703308 VO High-Performance Computing WS2022/2023
MPI - Message Passing Interface

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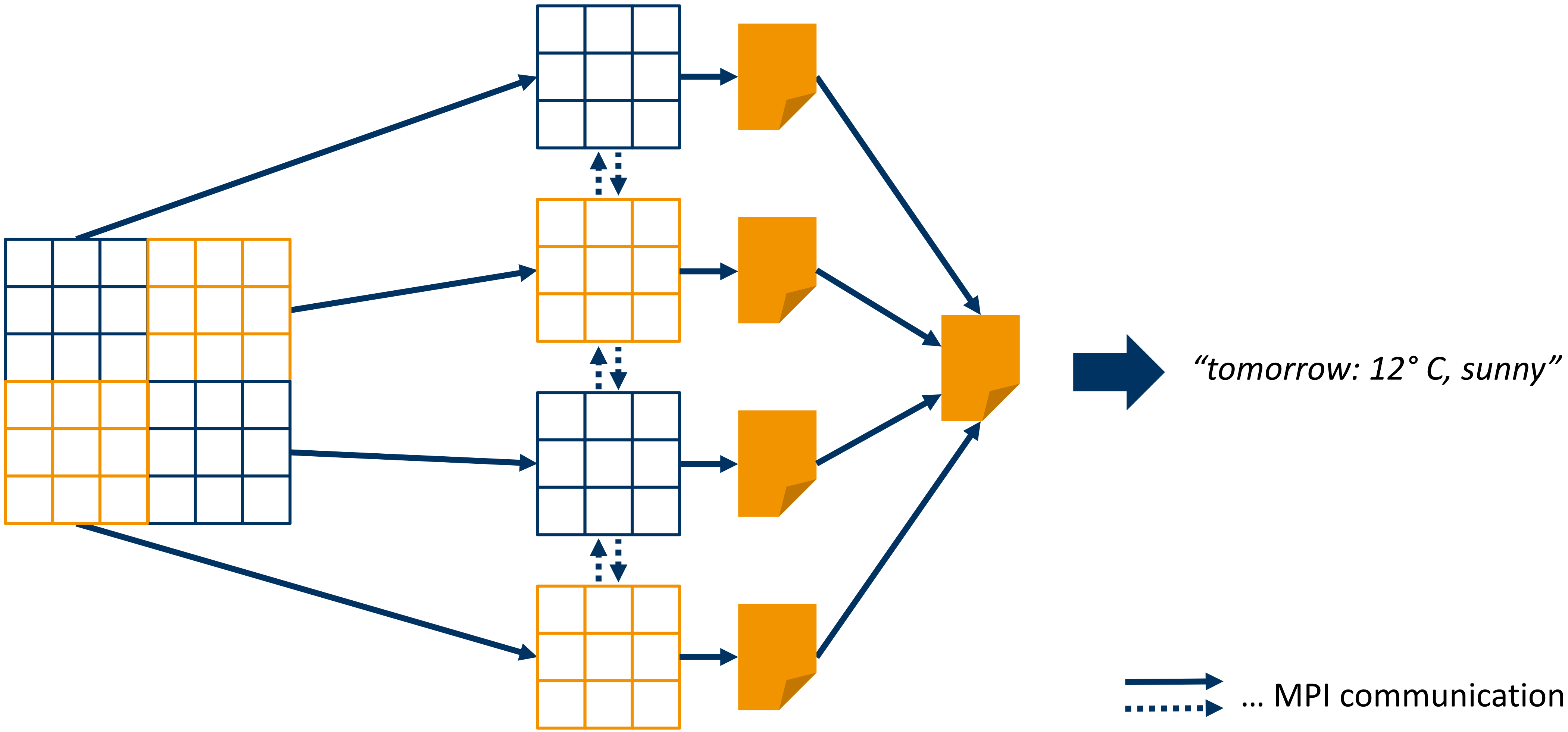
Overview

- general concepts about MPI
  - characteristics
  - programming model
  - startup
- point-to-point communication
- collective communication
- practical example

Motivation for using MPI: data distribution



Message Passing Interface (MPI)

- message passing library for distributed memory parallelism
- de-facto standard for C/C++ and Fortran
- maintained by the MPI Forum
  - initial release in 1994 (version 1.0)
  - updates in 1997 (2.0), 2012 (3.0), 2015 (3.1) and 202x (4.0)
  - specification updates slow, aim at stability and high TRL
    - “On June 30 2020, the MPI forum voted for version 3.3 of these voting rules (effective June 30th, 2020).”

MPI implementations

- OpenMPI
  - open source
  - merge of multiple previous MPI implementations
  - default on many systems

- MPICH
  - also open source
  - basis for many vendor implementations such as Intel, IBM, Cray, Microsoft, …
    - default on many systems

- Do not confuse implementation versions with specification versions!
- Do not confuse implementation adherence with specification adherence!

Main characteristics

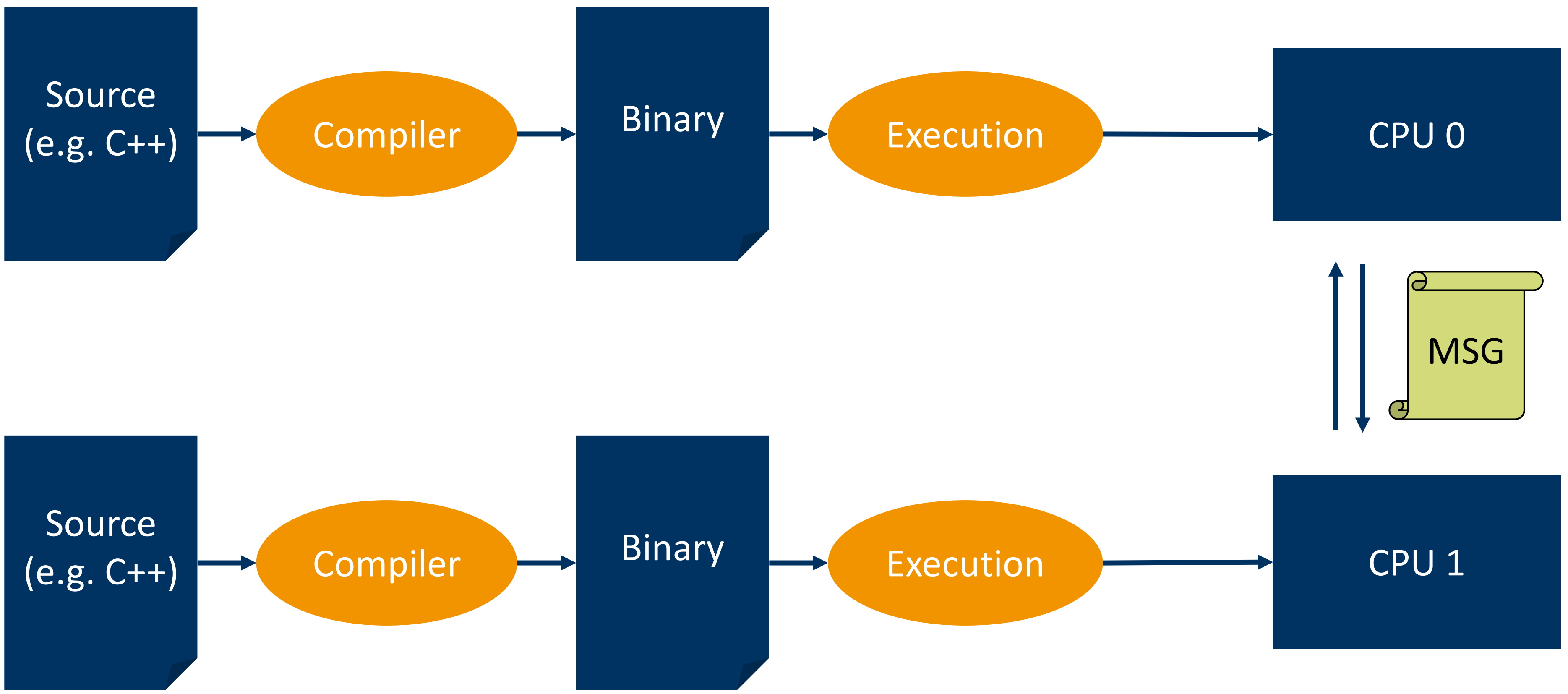
- offers specific tools for
  - sending and receiving messages
  - waiting and synchronization
  - identification of individual processes
  - …
- additional convenience tools for
  - partitioning and distributing data
  - organizing processes in structures
  - large-scale I/O operations
  - …

Main characteristics cont'd

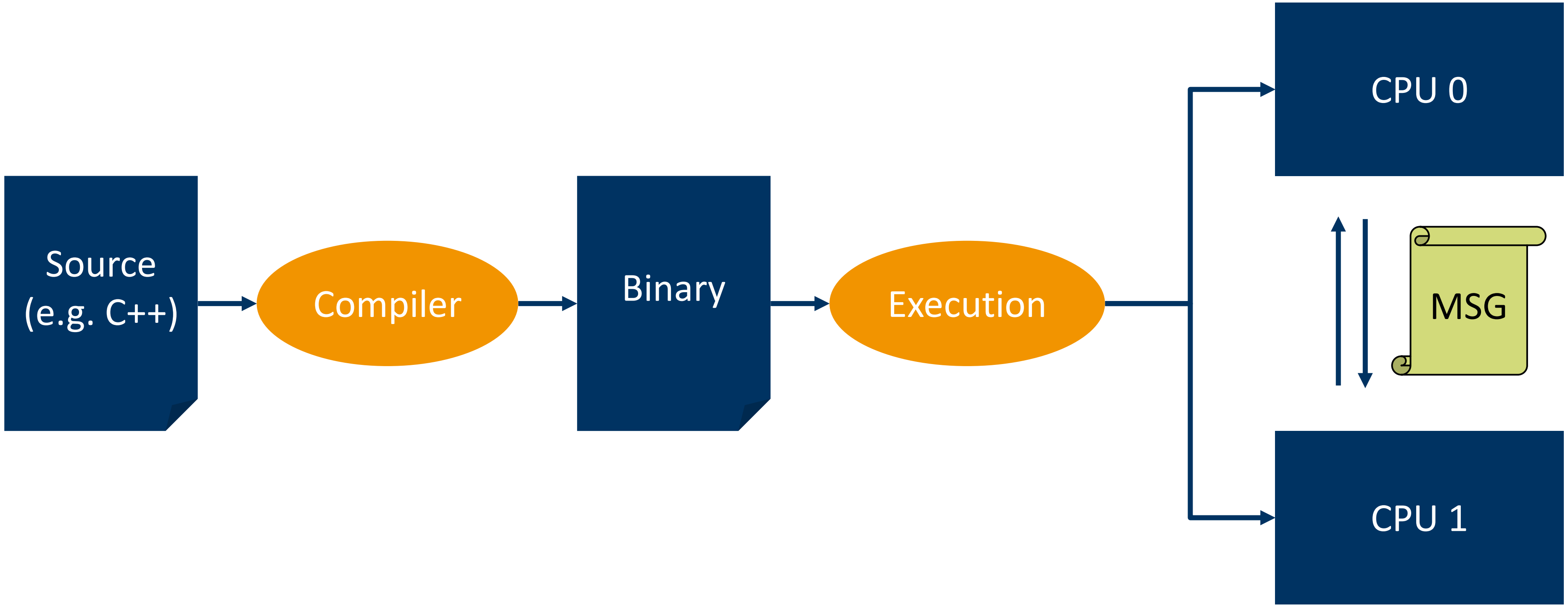
- a lot of user responsibility
  - explicit parallelism and communication
  - program correctness
  - performance optimization
    - (non-)blocking
    - (a)synchronous

- a lot of advantages
  - available everywhere
  - several implementations
  - portable to many architectures
  - very high performance

Recap: MIMD: MPMD



Recap: MIMD: SPMD



MPMD through SPMD

- many MPI implementations support only SPMD
- SPMD can emulate MPMD

```
int main() {
    // get id information
    int cpuID = ...;
    if(cpuID==0) {
        ... // program A
    } else {
        ... // program B
    }
}
```

Parallelism requires two mechanisms

- a mechanism for spawning processes
  - multiple ways of achieving this
  - we won't look at this in too much detail
  - simply rely on `mpiexec` to do the work for you

- a mechanism for sending and receiving messages
  - many, many ways of exchanging messages
  - we will definitely look at this in a lot of detail
  - tons of functionality to choose from, as we'll see in a bit

Compiler and execution wrappers

- `mpicc` / `mpic++` for compiling
  - OpenMPI: `--showme` prints compiler flags
  - passes all additional compiler flags to backend compiler (e.g. `mpicc -g`)
- `mpiexec` for running
  - formerly `mpirun`, but `mpiexec` is standardized

Startup procedure of an MPI application

SLURM job submission

- allocates resources
- sets environment
- calls mpiexec

mpiexec

- reads SLURM environment
- connects to nodes
- spawns processes

MPI function calls

- identify processes
- exchange messages
- synchronize

Hello world in MPI

```c
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
    MPI_Init(&argc, &argv); // initialize the MPI environment
    int size;
    MPI_Comm_size(MPI_COMM_WORLD, &size); // get the number of ranks
    int rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &rank); // get the rank of the caller
    printf("Hello world from rank %d of %d\n", rank, size);
    MPI_Finalize(); // cleanup
}
```

Setup and teardown

- `int MPI_Init( int* argc, char*** argv )`
  - must be called by every process before calling any other MPI function
  - initializes the MPI library
- `int MPI_Finalize( void )`
  - must be the last MPI function called by every process
  - user must ensure completion of all locally (!) pending communication
  - performs library cleanup

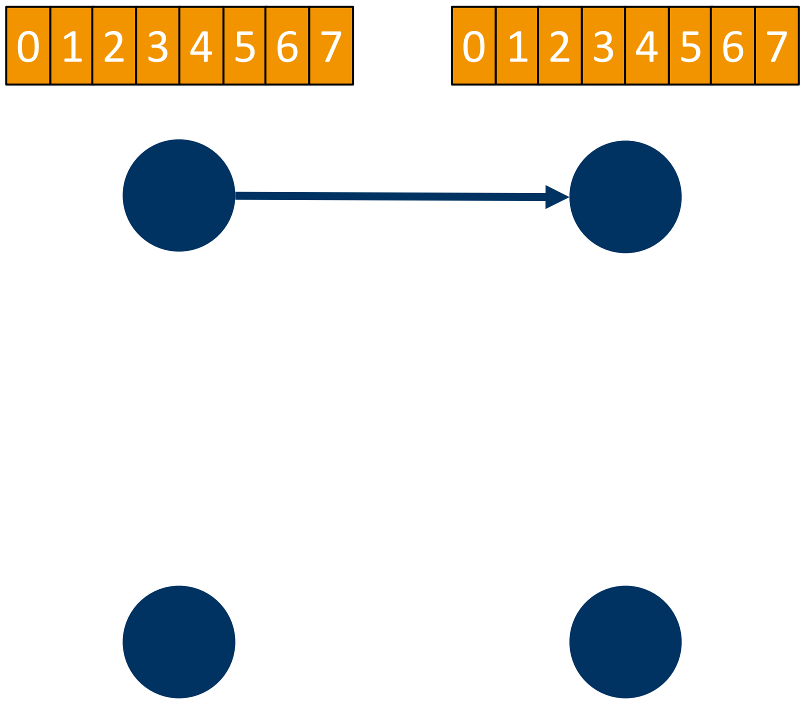
Who am I talking to?

- in MPI-speak, processes are known as “*ranks*”
  - numbered from 0 to N-1
  - own rank can be queried with
    `int MPI_Comm_rank( MPI_Comm comm, int* rank )`
  - number of ranks can be queried with
    `int MPI_Comm_size( MPI_Comm comm, int* size)`
- almost all MPI semantics are relative to a “*communicator*” or “*group*”
  - identifies a set of ranks
  - always available: `MPI_COMM_WORLD` (=everyone)
  - new communicators and groups that hold subsets of ranks can be created
  - when developing a library, always create your own communicator!
    - frequent MPI programming pattern

Point-to-Point Communication

Point-to-point communication

- `MPI_Send(…)/MPI_Recv(…)`
  - single sender, single receiver ("*point-to-point*")
- simplest form of communication available
  - not necessarily the best
- multiple different types
  - (a)synchronous
  - (non-)blocking



MPI_Send

- `int MPI_Send(const void* buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
  - `buf`: source buffer to send data from
  - `count`: number of data elements to send
  - `datatype`: type of data to send
  - `dest`: destination rank
  - `tag`: user-defined message type or category
  - `comm`: communicator

- `MPI_Send(&number, 1, MPI_INT, 1, 42, MPI_COMM_WORLD);`

MPI_Recv

- `int MPI_Recv(void* buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status* status)`
  - `buf`: destination buffer to save data to
  - `count`: number of data elements to receive
  - `datatype`: type of data to receive
  - `source`: source rank
  - `tag`: user-defined message type or category
  - `comm`: communicator
  - `status`: holds additional information (e.g. rank of sender or tag of message)

- `MPI_Recv(&number, 1, MPI_INT, 0, 42, MPI_COMM_WORLD, MPI_STATUS_IGNORE);`

Basic send/receive example

```
int number;
if (rank == 0) {
    number = -1;
    MPI_Send(&number, 1, MPI_INT, 1, 42, MPI_COMM_WORLD);
} else if (rank == 1) {
    MPI_Recv(&number, 1, MPI_INT, 0, 42, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    printf(“Rank 1: Received %d from rank 0\n", number);
}
```

Side note: MPI data type conversion

- "representation conversion"
  - changes the binary representation of some data
  - c.f. C++ reinterpret casts
  - allowed in MPI, required by supporting heterogeneous architectures
    - e.g. sender is ARM, receiver is x86, …
    - e.g. big-endian vs. little-endian, ASCII vs. EBCDIC, …

- "type conversion"
  - converts the actual data type, e.g. from float to integer
  - c.f. C++ numeric casts
  - not allowed in MPI

Predefined MPI constants

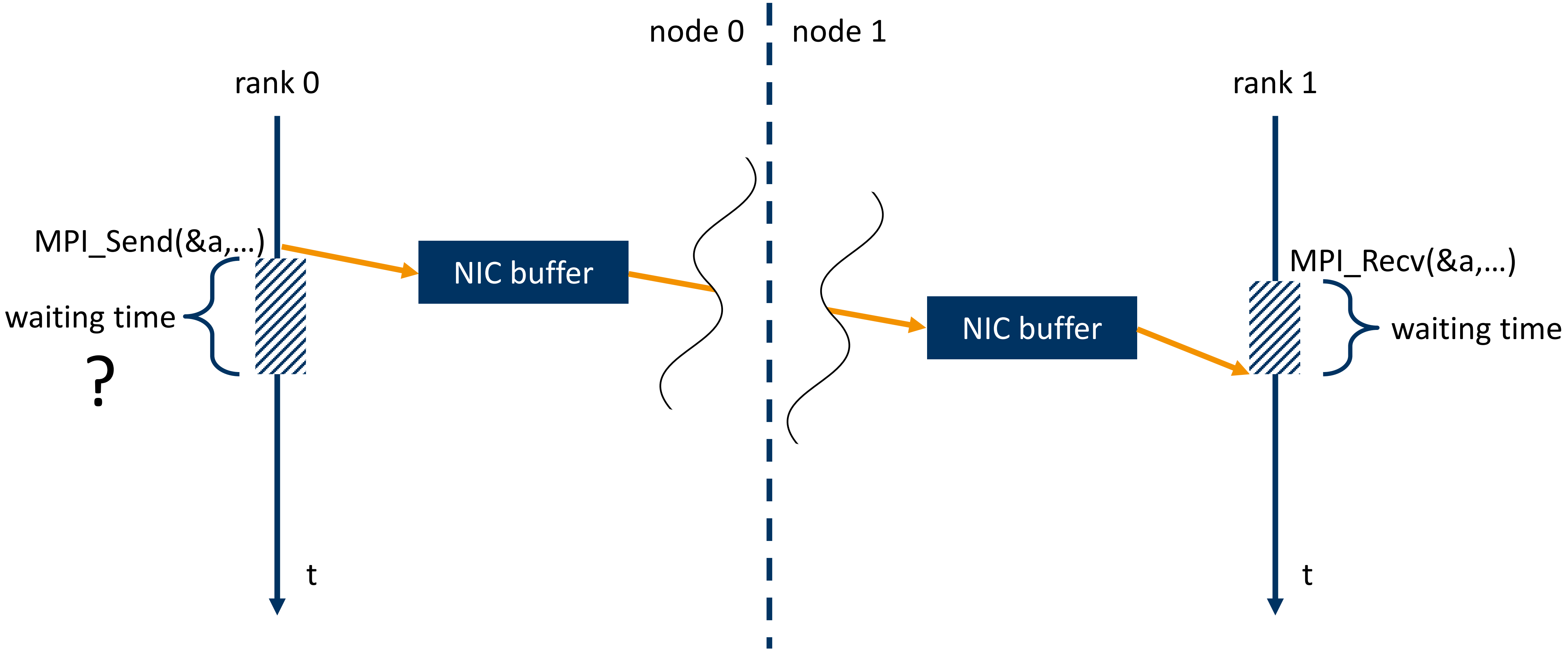
- datatypes
  - `MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_BYTE, MPI_CHAR, …`
- wildcards & misc
  - `MPI_ANY_SOURCE`
  - `MPI_ANY_TAG`
  - `MPI_COMM_WORLD`
  - `MPI_STATUS_IGNORE`
  - …

(Non-)Blocking and (a)synchronous communication

- distinguish two important properties
  - When does the MPI function call return?
    - Can I overwrite the send buffer?
    - When is all the data in the receive buffer?
  - When does the corresponding message transfer happen?
    - Do I need to wait for the receiver to get the entire message?
    - Do I need to wait for the receiver to begin receiving?

```
if (rank == 0) {
    MPI_Send(&number, ...);
} else if (rank == 1) {
    MPI_Recv(&number, ...);
}
```

(Non-)Blocking and (a)synchronous communication cont'd



Blocking vs. non-blocking communication

- blocking point-to-point: `MPI_Send()` and `MPI_Recv()`
  - allows to re-use send buffer after send call returns
  - allows to read receive buffer after receive call returns

```
if (rank == 0) {
    MPI_Send(&number, ...);
    // re-use number here
} else if (rank == 1) {
    MPI_Recv(&number, ...);
    // use number here
}
```

Blocking vs. non-blocking communication cont'd

- non-blocking point-to-point: `MPI_Isend()` and `MPI_Irecv()`
  - send and receive return (almost) Immediately
  - `MPI_Wait()` call blocks until buffer can be read/re-used

```
MPI_Request request;
if (rank == 0) {
  MPI_Isend(&number, ..., &request);
  MPI_Wait(&request, MPI_STATUS_IGNORE);
  // re-use number here
} else if (rank == 1) {
  MPI_Irecv(&number, ..., &request);
  MPI_Wait(&request, MPI_STATUS_IGNORE);
  // re-use number here
}
```

(A)Synchronous send modes

- `MPI_Ssend()` – synchronous mode
  - will wait for matching receive
- `MPI_Bsend()` – buffered mode
  - will buffer, won't wait for a matching receive
- `MPI_Rsend()` – ready mode
  - requires an already posted, matching receive (developer responsibility!)
- `MPI_Send()` – standard mode
  - may buffer (depends on message size)
  - may or may not wait for matching receive

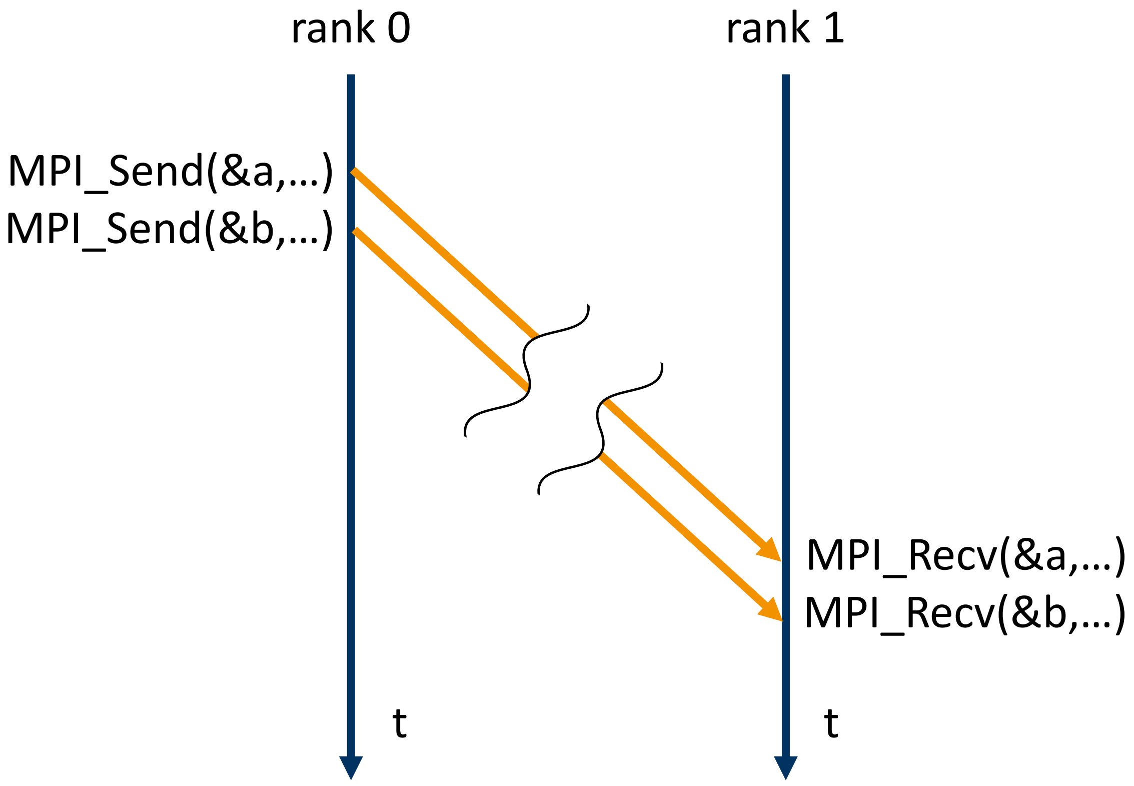
- and there are also non-blocking variants for ALL of them…

Message order preservation

- messages do NOT overtake each other if
  - same communicator
  - same source rank
  - same destination rank

- regardless of blocking or synchronization mode

- mandated by MPI specification



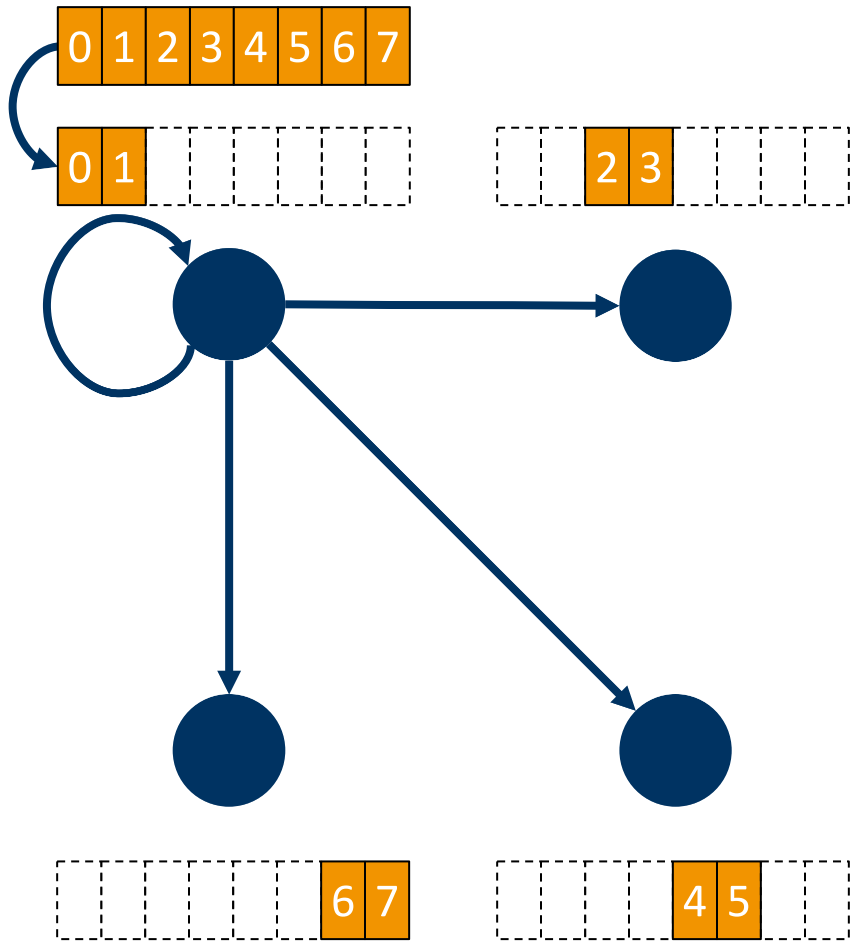
Collective Communication

Collective communication

- convenience function for frequently-used programming patterns (e.g. distributing data)
  - can involve several ranks at the same time, not just 2
  - must be called by ALL ranks in the communicator
  - must be called in-order by all ranks (no interleaving of multiple collective communication calls!)
  - is locally finished when local operation has finished
  - is globally finished when all participating ranks are finished
  - available as blocking and non-blocking variants (but cannot be mixed!)

MPI_Scatter/MPI_Scatterv

- sends chunks of data to multiple ranks, including root itself
- simple way of partitioning and distributing data
- MPI_Scatterv() allows varying counts of elements to be distributed to each rank



MPI_Scatter

- `int MPI_Scatter(const void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`
  - `sendbuf`: source buffer to send data from
  - `sendcount`: number of data elements to send to each rank
  - `sendtype`: type of data to send
  - `recvbuf`: destination buffer to save data to
  - `recvcount`: number of data elements to receive at each rank
  - `recvtype`: type of data to receive
  - `root`: rank of the sender
  - `comm`: communicator

Scatter example

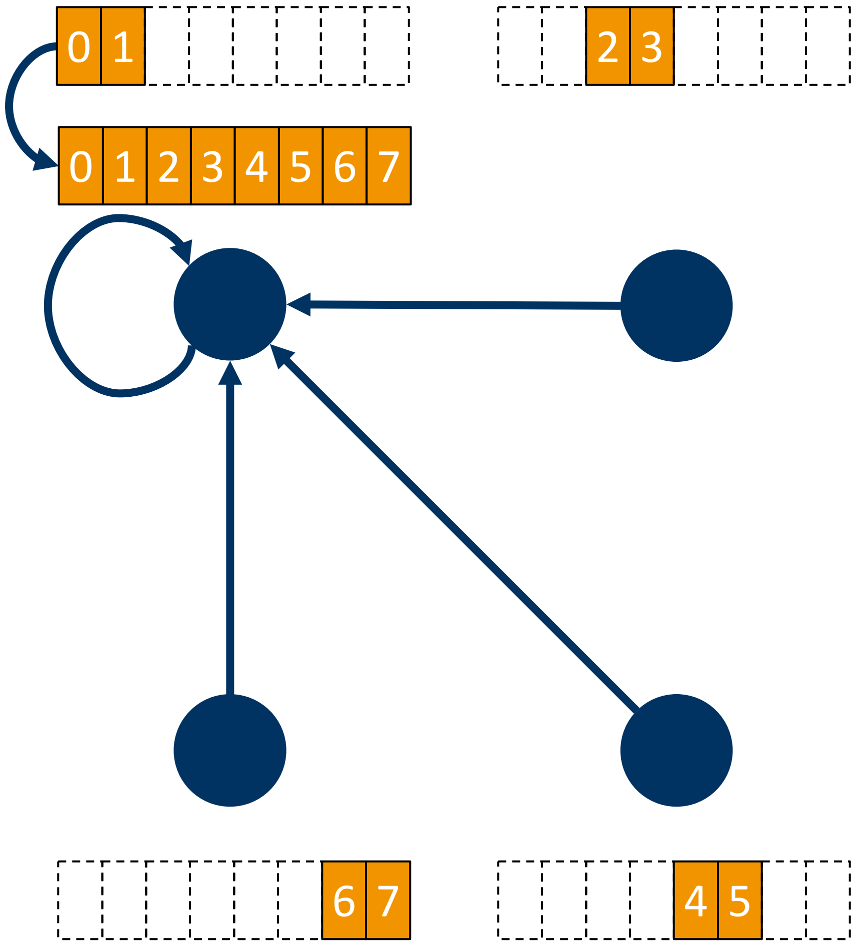
```
int globaldata[4];

if(rank==0) {
    for(int i = 0; i < 4; i++) {
        globaldata[i] = ...
    }
}

int localdata;
MPI_Scatter(globaldata, 1, MPI_INT, &localdata, 1, MPI_INT, 0,
  MPI_COMM_WORLD);
```

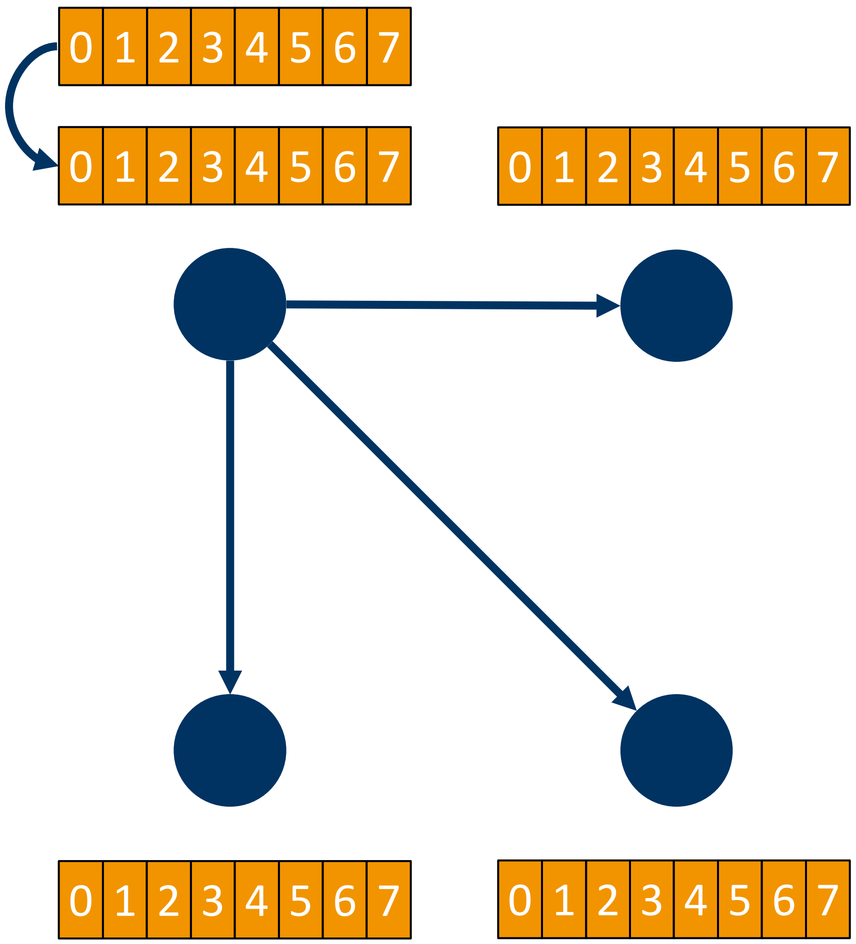
MPI_Gather/MPI_Gatherv

- sends chunks of data from multiple ranks, including root itself, to root
- simple way of collecting data
- MPI_Gatherv() allows varying counts of elements to be collected from each rank



MPI_Bcast

- broadcast operation
- sends copies of data to multiple ranks

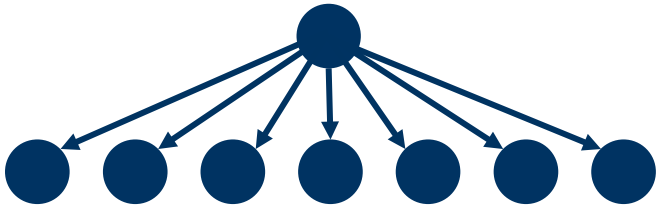


Q: emulating broadcast with point-to-point?

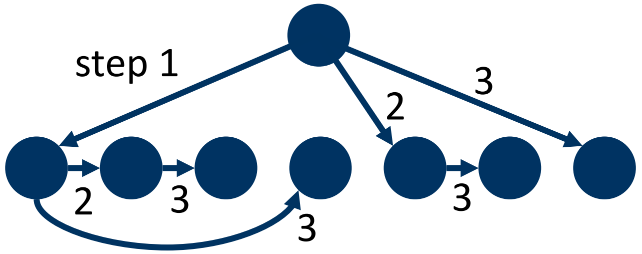
```
MPI_Bcast(&buf, 1, MPI_INT, 0, MPI_COMM_WORLD);
// ################ or instead: ################
if (rank == 0) {
    for (int i = 0; i < size; i++) {
        if (i != rank) {
            MPI_Send(&buf, 1, MPI_INT, i, 0, MPI_COMM_WORLD);
        }
    }
} else {
    MPI_Recv(&buf, 1, MPI_INT, 0, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

Collective communication patterns

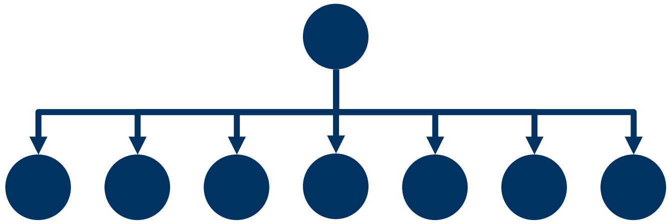
- chosen automatically at runtime by MPI implementation
- may depend on multiple parameters, including
  - type of operation (e.g. broadcast)
  - number and location of ranks
  - size and structure of data
  - hardware capabilities



sequential algorithm
O(num_ranks)



tree-based algorithm
e.g. $O(\log_2(\text{num\_ranks}))$



hardware operation
O(1)

Barrier

- `int MPI_Barrier(MPI_Comm comm)`
  - `comm`: communicator

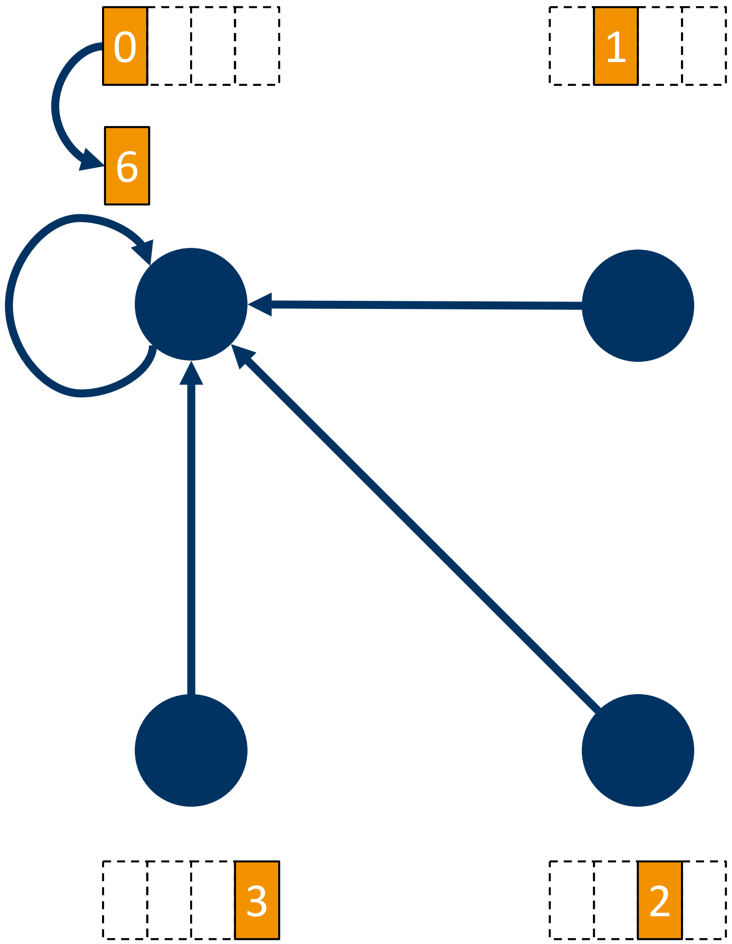
- causes all ranks to wait until everyone reached the barrier
  - normally not needed: explicit data communication usually also inherently synchronizes
  - often used for debugging and profiling
    - Don’t forget to remove in production/release!

MPI_Reduce

- aggregate data from multiple ranks, including root itself, to root
  - e.g. MPI_SUM
  - may use optimized collective communication patterns
- requires associative reduction operation $\circ$ such that e.g.

$$(x_0 \circ x_1) \circ (x_2 \circ x_3) = \big((x_0 \circ x_1) \circ x_2\big) \circ x_3$$

- be careful with floating point types!



MPI_Reduce cont'd

- `int MPI_Reduce(const void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)`
  - `sendbuf`: source buffer to reduce data from
  - `recvbuf`: destination buffer to reduce data into
  - `count`: number of data elements in source and destination buffers
  - `datatype`: type of data to reduce
  - `op`: reduction operation
  - `root`: rank of the destination of aggregated result
  - `comm`: communicator

Available reduction operations

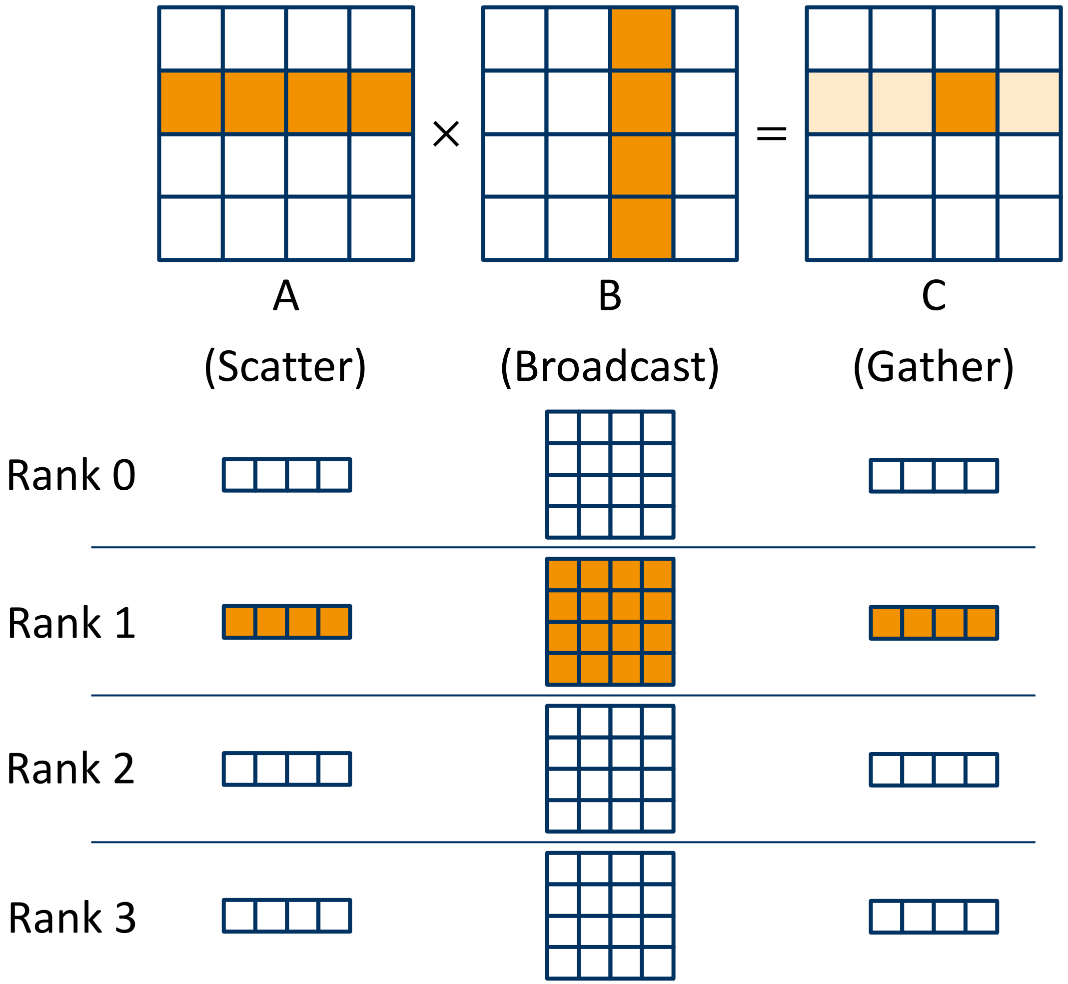
- several pre-defined
  - `MPI_MAX, MPI_MIN`
  - `MPI_SUM, MPI_PROD`
  - `MPI_LAND, MPI_LOR, MPI_LXOR`
  - `MPI_BAND, MPI_BOR, MPI_BXOR`
  - `MPI_MAXLOC, MPI_MINLOC`
- All pre-defined operations are associative and commutative

- also user-defined ops are possible
  - must be associative
  - may be commutative
  - requires a specific function signature
  - needs to be registered as an MPI handle

Additonal MPI functions

- `MPI_Wtime`
  - returns time in seconds since an arbitrary time in the past (**W**all clock time)
- `MPI_Sendrecv`
  - convenience wrapper for blocking send and receive
- `MPI_Allreduce/MPI_Allgather/…`
  - same as non-all versions, but result is available everywhere (performance impact!)
- `MPI_Scan/MPI_Exscan`
  - inclusive and exclusive prefix reductions
- `MPI_Wait/MPI_Test`
  - blocking/non-blocking check whether pending operation completed
- `MPI_Probe/MPI_Iprobe`
  - blocking/non-blocking check for new message without actually receiving it

Example code: naïve matrix multiplication




```c
#include <mpi.h>
#include <stdio.h>
#include <stdlib.h>

#define SIZE 4

int A[SIZE][SIZE];
int B[SIZE][SIZE];
int C[SIZE][SIZE];

void fill_matrix(int m[SIZE][SIZE]);
void print_matrix(int m[SIZE][SIZE]);
```

Example code: naïve matrix multiplication cont'd

```
int myRank, numProcs;

MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myRank);
MPI_Comm_size(MPI_COMM_WORLD, &numProcs);
// if matrix size not divisible
if(SIZE % numProcs != 0) {
    MPI_Finalize();
    return EXIT_FAILURE;
}
// root generates input data
if(myRank == 0) {
    fill_matrix(A);
    fill_matrix(B);
}
```

```
// compute boundaries of local computation
int start = myRank*SIZE/numProcs;
int end = (myRank+1)*SIZE/numProcs;

// distribute rows of A to everyone
MPI_Scatter(A, SIZE*SIZE/numProcs, MPI_INT,
  A[start], SIZE*SIZE/numProcs, MPI_INT, 0,
  MPI_COMM_WORLD);

// send entire matrix B to everyone
MPI_Bcast(B, SIZE*SIZE, MPI_INT, 0,
  MPI_COMM_WORLD);
```

Example code: naïve matrix multiplication cont'd

```c
// local computation of every rank
for(int i = start; i < end; i++) {
    for(int j = 0; j < SIZE; j++) {
        C[i][j] = 0;
        for(int k = 0; k < SIZE; k++) {
            C[i][j] += A[i][k] * B[k][j];
        }
    }
}
```

```c
// gather result rows back to root
MPI_Gather(C[start], SIZE*SIZE/numProcs,
  MPI_INT, C, SIZE*SIZE/numProcs, MPI_INT, 0,
  MPI_COMM_WORLD);

if(myRank == 0) { print_matrix(C); }

MPI_Finalize();

return EXIT_SUCCESS;
```

Submitting to a cluster (SLURM & SGE)

```
#!/bin/bash

# submission partition
#SBATCH --partition std.q
# name of the job
#SBATCH --job-name my_test_job
# redirect output stream to this file
#SBATCH --output output.dat
# specify parallel environment
#SBATCH --ntasks 8
#SBATCH --ntasks-per-node 2

srun /path/to/application
# or
mpiexec -n $SLURM_NTASKS /path/to/application
```

```
#!/bin/bash

# submission queue
#$ -q std.q
# change to current directory
#$ -cwd
# name of the job
#$ -N my_test_job
# redirect output stream to this file
#$ -o output.dat
# join the output and error stream
#$ -j yes
# specify parallel environment
#$ -pe openmpi-2perhost 8

mpiexec –n 8 /path/to/application
```

Summary

- general concepts about MPI
  - characteristics
  - program model
  - startup
- point-to-point communication
- collective communication
- practical example (matrix multiplication)