



# High Performance Linear Algebra

Lecture 9: Basic functions of MPI — Part 2

Ph.D. program in High Performance Scientific Computing

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# Last time on High Performance Linear Algebra

## 1 Last time on High Performance Linear Algebra

- During the last lecture we have introduced the basics of parallel programming using the **Message Passing Interface (MPI)** paradigm.
- We have discussed the main features of MPI and we have seen how to setup a simple MPI environment.
- We have also discussed the usage of SLURM to handle queues on HPC systems.

Today we will continue our discussion on MPI by introducing some of the most used MPI functions.



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## MPI Timers

2 Message Passing Interface (MPI)

- `MPI_Wtime()` returns a double-precision wall-clock time in seconds
- `MPI_Wtick()` returns the resolution of `MPI_Wtime()`
- Suitable for measuring elapsed time of code regions (not CPU time)
- Call `MPI_Init` before and `MPI_Finalize` after using timers

### CPU time vs Wall-clock time

CPU time measures the time a CPU spends executing a program, while wall-clock time measures the real-world elapsed time from start to finish, including waiting times and delays. To **measure performance** in parallel computing, wall-clock time is often more relevant as it reflects the actual time users experience.



## Example: Timing a Loop

2 Message Passing Interface (MPI)

```
program timing_example
use mpi
implicit none
integer :: ierr, rank, nprocs, i
real(kind=8) :: t0, t1, elapsed

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)

call MPI_Barrier(MPI_COMM_WORLD, ierr) ! synchronize start
t0 = MPI_Wtime()
```



## Example: Timing a Loop

2 Message Passing Interface (MPI)

```
do i = 1, 10**7
    call random_seed() ! dummy work
end do

call MPI_Barrier(MPI_COMM_WORLD, ierr) ! synchronize end
t1 = MPI_Wtime()

elapsed = t1 - t0
print '(A,I3,A,F8.4)', 'Rank ', rank, ' elapsed: ', elapsed

call MPI_Finalize(ierr)
end program timing_example
```



# Barriers and Timing Best Practices

## 2 Message Passing Interface (MPI)

- **Barriers** (`MPI_Barrier`) force all ranks to synchronize
- Use barriers to align start/end of timed regions; avoid overuse
- Prefer `MPI_Reduce` (e.g., `MPI_MAX`) to collect max elapsed time across ranks
- Run multiple iterations and average to smooth variability



## Example: Timing with Reduction

2 Message Passing Interface (MPI)

```
program timing_reduce
use mpi
implicit none
integer :: ierr, rank, root
real(kind=8) :: t0, t1, tlocal, tmax

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
root = 0
call MPI_Barrier(MPI_COMM_WORLD, ierr)
t0 = MPI_Wtime()
call MPI_Bcast(tlocal, 1, MPI_DOUBLE_PRECISION, root, MPI_COMM_WORLD,
   ↴ ierr)
```



## Example: Timing with Reduction

2 Message Passing Interface (MPI)

```
call MPI_Barrier(MPI_COMM_WORLD, ierr)
t1 = MPI_Wtime()

tlocal = t1 - t0
call MPI_Reduce(tlocal, tmax, 1, MPI_DOUBLE_PRECISION, MPI_MAX, root,
                MPI_COMM_WORLD, ierr)

if (rank == root) then
    print *, 'Max elapsed across ranks: ', tmax
end if

call MPI_Finalize(ierr)
end program timing_reduce
```



# The Cost of Communication

## 2 Message Passing Interface (MPI)

- Communication overhead increases with the number of processes
- Two main components: **latency** and **bandwidth**
  - **Latency:** time to initiate a message (startup cost)
  - **Bandwidth:** data transfer rate once communication starts
- Total communication time:  $T_{\text{comm}} = \alpha + \frac{N}{\beta}$ 
  - $\alpha$ : latency (message startup cost)
  - $\beta$ : reciprocal of the bandwidth
  - $N$ : message size in bytes

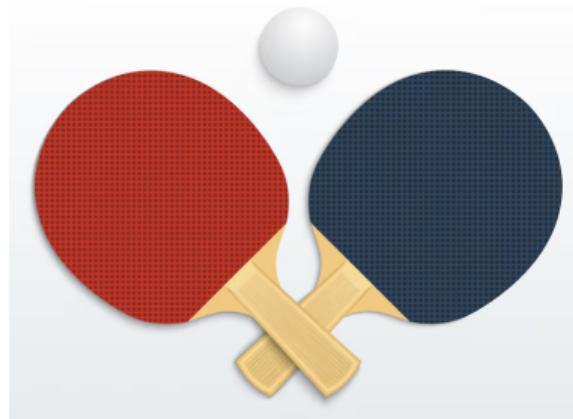


## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

The first measure we can do is to evaluate the scaling of point-to-point communication costs with respect to the number of MPI ranks.

- 💡 An idea is to implement a simple benchmark that implements a **ping-pong test** between two MPI ranks, where rank 0 sends a message to rank  $n - 1$ , which immediately sends it back.



- ⌚ The time taken for this round-trip communication is measured and reported.



# Scaling Communication Costs: Point-to-Point Example

## 2 Message Passing Interface (MPI)

```
program test_mpi_pingpong
use mpi
implicit none
integer :: ierr, rank, nprocs
integer :: n, i, niter
real(kind=8), allocatable :: sendbuf(:), recvbuf(:)
real(kind=8) :: t_start, t_end, t_local, t_avg, t_max
call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
! -----
! Fixed problem size (strong scaling)
! -----
```



# Scaling Communication Costs: Point-to-Point Example

## 2 Message Passing Interface (MPI)

```
n = 1000000      ! number of double-precision elements
niter = 100      ! number of repetitions
allocate(sendbuf(n), recvbuf(n))
sendbuf = 1.0d0
recvbuf = 0.0d0
```

We perform a warm-up phase to avoid measuring initial overheads,

```
! Warm-up (not timed)
if (rank == 0) then
  call MPI_Send(sendbuf, n, MPI_DOUBLE_PRECISION, nprocs-1, 0,
    MPI_COMM_WORLD, ierr)
  call MPI_Recv(recvbuf, n, MPI_DOUBLE_PRECISION, nprocs-1, 0,
    MPI_COMM_WORLD, MPI_STATUS_IGNORE, ierr)
else if (rank == nprocs-1) then
```



# Scaling Communication Costs: Point-to-Point Example

## 2 Message Passing Interface (MPI)

```
call MPI_Recv(recvbuf, n, MPI_DOUBLE_PRECISION, 0, 0, MPI_COMM_WORLD,
  ↴ MPI_STATUS_IGNORE, ierr)
call MPI_Send(sendbuf, n, MPI_DOUBLE_PRECISION, 0, 0, MPI_COMM_WORLD,
  ↴ ierr)
end if
call MPI_Barrier(MPI_COMM_WORLD, ierr)
```

then we perform the ping-pong test for a number of iterations, measuring the time taken for each round-trip communication.



# Scaling Communication Costs: Point-to-Point Example

## 2 Message Passing Interface (MPI)

```
t_local = 0.0d0
do i = 1, niter
  call MPI_BARRIER(MPI_COMM_WORLD, ierr)
  t_start = MPI_Wtime()
  if (rank == 0) then
    call MPI_Send(sendbuf, n, MPI_DOUBLE_PRECISION, nprocs-1, 0,
                 MPI_COMM_WORLD, ierr)
    call MPI_Recv(recvbuf, n, MPI_DOUBLE_PRECISION, nprocs-1, 0,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE, ierr)
  else if (rank == nprocs-1) then
    call MPI_Recv(recvbuf, n, MPI_DOUBLE_PRECISION, 0, 0,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE, ierr)
    call MPI_Send(sendbuf, n, MPI_DOUBLE_PRECISION, 0, 0,
                 MPI_COMM_WORLD, ierr)
```



## Scaling Communication Costs: Point-to-Point Example

2 Message Passing Interface (MPI)

```
end if
t_end = MPI_Wtime()
t_local = t_local + (t_end - t_start)
end do
t_avg = t_local / niter
```

Finally, we compute the average time and bandwidth, reporting the results from rank 0.

```
! Take the maximum time across all ranks
call MPI_Reduce(t_avg, t_max, 1, MPI_DOUBLE_PRECISION, MPI_MAX, 0,
                MPI_COMM_WORLD, ierr)
if (rank == 0) then
    print *, "MPI Ping-Pong strong scaling test"
    print *, "Message size (MB): ", n * 8.0d0 / 1.0d6
    print *, "MPI ranks : ", nprocs
```



# Scaling Communication Costs: Point-to-Point Example

## 2 Message Passing Interface (MPI)

```
print *, "Avg Ping-Pong time (s): ", t_max
print *, "Avg Bandwidth (GB/s): ", (n * 8.0d0 * 2.0d0) / (t_max *
    ↪ 1.0d9)
print *, "Avg Bandwidth (GBit/s): ", (n * 8.0d0 * 8.0d0 * 2.0d0) /
    ↪ (t_max * 1.0d9)
end if
deallocate(sendbuf, recvbuf)
call MPI_Finalize(ierr)
end program test_mpi_pingpong
```



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

We recall that the bandwidth is computed as the total data transferred (send + receive) divided by the time taken, i.e.,

$$\text{Bandwidth} \approx \frac{N \times 2}{T_{\text{comm}}}$$

where  $N$  is the message size in bytes and  $T_{\text{comm}}$  is the average time taken for the ping-pong communication.

We have an array of size  $n$  double-precision elements, so the message size in bytes is  $N = n \times 8$  bytes, and the total data transferred in the ping-pong test is  $N \times 2$  bytes and we multiply by 8 to convert to bits.



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

To run this benchmark on a HPC system with SLURM, we use the Amelia cluster at IAC-CNR.

This is a machine whose nodes are equipped with Intel Xeon Gold 6338 processors (32 cores per socket, 2 sockets per node), connected via an InfiniBand HDR200 network with a **theoretical peak bandwidth of 200 Gbit s<sup>-1</sup>**.

We write a SLURM script to run the benchmark with different numbers of MPI ranks,

```
#!/bin/bash
#SBATCH --job-name=pingpong_strong_64ppn
#SBATCH --nodes=7
#SBATCH --ntasks-per-node=64
#SBATCH --time=00:20:00
#SBATCH --partition=prod-gn
#SBATCH --mem=900Gb
#SBATCH --output=pingpong_%j.out
#SBATCH --error=pingpong_%j.err
```



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

We load the necessary modules and compile the Fortran code using mpifort,

```
module load intel/gcc-12.2.1/openmpi-4.1.6
```

And then use bash loops to run the benchmark with different numbers of MPI ranks,

```
for NODES in $(seq 1 7); do
    NTASKS=$((NODES * 64))
    echo "Running Ping-Pong with:"
    echo "  Nodes : $NODES"
    echo "  Tasks : $NTASKS (64 per node)"
    mpirun --bind-to core --map-by ppr:64:node --mca btl ^openib --mca pml
    ↳ ucx -x UCX_NET_DEVICES='mlx5_0:1' -np $NTASKS ./pingpong
done
```

The script can be submitted to the SLURM queue using the command:

```
sbatch runner-pingpong.sh.
```



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

We have passed several options to `mpirun` to optimize the communication performance:

- `--bind-to core`: binds each MPI process to a specific CPU core to reduce context switching and improve cache utilization.
- `--map-by ppr:64:node`: maps 64 MPI processes per node, ensuring an even distribution of processes across the available nodes.
- `--mca btl ^openib`: disables the OpenIB BTL (Byte Transfer Layer) to avoid potential issues with certain InfiniBand configurations.
- `--mca pml ucx`: selects the UCX (Unified Communication X) PML (Point-to-Point Messaging Layer) for improved performance on high-speed networks.
- `-x UCX_NET_DEVICES='mlx5_0:1'`: specifies the network devices to be used by UCX for communication, optimizing data transfer over the InfiniBand network.

?

The last three options are relevant only to the specific network configuration of the Amelia cluster, thus they might not be necessary on other systems.



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

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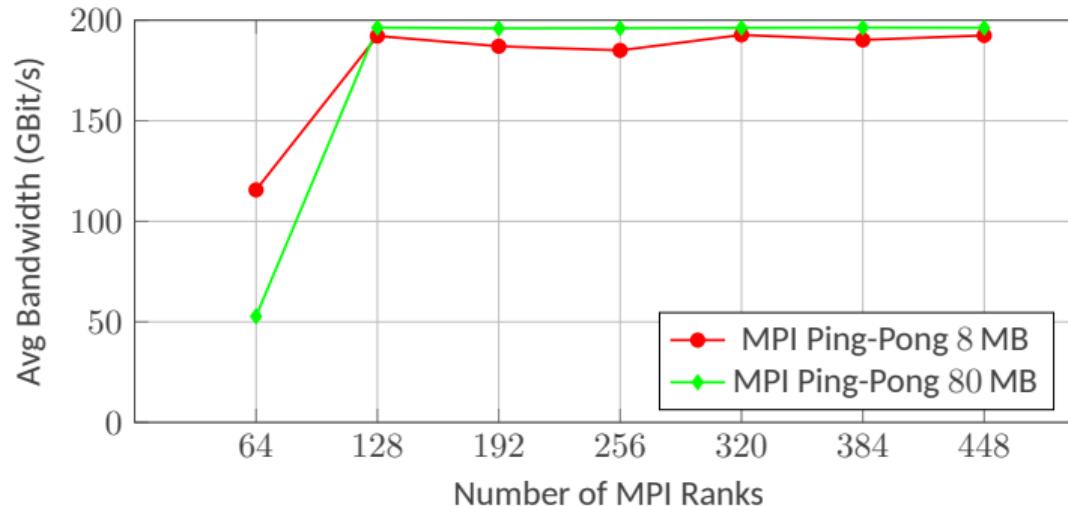
**⚠** The first two options are important for what we are doing, because they ensure that we really use the network as expected.



## Scaling Communication Costs: Point-to-Point Example

### 2 Message Passing Interface (MPI)

We increase the number of MPI ranks from 64 to 448 (7 nodes with 64 ranks each).



The average ping-pong bandwidth approaches the theoretical peak bandwidth of the InfiniBand HDR200 network ( $200 \text{ Gbit s}^{-1}$ ).



## Exercise

### 2 Message Passing Interface (MPI)

There are a number of possible exercises you can do to further explore the ping-pong benchmark

1. Vary the message size and perform linear regression to estimate the latency and bandwidth parameters ( $\alpha$  and  $\beta$ ) of the communication model.
2. Implement a similar benchmark using non-blocking communication (e.g., `MPI_Isend` and `MPI_Irecv`).
3. Benchmark what happens when you use MPI ranks on different nodes versus on the same node.
4. Explore the impact of different MPI implementations (e.g., OpenMPI vs MPICH vs Intel MPI) on communication performance.



# The problem of collective communications

## 2 Message Passing Interface (MPI)

Let's review the idea of the Broadcast operation. Algorithmically, we can implement it as:

```
if (my_rank == 0) then
    do i = 1, p-1
        call MPI_Send(a, 1, MPI_REAL, i, tag, MPI_COMM_WORLD, ierr)
    end do
else
    call MPI_Recv(a, 1, MPI_REAL, 0, tag, MPI_COMM_WORLD,
                  MPI_STATUS_IGNORE, ierr)
end if
```

- This is a **collective communication** since *all* processes participate in its implementation;
- Just from a software engineering perspective, it makes sense to encapsulate it in a function: the MPI\_Bcast.



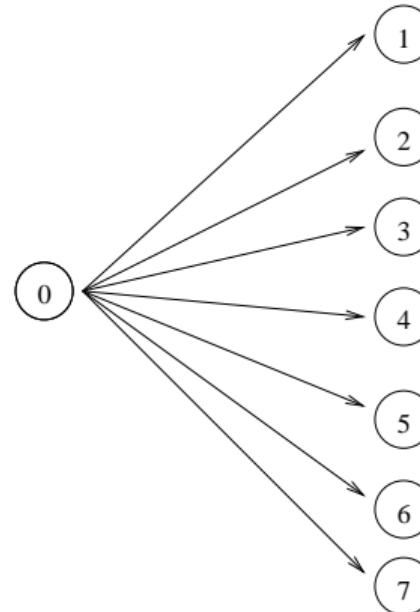
# How much does it cost?

2 Message Passing Interface (MPI)

- With fast networks, cost for 1 float is dominated by latency  $\alpha$ ;
- Cost of this algorithm is therefore

$$T(p) \approx \alpha \cdot (p - 1)$$

or, linear in  $p$ .





## Can we do any better?

### 2 Message Passing Interface (MPI)

Let's make some assumptions about the network:

- The cost of communication between any two network nodes is uniform, and is given by  $\alpha + N/\beta$ ;
- In particular, it is *possible* to send a message between *any* two nodes<sup>1</sup>
- The network is capable of sustaining multiple messages (*noisy topology*) at the same time, provided pairs of nodes involved in the messages do not overlap.

The latter assumption is especially important: we can improve communication if we can have multiple messages “flying” through the network at the same time.

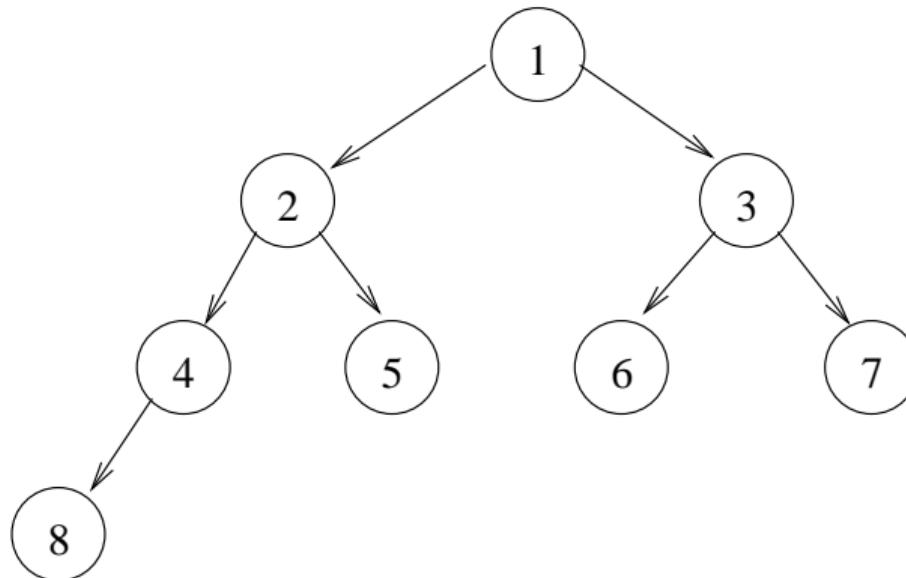
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<sup>1</sup>Historically there existed networks where only neighbouring nodes could exchange messages



## Tree broadcast — simple minded

2 Message Passing Interface (MPI)





## Tree broadcast — simple minded

2 Message Passing Interface (MPI)

Assume processes are numbered from 1:

- Each process  $i$  (except 1) receives from  $\lfloor (p - 1)/2 \rfloor$ ;
- Each process such that  $2i \leq p$  sends first to process  $2i$ , then to process  $2i + 1$ .

Cost:

$$T(p) \approx 2 \log(p),$$

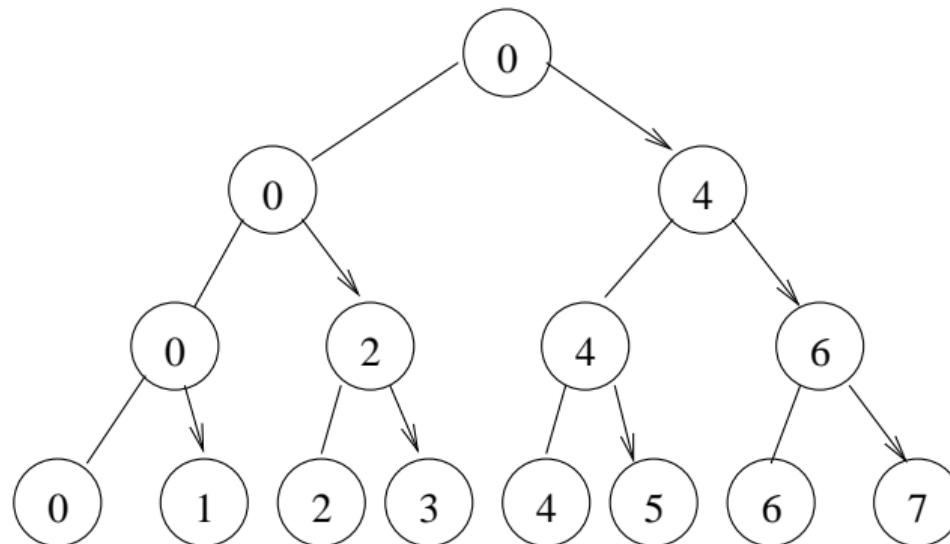
or logarithmic in  $p$ . To be precise, with  $p > 1$  then

$$T(p) = \begin{cases} 0 & \text{for } p = 1 \\ 2 \cdot (k - 1) + 1 & \text{for } p = 2^k, k > 0 \\ 2 \cdot \lfloor \log_2(p) \rfloor & \text{otherwise} \end{cases}$$



# Tree broadcast — Recursive Doubling

2 Message Passing Interface (MPI)





## Tree broadcast — Recursive Doubling

2 Message Passing Interface (MPI)

- Consider that there are  $p$  processes with root  $\text{o}$ ;
- Set  $K$  the minimum power of 2 such that  $K \geq p$ ;
- Process  $\text{o}$  sends to process  $K/2$ ;
- Divide the processes in two groups: from  $\text{o}$  to  $K/2 - 1$ , and from  $K/2$  to  $\min(p - 1, K - 1)$ ;
- Apply recursively to:
  - Processes  $\text{o}$  to  $K/2 - 1$  with root  $\text{o}$ ;
  - Processes  $K/2$  to  $\min(p - 1, K - 1)$  with root  $K/2$ .

Cost:

$$T(p) = \lceil \log(p) \rceil,$$

or logarithmic in  $p$ .



# Collective communications

## 2 Message Passing Interface (MPI)

Considerations for collective communications:

- Their functionality can be defined in terms of simple loops;
- There exist much better implementations;
- The **optimal implementation** for a given collective depends on:
  - The operation;
  - The network interface;
  - The network topology;
  - The amount of data.

A good MPI implementation will switch internally among different algorithms where appropriate (another advantage of encapsulating the collective)



## Collective communications

2 Message Passing Interface (MPI)

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☞ Let us try and take some measurements of the broadcast operation to see how its cost scales with the number of MPI ranks.



# Scaling Communication Costs: Broadcast Example

## 2 Message Passing Interface (MPI)

```
program test_mpi_bcast_latency
use mpi
implicit none

integer :: ierr, rank, nprocs
integer :: root
integer :: n, i, niter
real(kind=8), allocatable :: buffer(:)
real(kind=8) :: t_start, t_end, t_local, t_avg, t_max

call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
```



# Scaling Communication Costs: Broadcast Example

## 2 Message Passing Interface (MPI)

```
root = 0
! Small message size for latency measurement
n = 1           ! single element for pure latency
niter = 10000    ! more iterations for better statistics
allocate(buffer(n))
if (rank == root) then
    buffer = 1.0d0
else
    buffer = 0.0d0
end if
! Warm-up (not timed)
call MPI_Bcast(buffer, n, MPI_DOUBLE_PRECISION, root, MPI_COMM_WORLD,
   ierr)
```



# Scaling Communication Costs: Broadcast Example

## 2 Message Passing Interface (MPI)

```
call MPI_BARRIER(MPI_COMM_WORLD, ierr)
t_local = 0.0d0
call MPI_BARRIER(MPI_COMM_WORLD, ierr)
t_start = MPI_Wtime()
do i = 1, niter
    call MPI_Bcast(buffer, n, MPI_DOUBLE_PRECISION, root,
                   MPI_COMM_WORLD, ierr)
end do
t_end = MPI_Wtime()
    t_local = t_local + (t_end - t_start)
t_avg = (t_end - t_start) / niter
! Take the maximum latency across all ranks
call MPI_Reduce(t_avg, t_max, 1, MPI_DOUBLE_PRECISION, MPI_MAX, root,
                MPI_COMM_WORLD, ierr)
```



# Scaling Communication Costs: Broadcast Example

## 2 Message Passing Interface (MPI)

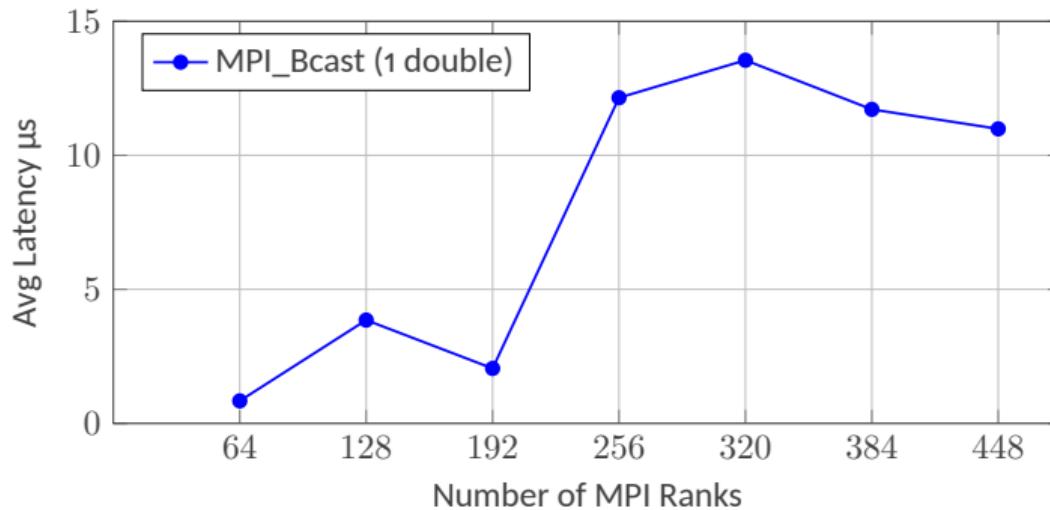
```
if (rank == root) then
    print *, "MPI_Bcast latency test"
    print *, "MPI ranks           : ", nprocs
    print *, "Avg Bcast latency (us): ", t_max * 1.0d6
end if
deallocate(buffer)
call MPI_Finalize(ierr)
end program test_mpi_bcast_latency
```



## Scaling Communication Costs: Broadcast Example

2 Message Passing Interface (MPI)

We run the benchmark on the Amelia cluster at IAC-CNR, (20 nodes with 64 ranks each).



The observed MPI\_Bcast latency shows a non-monotonic scaling trend as the number of MPI ranks increases.



# Interpreting Broadcast Scaling Behavior

2 Message Passing Interface (MPI)

This behavior is expected and reflects the internal algorithm selection.

- **1 node (64 ranks):** Extremely low latency due to shared-memory communication.
- **2-3 nodes (128-192 ranks):** Transition to inter-node communication with efficient tree-based collectives.
- **4-5 nodes (256-320 ranks):** Sudden increase in latency caused by algorithm switching and network contention.
- **6-7 nodes (384-448 ranks):** Stabilization as MPI switches to scalable hierarchical broadcast algorithms.

Overall, broadcast latency is dominated by **collective startup costs** rather than message size, and is strongly influenced by **communicator size, topology awareness**, and **algorithm thresholds**.



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- ▶ Restarting with BLAS: Level 1 routines
  - How do we distribute vectors?
  - Creation and destruction



## Restarting with BLAS: Level 1 routines

### 3 Restarting with BLAS: Level 1 routines

The first operation we are going to consider are the level-1 BLAS routines, which we recall are **vector-vector operations**.

- Vector scaling:  $\mathbf{y} \leftarrow \alpha \mathbf{y}$  (DSCAL)
- Vector addition:  $\mathbf{y} \leftarrow \mathbf{y} + \alpha \mathbf{x}$  (DAXPY)
- Vector dot product:  $\alpha \leftarrow \mathbf{x}^T \mathbf{y}$  (DDOT)
- Vector norm:  $\alpha \leftarrow \|\mathbf{x}\|_2$  (DNRM2)

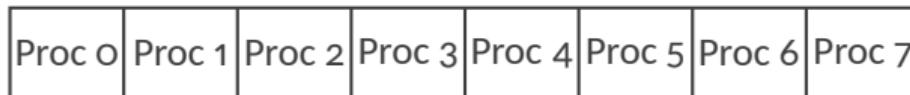
In our model, **each process holds a local portion of the vectors**, this means that for a vector of size  $N$  distributed over  $P$  processes, each process holds a local vector of size  $N/P$ .



# How do we distribute vectors?

3 Restarting with BLAS: Level 1 routines

The **basic idea** can be represented with an easy picture:



Full Vector of Size  $N$  divided across  $P = 8$  Processes

This permits us to:

- Perform local computations on each process independently;
- Know what data is stored where with a closed-form formula:

Process  $p$  holds elements  $\left[ p \cdot \frac{N}{P}, (p + 1) \cdot \frac{N}{P} - 1 \right]$



# Implementing vector distribution

## 3 Restarting with BLAS: Level 1 routines

To implement this distribution in code, we need to:

- Initialize MPI and get the rank and size of the communicator;
- Determine the global vector size  $N$  and compute the local size  $N/P$ ;
- Allocate local arrays for each process to hold its portion of the vector;

The initialization code looks always the same:

```
call MPI_Init(ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
```

To **compute the local size** and allocate the local vector we can use a simple-minded block distribution.



## Implementing vector distribution: block distribution

### 3 Restarting with BLAS: Level 1 routines

Assuming  $N$  is divisible by  $P$ , the local size is simply:

$$N_{\text{local}} = \frac{N}{P}$$

In the general case, we can compute the local size as:

$$N_{\text{local}} = \left\lfloor \frac{N + P - 1 - p}{P} \right\rfloor$$

where  $p$  is the rank of the process. This formula ensures that the last process gets any remaining elements if  $N$  is not perfectly divisible.

We can implement this as a function:

```
function compute_local_size(N, P, p) result(n_local)
    integer, intent(in) :: N, P, p
    integer :: n_local
    n_local = (N + P - 1 - p) / P
end function compute_local_size
```



# Implementing Level-1 BLAS: a type for distributed vectors

## 3 Restarting with BLAS: Level 1 routines

The first thing we need to do is to create a distributed vector datatype, this can be done using the **object-oriented** functionalities of Fortran:

```
type :: mpi_ddistributed_vector
    integer :: n_local(1) ! number of local elements
    integer :: n_global    ! total number of global elements
    integer :: comm         ! MPI communicator
    real(real64), allocatable :: data(:) ! local data array
end type mpi_ddistributed_vector
```

The **type** encapsulates all necessary information about the distributed vector, including *local size*, *global size*, *communicator*, and *local data array*.



# Implementing Level-1 BLAS: type-bound procedures

## 3 Restarting with BLAS: Level 1 routines

In Fortran a **type** can have **type-bound procedures**, which are functions or subroutines associated with the type. These are declared within the **contains** section of the type definition.

```
type :: mpi_ddistributed_vector
  <Type members>
contains
  <Type bound procedure are declared here>
end type mpi_ddistributed_vector
```

For our distributed vector type, we need to start by implementing:

- A **constructor** to initialize the distributed vector;
- A **destructor** to free resources;



# Implementing Level-1 BLAS: Constructor

## 3 Restarting with BLAS: Level 1 routines

The **constructor** initializes the distributed vector by computing the local size, allocating the local data array, and setting the global size and communicator.

- We add the following type-bound procedure to the type:

```
procedure, pass(this) :: dinit
```

- The implementation of the constructor is then inserted in the **contains** part

```
subroutine dinit(this, comm, n_global)
use mpi
use iso_fortran_env, only: error_unit
implicit none
class(MPI_Distributed_Vec), intent(inout) :: this
integer, intent(in) :: comm
integer, intent(in) :: n_global
end subroutine dinit
```



# Implementing Level-1 BLAS: Constructor

## 3 Restarting with BLAS: Level 1 routines

The **type constructor** has a default variable `this` that refers to the instance of the type being initialized.

```
integer :: ierr, rank, nprocs  
this%comm = comm  
this%n_global = n_global  
call MPI_Comm_rank(this%comm, rank, ierr)  
call MPI_Comm_size(this%comm, nprocs,  
      ierr)  
this%n_local =  
      compute_local_size(this%n_global,  
      nprocs, rank)  
allocate(this%data(this%n_local),  
      stat=ierr)
```

- We assign the communicator and global size to the type members;
- We get the rank and size of the communicator;
- We compute the local size using the previously defined function;
- We allocate the local data array based on the computed local size.

We should also include **error handling** for the allocation.



# Implementing Level-1 BLAS: Constructor (error handling)

## 3 Restarting with BLAS: Level 1 routines

The **error handling** for the allocation can be done by checking the status of the allocation.

```
if (ierr /= 0) then
    write(error_unit, *) "Error allocating local data array on rank ", rank
    call MPI_Abort(this%comm, ierr, ierr)
end if
```

The MPI\_Abort function is called to **terminate the MPI program** if the allocation fails, ensuring that all processes are informed of the error, and that the *program fails and exits gracefully*.



# Implementing Level-1 BLAS: Destructor

## 3 Restarting with BLAS: Level 1 routines

The **destructor** is responsible for freeing the resources allocated to the distributed vector.

- ⟨/⟩ We add use the **final** keyword in the type bound procedures to define the destructor:

```
final :: dfinalize
```

- ⟨/⟩ The implementation of the destructor is then inserted in che **contains** part

```
subroutine dfinalize(this)
    type(MPI_Distributed_Vec), intent(inout) :: this
    if (allocated(this%data)) then
        deallocate(this%data)
    end if
end subroutine dfinalize
```



# The creation and destruction of distributed vectors

## 3 Restarting with BLAS: Level 1 routines

With the constructor and destructor defined, we can now create and destroy distributed vector instances easily.

```
integer :: n_global, rank, ierr
type(MPI_Distributed_Vec) :: x
call MPI_Init(ierr)
n_global = 1000000 ! Total number of elements
call x%dinit(MPI_COMM_WORLD, n_global)
call MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
if (rank == 0) then
    write(output_unit, *) "MPI ranks           : ", nprocs
    write(output_unit, *) "Global vector size : ", n_global
end if
call MPI_Barrier(MPI_COMM_WORLD, ierr)
write(output_unit, *) "Rank ", rank, ": Local vector size : ", x%n_local
call MPI_Finalize(ierr)
```



## Conclusions and next steps

### 4 Conclusions and next steps

Today we have:

- ✓ Reviewed the concept of communication costs in MPI;
- ✓ Implemented a point-to-point ping-pong benchmark to measure communication latency and bandwidth;
- ✓ Explored the scaling behavior of collective communications using a broadcast benchmark;
- ✓ Introduced the concept of distributed vectors and how to implement them in Fortran using object-oriented programming.

Next steps:

- + Implement Level-1 BLAS operations (vector scaling, addition, dot product, norm) for distributed vectors;
- + Explore Level-2 and Level-3 BLAS operations