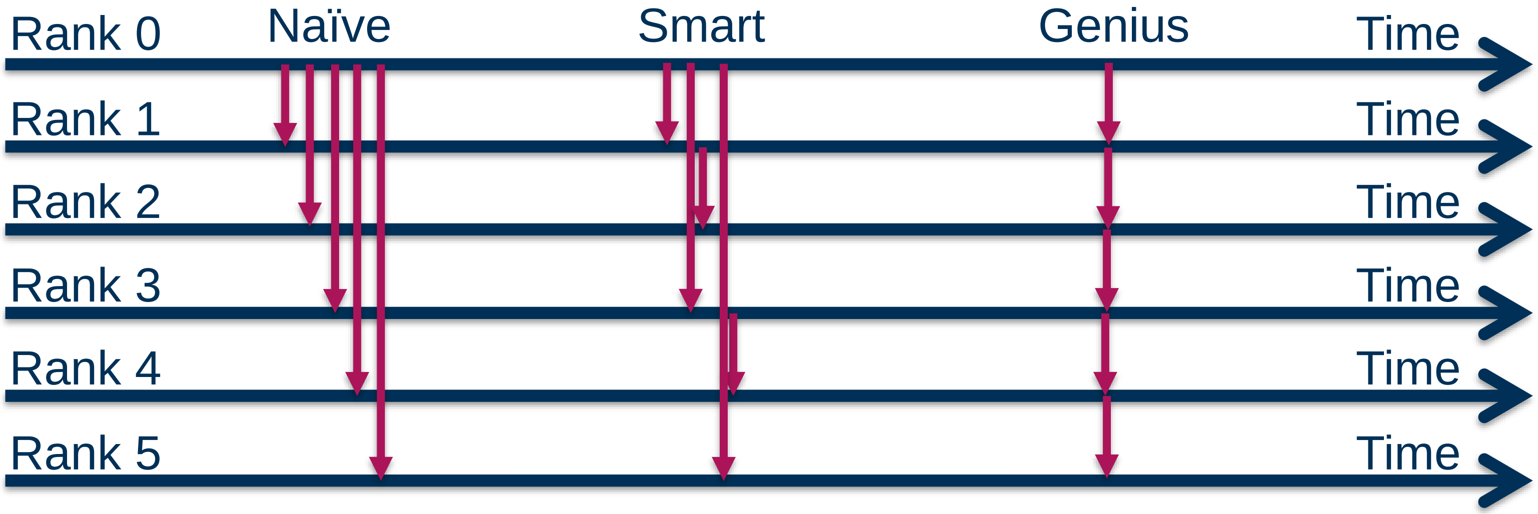
- Collective operations implement common SPMD patterns portably
- Platform/Vendor-specific implementation, but standard behaviour
- Example: Broadcast
  - Naïve: root sends separate message to every other rank, O(#ranks)
  - Smart: tree-based hierarchical communication, O(log(#ranks))
  - Genius: pipelined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