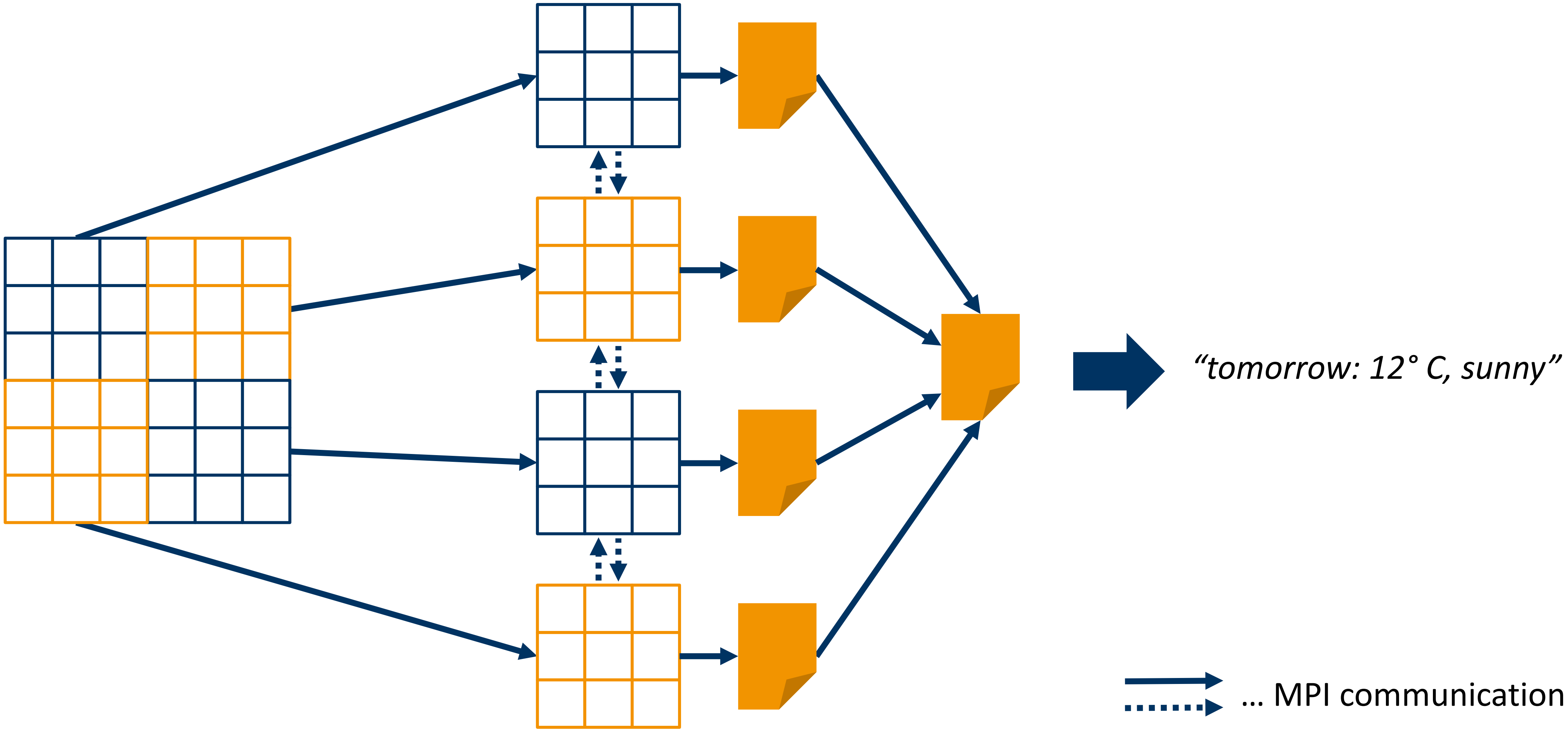
703308 VO High-Performance Computing
MPI - Message Passing Interface

Philipp Gschwandtner

Overview

- general concepts about MPI
  - characteristics
  - programming model
  - startup
- point-to-point communication
- collective communication
- practical example
- Tales from the proseminar: `osu_latency` on LCC3

Motivation for using MPI: data distribution



“tomorrow: 12° C, sunny”

… MPI communication

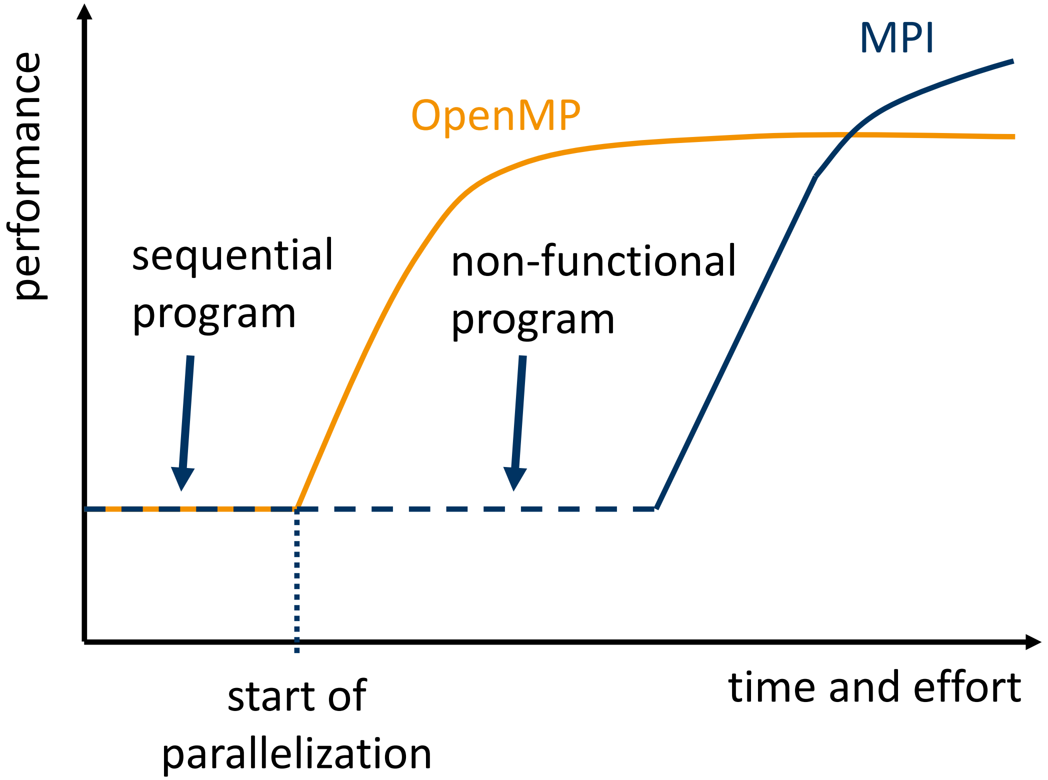
Message Passing Interface (MPI)

- 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), 2021 (4.0), 2023 (4.1), 202x (5.0)
  - 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).”

How does it compare to OpenMP?

- MPI – Message Passing Interface
  - distributed memory programming model
  - library: steeper learning curve compared to OpenMP
  - much higher obtainable performance and maximum memory footprint

- OpenMP – Open MultiProcessing
  - shared memory programming model
  - compiler-based: much easier to get working parallel programs, allows incremental parallelization
  - lower obtainable performance and maximum memory footprint



MPI implementations

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

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

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

- https://www.mpi-forum.org/implementation-status/

Main characteristics

- offers specific tools for
  - sending and receiving messages
  - waiting and synchronization
  - identification of individual processes
  - …

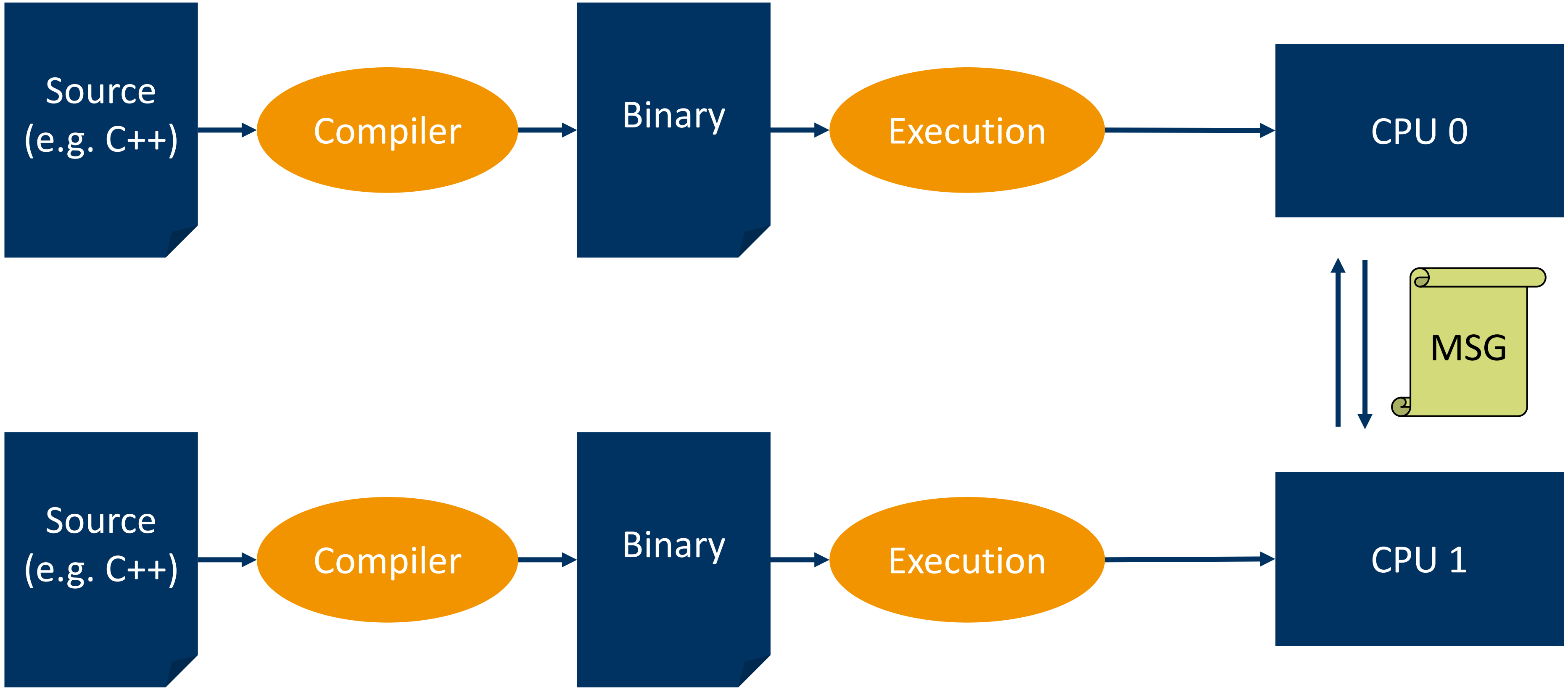
- additional convenience tools for
  - partitioning and distributing data
  - organizing processes in structures
  - large-scale I/O operations
  - …

Main characteristics cont'd

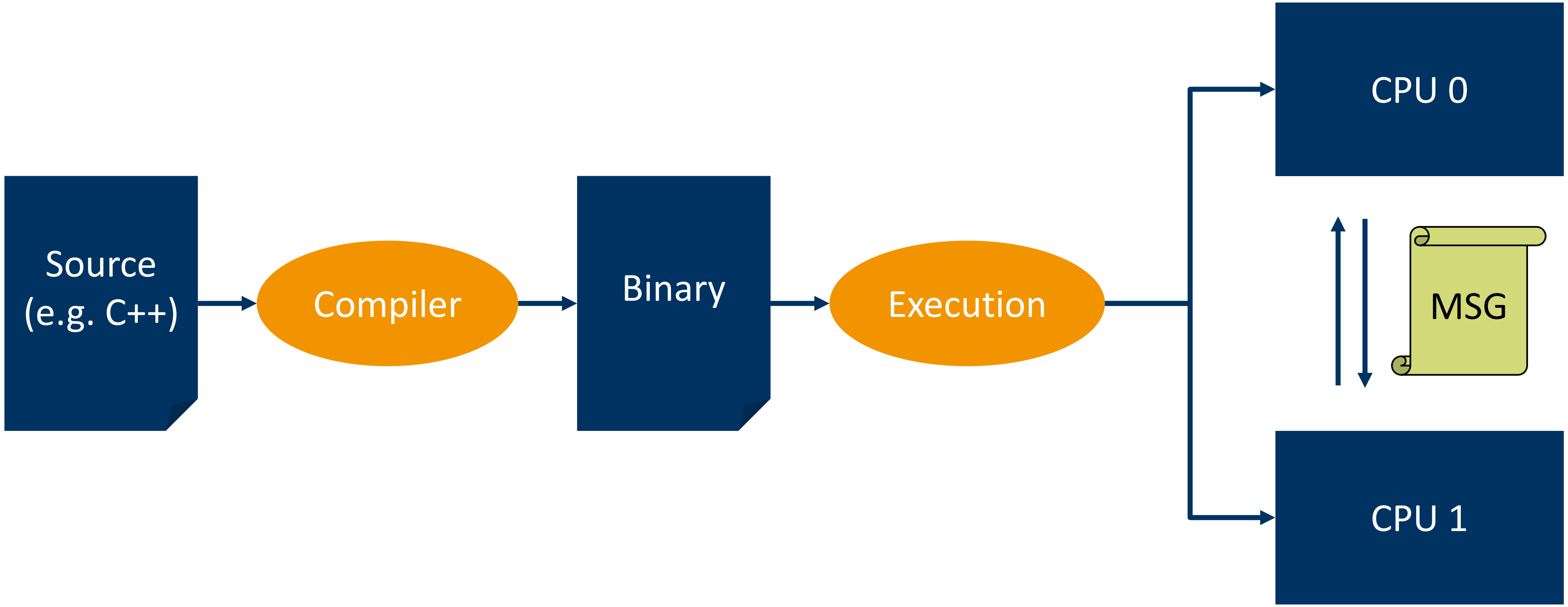
- a lot of user responsibility
  - explicit parallelism and communication
  - program correctness
  - performance optimization
    - (non-)blocking
    - (a)synchronous

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

Recap: MIMD: MPMD

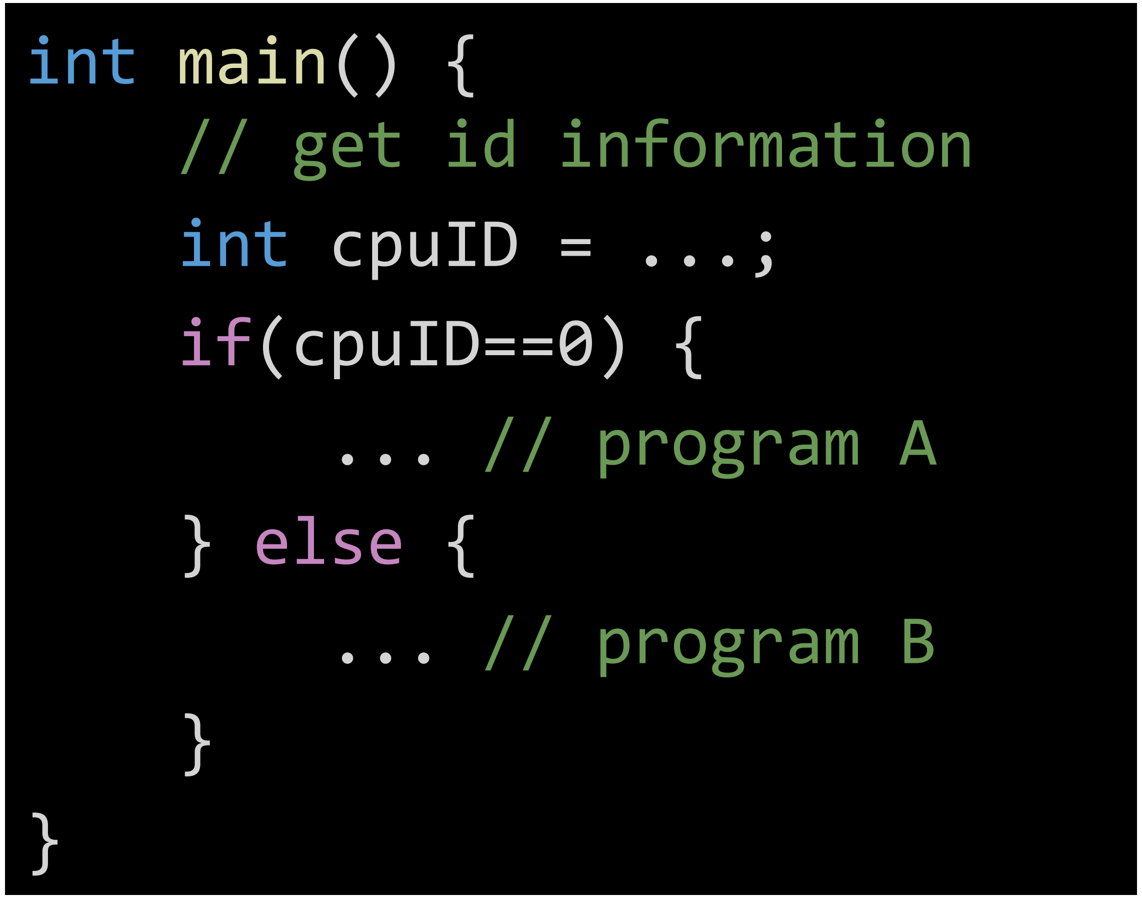


Recap: MIMD: SPMD



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

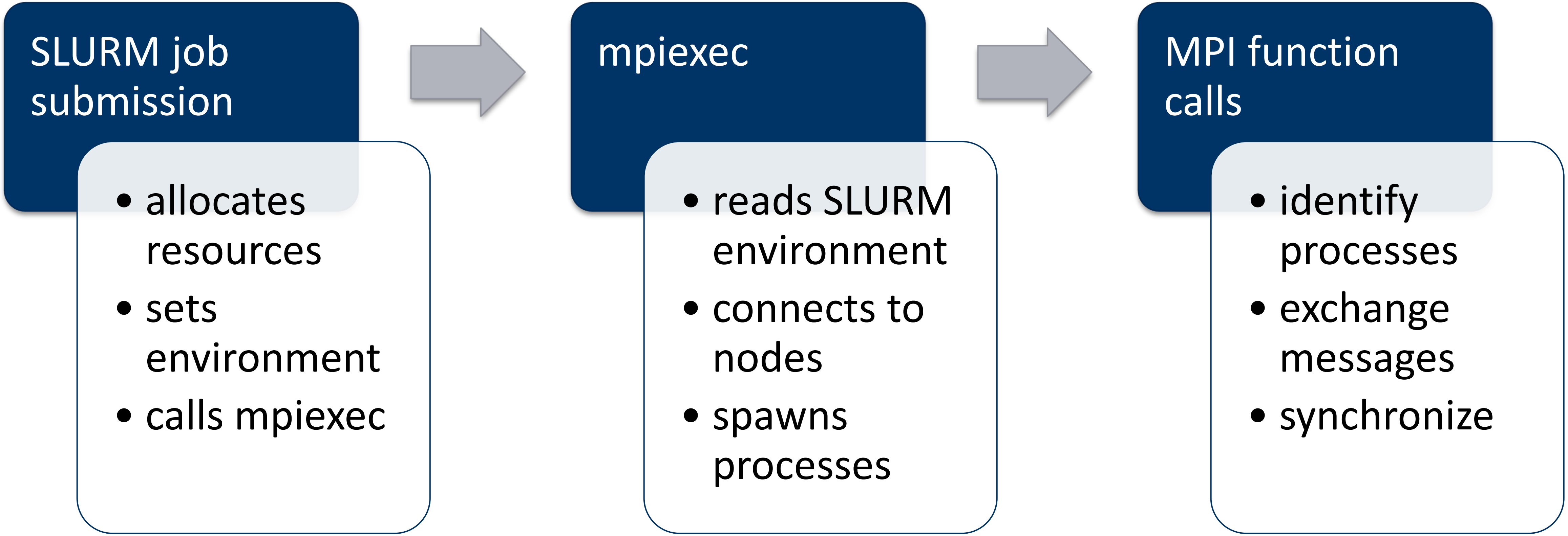
- a mechanism for sending and receiving messages
  - many ways of exchanging messages
  - we will definitely look at this in a lot of detail
  - tons of functionality to choose from, as we’ll see in a bit

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
  - alternatively `srun` or whatever the platform documentation recommends

Startup procedure of an MPI application



SLURM job submission

- allocates resources
- sets environment
- calls mpiexec

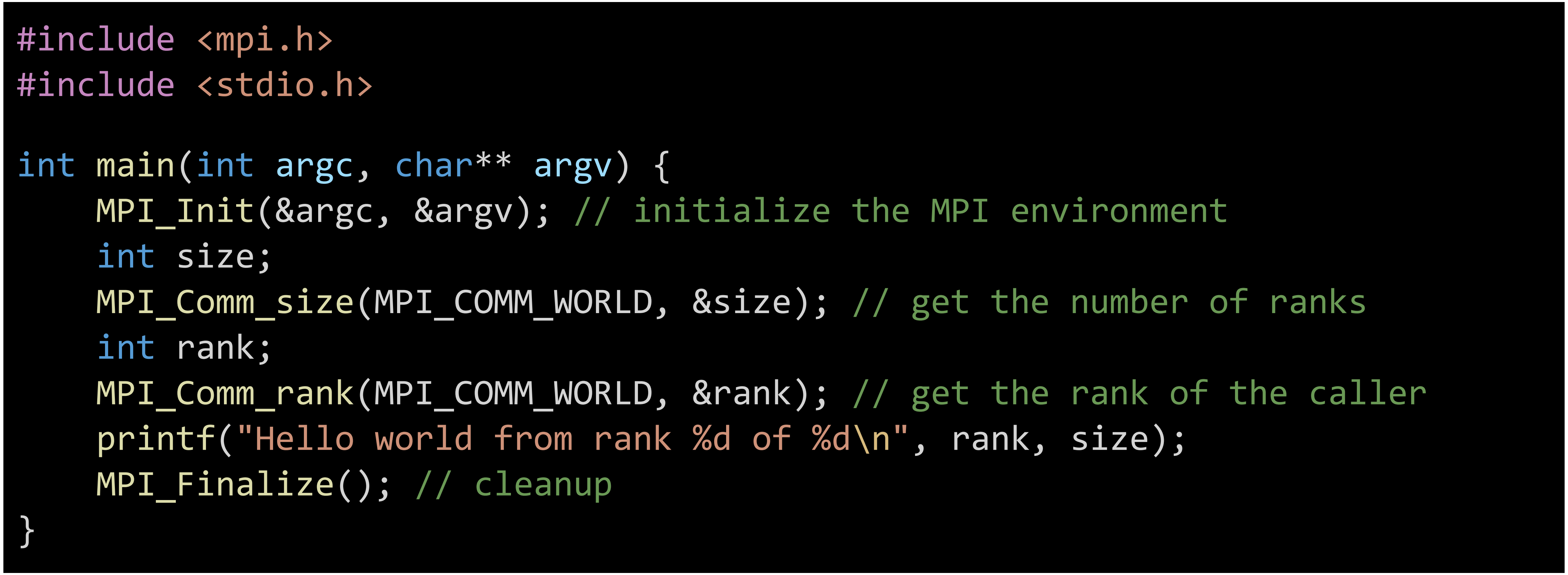
mpiexec

- 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?

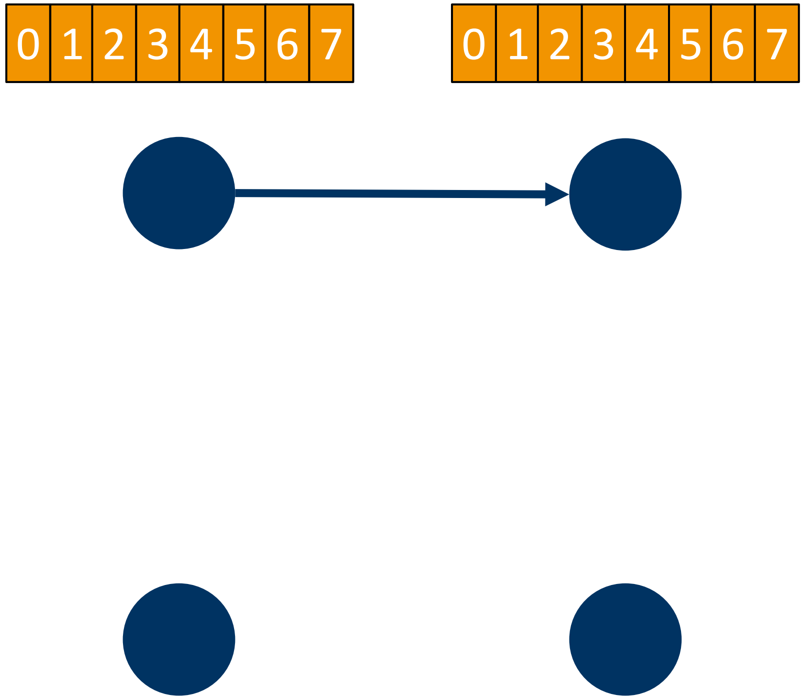
- in MPI-speak, processes are known as “*ranks*”
  - numbered from 0 to N-1
  - own rank can be queried with
    `int MPI_Comm_rank(MPI_Comm comm, int* rank)`
  - number of ranks can be queried with
    `int MPI_Comm_size(MPI_Comm comm, int* size)`

- 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 data without changing semantics
  - allowed in MPI, required for supporting heterogeneous architectures
    - e.g. sender is ARM, receiver is x86, …
    - e.g. big-endian vs. little-endian, ASCII vs. EBCDIC, …

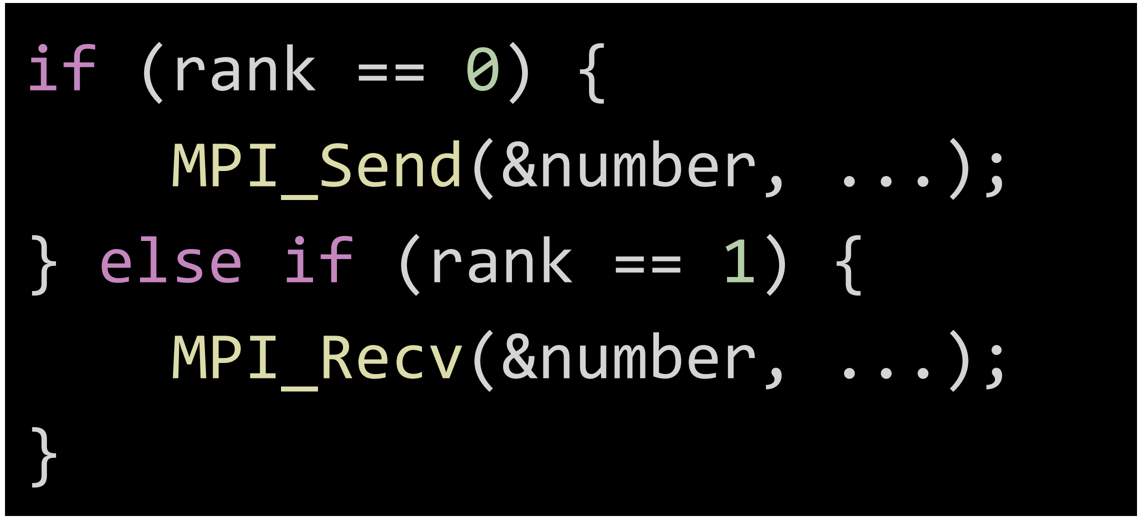
- “type conversion”
  - converts the actual data type, e.g. from float to integer
  - c.f. C++ numeric casts
  - not allowed in MPI, might change semantics

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`
  - …

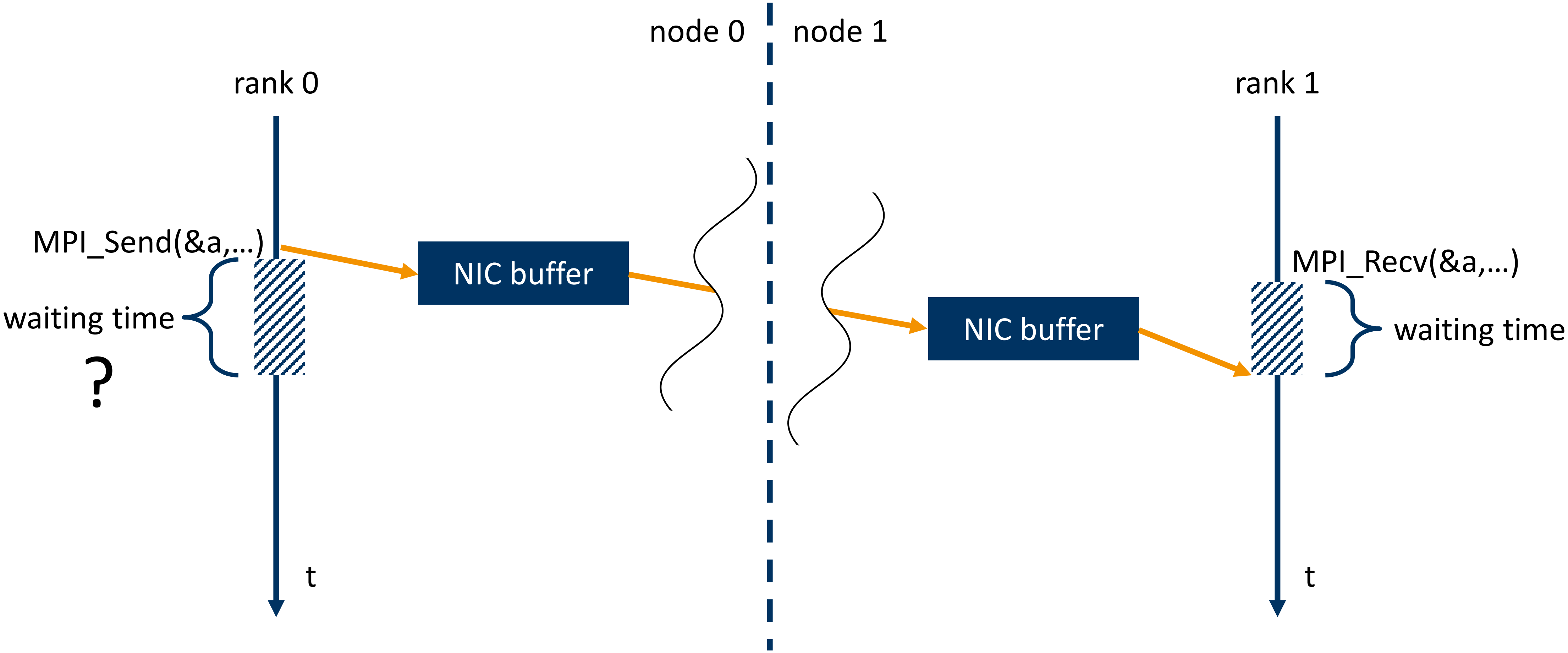
(Non-)Blocking and (a)synchronous communication

- 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

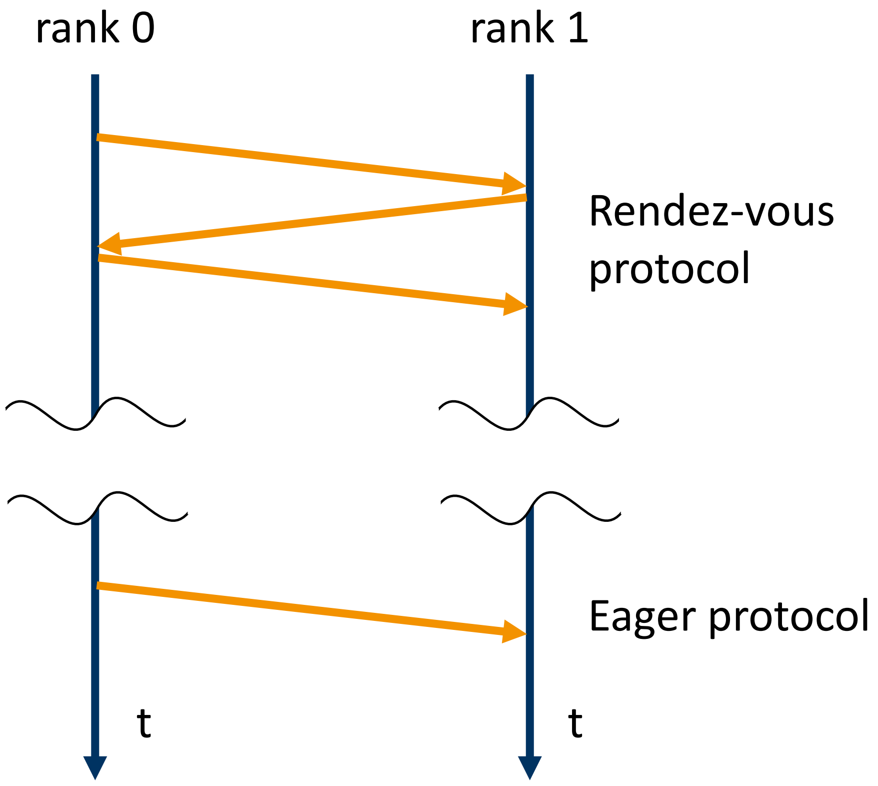
- non-blocking point-to-point: `MPI_Isend()` and `MPI_Irecv()`
  - send and receive return (almost) Immediately
  - `MPI_Wait()` call blocks until buffer can be read/re-used

```
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 (dangerous, 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…

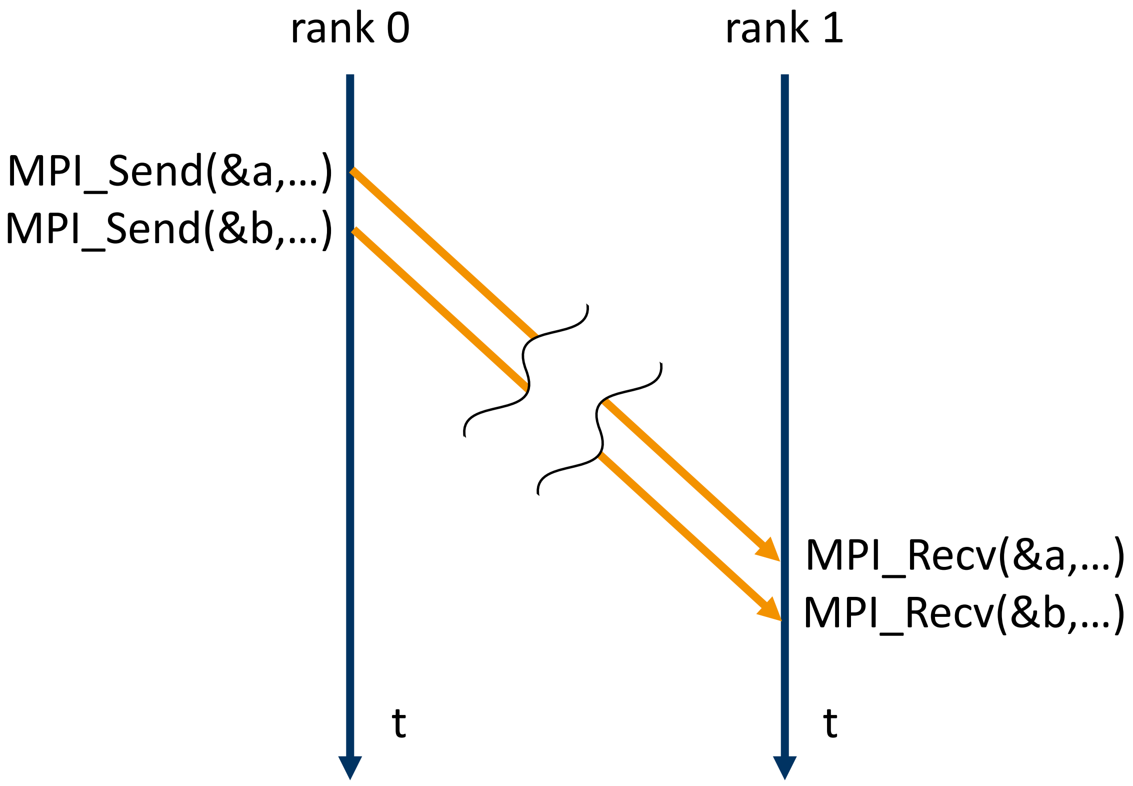


Message order preservation

- 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



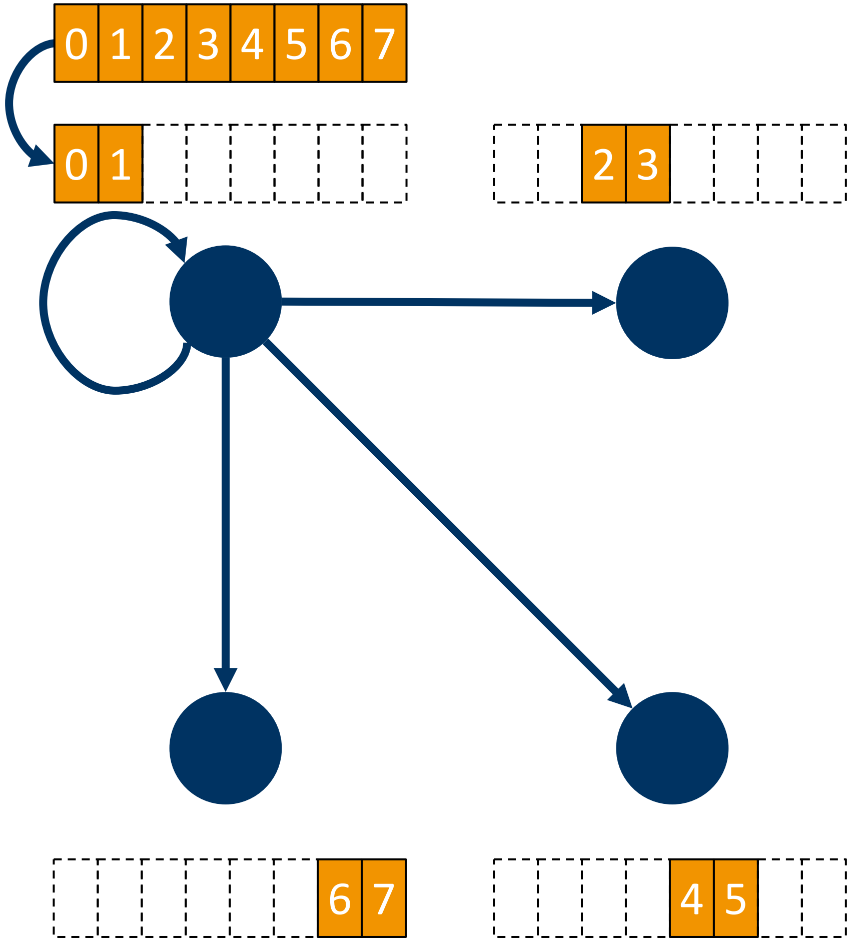
Collective Communication

Collective communication

- convenience functions 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

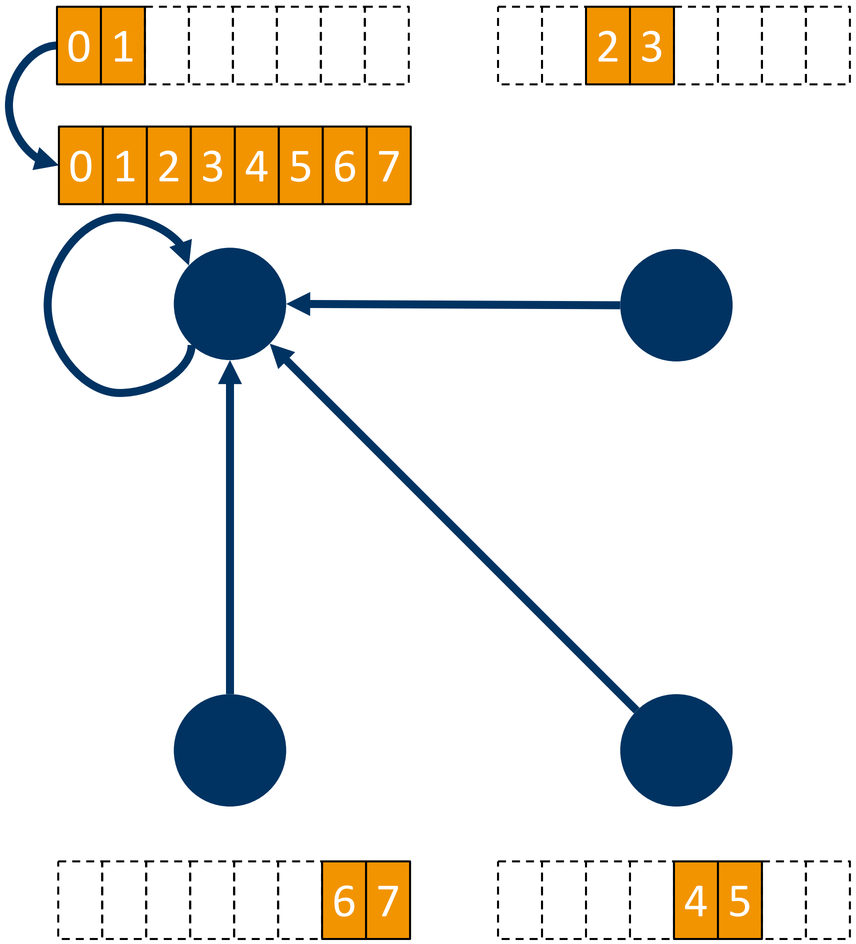
-
  ```
  int MPI_Scatter(const void* sendbuf, int sendcount,
    MPI_Datatype sendtype, void* recvbuf, int recvcount,
    MPI_Datatype recvtype, int root, MPI_Comm comm)
  ```
  - `sendbuf`: source buffer to send data from
  - `sendcount`: number of data elements to send to each rank
  - `sendtype`: 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);
```

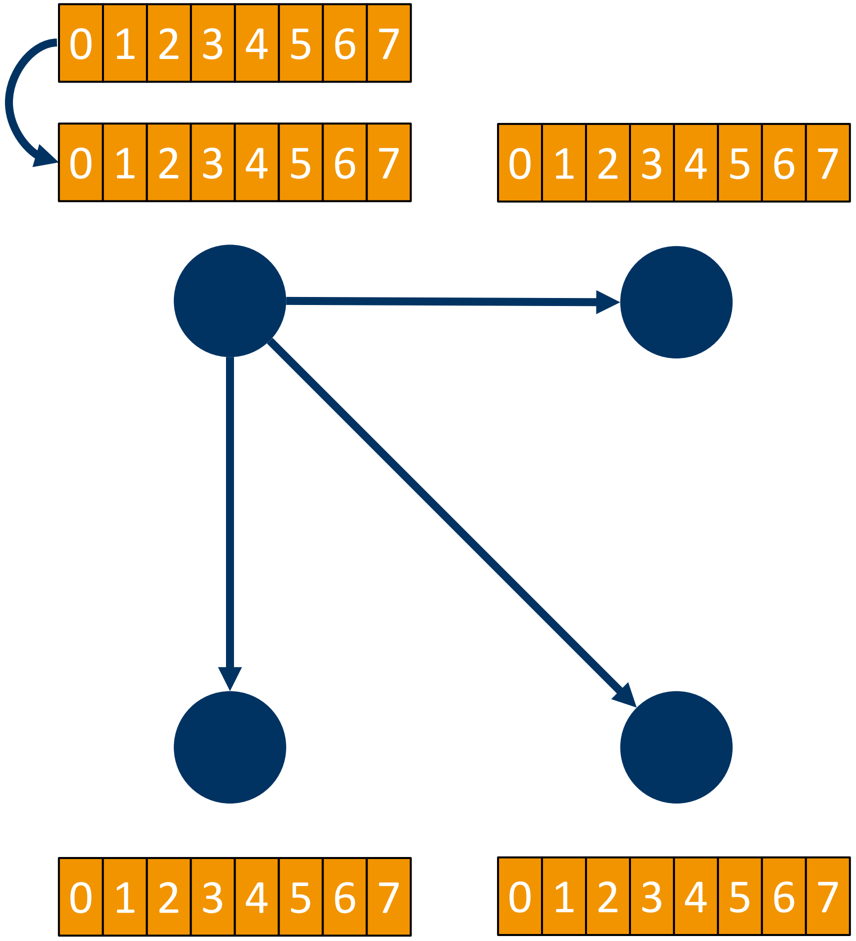
MPI_Gather/MPI_Gatherv

- 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

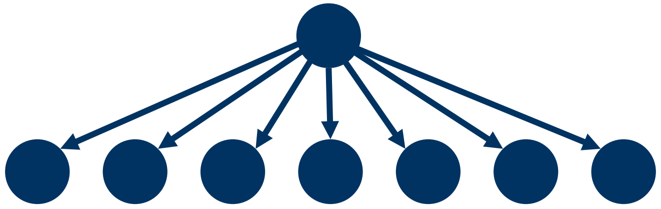


Q: emulating broadcast with point-to-point?

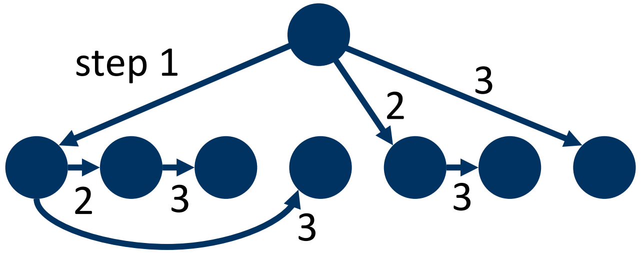
```c
MPI_Bcast(&buf, 1, MPI_INT, 0, MPI_COMM_WORLD);
// ################ or instead: ################
if (rank == 0) {
    for (int i = 0; i < size; i++) {
        if (i != rank) {
            MPI_Send(&buf, 1, MPI_INT, i, 0, MPI_COMM_WORLD);
        }
    }
} else {
    MPI_Recv(&buf, 1, MPI_INT, 0,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

Collective communication patterns

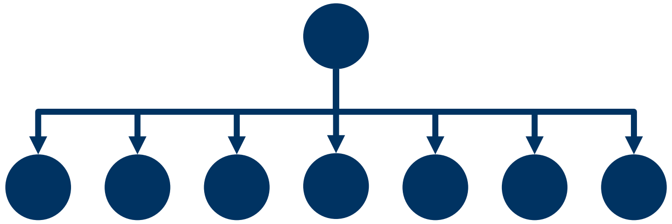
- might be chosen automatically at runtime by MPI implementation
- may depend on multiple parameters, including
  - type of operation (e.g. broadcast)
  - number and location of ranks
  - size and structure of data
  - hardware capabilities



sequential algorithm
O(num_ranks)



tree-based algorithm
e.g. O(log$_2$(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!

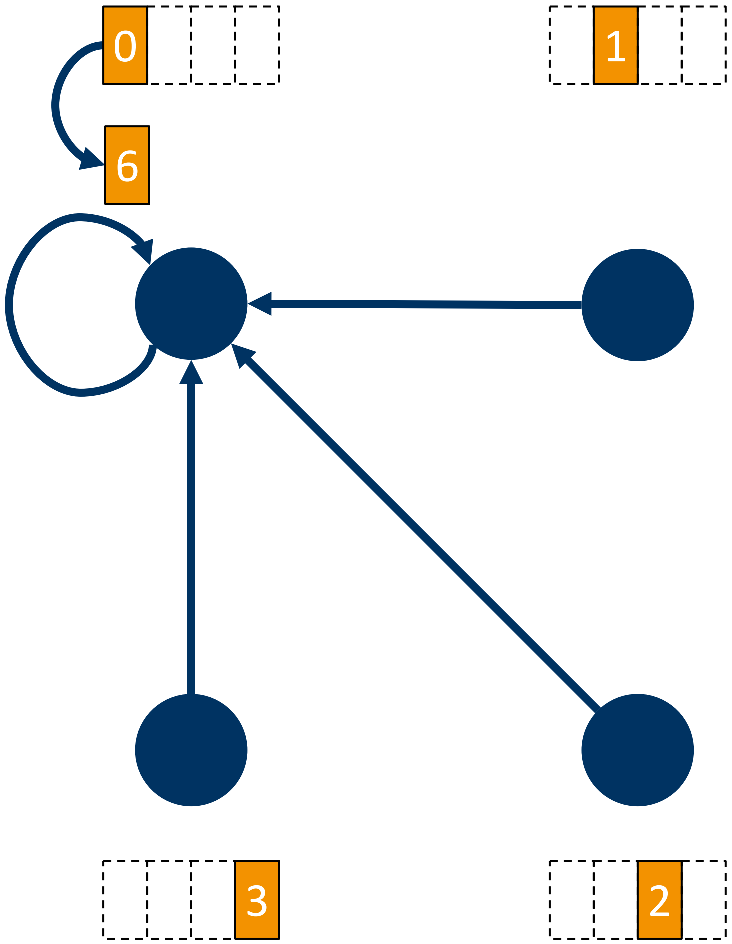
MPI_Reduce

- aggregate data from multiple ranks, including root itself, to root
  - e.g. MPI_SUM
  - may use optimized collective communication patterns

- assumes 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`

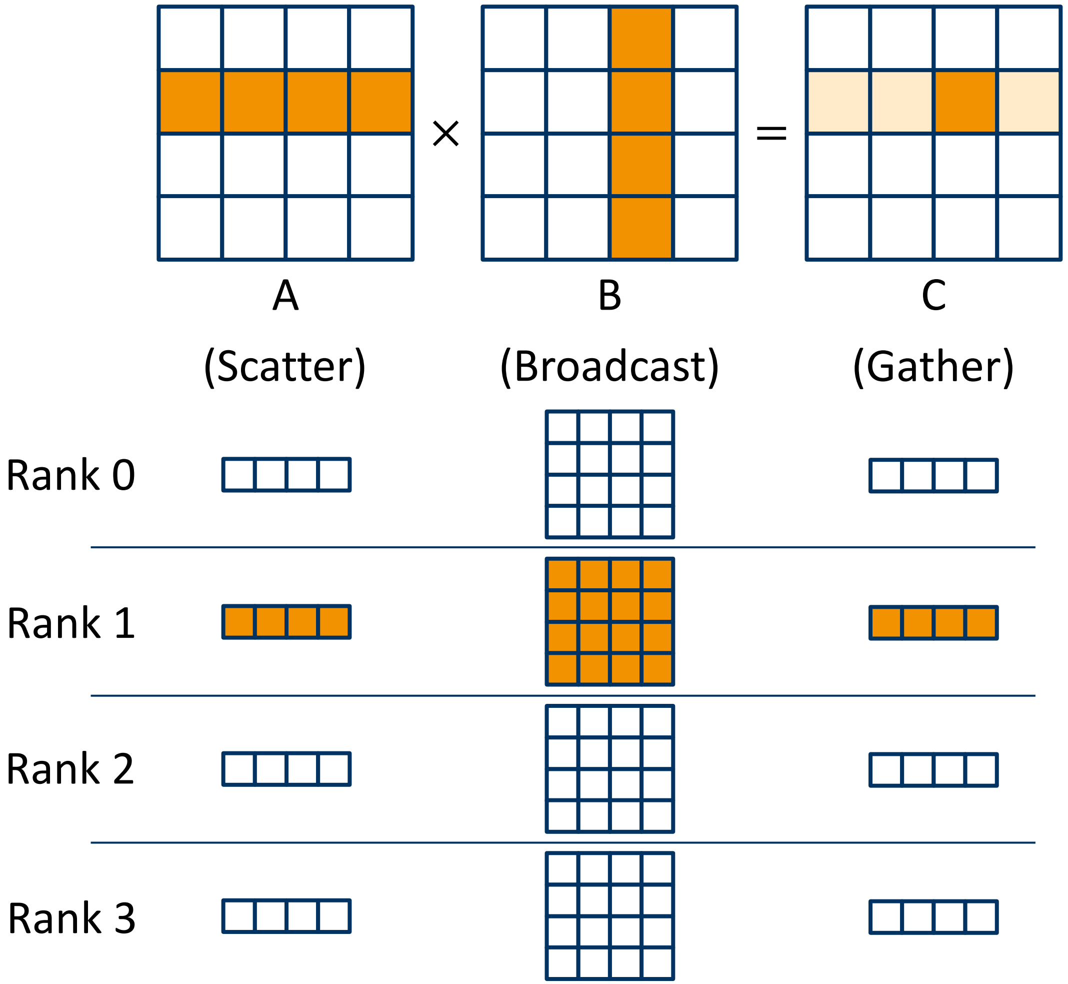
- All pre-defined operations are associative and commutative

- 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



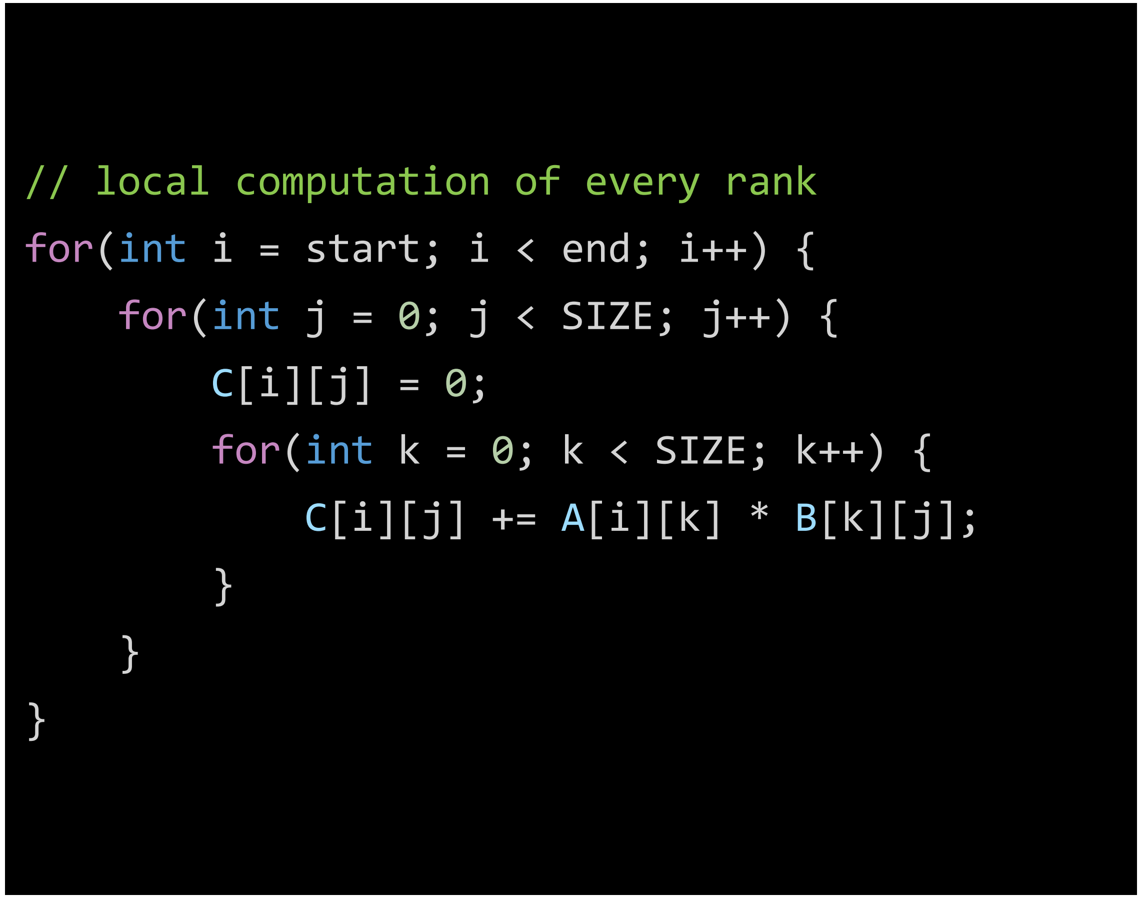
```
#include <mpi.h>
#include <stdio.h>
#include <stdlib.h>

#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

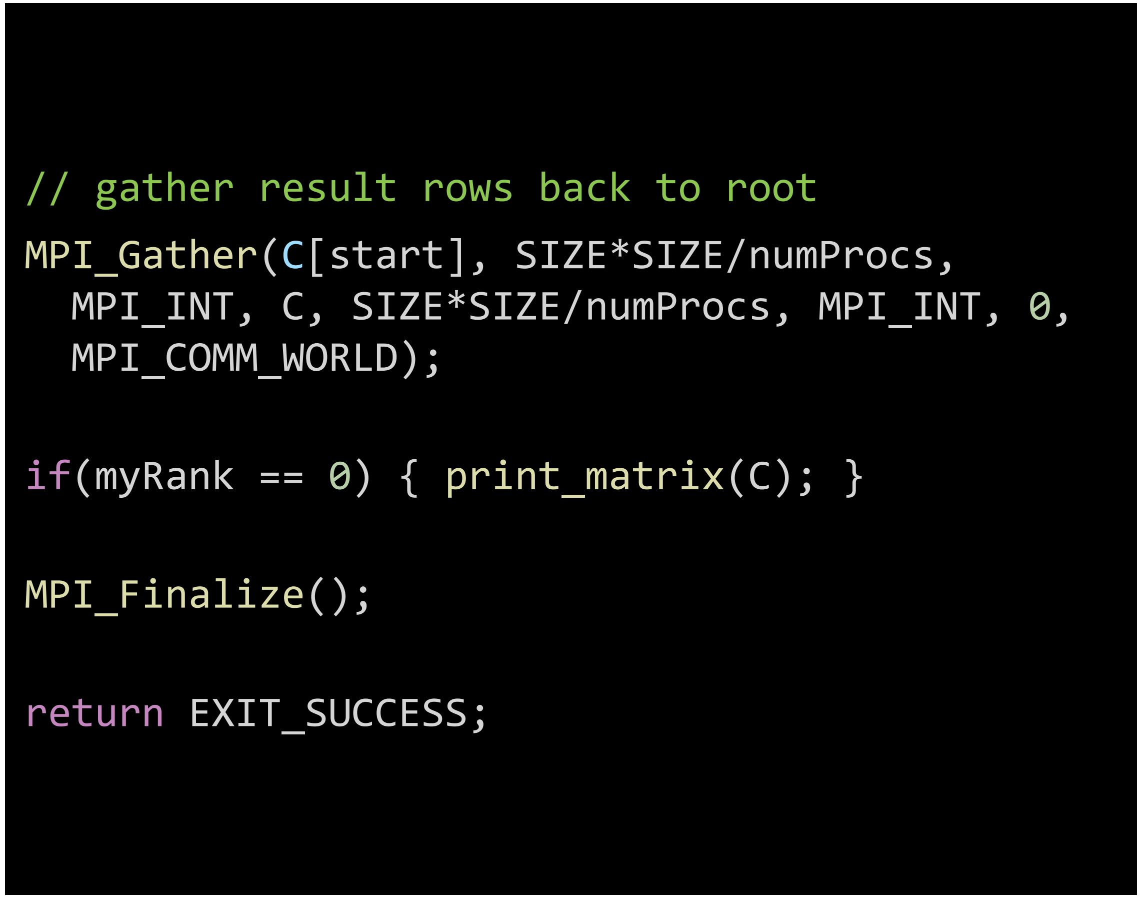
```c
int myRank, numProcs;

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);
}
```

```c
// 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



```
// 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];
        }
    }
}
```



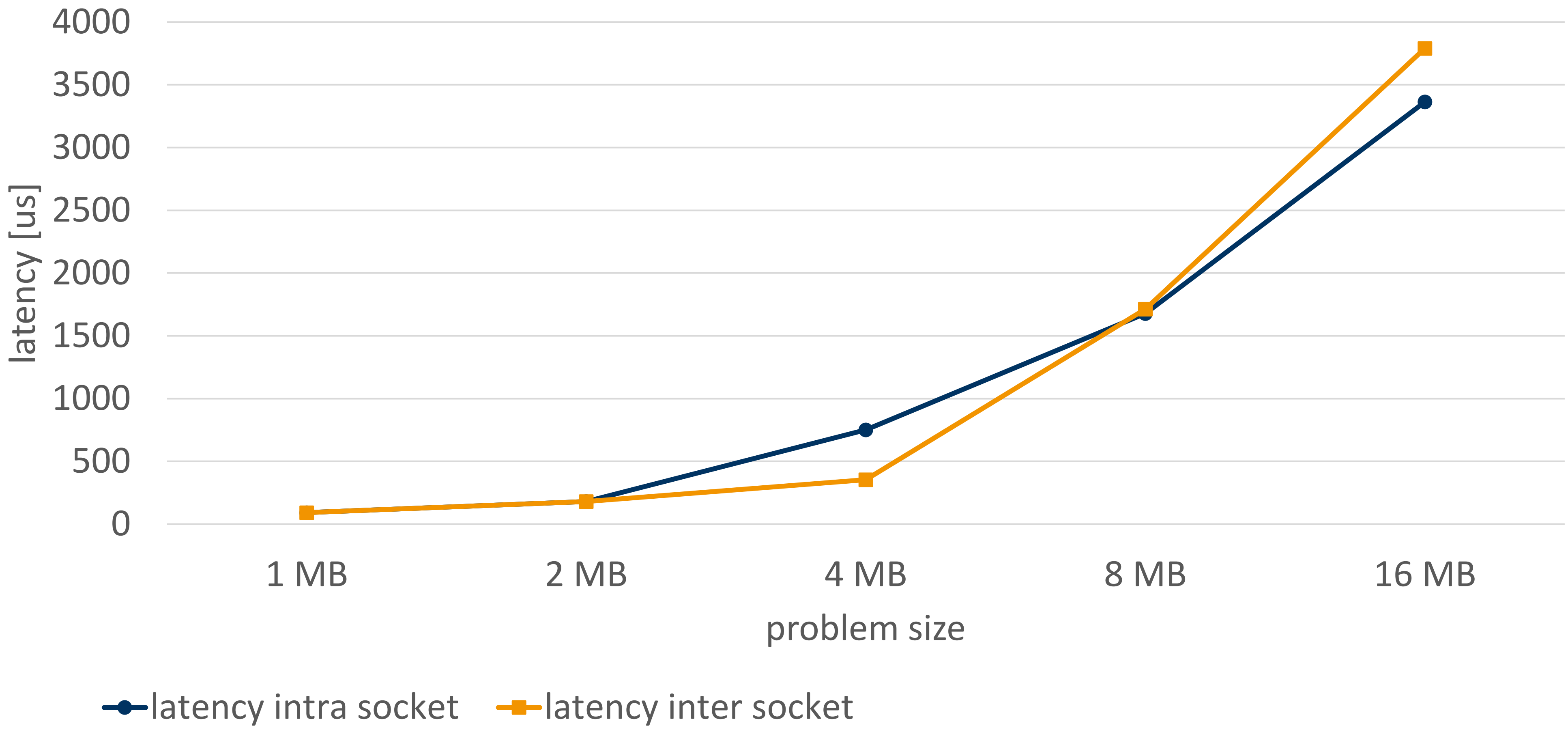
```
// gather result rows back to root
MPI_Gather(C[start], SIZE*SIZE/numProcs,
  MPI_INT, C, SIZE*SIZE/numProcs, MPI_INT, 0,
  MPI_COMM_WORLD);

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

MPI_Finalize();

return EXIT_SUCCESS;
```

Submitting to a cluster (SLURM & SGE)

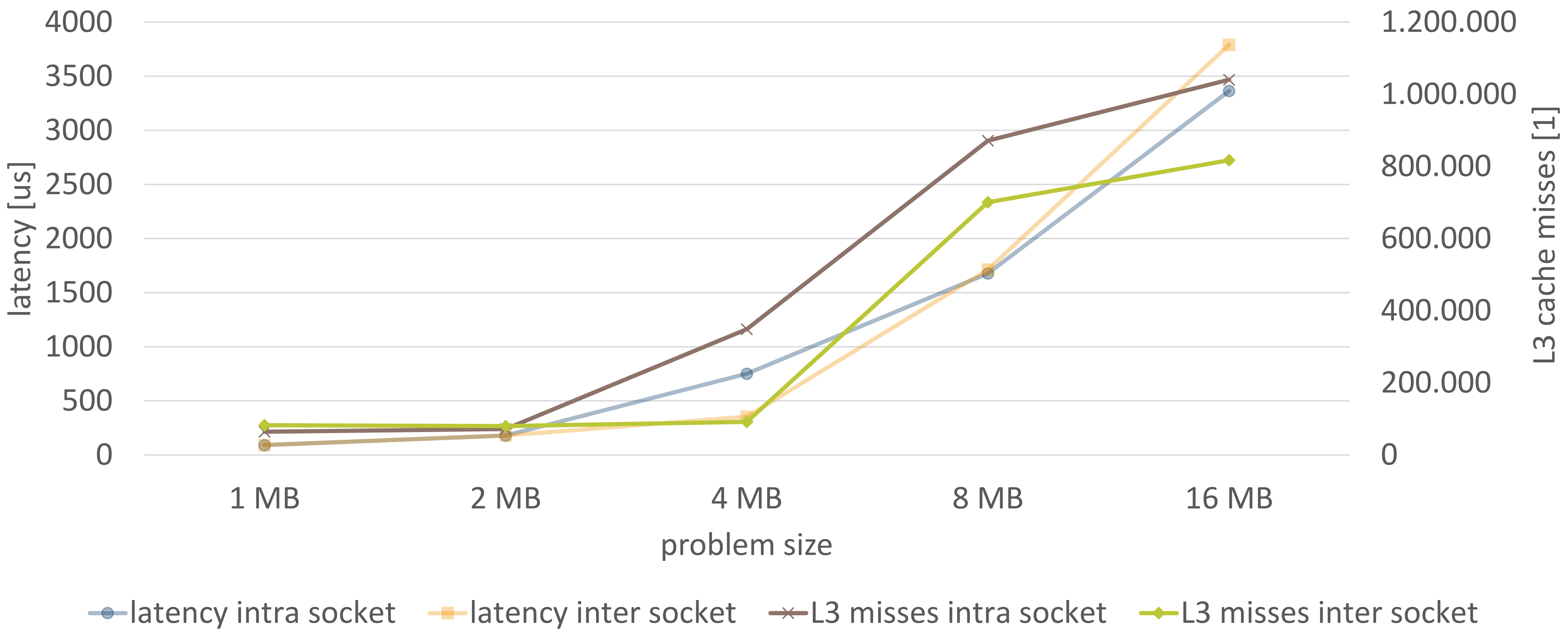
```
#!/bin/bash

# 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
```

Tales from the proseminar: `osu_latency` on LCC3



Tales from the proseminar: `osu_latency` on LCC3



Tales from the proseminar: `osu_latency` on LCC3 (WIP!)

	mpiexec						mpirun						srun					
	intel-mpi_2019.10.317-gcc-8.5.0	openmpi_3.1.6-gcc-12.2.0	openmpi_4.1.4-gcc-12.2.0	openmpi_4.1.4-gcc-8.5.0	openmpi_4.1.4-intel-2021.7.1	openmpi_4.1.4-oneapi-2022.2.1	intel-mpi_2019.10.317-gcc-8.5.0	openmpi_3.1.6-gcc-12.2.0	openmpi_4.1.4-gcc-12.2.0	openmpi_4.1.4-gcc-8.5.0	openmpi_4.1.4-intel-2021.7.1	openmpi_4.1.4-oneapi-2022.2.1	intel-mpi_2019.10.317-gcc-8.5.0	openmpi_3.1.6-gcc-12.2.0	openmpi_4.1.4-gcc-12.2.0	openmpi_4.1.4-gcc-8.5.0	openmpi_4.1.4-intel-2021.7.1	openmpi_4.1.4-oneapi-2022.2.1
0	1,80	1,66	95,88	69,47	28,93	85,42	1,81	1,66	79,14	56,00	97,42	80,42		1,67	71,90	78,34	66,89	92,06
1	1,76	1,63	95,62	70,13	40,54	86,30	1,78	1,63	28,03	86,42	82,59	85,00		1,63	71,16	76,03	83,24	87,43
2	1,78	1,62	94,80	62,64	75,30	86,50	1,77	1,64	26,43	86,48	85,01	77,27		1,63	71,98	78,50	82,65	58,13
4	1,74	1,61	95,21	40,60	95,26	83,93	1,76	1,62	31,36	66,64	93,13	28,45		1,62	73,02	78,09	86,48	75,57
8	1,75	1,62	91,95	34,66	95,93	64,33	1,77	1,62	26,62	25,96	97,88	84,32		1,63	69,35	74,28	86,32	92,21
16	1,75	1,62	94,23	51,73	93,17	86,81	1,76	1,62	27,07	26,12	96,36	84,41		1,63	72,14	69,28	86,04	91,93
32	1,76	1,62	93,55	27,47	94,14	87,76	1,78	1,63	27,01	44,32	99,08	85,11		1,64	72,14	77,91	84,58	89,96
64	1,90	1,76	96,35	60,40	45,49	85,40	1,92	1,76	27,84	87,75	99,55	85,52		1,78	73,94	78,47	87,38	79,77
128	2,53	2,43	96,78	26,83	35,30	88,23	2,53	2,43	67,60	91,09	90,25	88,17		2,41	75,87	80,22	88,34	95,52
256	2,68	2,58	99,64	59,55	34,41	90,81	2,70	2,58	88,90	98,05	101,17	91,23		2,56	80,46	87,47	91,85	98,71
512	2,96	2,86	107,64	82,11	110,03	100,77	2,97	2,86	93,53	103,54	112,58	97,99		2,84	83,85	94,60	97,54	104,10
1024	3,52	3,41	120,97	98,86	106,42	112,24	3,52	3,41	107,47	118,41	126,83	106,49		3,40	97,34	106,20	112,88	114,55
2048	4,54	4,48	113,75	172,84	108,50	146,21	4,55	4,48	144,54	126,49	117,29	141,24		4,44	192,35	153,77	147,66	137,15
4096	6,58	6,57	251,72	256,34	247,65	244,15	6,58	6,58	269,62	230,88	224,56	284,89		6,56	282,53	239,24	275,62	274,82
8192	8,47	8,43	250,83	248,67	250,95	249,15	8,47	8,45	248,30	248,97	254,67	247,43		8,42	261,81	240,03	251,19	250,45
16384	11,12	11,10	328,66	321,86	334,00	323,64	11,14	11,10	332,36	335,69	328,07	333,04		11,12	313,01	340,97	330,24	333,83
32768	16,44	16,17	492,69	483,37	494,25	490,36	16,27	16,16	490,37	497,96	500,31	491,88		16,16	484,16	487,69	501,96	492,64
65536	26,62	26,27	362,85	296,98	260,67	376,14	26,47	26,21	353,66	331,07	265,20	329,14		26,21	390,03	284,66	379,37	318,44
131072	46,24	45,86	488,97	428,50	398,00	460,38	46,22	45,86	445,32	451,03	408,62	420,09		45,79	496,38	427,23	487,01	408,33
262144	85,68	84,46	555,13	491,73	487,80	545,97	85,67	83,83	551,87	518,01	425,43	514,13		84,51	563,26	500,48	551,89	481,68
524288	164,97	161,19	770,21	734,66	662,11	740,81	165,59	161,27	738,98	728,89	666,06	742,23		161,10	762,28	661,29	848,54	703,71
1048576	324,72	315,54	1095,23	958,25	996,85	1057,35	324,32	315,51	1053,36	1037,02	955,35	944,12		315,53	1170,47	998,66	1073,28	1008,58
2097152	625,85	624,34	1874,31	1453,91	1289,10	1763,01	626,02	624,43	1815,92	1769,04	1280,92	1492,41		624,48	2025,38	1390,87	1603,72	1669,82
4194304	1243,62	1243,62	3420,45	2699,88	2327,88	3177,13	1243,86	1243,49	3290,81	2947,66	2329,35	2736,99		1243,16	3706,90	2748,61	2925,97	3087,45

Summary

- general concepts about MPI
  - characteristics
  - programming model
  - startup
- point-to-point communication
- collective communication
- practical example
- Tales from the proseminar: `osu_latency` on LCC3