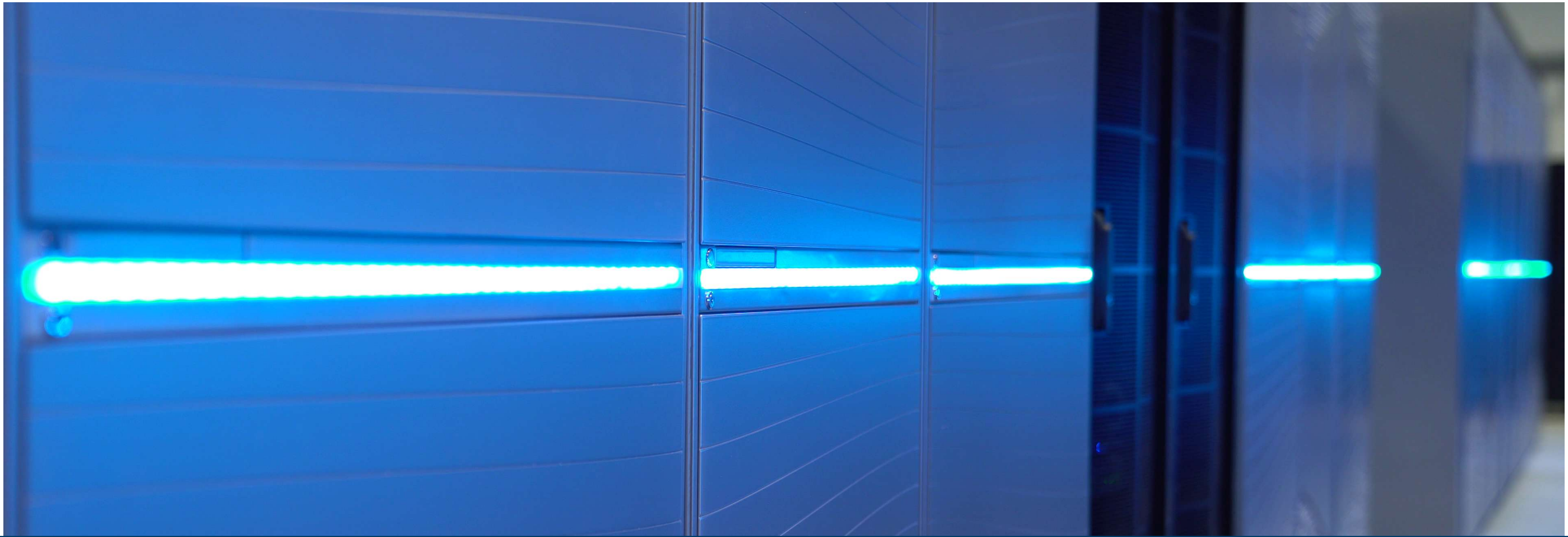

INTRODUCTION TO PARALLEL PROGRAMMING WITH MPI AND OPENMP

14–18 February 2022 | Benedikt Steinbusch | Jülich Supercomputing Centre

JÜLICH Forschungszentrum

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CONTENTS

TIMETABLE

	Day 1	**Day 2**	**Day 3**	**Day 4**	**(Day 5)**
09:00 10:30	Fundamentals of Parallel Computing	Blocking Collective Communication	I/O	First Steps with OpenMP	Tutorial
			☕		
11:00 12:30	First Steps with MPI	Nonblocking Collective Comm.	I/O	Low-Level Constructs	Tutorial
			🍴		
13:30 14:30	Blocking P2P Communication	Derived Datatypes	Tools & Communicators	Loop Worksharing	Tutorial
			☕		
15:00 16:30	Nonblocking P2P Communication	Derived Datatypes	Thread Compliance	Task Worksharing	Tutorial

PART I

FUNDAMENTALS OF PARALLEL COMPUTING

1 MOTIVATION

PARALLEL COMPUTING

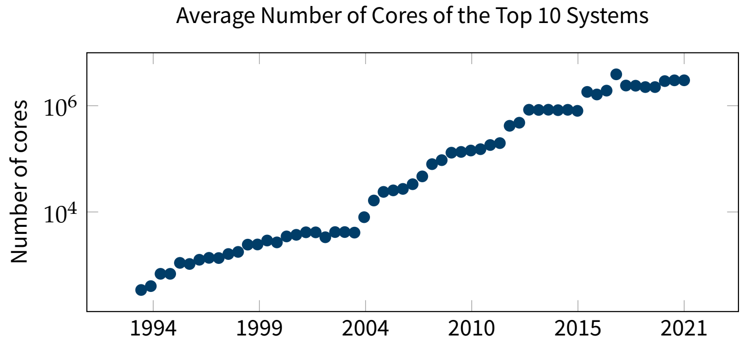
> Parallel computing is a type of computation in which many calculations or the execution of processes are carried out simultaneously. (Wikipedia[1])

WHY AM I HERE?

The Way Forward

- Frequency scaling has stopped
- Performance increase through more parallel hardware
- Treating scientific problems
  - of larger scale
  - in higher accuracy
  - of a completely new kind

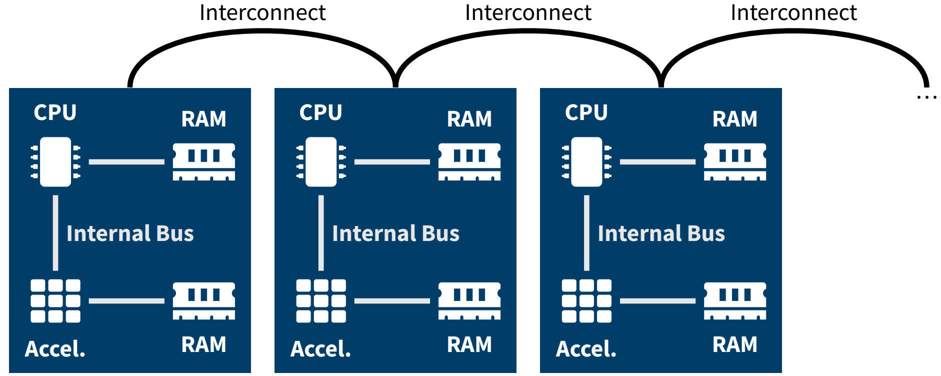
PARALLELISM IN THE TOP 500 LIST



[1]Wikipedia. *Parallel computing — Wikipedia, The Free Encyclopedia*. 2017. URL: `https://en.wikipedia.org/w/index.php?title=Parallel_computing&oldid=787466585` (visited on 06/28/2017).

2 HARDWARE

A MODERN SUPERCOMPUTER



PARALLEL COMPUTATIONAL UNITS

Implicit Parallelism

- Parallel execution of different (parts of) processor instructions
- Happens automatically
- Can only be influenced indirectly by the programmer

Multi-core / Multi-CPU

- Found in commodity hardware today
- Computational units share the same memory

Cluster

- Found in computing centers
- Independent systems linked via a (fast) interconnect
- Each system has its own memory

Accelerators

- Strive to perform certain tasks faster than is possible on a general purpose CPU
- Make different trade-offs
- Often have their own memory
- Often not autonomous

Vector Processors / Vector Units

- Perform same operation on multiple pieces of data simultaneously
- Making a come-back as SIMD units in commodity CPUs (AVX-512) and GPGPU

MEMORY DOMAINS

Shared Memory

- All memory is directly accessible by the parallel computational units
- Single address space
- Programmer might have to synchronize access

Distributed Memory

- Memory is partitioned into parts which are private to the different computational units
- "Remote" parts of memory are accessed via an interconnect
- Access is usually nonuniform

3 SOFTWARE

PROCESSES & THREADS & TASKS

Abstractions for the independent execution of (part of) a program.

Process
Usually, multiple processes, each with their own associated set of resources (memory, file descriptors, etc.), can coexist

Thread

- Typically "smaller" than processes
- Often, multiple threads per one process
- Threads of the same process can share resources

Task

- Typically "smaller" than threads
- Often, multiple tasks per one thread
- Here: user-level construct

DISTRIBUTED STATE & MESSAGE PASSING

Distributed State
Program state is partitioned into parts which are private to the different processes.

Message Passing

- Parts of program state are transferred from one process to another for coordination
- Primitive operations are active send and active receive

MPI

- Implements a form of Distributed State and Message Passing
- (But also Shared State and Synchronization)

SHARED STATE & SYNCHRONIZATION

Shared State
The whole program state is directly accessible by the parallel threads.

Synchronization

- Threads can manipulate shared state using common loads and stores
- Establish agreement about progress of execution using synchronization primitives, e.g. barriers, critical sections, …

OpenMP

- Implements Shared State and Synchronization
- (But also higher level constructs)

PART II

FIRST STEPS WITH MPI

4 WHAT IS MPI?

> MPI (**M**essage-**P**assing **I**nterface) is a message-passing library interface specification. […] MPI addresses primarily the message-passing parallel programming model, in which data is moved from the address space of one process to that of another process through cooperative operations on each process. (MPI Forum[2])

- Industry standard for a message-passing programming model
- Provides *specifications* (no implementations)
- Implemented as a library with language bindings for Fortran and C
- Portable across different computer architectures

[2] Message Passing Interface Forum. *MPI: A Message-Passing Interface Standard*. Version 4.0. June 9, 2021. URL: `https://www.mpi-forum.org/docs/mpi-4.0/mpi40-report.pdf`.

Current version of the standard: 4.0 (June 2021)

BRIEF HISTORY

<1992 several message-passing libraries were developed, PVM, P4,…

1992 At SC92, several developers for message-passing libraries agreed to develop a standard for message-passing

1994 MPI-1.0 standard published

1997 MPI-2.0 standard adds process creation and management, one-sided communication, extended collective communication, external interfaces and parallel I/O

2008 MPI-2.1 combines MPI-1.3 and MPI-2.0

2009 MPI-2.2 corrections and clarifications with minor extensions

2012 MPI-3.0 nonblocking collectives, new one-sided operations, Fortran 2008 bindings

2015 MPI-3.1 nonblocking collective I/O

2021 MPI-4.0 large counts, persistent collective communication, partitioned communication, session model

COVERAGE

1. Introduction to MPI ✓
2. MPI Terms and Conventions ✓
3. Point-to-Point Communication ✓
4. Partitioned Point-to-Point Communication
5. Datatypes ✓
6. Collective Communication ✓
7. Groups, Contexts, Communicators and Caching (✓)
8. Process Topologies (✓)
9. MPI Environmental Management (✓)
10. The `Info` Object
11. Process Initialization, Creation, and Management
12. One-Sided Communications
13. External interfaces (✓)
14. I/O ✓
15. Tool Support
16. …

LITERATURE & ACKNOWLEDGEMENTS

Literature

- Message Passing Interface Forum. *MPI: A Message-Passing Interface Standard*. Version 4.0. June 9, 2021. URL: `https://www.mpi-forum.org/docs/mpi-4.0/mpi40-report.pdf`
- William Gropp, Ewing Lusk, and Anthony Skjellum. *Using MPI. Portable Parallel Programming with the Message-Passing Interface*. 3rd ed. The MIT Press, Nov. 2014. 336 pp. ISBN: 9780262527392
- William Gropp et al. *Using Advanced MPI. Modern Features of the Message-Passing Interface*. 1st ed. Nov. 2014. 392 pp. ISBN: 9780262527637
- `https://www.mpi-forum.org`

Acknowledgements

- Rolf Rabenseifner for his comprehensive course on MPI and OpenMP
- Marc-André Hermanns, Florian Janetzko and Alexander Trautmann for their course material on MPI and OpenMP

5 TERMINOLOGY

PROCESS ORGANIZATION [MPI-4.0, 7.2]

Terminology: Process

An MPI program consists of autonomous processes, executing their own code, in an MIMD style.

Terminology: Rank

A unique number assigned to each process within a group (start at 0)

Terminology: Group

An ordered set of process identifiers

Terminology: Context

A property that allows the partitioning of the communication space

Terminology: Communicator

Scope for communication operations within or between groups, combines the concepts of group and context

OBJECTS [MPI-4.0, 2.5.1]

Terminology: Opaque Objects

Most objects such as communicators, groups, etc. are opaque to the user and kept in regions of memory managed by the MPI library. They are created and marked for destruction using dedicated routines. Objects are made accessible to the user via handle values.

Terminology: Handle

Handles are references to MPI objects. They can be checked for referential equality and copied, however copying a handle does not copy the object it refers to. Destroying an object that has operations pending will not disrupt those operations.

Terminology: Predefined Handles

MPI defines several constant handles to certain objects, e.g. `MPI_COMM_WORLD` a communicator containing all processes initially partaking in a parallel execution of a program.

6 INFRASTRUCTURE

COMPILING & LINKING [MPI-4.0, 19.1.7]

MPI libraries or system vendors usually ship compiler wrappers that set search paths and required libraries, e.g.:

C Compiler Wrappers

```
$ # Generic compiler wrapper shipped with e.g. OpenMPI
$ mpicc foo.c -o foo
$ # Vendor specific wrapper for IBM's XL C compiler on BG/Q
$ bgxlc foo.c -o foo
```

Fortran Compiler Wrappers

```
$ # Generic compiler wrapper shipped with e.g. OpenMPI
$ mpifort foo.f90 -o foo
$ # Vendor specific wrapper for IBM's XL Fortran compiler on BG/Q
$ bgxlf90 foo.f90 -o foo
```

However, neither the existence nor the interface of these wrappers is mandated by the standard.

PROCESS STARTUP [MPI-4.0, 11.5]

The MPI standard does not mandate a mechanism for process startup. It suggests that a command `mpiexec` with the following interface should exist:

Process Startup

```
$ # startup mechanism suggested by the standard
$ mpiexec -n <numprocs> <program>
$ # Slurm startup mechanism as found on JSC systems
$ srun -n <numprocs> <program>
```

LANGUAGE BINDINGS [MPI-4.0, 19, A]

C Language Bindings

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

Fortran Language Bindings

Consistent with F08 standard; good type-checking; highly recommended

```fortran
use mpi_f08
```

Not consistent with standard; so-so type-checking; not recommended

```fortran
use mpi
```

Not consistent with standard; no type-checking; strongly discouraged

```fortran
include 'mpif.h'
```

FORTRAN HINTS [MPI-4.0, 19.1.2 -- 19.1.4]

This course uses the Fortran 2008 MPI interface (**use** `mpi_f08`) which is not available in all MPI implementations. The Fortran 90 bindings differ from the Fortran 2008 bindings in the following points:

- All derived **type** arguments are instead **integer** (some are arrays of **integer** or have a non-default `kind`)
- Argument **intent** is not mandated by the Fortran 90 bindings
- The `ierror` argument is mandatory instead of **optional**
- Further details can be found in [MPI-4.0, 19.1]

MPI4PY HINTS

All exercises in the MPI part can be solved using Python with the `mpi4py` package. The slides do not show Python syntax, so here is a translation guide from the standard bindings to `mpi4py`.

- Everything lives in the `MPI` module (**from mpi4py import** `MPI`).

- Constants translate to attributes of that module: `MPI_COMM_WORLD` is `MPI.COMM_WORLD`.
- Central types translate to Python classes: `MPI_Comm` is `MPI.Comm`.
- Functions related to point-to-point and collective communication translate to methods on `MPI.Comm`: `MPI_Send` becomes `MPI.Comm.Send`.
- Functions related to I/O translate to methods on `MPI.File`: `MPI_File_write` becomes `MPI.File.Write`.
- Communication functions come in two flavors:
  - high level, uses `pickle` to (de)serialize python objects, method names start with lower case letters, e.g. `MPI.Comm.send`,
  - low level, uses MPI Datatypes and Python buffers, method names start with upper case letters, e.g. `MPI.Comm.Scatter`.

See also `https://mpi4py.readthedocs.io` and the built-in Python `help()`.

OTHER LANGUAGE BINDINGS

Besides the official bindings for C and Fortran mandated by the standard, unofficial bindings for other programming languages exist:

C++ Boost.MPI

MATLAB Parallel Computing Toolbox

Python pyMPI, mpi4py, pypar, MYMPI, …

R Rmpi, pdbMPI

julia MPI.jl

.NET MPI.NET

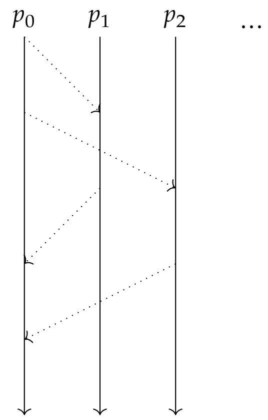
Java mpiJava, MPJ, MPJ Express

And many others, ask your favorite search engine.

7 BASIC PROGRAM STRUCTURE

WORLD ORDER IN MPI

- Program starts as N distinct processes.
- Stream of instructions might be different for each process.
- Each process has access to its own private memory.
- Information is exchanged between processes via messages.
- Processes may consist of multiple threads (see OpenMP part on day 4).



INITIALIZATION [MPI-4.0, 11.2.1, 11.2.3]

Initialize MPI library, needs to happen before most other MPI functions can be used

C
```c
int MPI_Init(int *argc, char ***argv)
```

F08
```fortran
MPI_Init(ierror)
integer, optional, intent(out) :: ierror
```

Exception (can be used before initialization)

C
```c
int MPI_Initialized(int* flag)
```

F08
```fortran
MPI_Initialized(flag, ierror)
logical, intent(out) :: flag
integer, optional, intent(out) :: ierror
```

FINALIZATION [MPI-4.0, 11.2.2, 11.2.3]

Finalize MPI library when you are done using its functions

C
```c
int MPI_Finalize(void)
```

F08
```fortran
MPI_Finalize(ierror)
integer, optional, intent(out) :: ierror
```

Exception (can be used after finalization)

C
```c
int MPI_Finalized(int *flag)
```

F08
```fortran
MPI_Finalized(flag, ierror)
logical, intent(out) :: flag
integer, optional, intent(out) :: ierror
```

PREDEFINED COMMUNICATORS

After `MPI_Init` has been called, `MPI_COMM_WORLD` is a valid handle to a predefined communicator that includes all processes available for communication. Additionally, the handle `MPI_COMM_SELF` is a communicator that is valid on each process and contains only the process itself.

C
```c
MPI_Comm MPI_COMM_WORLD;
MPI_Comm MPI_COMM_SELF;
```

F08
```fortran
type(MPI_Comm) :: MPI_COMM_WORLD
type(MPI_Comm) :: MPI_COMM_SELF
```

COMMUNICATOR SIZE [MPI-4.0, 7.4.1]

Determine the total number of processes in a communicator

C
```c
int MPI_Comm_size(MPI_Comm comm, int *size)
```

F08
```fortran
MPI_Comm_size(comm, size, ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(out) :: size
integer, optional, intent(out) :: ierror
```

Examples

C
```c
int size;
int ierror = MPI_Comm_size(MPI_COMM_WORLD, &size);
```

F08
```fortran
integer :: size
call MPI_Comm_size(MPI_COMM_WORLD, size)
```

PROCESS RANK [MPI-4.0, 7.4.1]

Determine the rank of the calling process within a communicator

C
```c
int MPI_Comm_rank(MPI_Comm comm, int *rank)
```

F08
```fortran
MPI_Comm_rank(comm, rank, ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(out) :: rank
integer, optional, intent(out) :: ierror
```

Examples

C
```c
int rank;
int ierror = MPI_Comm_rank(MPI_COMM_WORLD, &rank);
```

F08
```fortran
integer :: rank
call MPI_Comm_rank(MPI_COMM_WORLD, rank)
```

ERROR HANDLING [MPI-4.0, 9.3, 9.4, 9.5]

- Flexible error handling through error handlers which can be attached to
  - Communicators
  - Files
  - Windows (not part of this course)
- Error handlers can be

  `MPI_ERRORS_ARE_FATAL` Errors encountered in MPI routines abort execution

  `MPI_ERRORS_RETURN` An error code is returned from the routine

  Custom error handler A user supplied function is called on encountering an error
- By default
  - Communicators use `MPI_ERRORS_ARE_FATAL`
  - Files use `MPI_ERRORS_RETURN`
  - Windows use `MPI_ERRORS_ARE_FATAL`

8 EXERCISES

EXERCISE STRATEGIES

Solving

- Do not have to solve all exercises, one per section would be good
- Exercise description tells you what MPI functions/OpenMP directives to use
- Work in pairs on harder exercises
- If you get stuck
  - ask us
  - peek at solution
- `CMakeLists.txt` is included

Solutions
`exercises/{C|C++|Fortran|Python}/`:

- Most of the algorithm is there, you add MPI/OpenMP

`hard` Almost empty files you add algorithm and MPI/OpenMP

`solutions` Fully solved exercises, if you are completely stuck or for comparison

EXERCISES

Exercise 1 – First Steps
1.1 Output of Ranks

Write a program `print_rank.{c|cxx|f90|py}` that has each process printing its rank.

```
I am process 0
I am process 1
I am process 2
```

Use: `MPI_Init`, `MPI_Finalize`, `MPI_Comm_rank`

1.2 Output of ranks and total number of processes

Write a program `print_rank_conditional.{c|cxx|f90|py}` in such a way that process 0 writes out the total number of processes

```
I am process 0 of 3
I am process 1
I am process 2
```

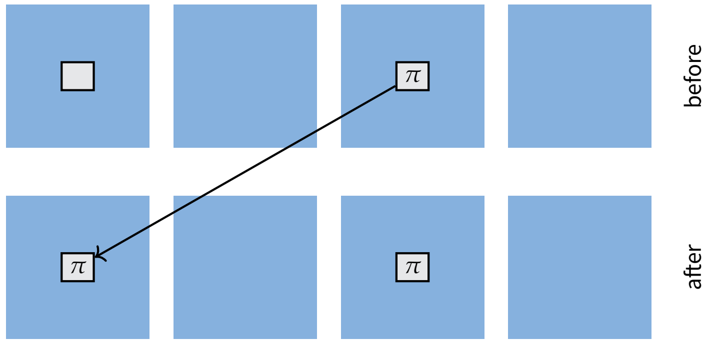
Use: `MPI_Comm_size`

PART III

BLOCKING POINT-TO-POINT COMMUNICATION

9 INTRODUCTION

MESSAGE PASSING



BLOCKING & NONBLOCKING PROCEDURES

Terminology: Blocking

A procedure is blocking if return from the procedure indicates that the user is allowed to reuse resources specified in the call to the procedure.

Terminology: Nonblocking

If a procedure is nonblocking it will return as soon as possible. However, the user is not allowed to reuse resources specified in the call to the procedure before the communication has been completed using an appropriate completion procedure.

Examples:

- Blocking: Telephone call ☎
- Nonblocking: Email @

PROPERTIES

- Communication between two processes within the same communicator

  Caution: A process can send messages to itself.
- A *source* process sends a message to a destination process using an MPI *send* routine

- A *destination* process needs to post a receive using an MPI *receive* routine
- The source process and the destination process are specified by their ranks in the communicator
- Every message sent with a point-to-point operation needs to be matched by a receive operation

10 SENDING

SENDING MESSAGES [MPI-4.0, 3.2.1]

*
```
MPI_Send( <buffer>, <destination> )
```

C
```c
int MPI_Send(const void* buf, int count, MPI_Datatype datatype,
↪ int dest, int tag, MPI_Comm comm)
```

F08
```fortran
MPI_Send(buf, count, datatype, dest, tag, comm, ierror)
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count, dest, tag
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

MESSAGES [MPI-4.0, 3.2.2, 3.2.3]

A message consists of two parts:

Terminology: Envelope

- Source process `source`
- Destination process `dest`
- Tag `tag`
- Communicator `comm`

Terminology: Data

Message data is read from/written to buffers specified by:

- Address in memory `buf`
- Number of elements found in the buffer `count`
- Structure of the data `datatype`

DATA TYPES [MPI-4.0, 3.2.2, 3.3, 5.1]

Terminology: Data Type

Describes the structure of a piece of data

Terminology: Basic Data Types

Named by the standard, most correspond to basic data types of C or Fortran

C type	MPI basic data type
signed int	`MPI_INT`
float	`MPI_FLOAT`
char	`MPI_CHAR`
…	

Fortran type	MPI basic data type
integer	`MPI_INTEGER`
real	`MPI_REAL`
character	`MPI_CHARACTER`
…	

Terminology: Derived Data Type

Data types which are not basic datatypes. These can be constructed from other (basic or derived) datatypes.

DATA TYPE MATCHING [MPI-4.0, 3.3]

Terminology: Untyped Communication

- Contents of send and receive buffers are declared as `MPI_BYTE`.
- Actual contents of buffers can be any type (possibly different).
- Use with care.

Terminology: Typed Communication

- Type of buffer contents must match MPI data type (e.g. in C **`int`** and `MPI_INT`).
- Data type on send must match data type on receive operation.
- Allows data conversion when used on heterogeneous systems.

Terminology: Packed data

See [MPI-4.0, 5.2]

11 EXERCISES

Exercise 2 – Point-to-Point Communication
2.1 Send

In the file `send_receive.{c|cxx|f90|py}` implement the function/subroutine `send(msg, dest)`. It should use `MPI_Send` to send the integer `msg` to the process with rank number `dest` in `MPI_COMM_WORLD`. For the tag value, use the answer to the ultimate question of life, the universe, and everything (42)[3].

Use: `MPI_Send`

12 RECEIVING

RECEIVING MESSAGES [MPI-4.0, 3.2.4]

```
MPI_Recv( <buffer>, <source> ) -> <status>
```

```c
int MPI_Recv(void* buf, int count, MPI_Datatype datatype, int
    source, int tag, MPI_Comm comm, MPI_Status *status)
```

```fortran
MPI_Recv(buf, count, datatype, source, tag, comm, status,
    ierror)
type(*), dimension(..) :: buf
integer, intent(in) :: count, source, tag
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- `count` specifies the *capacity* of the buffer
- Wildcard values are permitted (`MPI_ANY_SOURCE` & `MPI_ANY_TAG`)

THE MPI_STATUS TYPE [MPI-4.0, 3.2.5]

Contains information about received messages

```c
MPI_Status status;
status.MPI_SOURCE
status.MPI_TAG
status.MPI_ERROR
```

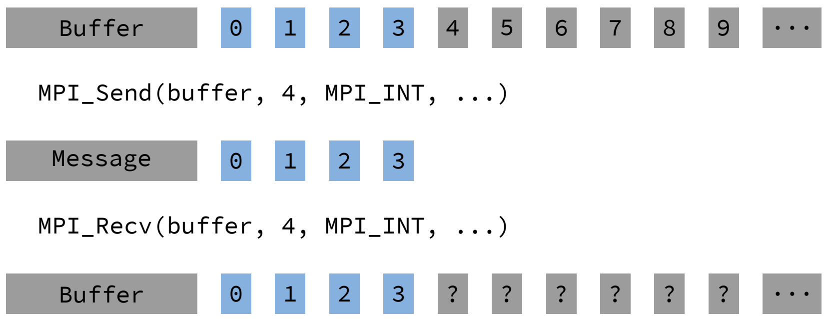
```fortran
type(MPI_status) :: status
status%MPI_SOURCE
status%MPI_TAG
status%MPI_ERROR
```

```c
int MPI_Get_count(const MPI_Status *status, MPI_Datatype
    datatype, int *count)
```

```fortran
MPI_Get_count(status, datatype, count, ierror)
type(MPI_Status), intent(in) :: status
type(MPI_Datatype), intent(in) :: datatype
integer, intent(out) :: count
integer, optional, intent(out) :: ierror
```

Pass `MPI_STATUS_IGNORE` to `MPI_Recv` if not interested.

MESSAGE ASSEMBLY



PROBE [MPI-4.0, 3.8.1]

```
MPI_Probe( <source> ) -> <status>
```

```c
int MPI_Probe(int source, int tag, MPI_Comm comm, MPI_Status
    *status)
```

```fortran
MPI_Probe(source, tag, comm, status, ierror)
integer, intent(in) :: source, tag
type(MPI_Comm), intent(in) :: comm
type(MPI_Status), intent(out) :: status
integer, optional, intent(out) :: ierror
```

Returns after a matching message is ready to be received.

- Same rules for message matching as receive routines
- Wildcards permitted for `source` and `tag`

[3]Douglas Adams. *The Hitchhiker's Guide to the Galaxy*. Pan Books, Oct. 12, 1979. ISBN: 0-330-25864-8.

- `status` contains information about message (e.g. number of elements)

13 EXERCISES

2.2 Receive

In the file `send_receive.{c|cxx|f90|py}` implement the function `recv(source)`. It should use `MPI_Recv` to receive a single integer from the process with rank number `source` in `MPI_COMM_WORLD`. Any tag value should be accepted. Use the received integer as the return value of `recv`. If you are not interested in the status value, use `MPI_STATUS_IGNORE`.

Use: `MPI_Recv`

14 COMMUNICATION MODES

SEND MODES [MPI-4.0, 3.4]

Synchronous send: `MPI_Ssend`
Only completes when the receive has started.

Buffered send: `MPI_Bsend`

- May complete before a matching receive is posted
- Needs a user-supplied buffer (see `MPI_Buffer_attach`)

Standard send: `MPI_Send`

- Either synchronous or buffered, leaves decision to MPI
- If buffered, an internal buffer is used

Ready send: `MPI_Rsend`

- Asserts that a matching receive has already been posted (otherwise generates an error)
- Might enable more efficient communication

RECEIVE MODES [MPI-4.0, 3.4]

Only one receive routine for all send modes:

Receive: `MPI_Recv`

- Completes when a message has arrived and message data has been stored in the buffer
- Same routine for all communication modes

All blocking routines, both send and receive, guarantee that buffers can be reused after control returns.

15 LARGE NUMBERS

LARGE COUNT AND LARGE BYTE DISPLACEMENT [MPI-4.0, 19.2]

Use of **`int`**/**`integer`** and `MPI_Aint`/**`integer`**`(MPI_ADDRESS_KIND)` problematic in certain situations.

New conventions for datatype use

- *Count* type arguments use the `MPI_Count`/**`integer`**`(MPI_COUNT_KIND)` datatype.
- *Byte displacements* are represented as
  - `MPI_Aint`/**`integer`**`(MPI_ADDRESS_KIND)` when applied to memory
  - `MPI_Offset`/**`integer`**`(MPI_OFFSET_KIND)` when applied to files
  - `MPI_Count`/**`integer`**`(MPI_COUNT_KIND)` when applied to either files or memory

Implementation strategy

- Procedures added beginning with MPI-4.0 follow the new conventions.
- Procedures which existed before MPI-4.0
  - in C get a counterpart with a `_c` suffix in the function name that follows the new convention
  - with **`use`** `mpi_f08` get a specific routine under the same generic name that follows the new convention
  - with **`use`** `mpi` and **`include`** `'mpif.h'` get no updated version.

LARGE COUNT EXAMPLE

```c
int MPI_Send(const void* buf, int count, MPI_Datatype datatype,
    int dest, int tag, MPI_Comm comm)

int MPI_Send_c(const void* buf, MPI_Count count, MPI_Datatype
    datatype, int dest, int tag, MPI_Comm comm)
```

```fortran
MPI_Send(buf, count, datatype, dest, tag, comm, ierror)
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count, dest, tag
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror

MPI_Send(buf, count, datatype, dest, tag, comm, ierror)
type(*), dimension(..), intent(in) :: buf
integer(MPI_COUNT_KIND), intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
integer, intent(in) :: dest, tag
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

F08

16 SEMANTICS

POINT-TO-POINT SEMANTICS [MPI-4.0, 3.5]

Order
In single threaded programs, messages are non-overtaking. Between any pair of processes, messages will be received in the order they were sent.

Progress
Out of a pair of matching send and receive operations, at least one is guaranteed to complete.

Fairness
Fairness is not guaranteed by the MPI standard.

Resource limitations
Resource starvation may lead to deadlock, e.g. if progress relies on availability of buffer space for standard mode sends.

17 PITFALLS

DEADLOCK

Structure of program prevents blocking routines from ever completing, e.g.:

Process 0

```fortran
call MPI_Ssend(..., 1, ...)
call MPI_Recv(..., 1, ...)
```

Process 1

```fortran
call MPI_Ssend(..., 0, ...)
call MPI_Recv(..., 0, ...)
```

Mitigation Strategies

- Changing communication structure (e.g. checkerboard)
- Using `MPI_Sendrecv`
- Using nonblocking routines

18 EXERCISES

2.3 Global Summation – Ring

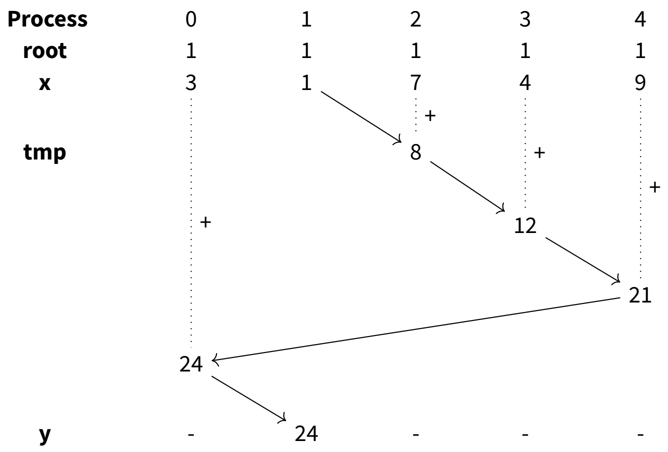
In the file `global_sum.{c|cxx|f90|py}` implement the function/subroutine `global_sum_ring(x, y, root, comm)`. It will be called by all processes on the communicator `comm` and on each one accepts an integer `x`. It should compute the global sum of all values of `x` across all processes and return the result in `y` (as the function return value in Python) only on the process with rank `root`.

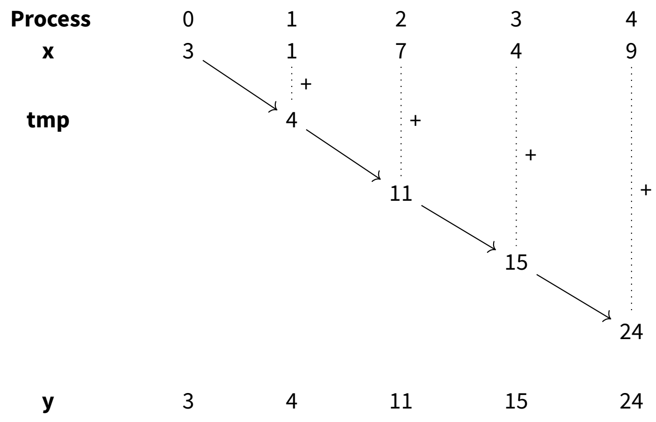
Use the following strategy:

1. The process with rank `root` starts by sending its value of `x` to the process with the next higher rank (wrap around to rank 0 on the process with the highest rank).
2. All other processes start by receiving the partial sum from the process with the next lower rank (or from the process with the highest rank on process 0)
3. Next, they add their value of `x` to the partial result and send it to the next process.
4. The `root` process eventually receives the global result which it will return in `y`.

The file contains a small `main()` function / **`program`** that can be used to test whether your implementation works.

Use: `MPI_Send`, `MPI_Recv` (and maybe `MPI_Sendrecv`)





Bonus

In the file `global_prefix_sum.{c|cxx|f90|py}` implement the function/subroutine `global_prefix_sum_ring(x, y, comm)`. It will be called by all processes on the communicator `comm` and on each one accepts an integer `x`. It should compute the global prefix sum of all values of `x` across all processes and return the results in `y` (as the function return value in Python), i.e. the `y` returned on a process is the sum of all the `x` contributed by processes with lower rank number and its own.

Use the following strategy:

1. Every process except for the one with rank 0 receives a partial result from the process with the next lower rank number
2. Add the local `x` to the partial result
3. Send the partial result to the process with the next higher rank number (except on the process with the highest rank number)
4. Return the partial result in `y`

The file contains a small `main()` function / **`program`** that can be used to test whether your implementation works.

Use: `MPI_Send`, `MPI_Recv`

PART IV

NONBLOCKING POINT-TO-POINT COMMUNICATION

19 INTRODUCTION

RATIONALE [MPI-4.0, 3.7]

Premise
Communication operations are split into *start* and *completion*. The *start* routine produces a *request handle* that represents the in-flight operation and is used in the *completion* routine. The user promises to refrain from accessing the contents of message buffers while the operation is in flight.

Benefit
A single process can have multiple nonblocking operations in flight at the same time. This enables communication patterns that would lead to deadlock if programmed using blocking variants of the same operations. Also, the additional leeway given to the MPI library *may* be utilized to, e.g.:

- overlap computation and communication
- overlap communication
- pipeline communication
- elide usage of buffers

20 START

INITIATION ROUTINES [MPI-4.0, 3.7.2]

Send

Synchronous `MPI_Issend`

Standard `MPI_Isend`

Buffered `MPI_Ibsend`

Ready `MPI_Irsend`

Receive

`MPI_Irecv`

Probe

`MPI_Iprobe`

- "I" is for immediate.
- Signature is similar to blocking counterparts with additional *request* object.
- Initiate operations and relinquish access rights to any buffer involved.

NONBLOCKING SEND [MPI-4.0, 3.7.2]

```
MPI_Isend( <buffer>, <destination> ) -> <request>
```

```c
int MPI_Isend(const void* buf, int count, MPI_Datatype
    datatype, int dest, int tag, MPI_Comm comm, MPI_Request
    *request)
```

```fortran
MPI_Isend(buf, count, datatype, dest, tag, comm, request,
    ierror)
type(*), dimension(..), intent(in), asynchronous :: buf
integer, intent(in) :: count, dest, tag
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
type(MPI_Request), intent(out) :: request
integer, optional, intent(out) :: ierror
```

NONBLOCKING RECEIVE [MPI-4.0, 3.7.2]

```
MPI_Irecv( <buffer>, <source> ) -> <request>
```

```c
int MPI_Irecv(void* buf, int count, MPI_Datatype datatype, int
    source, int tag, MPI_Comm comm, MPI_Request *request)
```

```fortran
MPI_Irecv(buf, count, datatype, source, tag, comm, request,
    ierror)
type(*), dimension(..), asynchronous :: buf
integer, intent(in) :: count, source, tag
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
type(MPI_Request), intent(out) :: request
integer, optional, intent(out) :: ierror
```

NONBLOCKING PROBE [MPI-4.0, 3.8.1]

```
MPI_Iprobe( <source> ) -> <status>?
```

```c
int MPI_Iprobe(int source, int tag, MPI_Comm comm, int *flag,
    MPI_Status *status)
```

```fortran
MPI_Iprobe(source, tag, comm, flag, status, ierror)
integer, intent(in) :: source, tag
type(MPI_Comm), intent(in) :: comm
logical, intent(out) :: flag
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Does not follow start/completion model.
- Uses true/false flag to indicate availability of a message.

21 COMPLETION

WAIT [MPI-4.0, 3.7.3]

```
MPI_Wait( <request> ) -> <status>
```

```c
int MPI_Wait(MPI_Request *request, MPI_Status *status)
```

```fortran
MPI_Wait(request, status, ierror)
type(MPI_Request), intent(inout) :: request
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Blocks until operation associated with `request` is completed
- To wait for the completion of several pending operations

  `MPI_Waitall` All events complete

  `MPI_Waitsome` At least one event completes

  `MPI_Waitany` Exactly one event completes

TEST [MPI-4.0, 3.7.3]

```
MPI_Test( <request> ) -> <status>?
```

```c
int MPI_Test(MPI_Request *request, int *flag, MPI_Status
    *status)
```

```fortran
MPI_Test(request, flag, status, ierror)
type(MPI_Request), intent(inout) :: request
logical, intent(out) :: flag
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Does not block
- `flag` indicates whether the associated operation has completed
- Test for the completion of several pending operations

  `MPI_Testall` All events complete

  `MPI_Testsome` At least one event completes

  `MPI_Testany` Exactly one event completes

FREE [MPI-4.0, 3.7.3]

```
MPI_Request_free( <request> )
```

```c
int MPI_Request_free(MPI_Request *request)
```

```fortran
MPI_Request_free(request, ierror)
type(MPI_Request), intent(inout) :: request
integer, optional, intent(out) :: ierror
```

- Marks the request for deallocation
- Invalidates the request handle
- Operation is allowed to complete
- Completion cannot be checked for

CANCEL [MPI-4.0, 3.8.4]

```
MPI_Cancel( <request> )
```

```c
int MPI_Cancel(MPI_Request *request)
```

```fortran
MPI_Cancel(request, ierror)
type(MPI_Request), intent(in) :: request
integer, optional, intent(out) :: ierror
```

- Marks an operation for cancellation
- Request still has to be completed via `MPI_Wait`, `MPI_Test` or `MPI_Request_free`
- Operation is either cancelled completely or succeeds (indicated in status value)

22 REMARKS

BLOCKING VS. NONBLOCKING OPERATIONS

- A blocking send can be paired with a nonblocking receive and vice versa
- Nonblocking sends can use any mode, just like the blocking counterparts
  - Synchronization of `MPI_Issend` is enforced at completion (wait or test)
  - Asserted readiness of `MPI_Irsend` must hold at start of operation
- A nonblocking operation immediately followed by a matching wait is equivalent to the blocking operation

The Fortran Language Bindings and nonblocking operations

- Arrays with subscript triplets (e.g. `a(1:100:5)`) can only be reliably used as buffers if the compile time constant `MPI_SUBARRAYS_SUPPORTED` equals `.true.` [MPI-4.0, 19.1.12]
- Arrays with vector subscripts must not be used as buffers [MPI-4.0, 19.1.13]
- Fortran compilers may optimize your program beyond the point of being correct. Communication buffers should be protected by the **`asynchronous`** attribute (make sure `MPI_ASYNC_PROTECTS_NONBLOCKING` is `.true.`) [MPI-4.0, 19.1.16–19.1.20]

OVERLAPPING COMMUNICATION

- Main benefit is overlap of *communication* with *communication*
- Overlap with computation
  - Progress may only be done inside of MPI routines
  - Not all platforms perform significantly better than well placed blocking communication
  - If hardware support is present, application performance may significantly improve due to overlap
- General recommendation
  - Initiation of operations should be placed as early as possible
  - Completion should be placed as late as possible

23 EXERCISES

Exercise 3 – Nonblocking P2P Communication

3.1 Global Summation – Tree

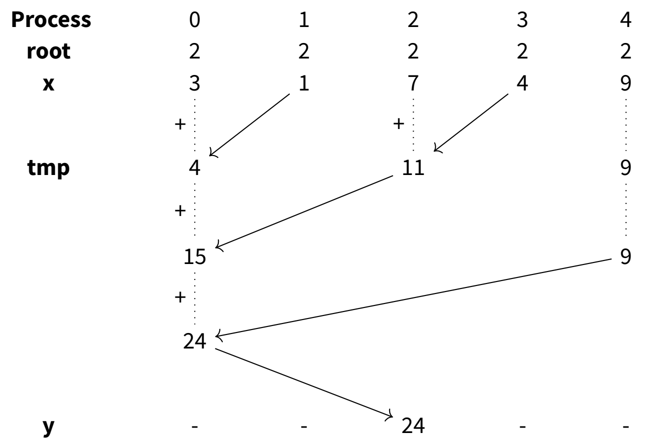
In the file `global_sum.{c|cxx|f90|py}`, implement a function/subroutine `global_sum_tree(x, y, root, comm)` that performs the same operation as the solution to exercise 2.3.

Use the following strategy:

1. On all processes, initialize the partial result for the sum to the local value of `x`.
2. Now proceed in rounds until only a single process remains:
   (a) Group processes into pairs – let us call them the left and the right process.
   (b) The right process sends its partial result to the left process.
   (c) The left process receives the partial result and adds it to its own one.
   (d) The left process continues on into the next round, the right one does not.
3. The process that made it to the last round now has the global result which it sends to the process with rank `root`.
4. The `root` process receives the global result and returns it in `y`.

Modify the `main()` function / **`program`** so that the new function/subroutine `global_sum_tree()` is also tested and check your implementation.

Use: `MPI_Irecv`, `MPI_Wait`



Bonus

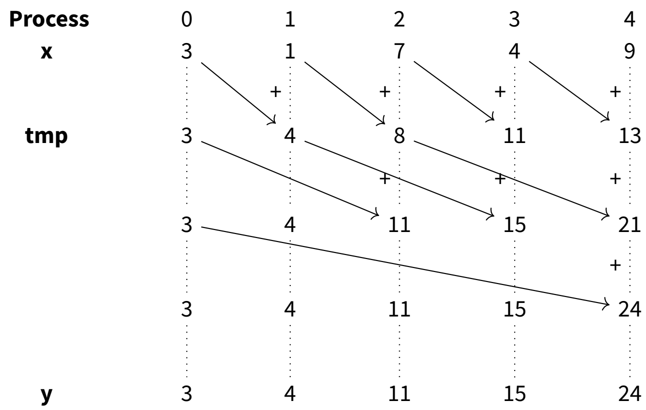
In the file `global_prefix_sum.{c|cxx|f90|py}`, implement a function/subroutine `global_prefix_sum_tree(x, y, comm)` that performs the same operation as `global_prefix_sum_ring`.

Use the following strategy:

1. On all processes, initialize the partial result for the sum to the local value of `x`.
2. Repeat the following steps with distance d starting at 1
   (a) Send partial results to the process `r + d` if that process exists (`r` is rank number)
   (b) Receive partial result from process `r - d` if that process exists and add it to the local partial result
   (c) If either process exists increase d by a factor of two and continue, otherwise return the partial result in y

Modify the `main()` function / **`program`** so that the new function/subroutine `global_prefix_sum_tree()` is also tested and check your implementation.

Use: `MPI_Sendrecv`



PART V

COLLECTIVE COMMUNICATION

24 INTRODUCTION

COLLECTIVE [MPI-4.0, 2.4, 6.1]

Terminology: Collective

A procedure is collective if all processes in a group need to invoke the procedure.

- Collective communication implements certain communication patterns that involve all processes in a group
- Synchronization may or may not occur (except for `MPI_Barrier`)
- No tags are used
- No `MPI_Status` values are returned
- Receive buffer size must match the total amount of data sent (c.f. point-to-point communication where receive buffer capacity is allowed to exceed the message size)
- Point-to-point and collective communication do not interfere

CLASSIFICATION [MPI-4.0, 6.2.2]

One-to-all
`MPI_Bcast`, `MPI_Scatter`, `MPI_Scatterv`

All-to-one
`MPI_Gather`, `MPI_Gatherv`, `MPI_Reduce`

All-to-all
`MPI_Allgather`, `MPI_Allgatherv`, `MPI_Alltoall`, `MPI_Alltoallv`, `MPI_Alltoallw`, `MPI_Allreduce`, `MPI_Reduce_scatter`, `MPI_Barrier`

Other
`MPI_Scan`, `MPI_Exscan`

25 REDUCTIONS

GLOBAL REDUCTION OPERATIONS [MPI-4.0, 6.9]

Associative operations over distributed data

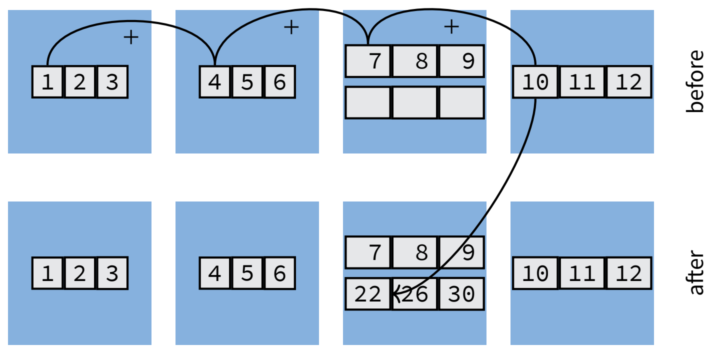
$d_0 \oplus d_1 \oplus d_2 \oplus \ldots \oplus d_{n-1}$, where
d_i, data of process with rank i
$\oplus$, associative operation

Examples for $\oplus$:

- Sum $+$ and product $\times$
- Maximum max and minimum min
- User-defined operations

Caution: Order of application is not defined, watch out for floating point rounding.

REDUCE [MPI-4.0, 6.9.1]

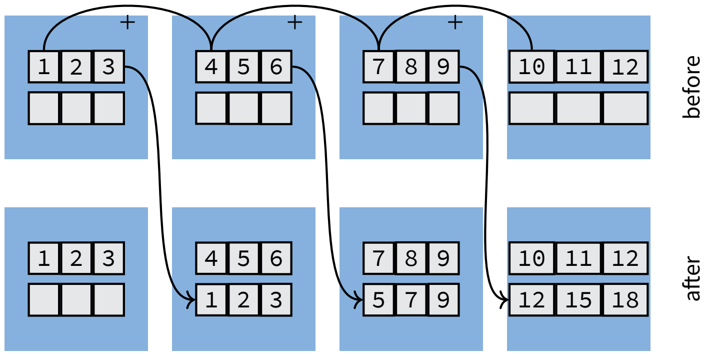


```
MPI_Reduce( <send buffer>, <receive buffer>, <operation>,
  <root> )
```

```c
int MPI_Reduce(const void* sendbuf, void* recvbuf, int count,
  MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)
```

```fortran
MPI_Reduce(sendbuf, recvbuf, count, datatype, op, root, comm,
  ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: count, root
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Op), intent(in) :: op
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

EXCLUSIVE SCAN [MPI-4.0, 6.11.2]




```
MPI_Exscan( <send buffer>, <receive buffer>, <operation>,
  <communicator> )
```

```c
int MPI_Exscan(const void* sendbuf, void* recvbuf, int count,
  MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)
```

```fortran
MPI_Exscan(sendbuf, recvbuf, count, datatype, op, comm,
  ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Op), intent(in) :: op
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

PREDEFINED OPERATIONS [MPI-4.0, 6.9.2]

Name	Meaning
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical and
MPI_BAND	Bitwise and
MPI_LOR	Logical or
MPI_BOR	Bitwise or
MPI_LXOR	Logical exclusive or
MPI_BXOR	Bitwise exclusive or
MPI_MAXLOC	Maximum and the first rank that holds it [MPI-4.0, 6.9.4]
MPI_MINLOC	Minimum and the first rank that holds it [MPI-4.0, 6.9.4]

26 REDUCTION VARIANTS

REDUCTION VARIANTS [MPI-4.0, 6.9 -- 6.11]

Routines with extended or combined functionality:

- `MPI_Allreduce`: perform a global reduction and replicate the result onto all ranks
- `MPI_Reduce_scatter`: perform a global reduction then scatter the result onto all ranks
- `MPI_Scan`: perform a global prefix reduction, include own data in result

27 EXERCISES

Exercise 4 – Collective Communication

4.1 Global Summation – `MPI_Reduce`

In the file `global_sum.{c|cxx|f90|py}` implement the function/subroutine `global_sum_reduce(x, y, root, comm)` that performs the same operation as the solution to exercise 2.3.

Since `global_sum_...` is a specialization of `MPI_Reduce`, it can be implemented by calling `MPI_Reduce`, passing on the function arguments in the correct way and selecting the correct MPI datatype and reduction operation.

Use: `MPI_Reduce`

Bonus

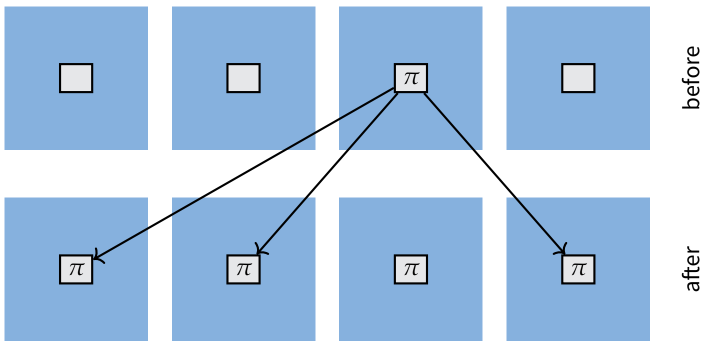
In the file `global_prefix_sum.{c|cxx|f90|py}` implement the function/subroutine `global_prefix_sum_scan(x, y, comm)` that performs the same operation as `global_prefix_sum_ring`.

Since `global_prefix_sum_...` is a specialization of `MPI_Scan`, it can be implemented by calling `MPI_Scan`, passing on the function arguments in the correct way and selecting the correct MPI datatype and reduction operation.

Use: `MPI_Scan`

28 DATA MOVEMENT

BROADCAST [MPI-4.0, 6.4]



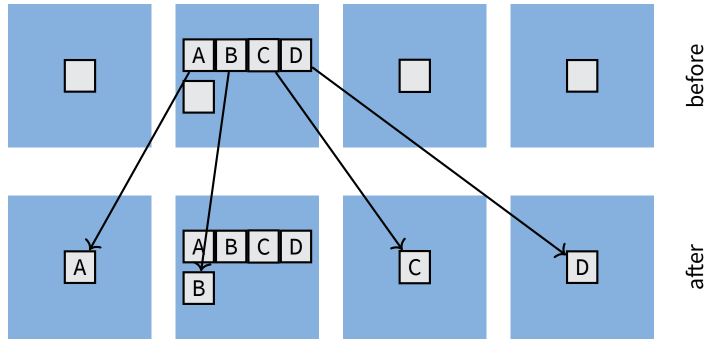
C

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

F08

```fortran
MPI_Bcast(buffer, count, datatype, root, comm, ierror)
type(*), dimension(..) :: buffer
integer, intent(in) :: count, root
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

SCATTER [MPI-4.0, 6.6]



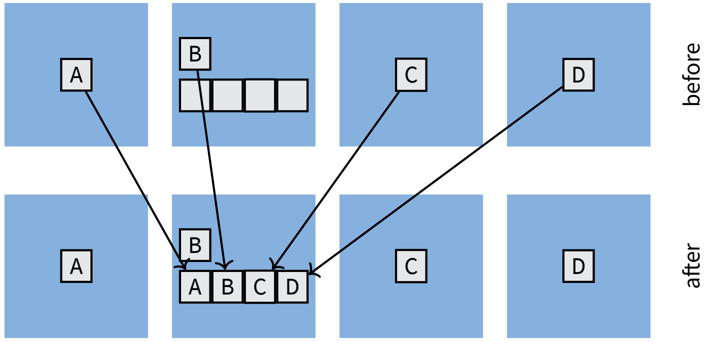
C

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

F08

```fortran
MPI_Scatter(sendbuf, sendcount, sendtype, recvbuf, recvcount,
    recvtype, root, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: sendcount, recvcount, root
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

GATHER [MPI-4.0, 6.5]



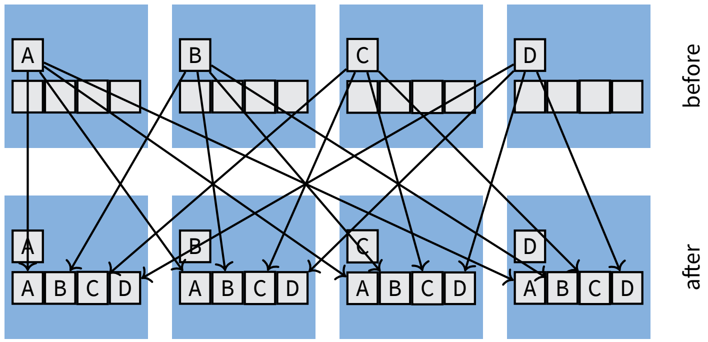
C

```c
int MPI_Gather(const void* sendbuf, int sendcount,
  ↪ MPI_Datatype sendtype, void* recvbuf, int recvcount,
  ↪ MPI_Datatype recvtype, int root, MPI_Comm comm)
```

F08

```fortran
MPI_Gather(sendbuf, sendcount, sendtype, recvbuf, recvcount,
  ↪ recvtype, root, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: sendcount, recvcount, root
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

GATHER-TO-ALL [MPI-4.0, 6.7]



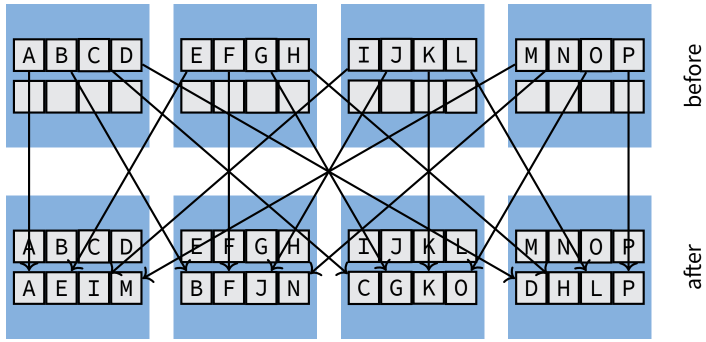
C

```c
int MPI_Allgather(const void* sendbuf, int sendcount,
  ↪ MPI_Datatype sendtype, void* recvbuf, int recvcount,
  ↪ MPI_Datatype recvtype, MPI_Comm comm)
```

F08

```fortran
MPI_Allgather(sendbuf, sendcount, sendtype, recvbuf, recvcount,
  ↪ recvtype, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: sendcount, recvcount
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

ALL-TO-ALL SCATTER/GATHER [MPI-4.0, 6.8]



C

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

F08

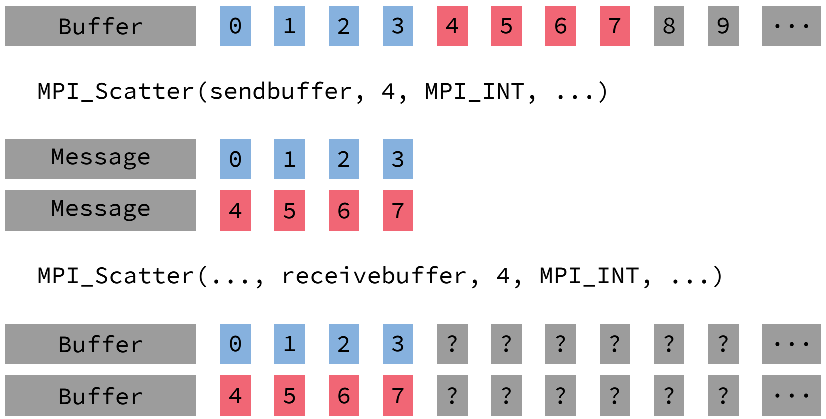
```fortran
MPI_Alltoall(sendbuf, sendcount, sendtype, recvbuf, recvcount,
  ↪ recvtype, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: sendcount, recvcount
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

DATA MOVEMENT SIGNATURES

```
MPI_Collective(<send buffer>, <receive buffer>, <root or communicator>)
```

- Both `send buffer` and `receive buffer` are address, count, datatype
- In One-to-all / All-to-one pattern
  - Specify `root` process by rank number
  - `send buffer` / `receive buffer` is only read / written on `root` process
- Buffers hold either one or n messages, where n is the number of processes
- If multiple messages are sent from / received into a buffer, associated `count` specifies the number of elements in a single message

MESSAGE ASSEMBLY



29 DATA MOVEMENT VARIANTS

DATA MOVEMENT VARIANTS [MPI-4.0, 6.5 -- 6.8]

Routines with variable counts (and datatypes):

- `MPI_Scatterv`: scatter into parts of variable length
- `MPI_Gatherv`: gather parts of variable length
- `MPI_Allgatherv`: gather parts of variable length onto all processes
- `MPI_Alltoallv`: exchange parts of variable length between all processes
- `MPI_Alltoallw`: exchange parts of variable length and datatype between all processes

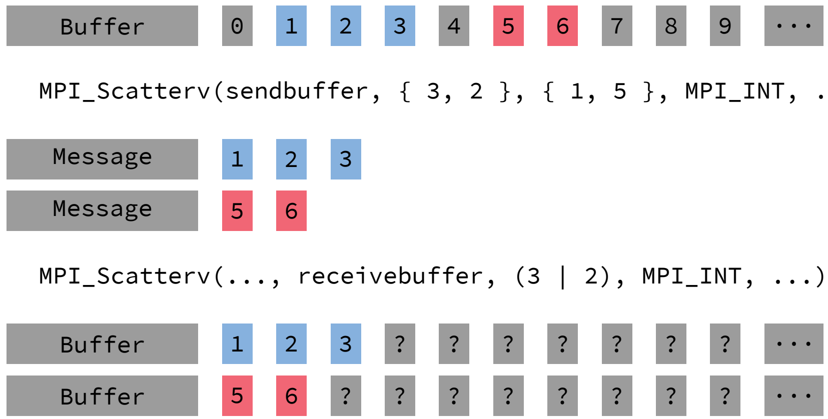
DATA MOVEMENT SIGNATURES

```
MPI_Collectivev(<send buffer>, <receive buffer>, <root or communicator>)
```

- Same high-level pattern as before
- Difference: for buffers holding n messages, can specify, for every message
  - An individual `count` of message elements
  - A `displacement` (in units of message elements) from the beginning of the buffer at which to start taking elements

Caution: The blocks for different messages in send buffers can overlap. In receive buffers, they must not.

MESSAGE ASSEMBLY



30 EXERCISES

4.2 Redistribution of Points with Collectives

In the file `redistribute.{c|cxx|f90|py}` implement the function `redistribute` which should work as follows:

1. All processes call the function collectively and pass in an array of random numbers – the points – from a uniform random distribution on $[0, 1)$.
2. Partition $[0, 1)$ among the `nranks` processes: process i gets partition $[i/nranks, (i+1)/nranks)$.

3. Redistribute the points, so that every process is left with only those points that lie inside its partition and return them from the function.

Guidelines:

- Use collectives, either `MPI_Gather` and `MPI_Scatter` or `MPI_Alltoall(v)` (see below)
- It helps to partition the points so that consecutive blocks can be sent to other processes
- `MPI_Alltoall` can be used to distribute the information that is needed to call `MPI_Alltoallv`
- Dynamic memory management could be necessary

The file contains tests that will check your implementation.

Use: `MPI_Alltoall`, `MPI_Alltoallv`

ALL-TO-ALL WITH VARYING COUNTS

C

```c
MPI_Alltoallv(const void* sendbuf, const int sendcounts[],
    const int sdispls[], MPI_Datatype sendtype, void* recvbuf,
    const int recvcounts[], const int rdispls[], MPI_Datatype
    recvtype, MPI_Comm comm)
```

F08

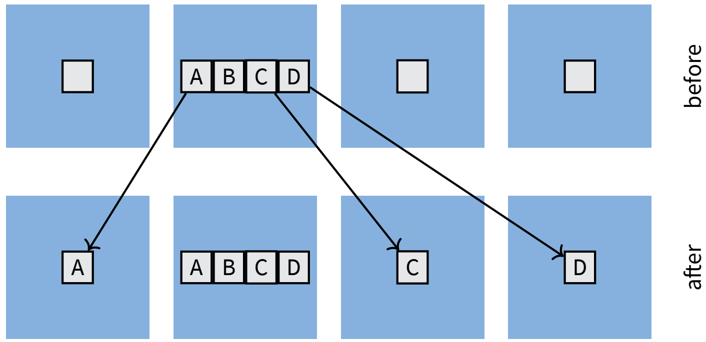
```fortran
MPI_Alltoallv(sendbuf, sendcounts, sdispls, sendtype, recvbuf,
    recvcounts, rdispls, recvtype, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
type(*), dimension(..) :: recvbuf
integer, intent(in) :: sendcounts(*), sdispls(*),
    recvcounts(*), rdispls(*)
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

31 IN PLACE MODE

IN PLACE MODE

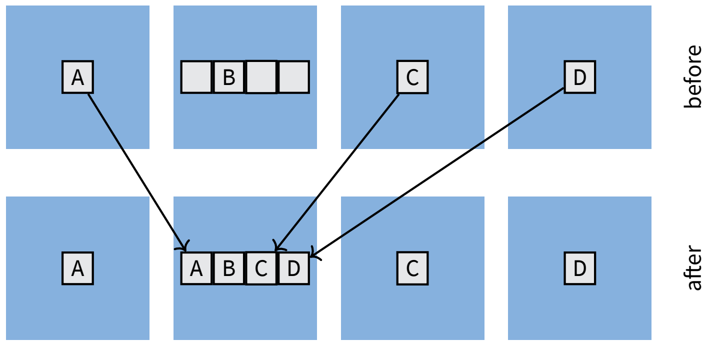
- Collectives can be used in *in place mode* with only one buffer to conserve memory
- The special value `MPI_IN_PLACE` is used in place of either the send or receive buffer address
- `count` and `datatype` of that buffer are ignored

IN PLACE SCATTER



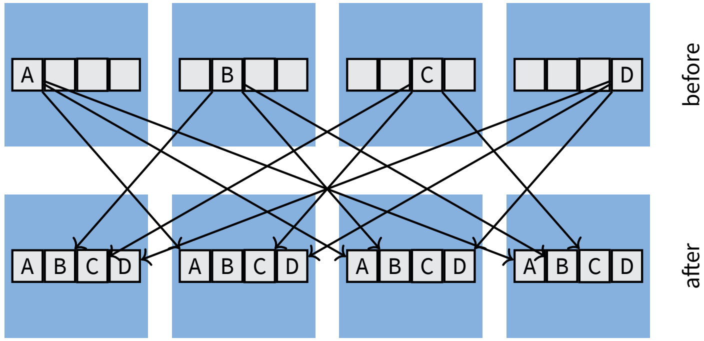
If `MPI_IN_PLACE` is used for `recvbuf` on the root process, `recvcount` and `recvtype` are ignored and the root process does not send data to itself

IN PLACE GATHER



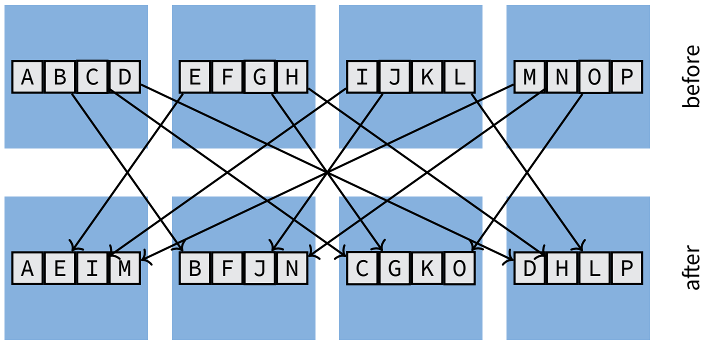
If `MPI_IN_PLACE` is used for `sendbuf` on the root process, `sendcount` and `sendtype` are ignored on the root process and the root process will not send data to itself.

IN PLACE GATHER-TO-ALL



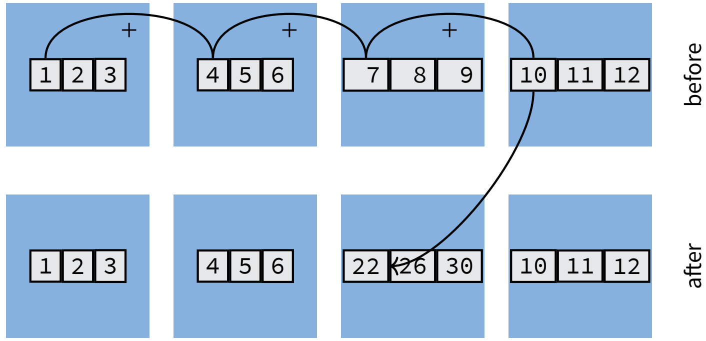
If MPI_IN_PLACE is used for sendbuf on all processes, sendcount and sendtype are ignored and the input data is assumed to already be in the correct position in recvbuf.

IN PLACE ALL-TO-ALL SCATTER/GATHER



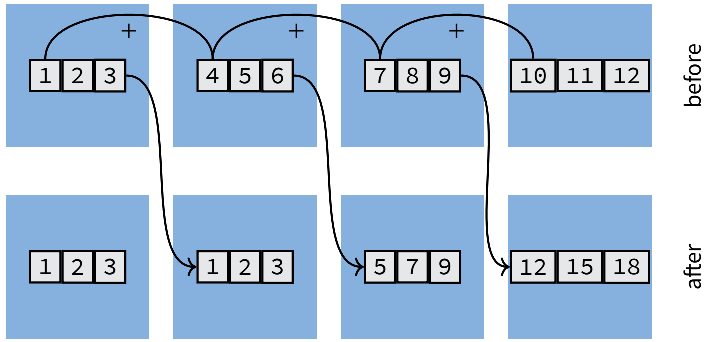
If MPI_IN_PLACE is used for sendbuf on all processes, sendcount and sendtype are ignored and the input data is assumed to already be in the correct position in recvbuf.

IN PLACE REDUCE



If MPI_IN_PLACE is used for sendbuf on the root process, the input data for the root process is taken from recvbuf.

IN PLACE EXCLUSIVE SCAN



If MPI_IN_PLACE is used for sendbuf on all the processes, the input data is taken from recvbuf and replaced by the results.

32 SYNCHRONIZATION

BARRIER [MPI-4.0, 6.3]

C
```c
int MPI_Barrier(MPI_Comm comm)
```

F08
```fortran
MPI_Barrier(comm, ierror)
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

Explicitly synchronizes all processes in the group of a communicator by blocking until all processes have entered the procedure.

33 LARGE NUMBERS

LARGE COUNT EXAMPLE

```c
int MPI_Scatterv(const void* sendbuf, const int sendcounts[], const int displs[], MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)

int MPI_Scatterv_c(const void* sendbuf, const MPI_Count sendcounts[], const MPI_Aint displs[], MPI_Datatype sendtype, void* recvbuf, MPI_Count recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)
```

C

```fortran
MPI_Scatterv(sendbuf, sendcounts, displs, sendtype, recvbuf, recvcount, recvtype, root, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
integer, intent(in) :: sendcounts(*), displs(*), recvcount, root
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(*), dimension(..) :: recvbuf
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

F08

```fortran
MPI_Scatterv(sendbuf, sendcounts, displs, sendtype, recvbuf, recvcount, recvtype, root, comm, ierror)
type(*), dimension(..), intent(in) :: sendbuf
integer(MPI_COUNT_KIND), intent(in) :: sendcounts(*), recvcount
integer(MPI_ADDRESS_KIND), intent(in) :: displs(*)
type(MPI_Datatype), intent(in) :: sendtype, recvtype
type(*), dimension(..) :: recvbuf
integer, intent(in) :: root
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

F08

34 NONBLOCKING COLLECTIVE COMMUNICATION

PROPERTIES

Properties similar to nonblocking point-to-point communication

1. Initiate communication
   - Routine names: `MPI_I...` (I for immediate)
   - Nonblocking routines return before the operation has completed.
   - Nonblocking routines have the same arguments as their blocking counterparts plus an extra `request` argument.
2. User-application proceeds with something else
3. Complete operation
   - Same completion routines (`MPI_Test`, `MPI_Wait`, ...)

Caution: Nonblocking collective operations cannot be matched with blocking collective operations.

Nonblocking Barrier

Barrier is entered through `MPI_Ibarrier` (which returns immediately). Completion (e.g. `MPI_Wait`) blocks until all processes have entered.

NONBLOCKING BROADCAST [MPI-4.0, 6.12.2]

Blocking operation

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

C

Nonblocking operation

```c
int MPI_Ibcast(void* buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm, MPI_Request* request)
```

C

```fortran
MPI_Bcast(buffer, count, datatype, root, comm, ierror)
type(*), dimension(..) :: buffer
integer, intent(in) :: count, root
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
integer, optional, intent(out) :: ierror
```

F08

```fortran
MPI_Ibcast(buffer, count, datatype, root, comm, request,
↪ ierror)
type(*), dimension(..), asynchronous :: buffer
integer, intent(in) :: count, root
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Comm), intent(in) :: comm
type(MPI_Request), intent(out) :: request
integer, optional, intent(out) :: ierror
```
F08

PART VI

DERIVED DATATYPES

35 INTRODUCTION

MOTIVATION [MPI-4.0, 5.1]

Reminder: Buffer

- Message buffers are defined by a triple (`address`, `count`, `datatype`).
- Basic data types restrict buffers to homogeneous, contiguous sequences of values in memory.

Scenario A

Problem: Want to communicate data describing particles that consists of a position (3 `double`) and a particle species (encoded as an `int`).

Solution(?): Communicate positions and species in two separate operations.

Scenario B

Problem: Have an array `real :: a(:)`, want to communicate only every second entry `a(1:n:2)`.

Solution(?): Copy data to a temporary array.

Derived datatypes are a mechanism for describing arrangements of data in buffers. Gives the MPI library the opportunity to employ the optimal solution.

TYPE MAP & TYPE SIGNATURE [MPI-4.0, 5.1]

Terminology: Type map

A *general datatype* is described by its *type map*, a sequence of pairs of *basic datatype* and *displacement*:

$$Typemap = \{(type_0, disp_0), \ldots, (type_{n-1}, disp_{n-1})\}$$

Terminology: Type signature

A *type signature* describes the contents of a message read from a buffer with a *general datatype*:

$$Typesig = \{type_0, \ldots, type_{n-1}\}$$

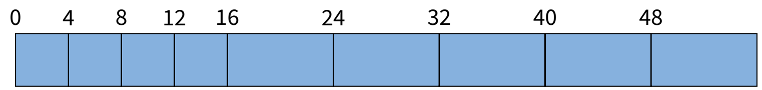
Type matching is done based on *type signatures* alone.

EXAMPLE

```c
struct heterogeneous {
  int i[4];
  double d[5];
}
```
C

```fortran
type, bind(C) :: heterogeneous
  integer :: i(4)
  real(real64) :: d(5)
end type
```
F08

	Basic Datatype	
0	MPI_INT	MPI_INTEGER
4	MPI_INT	MPI_INTEGER
8	MPI_INT	MPI_INTEGER
12	MPI_INT	MPI_INTEGER
16	MPI_DOUBLE	MPI_REAL8
24	MPI_DOUBLE	MPI_REAL8
32	MPI_DOUBLE	MPI_REAL8
40	MPI_DOUBLE	MPI_REAL8
48	MPI_DOUBLE	MPI_REAL8



36 CONSTRUCTORS

TYPE CONSTRUCTORS [MPI-4.0, 5.1]

A new derived type is constructed from an existing type `oldtype` (basic or derived) using type constructors. In order of increasing generality/complexity:

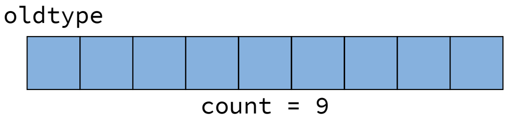
1. `MPI_Type_contiguous` n consecutive instances of `oldtype`
2. `MPI_Type_vector` n blocks of m instances of `oldtype` with stride s
3. `MPI_Type_indexed_block` n blocks of m instances of `oldtype` with displacement d_i for each $i = 1, \dots, n$
4. `MPI_Type_indexed` n blocks of m_i instances of `oldtype` with displacement d_i for each $i = 1, \dots, n$
5. `MPI_Type_create_struct` n blocks of m_i instances of `oldtype`$_i$ with displacement d_i for each $i = 1, \dots, n$
6. `MPI_Type_create_subarray` n dimensional subarray out of an array with elements of type `oldtype`
7. `MPI_Type_create_darray` distributed array with elements of type `oldtype`

CONTIGUOUS DATA [MPI-4.0, 5.1.2]

C
```c
int MPI_Type_contiguous(int count, MPI_Datatype oldtype,
  MPI_Datatype* newtype)
```

F08
```fortran
MPI_Type_contiguous(count, oldtype, newtype, ierror)
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

- Simple concatenation of `oldtype`
- Results in the same access pattern as using `oldtype` and specifying a buffer with `count` greater than one.



STRUCT DATA [MPI-4.0, 5.1.2]

C
```c
int MPI_Type_create_struct(int count, const int
  array_of_blocklengths[], const MPI_Aint
  array_of_displacements[], const MPI_Datatype
  array_of_types[], MPI_Datatype* newtype)
```

F08
```fortran
MPI_Type_create_struct(count, array_of_blocklengths,
  array_of_displacements, array_of_types, newtype, ierror)
integer, intent(in) :: count, array_of_blocklengths(count)
integer(kind=MPI_ADDRESS_KIND), intent(in) ::
  array_of_displacements(count)
type(MPI_Datatype), intent(in) :: array_of_types(count)
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

Caution: Fortran derived data types must be declared **sequence** or **bind**(C), see [MPI-4.0, 19.1.15].

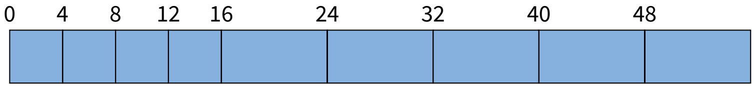
EXAMPLE

C
```c
struct heterogeneous {
  int i[4];
  double d[5];
}

count = 2;
array_of_blocklengths[0] = 4;
array_of_displacements[0] = 0;
array_of_types[0] = MPI_INT;
array_of_blocklengths[1] = 5;
array_of_displacements[1] = 16;
array_of_types[1] = MPI_DOUBLE;
```

```fortran
type, bind(C) :: heterogeneous
  integer :: i(4)
  real(real64) :: d(5)
end type

count = 2;
array_of_blocklengths(1) = 4
array_of_displacements(1) = 0
array_of_types(1) = MPI_INTEGER
array_of_blocklengths(2) = 5
array_of_displacements(2) = 16
array_of_types(2) = MPI_REAL8
```



SUBARRAY DATA [MPI-4.0, 5.1.3]

```c
int MPI_Type_create_subarray(int ndims, const int
↪ array_of_sizes[], const int array_of_subsizes[], const int
↪ array_of_starts[], int order, MPI_Datatype oldtype,
↪ MPI_Datatype* newtype)
```

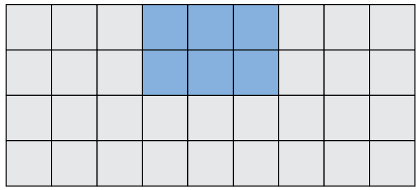
```fortran
MPI_Type_create_subarray(ndims, array_of_sizes,
↪ array_of_subsizes, array_of_starts, order, oldtype,
↪ newtype, ierror)
integer, intent(in) :: ndims, array_of_sizes(ndims),
↪ array_of_subsizes(ndims), array_of_starts(ndims), order
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

EXAMPLE

```c
ndims = 2;
array_of_sizes[] = { 4, 9 };
array_of_subsizes[] = { 2, 3 };
array_of_starts[] = { 0, 3 };
order = MPI_ORDER_C;
oldtype = MPI_INT;
```

```fortran
ndims = 2
array_of_sizes(:) = (/ 4, 9 /)
array_of_subsizes(:) = (/ 2, 3 /)
array_of_starts(:) = (/ 0, 3 /)
order = MPI_ORDER_FORTRAN
oldtype = MPI_INTEGER
```

An array with global size 4×9 containing a subarray of size 2×3 at offsets $0, 3$:



COMMIT & FREE [MPI-4.0, 5.1.9]

Before using a derived datatype in communication it needs to be committed

```c
int MPI_Type_commit(MPI_Datatype* datatype)
```

```fortran
MPI_Type_commit(datatype, ierror)
type(MPI_Datatype), intent(inout) :: datatype
integer, optional, intent(out) :: ierror
```

Marking derived datatypes for deallocation

```c
int MPI_Type_free(MPI_Datatype *datatype)
```

```fortran
MPI_Type_free(datatype, ierror)
type(MPI_Datatype), intent(inout) :: datatype
integer, optional, intent(out) :: ierror
```

37 EXERCISES

Exercise 5 – Derived Datatypes

5.1 Matrix Access – Diagonal

In the file `matrix_access.{c|cxx|f90|py}` implement the function/subroutine `get_diagonal` that extracts the elements on the diagonal of an $N \times N$ matrix into a vector:

$$\texttt{vector}_i = \texttt{matrix}_{i,i}, \quad i = 1 \ldots N.$$

Do not access the elements of either the matrix or the vector directly. Rather, use MPI datatypes for accessing your data. Assume that the matrix elements are stored in row-major order in C (all elements of the first row, followed by all elements of the second row, etc.), column-major order in Fortran.

Hint: `MPI_Sendrecv` on the `MPI_COMM_SELF` communicator can be used for copying the data.

Use: `MPI_Type_vector`

5.2 Matrix Access – Upper Triangle

In the file `matrix_access.{c|cxx|f90|py}` implement the function/subroutine `get_upper` that copies all elements on or above the diagonal of an $N \times N$ matrix to a second matrix and leaves all other elements untouched.

$$\mathtt{upper}_{i,j} = \mathtt{matrix}_{i,j}, \quad i = 1 \ldots N, j = i \ldots N$$

As in the previous exercise, do not access the matrix elements directly and assume row-major layout of the matrices in C, column-major order in Fortran. Make sure to un-comment the call to `test_get_upper()` to have your solution tested.

Hint: `MPI_Sendrecv` on the `MPI_COMM_SELF` communicator can be used for copying the data.

Use: `MPI_Type_indexed`

38 ADDRESS CALCULATION

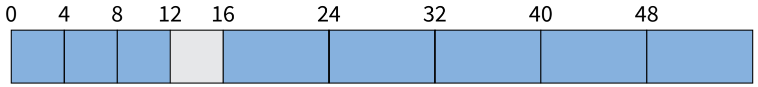
ALIGNMENT & PADDING

```c
struct heterogeneous {
  int i[3];
  double d[5];
}

count = 2;
array_of_blocklengths[0] = 3;
array_of_displacements[0] = 0;
array_of_types[0] = MPI_INT;
array_of_blocklengths[1] = 5;
array_of_displacements[1] = 16;
array_of_types[1] = MPI_DOUBLE;
```

```fortran
type, bind(C) :: heterogeneous
  integer :: i(3)
  real(real64) :: d(5)
end type

count = 2;
array_of_blocklengths(1) = 3
array_of_displacements(1) = 0
array_of_types(1) = MPI_INTEGER
array_of_blocklengths(2) = 5
array_of_displacements(2) = 16
array_of_types(2) = MPI_REAL8
```



ADDRESS CALCULATION [MPI-4.0, 5.1.5]

Displacements are calculated as the difference between the addresses at the start of a buffer and at a particular piece of data in the buffer. The address of a location in memory is found using:

```c
int MPI_Get_address(const void* location, MPI_Aint* address)
```

```fortran
MPI_Get_address(location, address, ierror)
type(*), dimension(..), asynchronous :: location
integer(kind=MPI_ADDRESS_KIND), intent(out) :: address
integer, optional, intent(out) :: ierror
```

Using the C operator & to determine addresses is discouraged, since it returns a pointer which is not necessarily the same as an address.

ADDRESS ARITHMETIC [MPI-4.0, 5.1.5]

Addition

```c
MPI_Aint MPI_Aint_add(MPI_Aint a, MPI_Aint b)
```

```fortran
integer(kind=MPI_ADDRESS_KIND) MPI_Aint_add(a, b)
integer(kind=MPI_ADDRESS_KIND), intent(in) :: a, b
```

Subtraction

```c
MPI_Aint MPI_Aint_diff(MPI_Aint a, MPI_Aint b)
```

```fortran
integer(kind=MPI_ADDRESS_KIND) MPI_Aint_diff(a, b)
integer(kind=MPI_ADDRESS_KIND), intent(in) :: a, b
```

EXAMPLE

```c
struct heterogeneous h;
MPI_Aint base, displ[2];
MPI_Datatype newtype;
MPI_Datatype types[2] = { MPI_INT, MPI_DOUBLE };
int blocklen[2] = { 3, 5 };

MPI_Get_address(&h, &base);
MPI_Get_address(&h.i, &displ[0]);
displ[0] = MPI_Aint_diff(displ[0], base);
MPI_Get_address(&h.d, &displ[1]);
displ[1] = MPI_Aint_diff(displ[1], base);
MPI_Type_create_struct(2, blocklen, displ, types, &newtype);
MPI_Type_commit(&newtype);
```

```fortran
type(heterogeneous) :: h
integer(kind=MPI_ADDRESS_KIND) :: base, displ(2)
type(MPI_Datatype) :: types(2), newtype
integer :: blocklen(2)

types = (/ MPI_INTEGER, MPI_REAL8 /)
blocklen = (/ 3, 5 /)

call MPI_Get_address(h, base)
call MPI_Get_address(h%i, displ(1))
displ(1) = MPI_Aint_diff(displ(1), base)
call MPI_Get_address(h%d, displ(2))
displ(2) = MPI_Aint_diff(displ(2), base)
call MPI_Type_create_struct(2, blocklen, displ, types,
 ↪ newtype)
call MPI_Type_commit(newtype)
```

39 PADDING

TYPE EXTENT [MPI-4.0, 5.1]

Terminology: Extent

The *extent* of a type is determined from its *lower bounds* and *upper bounds*:

$$\begin{aligned}
\mathit{Typemap} &= \{(\mathit{type}_0, \mathit{disp}_0), \dots, (\mathit{type}_{n-1}, \mathit{disp}_{n-1})\} \\
\mathrm{lb}\ \mathit{Typemap} &= \min_j \mathit{disp}_j \\
\mathrm{ub}\ \mathit{Typemap} &= \max_j (\mathit{disp}_j + \mathrm{sizeof}\ \mathit{type}_j) + \epsilon \\
\mathrm{extent}\ \mathit{Typemap} &= \mathrm{ub}\ \mathit{Typemap} - \mathrm{lb}\ \mathit{Typemap}
\end{aligned}$$

Extent and spacing

Let `t` be a type with type map `{(MPI_CHAR, 1)}` and `b` an array of **char**, `b = { 'a', 'b', 'c', 'd', 'e', 'f' }`, then `MPI_Send(b, 3, t, ...)` will result in a message `{'b', 'c', 'd'}` and not `{'b', 'd', 'f'}`.

Explicit padding can be added by *resizing* the type.

RESIZE [MPI-4.0, 5.1.7]

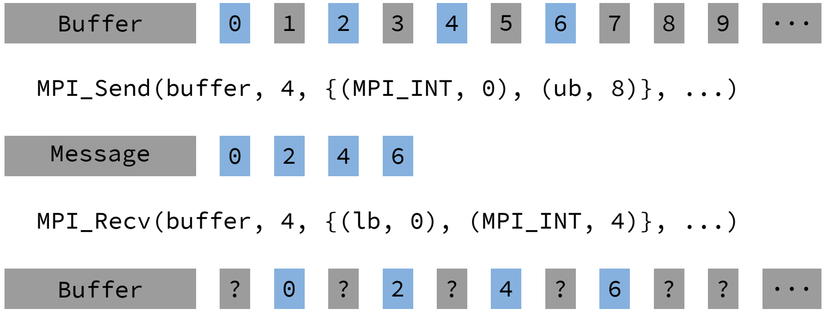
```c
int MPI_Type_create_resized(MPI_Datatype oldtype, MPI_Aint lb,
 ↪ MPI_Aint extent, MPI_Datatype* newtype)
```

```fortran
MPI_Type_create_resized(oldtype, lb, extent, newtype, ierror)
integer(kind=MPI_ADDRESS_KIND), intent(in) :: lb, extent
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

Creates a new derived type `newtype` with the same type map as `oldtype` but explicit lower bound `lb` and explicit upper bound `lb + extent`.

Extent and true extent of a type can be queried using `MPI_Type_get_extent` and `MPI_Type_get_true_extent`. The size of resulting messages can be queried with `MPI_Type_size`.

MESSAGE ASSEMBLY



40 LARGE NUMBERS

LARGE COUNT EXAMPLE

C

```c
int MPI_Type_create_hvector(int count, int blocklength,
  ↪ MPI_Aint stride, MPI_Datatype oldtype, MPI_Datatype*
  ↪ newtype)

int MPI_Type_create_hvector_c(MPI_Count count, MPI_Count
  ↪ blocklength, MPI_Count stride, MPI_Datatype oldtype,
  ↪ MPI_Datatype* newtype)
```

F08

```fortran
MPI_Type_create_hvector(count, blocklength, stride, oldtype,
  ↪ newtype, ierror)
integer, intent(in) :: count, blocklength
integer(KIND=MPI_ADDRESS_KIND), intent(in) :: stride
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror

MPI_Type_create_hvector(count, blocklength, stride, oldtype,
  ↪ newtype, ierror)
integer(KinD=MPI_COUNT_KIND), intent(in) :: count, blocklength,
  ↪ stride
type(MPI_Datatype), intent(in) :: oldtype
type(MPI_Datatype), intent(out) :: newtype
integer, optional, intent(out) :: ierror
```

41 EXERCISES

5.3 Structs

Given a definition of a datatype that represents a point in three-dimensional space with additional properties:

- 3 color values (`rgb`, integers)
- 3 coordinates (`xyz`, double precision)
- 1 tag (1 character)

write a function `point_datatype` in `struct.{c|cxx|f90}` or `struct_.py` that returns a committed MPI Datatype that describes the data layout. Your function will be tested by using the datatype you construct for copying an instance of the point type.

Modification: Change the order of the components of the point structure. Does your program still produce correct results?

Use: `MPI_Get_address`, `MPI_Aint_diff`, `MPI_Type_create_struct`, `MPI_Type_commit`

PART VII

INPUT/OUTPUT

42 INTRODUCTION

MOTIVATION

I/O on HPC Systems

- "This is not your parents' I/O subsystem"
- File system is a shared resource
  - Modification of metadata might happen sequentially
  - File system blocks might be shared among processes
- File system access might not be uniform across all processes
- Interoperability of data originating on different platforms

MPI I/O

- MPI already defines a language that describes data layout and movement
- Extend this language by I/O capabilities

- More expressive/precise API than POSIX I/O affords better chances for optimization

COMMON I/O STRATEGIES

Funnelled I/O

- + Simple to implement
- - I/O bandwidth is limited to the rate of this single process
- - Additional communication might be necessary
- - Other processes may idle and waste resources during I/O operations

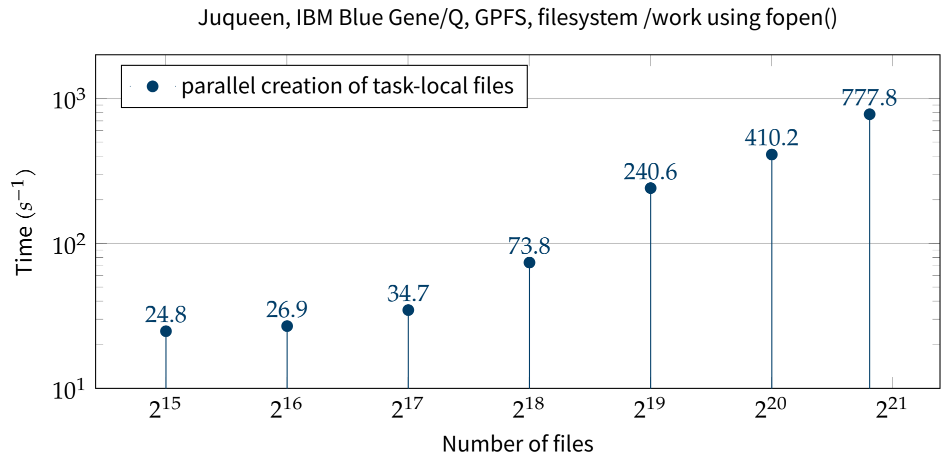
All or several processes use one file

- + Number of files is independent of number of processes
- + File is in canonical representation (no post-processing)
- - Uncoordinated client requests might induce time penalties
- - File layout may induce false sharing of file system blocks

Task-Local Files

- + Simple to implement
- + No explicit coordination between processes needed
- + No false sharing of file system blocks
- - Number of files quickly becomes unmanageable
- - Files often need to be merged to create a canonical dataset (post-processing)
- - File system might introduce implicit coordination (metadata modification)

SEQUENTIAL ACCESS TO METADATA



43 FILE MANIPULATION

FILE, FILE POINTER & HANDLE [MPI-4.0, 14.1]

Terminology: File

An MPI file is an ordered collection of typed data items.

Terminology: File Pointer

A file pointer is an implicit offset into a file maintained by MPI.

Terminology: File Handle

An opaque MPI object. All operations on an open file reference the file through the file handle.

OPENING A FILE [MPI-4.0, 14.2.1]

C

```c
int MPI_File_open(MPI_Comm comm, const char* filename, int
↪ amode, MPI_Info info, MPI_File* fh)
```

F08

```fortran
MPI_File_open(comm, filename, amode, info, fh, ierror)
type(MPI_Comm), intent(in) :: comm
character(len=*), intent(in) :: filename
integer, intent(in) :: amode
type(MPI_Info), intent(in) :: info
type(MPI_File), intent(out) :: fh
integer, optional, intent(out) :: ierror
```

- Collective operation on communicator `comm`
- Filename must reference the same file on all processes
- Process-local files can be opened using `MPI_COMM_SELF`
- `info` object specifies additional information (`MPI_INFO_NULL` for empty)

ACCESS MODE [MPI-4.0, 14.2.1]

`amode` denotes the access mode of the file and must be the same on all processes. It *must* contain exactly one of the following:

`MPI_MODE_RDONLY` read only access

`MPI_MODE_RDWR` read and write access

`MPI_MODE_WRONLY` write only access

and may contain some of the following:

`MPI_MODE_CREATE` create the file if it does not exist

`MPI_MODE_EXCL` error if creating file that already exists

`MPI_MODE_DELETE_ON_CLOSE` delete file on close

`MPI_MODE_UNIQUE_OPEN` file is not opened elsewhere

`MPI_MODE_SEQUENTIAL` access to the file is sequential

`MPI_MODE_APPEND` file pointers are set to the end of the file

Combine using bit-wise or (`|` operator in C, `ior` intrinsic in Fortran).

CLOSING A FILE [MPI-4.0, 14.2.2]

```c
int MPI_File_close(MPI_File* fh)
```

```fortran
MPI_File_close(fh, ierror)
type(MPI_File), intent(out) :: fh
integer, optional, intent(out) :: ierror
```

- Collective operation
- User must ensure that all outstanding nonblocking and split collective operations associated with the file have completed

DELETING A FILE [MPI-4.0, 14.2.3]

```c
int MPI_File_delete(const char* filename, MPI_Info info)
```

```fortran
MPI_File_delete(filename, info, ierror)
character(len=*), intent(in) :: filename
type(MPI_Info), intent(in) :: info
integer, optional, intent(out) :: ierror
```

- Deletes the file identified by `filename`
- File deletion is a local operation and should be performed by a single process
- If the file does not exist an error is raised
- If the file is opened by any process
  - all further and outstanding access to the file is implementation dependent
  - it is implementation dependent whether the file is deleted; if it is not, an error is raised

FILE PARAMETERS

Setting File Parameters

`MPI_File_set_size` Set the size of a file [MPI-4.0, 14.2.4]

`MPI_File_preallocate` Preallocate disk space [MPI-4.0, 14.2.5]

`MPI_File_set_info` Supply additional information [MPI-4.0, 14.2.8]

Inspecting File Parameters

`MPI_File_get_size` Size of a file [MPI-4.0, 14.2.6]

`MPI_File_get_amode` Acess mode [MPI-4.0, 14.2.7]

`MPI_File_get_group` Group of processes that opened the file [MPI-4.0, 14.2.7]

`MPI_File_get_info` Additional information associated with the file [MPI-4.0, 14.2.8]

I/O ERROR HANDLING [MPI-4.0, 9.3, 14.7]

Caution: Communication, by default, aborts the program when an error is encountered. I/O operations, by default, return an error code.

```c
int MPI_File_set_errhandler(MPI_File file, MPI_Errhandler
    errhandler)
```

F08

```
MPI_File_set_errhandler(file, errhandler, ierror)
type(MPI_File), intent(in) :: file
type(MPI_Errhandler), intent(in) :: errhandler
integer, optional, intent(out) :: ierror
```

- The default error handler for files is `MPI_ERRORS_RETURN`
- Success is indicated by a return value of `MPI_SUCCESS`
- `MPI_ERRORS_ARE_FATAL` aborts the program
- Can be set for each file individually or for all files by using `MPI_File_set_errhandler` on a special file handle, `MPI_FILE_NULL`

44 FILE VIEWS

FILE VIEW [MPI-4.0, 14.3]

Terminology: File View

A file view determines what part of the contents of a file is visible to a process. It is defined by a *displacement* (given in bytes) from the beginning of the file, an *elementary datatype* and a *file type*. The view into a file can be changed multiple times between opening and closing.

File Types and Elementary Types are Data Types

- Can be predefined or derived
- The usual constructors can be used to create derived file types and elementary types, e.g.
  - `MPI_Type_indexed`,
  - `MPI_Type_create_struct`,
  - `MPI_Type_create_subarray`
- Displacements in their typemap must be non-negative and monotonically nondecreasing
- Have to be committed before use

DEFAULT FILE VIEW [MPI-4.0, 14.3]

When newly opened, files are assigned a default view that is the same on all processes:

- Zero displacement
- File contains a contiguous sequence of bytes
- All processes have access to the entire file

File	0: byte	1: byte	2: byte	3: byte	...
Process 0	0: byte	1: byte	2: byte	3: byte	...
Process 1	0: byte	1: byte	2: byte	3: byte	...
...	0: byte	1: byte	2: byte	3: byte	...

ELEMENTARY TYPE [MPI-4.0, 14.3]

Terminology: Elementary Type

An elementary type (or *etype*) is the unit of data contained in a file. Offsets are expressed in multiples of etypes, file pointers point to the beginning of etypes. Etypes can be basic or derived.

Changing the Elementary Type

E.g. `etype = MPI_INT`:

File	0: int	1: int	2: int	3: int	...
Process 0	0: int	1: int	2: int	3: int	...
Process 1	0: int	1: int	2: int	3: int	...
...	0: int	1: int	2: int	3: int	...

FILE TYPE [MPI-4.0, 14.3]

Terminology: File Type

A file type describes an access pattern. It can contain either instances of the *etype* or holes with an extent that is divisible by the extent of the etype.

Changing the File Type

E.g. $Filetype_0 = \{(\texttt{int}, 0), (hole, 4), (hole, 8)\}$, $Filetype_1 = \{(hole, 0), (\texttt{int}, 4), (hole, 8)\}, \ldots$:

File	0: int	1: int	2: int	3: int	...
Process 0	0: int			1: int	
Process 1		0: int			...
...			0: int		

CHANGING THE FILE VIEW [MPI-4.0, 14.3]

```c
int MPI_File_set_view(MPI_File fh, MPI_Offset disp,
  ↪ MPI_Datatype etype, MPI_Datatype filetype, const char*
  ↪ datarep, MPI_Info info)
```

```fortran
MPI_File_set_view(fh, disp, etype, filetype, datarep, info,
  ↪ ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: disp
type(MPI_Datatype), intent(in) :: etype, filetype
character(len=*), intent(in) :: datarep
type(MPI_Info), intent(in) :: info
integer, optional, intent(out) :: ierror
```

- Collective operation
- `datarep` and extent of `etype` must match
- `disp`, `filetype` and `info` can be distinct
- File pointers are reset to zero
- May not overlap with nonblocking or split collective operations

DATA REPRESENTATION [MPI-4.0, 14.5]

- Determines the conversion of data in memory to data on disk
- Influences the interoperability of I/O between heterogeneous parts of a system or different systems

`"native"`
Data is stored in the file exactly as it is in memory

+ No loss of precision
+ No overhead
- On heterogeneous systems loss of transparent interoperability

`"internal"`
Data is stored in implementation-specific format

+ Can be used in a homogeneous *and* heterogeneous environment
+ Implementation will perform conversions if necessary
- Can incur overhead
- Not necessarily compatible between different implementations

`"external32"`
Data is stored in standardized data representation (big-endian IEEE)

+ Can be read/written also by non-MPI programs
- Precision and I/O performance may be lost due to type conversions between `native` and `external32` representations
- Not available in all implementations

45 DATA ACCESS

Three orthogonal aspects

1. Synchronism
   (a) Blocking
   (b) Nonblocking
   (c) Split collective
2. Coordination
   (a) Noncollective
   (b) Collective
3. Positioning
   (a) Explicit offsets
   (b) Individual file pointers
   (c) Shared file pointers

POSIX `read()` and `write()`
These are blocking, noncollective operations with individual file pointers.

SYNCHRONISM

Blocking I/O
Blocking I/O routines do not return before the operation is completed.

Nonblocking I/O

- Nonblocking I/O routines do not wait for the operation to finish
- A separate completion routine is necessary [MPI-4.0, 3.7.3, 3.7.5]
- The associated buffers must not be used while the operation is in flight

Split Collective

- “Restricted” form of nonblocking collective
- Buffers must not be used while in flight
- Does not allow other collective accesses to the file while in flight
- `begin` and `end` must be used from the same thread

COORDINATION

Noncollective
The completion depends only on the activity of the calling process.

Collective

- Completion may depend on activity of other processes
- Opens opportunities for optimization

POSITIONING [MPI-4.0, 14.4.1 -- 14.4.4]

Explicit Offset

- No file pointer is used
- File position for access is given directly as function argument

Individual File Pointers

- Each process has its own file pointer
- After access, pointer is moved to first *etype* after the last one accessed

Shared File Pointers

- All processes share a single file pointer
- All processes must use the same file view
- Individual accesses appear as if serialized (with an unspecified order)
- Collective accesses are performed in order of ascending rank

Combine the prefix `MPI_File_` with any of the following suffixes:

		coordination	
positioning	**synchronism**	noncollective	collective
explicit offsets	blocking	`read_at`, `write_at`	`read_at_all`, `write_at_all`
	nonblocking	`iread_at`, `iwrite_at`	`iread_at_all`, `iwrite_at_all`
	split collective	N/A	`read_at_all_begin`, `read_at_all_end`, `write_at_all_begin`, `write_at_all_end`
individual file pointers	blocking	`read`, `write`	`read_all`, `write_all`
	nonblocking	`iread`, `iwrite`	`iread_all`, `iwrite_all`
	split collective	N/A	`read_all_begin`, `read_all_end`, `write_all_begin`, `write_all_end`
shared file pointers	blocking	`read_shared`, `write_shared`	`read_ordered`, `write_ordered`
	nonblocking	`iread_shared`, `iwrite_shared`	N/A
	split collective	N/A	`read_ordered_begin`, `read_ordered_end`, `write_ordered_begin`, `write_ordered_end`

WRITING

blocking, noncollective, explicit offset [MPI-4.0, 14.4.2]

C
```c
int MPI_File_write_at(MPI_File fh, MPI_Offset offset, const
    void* buf, int count, MPI_Datatype datatype, MPI_Status
    *status)
```

F08
```fortran
MPI_File_write_at(fh, offset, buf, count, datatype, status,
    ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
integer, optional, intent(out) :: ierror
```

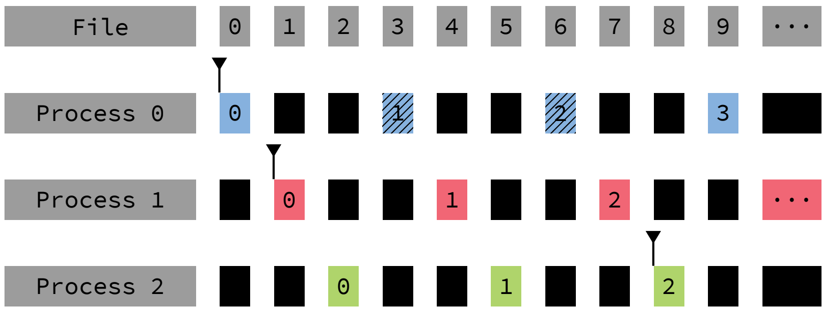
- Starting offset for access is explicitly given

- No file pointer is updated
- Writes `count` elements of `datatype` from memory starting at `buf`
- Typesig *datatype* = Typesig *etype* ... Typesig *etype*
- Writing past end of file increases the file size

EXAMPLE

blocking, noncollective, explicit offset [MPI-4.0, 14.4.2]

Process 0 calls `MPI_File_write_at(offset = 1, count = 2)`:



WRITING

blocking, noncollective, individual [MPI-4.0, 14.4.3]

C
```c
int MPI_File_write(MPI_File fh, const void* buf, int count,
    MPI_Datatype datatype, MPI_Status* status)
```

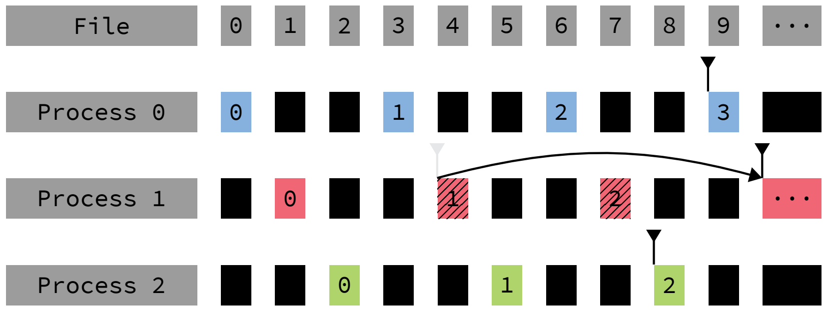
F08
```fortran
MPI_File_write(fh, buf, count, datatype, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Starts writing at the current position of the individual file pointer
- Moves the individual file pointer by the count of *etypes* written

EXAMPLE

blocking, noncollective, individual [MPI-4.0, 14.4.3]

With its file pointer at element 1, process 1 calls `MPI_File_write(count = 2)`:



WRITING

nonblocking, noncollective, individual [MPI-4.0, 14.4.3]

C
```c
int MPI_File_iwrite(MPI_File fh, const void* buf, int count,
    MPI_Datatype datatype, MPI_Request* request)
```

F08
```fortran
MPI_File_iwrite(fh, buf, count, datatype, request, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Request), intent(out) :: request
integer, optional, intent(out) :: ierror
```

- Starts the same operation as `MPI_File_write` but does not wait for completion
- Returns a `request` object that is used to complete the operation

WRITING

blocking, collective, individual [MPI-4.0, 14.4.3]

C
```c
int MPI_File_write_all(MPI_File fh, const void* buf, int count,
    MPI_Datatype datatype, MPI_Status* status)
```

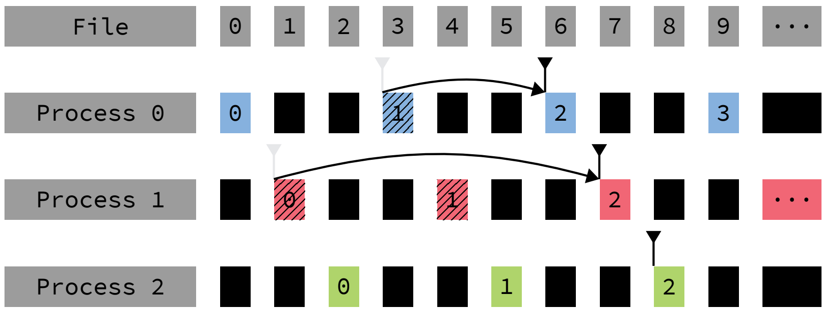
```F08
MPI_File_write_all(fh, buf, count, datatype, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Same signature as `MPI_File_write`, but collective coordination
- Each process uses its individual file pointer
- MPI can use communication between processes to funnel I/O

EXAMPLE

blocking, collective, individual [MPI-4.0, 14.4.3]

- With its file pointer at element 1, process 0 calls `MPI_File_write_all(count = 1)`,
- With its file pointer at element 0, process 1 calls `MPI_File_write_all(count = 2)`,
- With its file pointer at element 2, process 2 calls `MPI_File_write_all(count = 0)`:



WRITING

split-collective, individual [MPI-4.0, 14.4.5]

```C
int MPI_File_write_all_begin(MPI_File fh, const void* buf, int
    count, MPI_Datatype datatype)
```

```F08
MPI_File_write_all_begin(fh, buf, count, datatype, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
integer, optional, intent(out) :: ierror
```

- Same operation as `MPI_File_write_all`, but split-collective
- `status` is returned by the corresponding end routine

WRITING

split-collective, individual [MPI-4.0, 14.4.5]

```C
int MPI_File_write_all_end(MPI_File fh, const void* buf,
    MPI_Status* status)
```

```F08
MPI_File_write_all_end(fh, buf, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..), intent(in) :: buf
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- `buf` argument must match corresponding `begin` routine

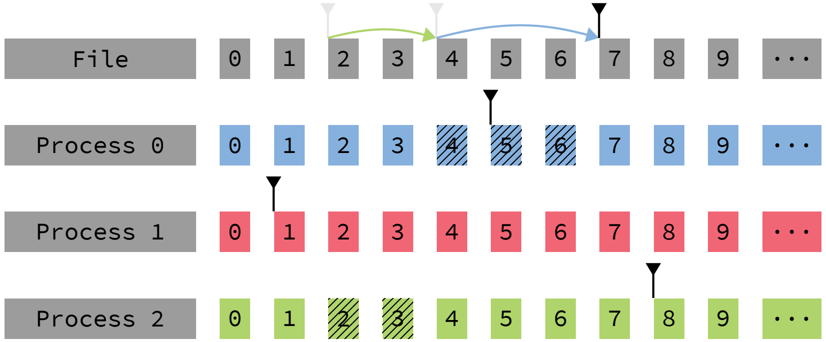
EXAMPLE

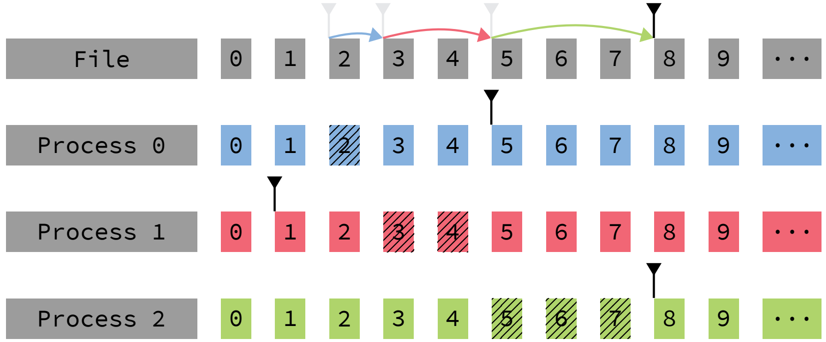
blocking, noncollective, shared [MPI-4.0, 14.4.4]

With the shared pointer at element 2,

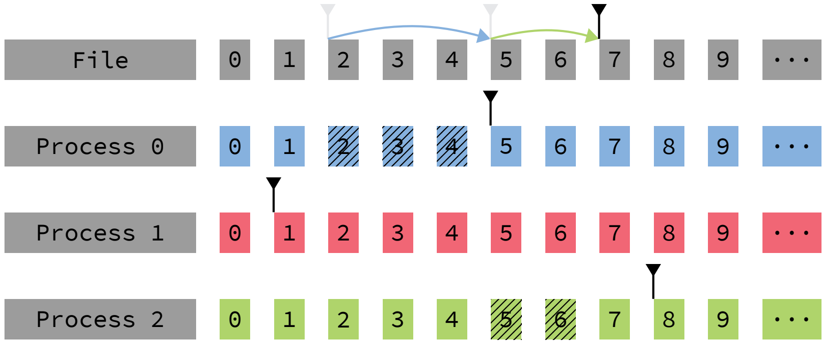
- process 0 calls `MPI_File_write_shared(count = 3)`,
- process 2 calls `MPI_File_write_shared(count = 2)`:

Scenario 1:





Scenario 2:



EXAMPLE

blocking, collective, shared [MPI-4.0, 14.4.4]

With the shared pointer at element 2,

- process 0 calls `MPI_File_write_ordered(count = 1)`,
- process 1 calls `MPI_File_write_ordered(count = 2)`,
- process 2 calls `MPI_File_write_ordered(count = 3)`:

READING

blocking, noncollective, individual [MPI-4.0, 14.4.3]

```c
int MPI_File_read(MPI_File fh, void* buf, int count,
↪ MPI_Datatype datatype, MPI_Status* status)
```

```fortran
MPI_File_read(fh, buf, count, datatype, status, ierror)
type(MPI_File), intent(in) :: fh
type(*), dimension(..) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Starts reading at the current position of the individual file pointer
- Reads up to `count` elements of `datatype` into the memory starting at `buf`
- `status` indicates how many elements have been read
- If `status` indicates less than `count` elements read, the end of file has been reached

FILE POINTER POSITION [MPI-4.0, 14.4.3]

```c
int MPI_File_get_position(MPI_File fh, MPI_Offset* offset)
```

```fortran
MPI_File_get_position(fh, offset, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(out) :: offset
integer, optional, intent(out) :: ierror
```

- Returns the current position of the individual file pointer in units of *etype*
- Value can be used for e.g.
  - return to this position (via seek)
  - calculate a displacement
- `MPI_File_get_position_shared` queries the position of the shared file pointer

SEEKING TO A FILE POSITION [MPI-4.0, 14.4.3]

C
```c
int MPI_File_seek(MPI_File fh, MPI_Offset offset, int whence)
```

F08
```fortran
MPI_File_seek(fh, offset, whence, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
integer, intent(in) :: whence
integer, optional, intent(out) :: ierror
```

- whence controls how the file pointer is moved:

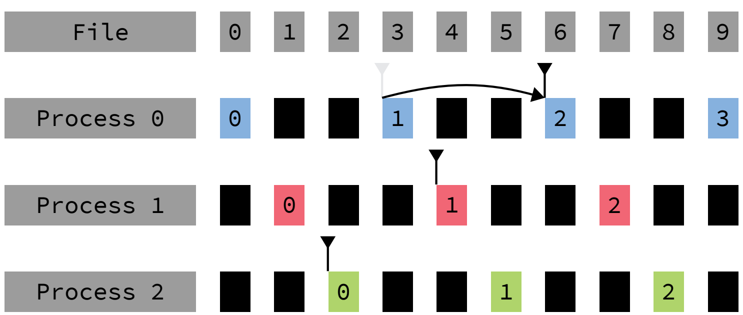
  `MPI_SEEK_SET` sets the file pointer to `offset`

  `MPI_SEEK_CUR` `offset` is relative to the current value of the pointer

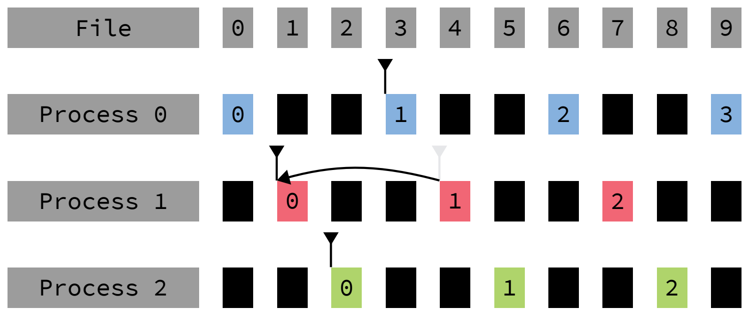
  `MPI_SEEK_END` `offset` is relative to the end of the file
- `offset` can be negative but the resulting position may not lie before the beginning of the file
- `MPI_File_seek_shared` manipulates the shared file pointer

EXAMPLE

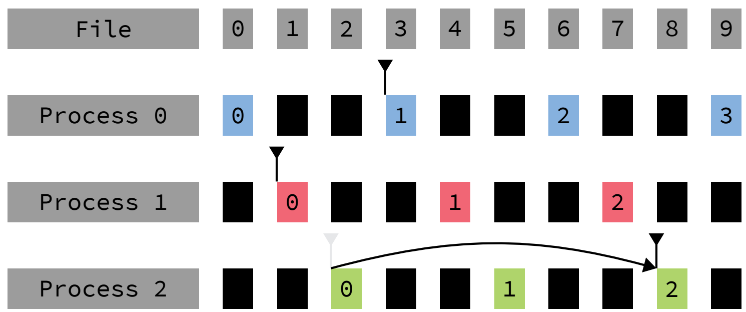
Process 0 calls `MPI_File_seek(offset = 2, whence = MPI_SEEK_SET)`:



Process 1 calls `MPI_File_seek(offset = -1, whence = MPI_SEEK_CUR)`:



Process 2 calls `MPI_File_seek(offset = -1, whence = MPI_SEEK_END)`:



CONVERTING OFFSETS [MPI-4.0, 14.4.3]

C
```c
int MPI_File_get_byte_offset(MPI_File fh, MPI_Offset offset,
  ↪ MPI_Offset* disp)
```

F08
```fortran
MPI_File_get_byte_offset(fh, offset, disp, ierror)
type(MPI_File), intent(in) :: fh
integer(kind=MPI_OFFSET_KIND), intent(in) :: offset
integer(kind=MPI_OFFSET_KIND), intent(out) :: disp
integer, optional, intent(out) :: ierror
```

- Converts a view relative offset (in units of *etype*) into a displacement in bytes from the beginning of the file

46 CONSISTENCY

CONSISTENCY [MPI-4.0, 14.6.1]

Terminology: Sequential Consistency

> If a set of operations is sequentially consistent, they behave as if executed in some serial order. The exact order is unspecified.

- To guarantee sequential consistency, certain requirements must be met
- Requirements depend on access path and file atomicity

Caution: Result of operations that are not sequentially consistent is implementation dependent.

ATOMIC MODE [MPI-4.0, 14.6.1]

Requirements for sequential consistency
Same file handle: always sequentially consistent

File handles from same open: always sequentially consistent

File handles from different open: not influenced by atomicity, see nonatomic mode

- Atomic mode is not the default setting
- Can lead to overhead, because MPI library has to uphold guarantees in general case

```c
int MPI_File_set_atomicity(MPI_File fh, int flag)
```

```fortran
MPI_File_set_atomicity(fh, flag, ierror)
type(MPI_File), intent(in) :: fh
logical, intent(in) :: flag
integer, optional, intent(out) :: ierror
```

NONATOMIC MODE [MPI-4.0, 14.6.1]

Requirements for sequential consistency
Same file handle: operations must be either nonconcurrent, nonconflicting, or both

File handles from same open: nonconflicting accesses are sequentially consistent, conflicting accesses have to be protected using `MPI_File_sync`

File handles from different open: all accesses must be protected using `MPI_File_sync`

Terminology: Conflicting Accesses

> Two accesses are conflicting if they touch overlapping parts of a file and at least one is writing.

```c
int MPI_File_sync(MPI_File fh)
```

```fortran
MPI_File_sync(fh, ierror)
type(MPI_File), intent(in) :: fh
integer, optional, intent(out) :: ierror
```

The Sync-Barrier-Sync construct

```c
// writing access sequence through one file handle
MPI_File_sync(fh0);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh0);
// ...
```

```c
// ...
MPI_File_sync(fh1);
MPI_Barrier(MPI_COMM_WORLD);
MPI_File_sync(fh1);
// access sequence to the same file through a different file
    handle
```

- `MPI_File_sync` is used to delimit sequences of accesses through different file handles
- Sequences that contain a write access may not be concurrent with any other access sequence

47 LARGE NUMBERS

LARGE COUNT EXAMPLE

```c
int MPI_File_read_at(MPI_File fh, MPI_Offset offset, void* buf,
    int count, MPI_Datatype datatype, MPI_Status* status)

int MPI_File_read_at_c(MPI_File fh, MPI_Offset offset, void*
    buf, MPI_Count count, MPI_Datatype datatype, MPI_Status*
    status)
```

```fortran
MPI_File_read_at(fh, offset, buf, count, datatype, status,
  ierror)
type(MPI_File), intent(in) :: fh
integer(KIND=MPI_OFFSET_KIND), intent(in) :: offset
type(*), dimension(..) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

```fortran
MPI_File_read_at(fh, offset, buf, count, datatype, status,
  ierror)
type(MPI_File), intent(in) :: fh
integer(KIND=MPI_OFFSET_KIND), intent(in) :: offset
type(*), dimension(..) :: buf
integer(KIND=MPI_COUNT_KIND), intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

48 EXERCISES

Exercise 6 – Data Access

6.1 Writing Data

In the file `rank_io.{c|cxx|f90|py}` write a function `write_rank` that takes a communicator as its only argument and does the following:

- Each process writes its own rank in the communicator to a common file `rank.dat` using `"native"` data representation.
- The ranks should be in order in the file: $0 \ldots n-1$.

Use: `MPI_File_open`, `MPI_File_set_errhandler`, `MPI_File_set_view`, `MPI_File_write_ordered`, `MPI_File_close`

6.2 Reading Data

In the file `rank_io.{c|cxx|f90|py}` write a function `read_rank` that takes a communicator as its only argument and does the following:

- The processes read the integers in the file in reverse order, i.e. process 0 reads the last entry, process 1 reads the one before, etc.
- Each process returns the rank number it has read from the function.

Careful: This function might be run on a communicator with a different number of processes. If there are more processes than entries in the file, processes with ranks larger than or equal to the number of file entries should return `MPI_PROC_NULL`.

Use: `MPI_File_seek`, `MPI_File_get_position`, `MPI_File_read`

6.3 Phone Book

The file `phonebook.dat` contains several records of the following form:

```c
struct dbentry {
  int key;
  int room_number;
  int phone_number;
  char name[200];
}
```

```fortran
type :: dbentry
  integer :: key
  integer :: room_number
  integer :: phone_number
  character(len=200) :: name
end type
```

In the file `phonebook.{c|cxx|f90|py}` write a function `look_up_by_room_number` that uses MPI I/O to find an entry by room number. Assume the file was written using `"native"` data representation. Use `MPI_COMM_SELF` to open the file. Return a `bool` or `logical` to indicate whether an entry has been found and fill an entry via pointer/intent out argument.

PART VIII

TOOLS

49 MUST

MUST

Marmot Umpire Scalable Tool

MUST

`https://itc.rwth-aachen.de/must/`

MUST checks for correct usage of MPI. It includes checks for the following classes of mistakes:

- Constants and integer values
- Communicator usage
- Datatype usage
- Group usage
- Operation usage
- Request usage
- Leak checks (MPI resources not freed before calling `MPI_Finalize`)
- Type mismatches
- Overlapping buffers passed to MPI
- Deadlocks resulting from MPI calls
- Basic checks for thread level usage (`MPI_Init_thread`)

MUST USAGE

Build your application:

```
$ mpicc -o application.x application.c
$ # or
$ mpif90 -o application.x application.f90
```

Replace the MPI starter (e.g. `srun`) with MUST's own `mustrun`:

```
$ mustrun -n 4 --must:mpiexec srun --must:np -n ./application.x
```

Different modes of operation (for improved scalability or graceful handling of application crashes) are available via command line switches.

Caution: MUST is not compatible with MPI's Fortran 2008 interface.

50 EXERCISES

Exercise 7 – MPI Tools

7.1 Must

Have a look at the file `must.{c|c++|f90}`. It contains a variation of the solution to exercise 2.3 – it should calculate the sum of all ranks and make the result available on all processes.

1. Compile the program and try to run it.
2. Use MUST to discover what is wrong with the program.
3. If any mistakes were found, fix them and go back to 1.

Note: `must.f90` uses the MPI Fortran 90 interface.

PART IX

COMMUNICATORS

51 INTRODUCTION

MOTIVATION

Communicators are a scope for communication within or between groups of processes. New communicators with different scope or topological properties can be used to accommodate certain needs.

- **Separation of communication spaces:** A software library that uses MPI underneath is used in an application that directly uses MPI itself. Communication due to the library should not conflict with communication due to the application.
- **Partitioning of process groups:** Parts of your software exhibit a collective communication pattern, but only across a subset of processes.
- **Exploiting inherent topology:** Your application uses a regular cartesian grid to discretize the problem and this translates into certain nearest neighbor communication patterns.

52 CONSTRUCTORS

DUPLICATE [MPI-4.0, 7.4.2]

C
```c
int MPI_Comm_dup(MPI_Comm comm, MPI_Comm *newcomm)
```

F08
```fortran
MPI_Comm_dup(comm, newcomm, ierror)
type(MPI_Comm), intent(in) :: comm
type(MPI_Comm), intent(out) :: newcomm
integer, optional, intent(out) :: ierror
```

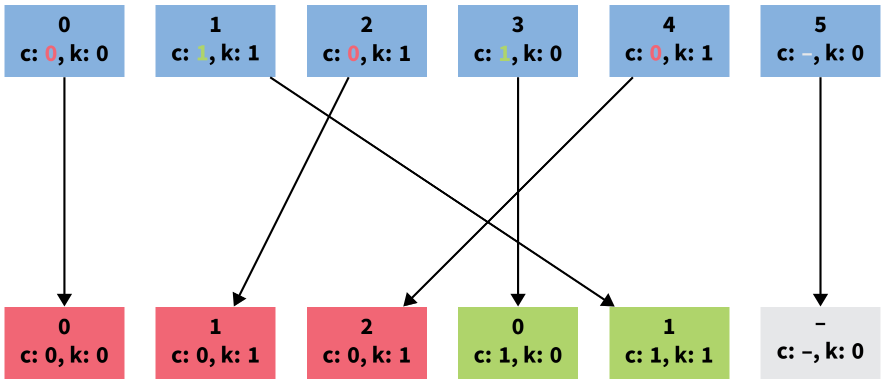
- Duplicates an existing communicator `comm`
- New communicator has the same properties but a new context

SPLIT [MPI-4.0, 7.4.2]

C
```
int MPI_Comm_split(MPI_Comm comm, int color, int key, MPI_Comm
    *newcomm)
```

F08
```
MPI_Comm_split(comm, color, key, newcomm, ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(in) :: color, key
type(MPI_Comm), intent(out) :: newcomm
integer, optional, intent(out) :: ierror
```

- Splits the processes in a communicator into disjoint subgroups
- Processes are grouped by `color`, one new communicator per distinct value
- Special color value `MPI_UNDEFINED` does not create a new communicator (`MPI_COMM_NULL` is returned in newcomm)
- Processes are ordered by ascending value of `key` in new communicator



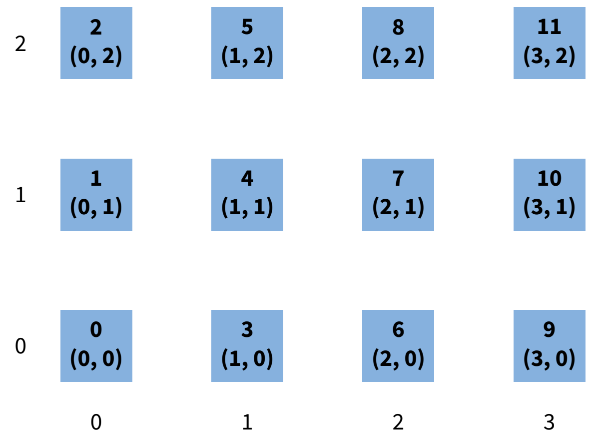
CARTESIAN TOPOLOGY [MPI-4.0, 8.5.1]

C
```
int MPI_Cart_create(MPI_Comm comm_old, int ndims, const int
    dims[], const int periods[], int reorder, MPI_Comm
    *comm_cart)
```

F08
```
MPI_Cart_create(comm_old, ndims, dims, periods, reorder,
    comm_cart, ierror)
type(MPI_Comm), intent(in) :: comm_old
integer, intent(in) :: ndims, dims(ndims)
logical, intent(in) :: periods(ndims), reorder
type(MPI_Comm), intent(out) :: comm_cart
integer, optional, intent(out) :: ierror
```

- Creates a new communicator with processes arranged on a (possibly periodic) Cartesian grid
- The grid has `ndims` dimensions and `dims[i]` points in dimension `i`
- If `reorder` is true, MPI is free to assign new ranks to processes

Input:
`comm_old` contains 12 processes (or more)
`ndims = 2`, `dims = [ 4, 3 ]`, `periods = [ .false., .false. ]` `reorder = .false.`
Output:
process 0–11: new communicator with topology as shown
process 12–: `MPI_COMM_NULL`



53 ACCESSORS

RANK TO COORDINATE [MPI-4.0, 8.5.5]

C
```
int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int
    coords[])
```

```fortran
MPI_Cart_coords(comm, rank, maxdims, coords, ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(in) :: rank, maxdims
integer, intent(out) :: coords(maxdims)
integer, optional, intent(out) :: ierror
```

Translates the rank of a process into its coordinate on the Cartesian grid.

COORDINATE TO RANK [MPI-4.0, 8.5.5]

```c
int MPI_Cart_rank(MPI_Comm comm, const int coords[], int
    *rank)
```

```fortran
MPI_Cart_rank(comm, coords, rank, ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(in) :: coords(*)
integer, intent(out) :: rank
integer, optional, intent(out) :: ierror
```

Translates the coordinate on the Cartesian grid of a process into its rank.

CARTESIAN SHIFT [MPI-4.0, 8.5.6]

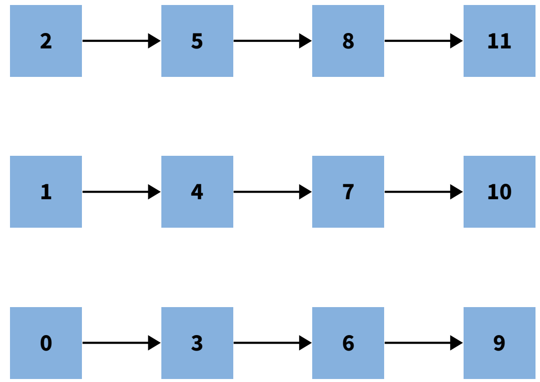
```c
int MPI_Cart_shift(MPI_Comm comm, int direction, int disp, int
    *rank_source, int *rank_dest)
```

```fortran
MPI_Cart_shift(comm, direction, disp, rank_source, rank_dest,
    ierror)
type(MPI_Comm), intent(in) :: comm
integer, intent(in) :: direction, disp
integer, intent(out) :: rank_source, rank_dest
integer, optional, intent(out) :: ierror
```

- Calculates the ranks of source and destination processes in a shift operation on a Cartesian grid
- `direction` gives the number of the axis (starting at 0)
- `disp` gives the displacement

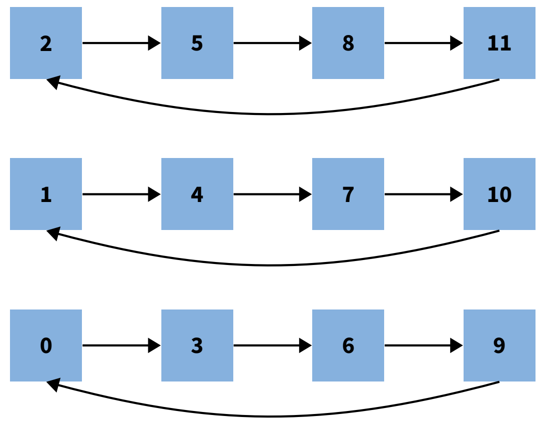
Input: `direction = 0`, `disp = 1`, not periodic

Output:
process 0: `rank_source = MPI_PROC_NULL`, `rank_dest = 3`
...
process 3: `rank_source = 0`, `rank_dest = 6`
...
process 9: `rank_source = 6`, `rank_dest = MPI_PROC_NULL`
...



Input: `direction = 0`, `disp = 1`, periodic

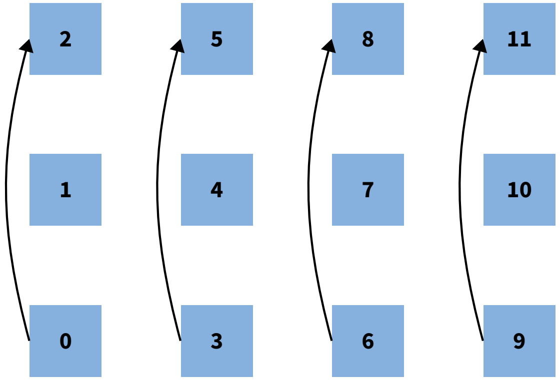
Output:
process 0: `rank_source = 9`, `rank_dest = 3`
...
process 3: `rank_source = 0`, `rank_dest = 6`
...
process 9: `rank_source = 6`, `rank_dest = 0`
...



Input: `direction = 1`, `disp = 2`, not periodic

Output:

process 0: `rank_source = MPI_PROC_NULL`, `rank_dest = 2`
process 1: `rank_source = MPI_PROC_NULL`, `rank_dest = MPI_PROC_NULL`
process 2: `rank_source = 0`, `rank_dest = MPI_PROC_NULL`
...



NULL PROCESSES [MPI-4.0, 3.10]

```c
int MPI_PROC_NULL = /* implementation defined */
```

```fortran
integer, parameter :: MPI_PROC_NULL = ! implementation defined
```

- Can be used as source or destination for point-to-point communication
- Communication with `MPI_PROC_NULL` has no effect
- May simplify code structure (communication with special source/destination instead of branch)
- `MPI_Cart_shift` returns `MPI_PROC_NULL` for out of range shifts

COMPARISON [MPI-4.0, 7.4.1]

```c
int MPI_Comm_compare(MPI_Comm comm1, MPI_Comm comm2, int
    *result)
```

```fortran
MPI_Comm_compare(comm1, comm2, result, ierror)
type(MPI_Comm), intent(in) :: comm1, comm2
integer, intent(out) :: result
integer, optional, intent(out) :: ierror
```

Compares two communicators. The result is one of:

`MPI_IDENT` The two communicators are the same.

`MPI_CONGRUENT` The two communicators consist of the same processes in the same order but communicate in different contexts.

`MPI_SIMILAR` The two communicators consist of the same processes in a different order.

`MPI_UNEQUAL` Otherwise.

54 DESTRUCTORS

FREE [MPI-4.0, 7.4.3]

```c
int MPI_Comm_free(MPI_Comm *comm)
```

```fortran
MPI_Comm_free(comm, ierror)
type(MPI_Comm), intent(inout) :: comm
integer, optional, intent(out) :: ierror
```

Marks a communicator for deallocation.

55 EXERCISES

Exercise 8 – Communicators

8.1 Cartesian Topology

In `global_sum_with_communicators.{c|cxx|f90|py}`, redo exercise 2.3 using a Cartesian communicator.

Use: `MPI_Cart_create`, `MPI_Cart_shift`, `MPI_Comm_free`

8.2 Split

In `global_sum_with_communicators.{c|cxx|f90|py}`, redo exercise 3.1 using a new split communicator per communication round.

Use: `MPI_Comm_split`

PART X

THREAD COMPLIANCE

56 INTRODUCTION

THREAD COMPLIANCE [MPI-4.0, 11.6]

- An MPI library is thread compliant if
  1. Concurrent threads can make use of MPI routines and the result will be as if they were executed in some order.
  2. Blocking routines will only block the executing thread, allowing other threads to make progress.
- MPI libraries are not required to be thread compliant
- Alternative initialization routines to request certain levels of thread compliance
- These functions are always safe to use in a multithreaded setting: `MPI_Initialized`, `MPI_Finalized`, `MPI_Query_thread`, `MPI_Is_thread_main`, `MPI_Get_version`, `MPI_Get_library_version`

57 ENABLING THREAD SUPPORT

THREAD SUPPORT LEVELS [MPI-4.0, 11.2.1]

The following predefined values are used to express all possible levels of thread support:

`MPI_THREAD_SINGLE` program is single threaded

`MPI_THREAD_FUNNELED` MPI routines are only used by the *main thread*

`MPI_THREAD_SERIALIZED` MPI routines are used by multiple threads, but not concurrently

`MPI_THREAD_MULTIPLE` MPI is thread compliant, no restrictions

`MPI_THREAD_SINGLE` < `MPI_THREAD_FUNNELED` < `MPI_THREAD_SERIALIZED` < `MPI_THREAD_MULTIPLE`

INITIALIZATION [MPI-4.0, 11.2.1]

C
```
int MPI_Init_thread(int* argc, char*** argv, int required,
↪ int* provided)
```

F08
```
MPI_Init_thread(required, provided, ierror)
integer, intent(in) :: required
integer, intent(out) :: provided
integer, optional, intent(out) :: ierror
```

- `required` and `provided` specify thread support levels
- If possible, `provided = required`
- Otherwise, if possible, `provided > required`
- Otherwise, `provided < required`
- `MPI_Init` is equivalent to `required = MPI_THREAD_SINGLE`

INQUIRY FUNCTIONS [MPI-4.0, 11.2.1]

Query level of thread support:

C
```
int MPI_Query_thread(int *provided)
```

F08
```
MPI_Query_thread(provided, ierror)
integer, intent(out) :: provided
integer, optional, intent(out) :: ierror
```

Check whether the calling thread is the *main thread*:

C
```
int MPI_Is_thread_main(int* flag)
```

F08
```
MPI_Is_thread_main(flag, ierror)
logical, intent(out) :: flag
integer, optional, intent(out) :: ierror
```

58 MATCHING PROBE AND RECEIVE

MATCHING PROBE [MPI-4.0, 3.8.2]

C
```
int MPI_Mprobe(int source, int tag, MPI_Comm comm,
↪ MPI_Message* message, MPI_Status* status)
```

F08
```
MPI_Mprobe(source, tag, comm, message, status, ierror)
integer, intent(in) :: source, tag
type(MPI_Comm), intent(in) :: comm
type(MPI_Message), intent(out) :: message
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Works like `MPI_Probe`, except for the returned `MPI_Message` value which may be used to receive exactly the probed message

- Nonblocking variant `MPI_Improbe` exists

MATCHED RECEIVE [MPI-4.0, 3.8.3]

```c
int MPI_Mrecv(void* buf, int count, MPI_Datatype datatype,
↪ MPI_Message* message, MPI_Status* status)
```

```fortran
MPI_Mrecv(buf, count, datatype, message, status, ierror)
type(*), dimension(..) :: buf
integer, intent(in) :: count
type(MPI_Datatype), intent(in) :: datatype
type(MPI_Message), intent(inout) :: message
type(MPI_Status) :: status
integer, optional, intent(out) :: ierror
```

- Receives the previously probed message `message`
- Sets the message handle to `MPI_MESSAGE_NULL`
- Nonblocking variant `MPI_Imrecv` exists

59 REMARKS

CLARIFICATIONS [MPI-4.0, 11.6.2]

Initialization and Finalization
Initialization and finalization of MPI should occur on the same thread, the *main thread*.

Request Completion
Multiple threads must not try to complete the same request (e.g. `MPI_Wait`).

Probe
In multithreaded settings, `MPI_Probe` might match a different message as a subsequent `MPI_Recv`.

PART XI

FIRST STEPS WITH OPENMP

60 WHAT IS OPENMP?

OpenMP is a specification for a set of compiler directives, library routines, and environment variables that can be used to specify high-level parallelism in Fortran and C/C++ programs. (*OpenMP FAQ*[4])

- Initially targeted SMP systems, now also DSPs, accelerators, etc.
- Provides *specifications* (not implementations)
- Portable across different platforms

Current version of the specification: 5.1 (November 2020)

BRIEF HISTORY

1997 FORTRAN version 1.0

1998 C/C++ version 1.0

1999 FORTRAN version 1.1

2000 FORTRAN version 2.0

2002 C/C++ version 2.0

2005 First combined version 2.5, memory model, internal control variables, clarifications

2008 Version 3.0, tasks

2011 Version 3.1, extended task facilities

2013 Version 4.0, thread affinity, SIMD, devices, tasks (dependencies, groups, and cancellation), improved Fortran 2003 compatibility

2015 Version 4.5, extended SIMD and devices facilities, task priorities

2018 Version 5.0, memory model, base language compatibility, allocators, extended task and devices facilities

2020 Version 5.1, support for newer base languages, loop transformations, compare-and-swap, extended devices facilities

2021 Version 5.2, reorganization of the specification and improved consistency

COVERAGE

- Overview of the OpenMP API (✓)
- Internal Control Variables (✓)
- Directive and Construct Syntax (✓)
- Base Language Formats and Restrictions (✓)
- Data Environment (✓)

[4] Matthijs van Waveren et al. *OpenMP FAQ*. version 3.0. June 6, 2018. URL: `https://www.openmp.org/about/openmp-faq/` (visited on 01/30/2019).

- Memory Management
- Variant Directives
- Informational and Utility Directives
- Loop Transformation Constructs
- Parallelism Generation and Control (✓)
- Work-Distribution Constructs (✓)
- Tasking Constructs (✓)
- Device Directives and Clauses
- Interoperability
- Synchronization Constructs and Clauses (✓)
- Cancellation Constructs
- Composition of Contstructs (✓)
- Runtime Library Routines (✓)
- OMPT Interface
- OMPD Interface
- Environment Variables (✓)

LITERATURE

Official Resources

- OpenMP Architecture Review Board. *OpenMP Application Programming Interface*. Version 5.2. Nov. 2021. URL: `https://www.openmp.org/wp-content/uploads/OpenMP-API-Specification-5-2.pdf`
- OpenMP Architecture Review Board. *OpenMP Application Programming Interface. Examples*. Version 5.1. Aug. 2021. URL: `https://www.openmp.org/wp-content/uploads/openmp-examples-5.1.pdf`
- `https://www.openmp.org`

Recommended by `https://www.openmp.org/resources/openmp-books/`

- Michael Klemm and Jim Cownie. *High Performance Parallel Runtimes*. De Gruyter Oldenbourg, 2021. ISBN: 9783110632729. DOI: `doi:10.1515/9783110632729`
- Timothy G. Mattson, Yun He, and Alice E. Koniges. *The OpenMP Common Core. Making OpenMP Simple Again*. 1st ed. The MIT Press, Nov. 19, 2019. 320 pp. ISBN: 9780262538862
- Ruud van der Pas, Eric Stotzer, and Christian Terboven. *Using OpenMP—The Next Step. Affinity, Accelerators, Tasking, and SIMD*. 1st ed. The MIT Press, Oct. 13, 2017. 392 pp. ISBN: 9780262534789

Additional Literature

- Michael McCool, James Reinders, and Arch Robison. *Structured Parallel Programming. Patterns for Efficient Computation*. 1st ed. Morgan Kaufmann, July 31, 2012. 432 pp. ISBN: 9780124159938

Older Works (`https://www.openmp.org/resources/openmp-books/`)

- Barbara Chapman, Gabriele Jost, and Ruud van der Pas. *Using OpenMP. Portable Shared Memory Parallel Programming*. 1st ed. Scientific and Engineering Computation. The MIT Press, Oct. 12, 2007. 384 pp. ISBN: 9780262533027
- Rohit Chandra et al. *Parallel Programming in OpenMP*. 1st ed. Morgan Kaufmann, Oct. 11, 2000. 231 pp. ISBN: 9781558606715
- Michael Quinn. *Parallel Programming in C with MPI and OpenMP*. 1st ed. McGraw-Hill, June 5, 2003. 544 pp. ISBN: 9780072822564
- Timothy G. Mattson, Beverly A. Sanders, and Berna L. Massingill. *Patterns for Parallel Programming*. 1st ed. Software Patterns. Sept. 15, 2004. 384 pp. ISBN: 9780321228116

61 TERMINOLOGY

THREADS & TASKS

Terminology: Thread

An execution entity with a stack and associated static memory, called *threadprivate memory*.

Terminology: OpenMP Thread

A *thread* that is managed by the OpenMP runtime system.

Terminology: Team

A set of one or more *threads* participating in the execution of a `parallel` *region*.

Terminology: Task

A specific instance of executable code and its data environment that the OpenMP imlementation can schedule for execution by threads.

LANGUAGE

Terminology: Base Language

A programming language that serves as the foundation of the OpenMP specification.

The following base languages are given in [OpenMP-5.1, 1.7]: C90, C99, C11, C18, C++98, C++11, C++14, C++17, C++20, Fortran 77, Fortran 90, Fortran 95, Fortran 2003, Fortran 2008, and a subset of Fortran 2018

Terminology: Base Program

A program written in the *base language*.

Terminology: OpenMP Program

A program that consists of a *base program* that is annotated with OpenMP *directives* or that calls OpenMP API runtime library routines.

Terminology: Directive

In C/C++, a *#pragma*, and in Fortran, a comment, that specifies *OpenMP program* behavior.

62 INFRASTRUCTURE

COMPILING & LINKING

Compilers that conform to the OpenMP specification usually accept a command line argument that turns on OpenMP support, e.g.:

Intel C Compiler OpenMP Command Line Switch

```
$ icc -qopenmp ...
```

GNU Fortran Compiler OpenMP Command Line Switch

```
$ gfortran -fopenmp ...
```

The name of this command line argument is not mandated by the specification and differs from one compiler to another.

Naturally, these arguments are then also accepted by the MPI compiler wrappers:

Compiling Programs with Hybrid Parallelization

```
$ mpicc -qopenmp ...
```

RUNTIME LIBRARY DEFINITIONS [OpenMP-5.1, 18.1]

C/C++ Runtime Library Definitions

Runtime library routines and associated types are defined in the `omp.h` header file.

C
```
#include <omp.h>
```

Fortran Runtime Library Definitions

Runtime library routines and associated types are defined in either a Fortran **include** file

F77
```
include "omp_lib.h"
```

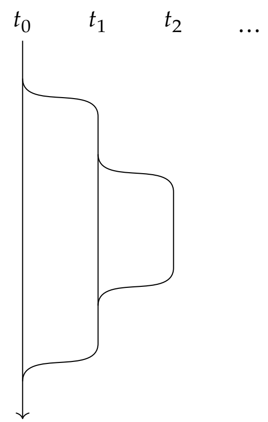
or a Fortran 90 module

F08
```
use omp_lib
```

63 BASIC PROGRAM STRUCTURE

WORLD ORDER IN OPENMP

- Program starts as one single-threaded process.
- Forks into teams of multiple threads when appropriate.
- Stream of instructions might be different for each thread.
- Information is exchanged via shared parts of memory.
- OpenMP threads may be nested inside MPI processes.



C AND C++ DIRECTIVE FORMAT [OpenMP-5.1, 3.1]

In C and C++, OpenMP directives are written using the *#pragma* method:

C
```
#pragma omp directive-name [clause[[,] clause]...]
```

- Directives are case-sensitive
- Applies to the next statement which must be a *structured block*

Terminology: Structured Block

An executable statement, possibly compound, with a single entry at the top and a single exit at the bottom, or an OpenMP *construct*.

FORTRAN DIRECTIVE FORMAT [OpenMP-5.1, 3.1.1, 3.1.2]

F08
```
sentinel directive-name [clause[[,] clause]...]
```

- Directives are case-insensitive

Fixed Form Sentinels

F08
```
sentinel = !$omp | c$omp | *$omp
```

- Must start in column 1
- The usual line length, white space, continuation and column rules apply
- Column 6 is blank for first line of directive, non-blank and non-zero for continuation

Free Form Sentinel

F08
```
sentinel = !$omp
```

- The usual line length, white space and continuation rules apply

CONDITIONAL COMPILATION [OpenMP-5.1, 3.3]

C Preprocessor Macro

C
```
#define _OPENMP yyyymm
```

`yyyy` and `mm` are the year and month the OpenMP specification supported by the compiler was published.

Fortran Fixed Form Sentinels

F08
```
!$ | *$ | c$
```

- Must start in column 1
- Only numbers or white space in columns 3–5
- Column 6 marks continuation lines

Fortran Free Form Sentinel

F08
```
!$
```

- Must only be preceded by white space
- Can be continued with ampersand

THE PARALLEL CONSTRUCT [OpenMP-5.1, 10.1]

C
```
#pragma omp parallel [clause[[,] clause]...]
  structured-block
```

F08
```
!$omp parallel [clause[[,] clause]...]
  structured-block
!$omp end parallel
```

- Creates a team of threads to execute the `parallel` region
- Each thread executes the code contained in the structured block
- Inside the region threads are identified by consecutive numbers starting at zero
- Optional clauses (explained later) can be used to modify behavior and data environment of the `parallel` region

THREAD COORDINATES [OpenMP-5.1, 18.2.2, 18.2.4]

Team size

C
```
int omp_get_num_threads(void);
```

F08
```
integer function omp_get_num_threads()
```

Returns the number of threads in the current team

Thread number

C
```
int omp_get_thread_num(void);
```

F08
```
integer function omp_get_thread_num()
```

Returns the number that identifies the calling thread within the current team (between zero and `omp_get_num_threads()`)

A FIRST OPENMP PROGRAM

C

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

int main(void) {
  printf("Hello from your main thread.\n");

  #pragma omp parallel
    printf("Hello from thread %d of %d.\n", omp_get_thread_num(), omp_get_num_threads());

  printf("Hello again from your main thread.\n");
}
```

Program Output

```
$ gcc -fopenmp -o hello_openmp.x hello_openmp.c
$ ./hello_openmp.x
Hello from your main thread.
Hello from thread 1 of 8.
Hello from thread 0 of 8.
Hello from thread 3 of 8.
Hello from thread 4 of 8.
Hello from thread 6 of 8.
Hello from thread 7 of 8.
Hello from thread 2 of 8.
Hello from thread 5 of 8.
Hello again from your main thread.
```

F08

```fortran
program hello_openmp
  use omp_lib
  implicit none

  print *, "Hello from your main thread."

  !$omp parallel
  print *, "Hello from thread ", omp_get_thread_num(), " of ", omp_get_num_threads(), "."
  !$omp end parallel

  print *, "Hello again from your main thread."
end program
```

64 EXERCISES

Exercise 9 – Warm Up

9.1 Generalized Vector Addition (axpy)

In the file `axpy.{c|c++|f90}`, fill in the missing body of the function/subroutine `axpy_serial(a, x, y, z[, n])` so that it implements the generalized vector addition (in serial, without making use of OpenMP):

$$\mathbf{z} = a\mathbf{x} + \mathbf{y}.$$

Compile the file into a program and run it to test your implementation.

9.2 Dot Product

In the file `dot.{c|c++|f90}`, fill in the missing body of the function/subroutine `dot_serial(x, y[, n])` so that it implements the dot product (in serial, without making use of OpenMP):

$$\texttt{dot}(\mathbf{x}, \mathbf{y}) = \sum_i x_i y_i.$$

Compile the file into a program and run it to test your implementation.

PART XII

LOW-LEVEL OPENMP CONCEPTS

65 INTRODUCTION

MAGIC

> Any sufficiently advanced technology is indistinguishable from magic.
> (Arthur C. Clarke[5])

INTERNAL CONTROL VARIABLES [OpenMP-5.1, 2]

Terminology: Internal Control Variable (ICV)

> A conceptual variable that specifies runtime behavior of a set of *threads* or *tasks* in an *OpenMP program*.

- Set to an initial value by the OpenMP implementation

[5] Arthur C. Clarke. *Profiles of the future : an inquiry into the limits of the possible*. London: Pan Books, 1973. ISBN: 9780330236195.

- Some can be modified through either environment variables (e.g. OMP_NUM_THREADS) or API routines (e.g. omp_set_num_threads())
- Some can be read through API routines (e.g. omp_get_max_threads())
- Some are inaccessible to the user
- Might have different values in different scopes (e.g. data environment, device, global)
- Some can be overridden by clauses (e.g. the num_threads() clause)
- Export OMP_DISPLAY_ENV=TRUE or call omp_display_env(1) to inspect the value of ICVs that correspond to environment variables [OpenMP-5.1, 18.15, 21.7]

PARALLELISM CLAUSES [OpenMP-5.1, 3.4, 10.1.2]

if Clause

```c
if([parallel :] scalar-expression)
```

```fortran
if([parallel :] scalar-logical-expression)
```

If *false*, the region is executed only by the encountering thread(s) and no additional threads are forked.

num_threads Clause

```c
num_threads(integer-expression)
```

```fortran
num_threads(scalar-integer-expression)
```

Requests a team size equal to the value of the expression (overrides the *nthreads-var* ICV)

EXAMPLE

A parallel directive with an if clause and associated structured block in C:

```c
#pragma omp parallel if( length > threshold )
{
  statement0;
  statement1;
  statement2;
}
```

A parallel directive with a num_threads clause and associated structured block in Fortran:

```fortran
!$omp parallel num_threads( 64 )
statement1
statement2
statement3
!$omp end parallel
```

CONTROLLING THE *nthreads-var* ICV

omp_set_num_threads API Routine [OpenMP-5.1, 18.2.1]

```c
void omp_set_num_threads(int num_threads);
```

```fortran
subroutine omp_set_num_threads(num_threads)
integer num_threads
```

Sets the ICV that controls the number of threads to fork for parallel regions (without num_threads clause) encountered subsequently.

omp_get_max_threads API Routine [OpenMP-5.1, 18.2.3]

```c
int omp_get_max_threads(void);
```

```fortran
integer function omp_get_max_threads()
```

Queries the ICV that controls the number of threads to fork.

THREAD LIMIT & DYNAMIC ADJUSTMENT

omp_get_thread_limit API Routine [OpenMP-5.1, 18.2.13]

```c
int omp_get_thread_limit(void);
```

```fortran
integer function omp_get_thread_limit()
```

Upper bound on the number of threads used in a program.

omp_get_dynamic and omp_set_dynamic API Routines [OpenMP-5.1, 18.2.6, 18.2.7]

```c
int omp_get_dynamic(void);
void omp_set_dynamic(int dynamic);
```

```
F08
logical function omp_get_dynamic()
subroutine omp_set_dynamic(dynamic)
logical dynamic
```

Enable or disable dynamic adjustment of the number of threads.

INSIDE OF A PARALLEL REGION?

omp_in_parallel API Routine [OpenMP-5.1, 18.2.5]

```
C
int omp_in_parallel(void);
```

```
F08
logical function omp_in_parallel()
```

Is this code being executed as part of a `parallel` region?

66 EXERCISES

Exercise 10 – Controlling `parallel`
10.1 Controlling the Number of Threads

Use `hello_openmp.{c|c++|f90}` to play around with the various ways to set the number of threads forked for a `parallel` region:

- The `OMP_NUM_THREADS` environment variable
- The `omp_set_num_threads` API routine
- The `num_threads` clause
- The `if` clause

Inspect the number of threads that are actually forked using `omp_get_num_threads`.

10.2 Limits of the OpenMP Implementation

Determine the maximum number of threads allowed by the OpenMP implementation you are using and check whether it supports dynamic adjustment of the number of threads.

67 DATA ENVIRONMENT

DATA-SHARING ATTRIBUTES [OpenMP-5.1, 5.1]

Terminology: Variable

A named data storage block, for which the value can be defined and redefined during the execution of a program.

Terminology: Private Variable

With respect to a given set of *task regions* that bind to the same `parallel` *region*, a *variable* for which the name provides access to a **different** block of storage for each *task region*.

Terminology: Shared Variable

With respect to a given set of *task regions* that bind to the same `parallel` *region*, a *variable* for which the name provides access to the **same** block of storage for each *task region*.

CONSTRUCTS & REGIONS

Terminology: Construct

An OpenMP *executable directive* (and for Fortran, the paired `end` *directive*, if any) and the associated statement, loop or *structured block*, if any, not including the code in any called routines. That is, the lexical extent of an *executable directive*.

Terminology: Region

All code encountered during a specific instance of the execution of a given *construct* or of an OpenMP library routine.

Terminology: Executable Directive

An OpenMP *directive* that is not declarative. That is, it may be placed in an executable context.

DATA-SHARING ATTRIBUTE RULES I [OpenMP-5.1, 5.1.1]

The rules that determine the data-sharing attributes of variables referenced from the inside of a construct fall into one of the following categories:

Pre-determined

- Variables with automatic storage duration declared inside the construct are private (C and C++)
- Objects with dynamic storage duration are shared (C and C++)
- Variables with static storage duration declared in the construct are shared (C and C++)
- Static data members are shared (C++)
- Loop iteration variables are private (Fortran)
- Implied-do indices and **`forall`** indices are private (Fortran)
- Assumed-size arrays are shared (Fortran)

Explicit

Data-sharing attributes are determined by explicit clauses on the respective constructs.

Implicit

If the data-sharing attributes are neither pre-determined nor explicitly determined, they fall back to the attribute determined by the `default` clause, or `shared` if no `default` clause is present.

DATA-SHARING ATTRIBUTE RULES II [OpenMP-5.1, 5.1.2]

The data-sharing attributes of variables inside regions, not constructs, are governed by simpler rules:

- Static variables (C and C++) and variables with the **`save`** attribute (Fortran) are shared
- File-scope (C and C++) or namespace-scope (C++) variables and common blocks or variables accessed through use or host association (Fortran) are shared
- Objects with dynamic storage duration are shared (C and C++)
- Static data members are shared (C++)
- Arguments passed by reference have the same data-sharing attributes as the variable they are referencing (C++ and Fortran)
- Implied-do indices, **`forall`** indices are private (Fortran)
- Local variables are private

THE SHARED CLAUSE [OpenMP-5.1, 5.4.2]

```
* shared(list)
```

- Declares the listed variables to be shared.
- The programmer must ensure that shared variables are alive while they are shared.
- Shared variables must not be part of another variable (i.e. array or structure elements).

THE PRIVATE CLAUSE [OpenMP-5.1, 5.4.3]

```
* private(list)
```

- Declares the listed variables to be private.
- All threads have their own new versions of these variables.
- Private variables must not be part of another variable.
- If private variables are of class type, a default constructor must be accessible. (C++)
- The type of a private variable must not be **`const`**-qualified, incomplete or reference to incomplete. (C and C++)
- Private variables must either be definable or allocatable. (Fortran)
- Private variables must not appear in **`namelist`** statements, variable format expressions or expressions for statement function definitions. (Fortran)
- Private variables must not be pointers with **`intent`**`(in)`. (Fortran)

FIRSTPRIVATE CLAUSE [OpenMP-5.1, 5.4.4]

```
* firstprivate(list)
```

Like private, but initialize the new versions of the variables to have the same value as the variable that exists before the construct.

- Non-array variables are initialized by copy assignment (C and C++)
- Arrays are initialize by element-wise assignment (C and C++)
- Copy constructors are invoked if present (C++)
- Non-**`pointer`** variables are initialized by assignment or not associated if the original variable is not associated (Fortran)
- **`pointer`** variables are initialized by pointer assignment (Fortran)

DEFAULT CLAUSE [OpenMP-5.1, 5.4.1]

C and C++

```
C default(shared | none)
```

Fortran

```
F08 default(private | firstprivate | shared | none)
```

Determines the data-sharing attributes for all variables referenced from inside of a region that have neither pre-determined nor explicit data-sharing attributes.

Caution: `default(none)` forces the programmer to make data-sharing attributes explicit if they are not pre-determined. This can help clarify the programmer's intentions to someone who does not have the implicit data-sharing rules in mind.

REDUCTION CLAUSE [OpenMP-5.1, 5.5.8]

*

```
reduction(reduction-identifier : list)
```

- Listed variables are declared private.
- At the end of the construct, the original variable is updated by combining the private copies using the operation given by `reduction-identifier`.
- `reduction-identifier` may be +, −, *, &, |, ^, &&, ||, `min` or `max` (C and C++) or an *identifier* (C) or an *id-expression* (C++)
- `reduction-identifier` may be a base language identifier, a user-defined operator, or one of +, −, *, `.and.`, `.or.`, `.eqv.`, `.neqv.`, `max`, `min`, `iand`, `ior` or `ieor` (Fortran)
- Private versions of the variable are initialized with appropriate values

68 EXERCISES

Exercise 11 – Data-sharing Attributes

11.1 Generalized Vector Addition (`axpy`)

In the file `axpy.{c|c++|f90}` add a new function/subroutine `axpy_parallel(a, x, y, z[, n])` that uses multiple threads to perform a generalized vector addition. Modify the main part of the program to have your function/subroutine tested.

Hints:

- Use the `parallel` construct and the necessary clauses to define an appropriate data environment.
- Use `omp_get_thread_num()` and `omp_get_num_threads()` to decompose the work.

69 THREAD SYNCHRONIZATION

- In MPI, exchange of data between processes implies synchronization through the message metaphor.
- In OpenMP, threads exchange data through shared parts of memory.
- Explicit synchronization is needed to coordinate access to shared memory.

Terminology: Data Race

A data race occurs when

- multiple threads write to the same memory unit without synchronization or
- at least one thread writes to and at least one thread reads from the same memory unit without synchronization.

- Data races result in unspecified program behavior.
- OpenMP offers several synchronization mechanism which range from high-level/general to low-level/specialized.

THE BARRIER CONSTRUCT [OpenMP-5.1, 15.3.1]

C

```
#pragma omp barrier
```

F08

```
!$omp barrier
```

- Threads are only allowed to continue execution of code after the `barrier` once all threads in the current team have reached the `barrier`.
- A barrier region must be executed by all threads in the current team or none.

THE CRITICAL CONSTRUCT [OpenMP-5.1, 15.2]

C

```
#pragma omp critical [(name)]
  structured-block
```

F08

```
!$omp critical [(name)]
  structured-block
!$omp end critical [(name)]
```

- Execution of `critical` regions with the same *name* are restricted to one thread at a time.
- *name* is a compile time constant.
- In C, *names* live in their own name space.
- In Fortran, *names* of critical regions can collide with other identifiers.

LOCK ROUTINES [OpenMP-5.1, 18.9]

C

```
void omp_init_lock(omp_lock_t* lock);
void omp_destroy_lock(omp_lock_t* lock);
void omp_set_lock(omp_lock_t* lock);
void omp_unset_lock(omp_lock_t* lock);
```

```
subroutine omp_init_lock(svar)
subroutine omp_destroy_lock(svar)
subroutine omp_set_lock(svar)
subroutine omp_unset_lock(svar)
integer(kind = omp_lock_kind) :: svar
```
F08

- Like `critical` sections, but identified by runtime value rather than global name
- Locks must be `shared` between threads
- Initialize a lock before first use
- Destroy a lock when it is no longer needed
- Lock and unlock using the `set` and `unset` routines
- `set` blocks if lock is already set

THE ATOMIC AND FLUSH CONSTRUCTS [OpenMP-5.1, 15.8.4, 15.8.5]

- `barrier`, `critical`, and locks implement synchronization between general blocks of code
- If blocks become very small, synchronization overhead could become an issue
- The `atomic` and `flush` constructs implement low-level, fine grained synchronization for certain limited operations on scalar variables:
  - `read`
  - `write`
  - `update`, writing a new value based on the old value
  - `capture`, like update and the old or new value is available in the subsequent code
- Correct use requires knowledge of the OpenMP Memory Model [OpenMP-5.1, 1.4]
- See also: C11 and C++11 Memory Models

70 EXERCISES

Exercise 12 – Thread Synchronization
12.1 Dot Product

In the file `dot.{c|c++|f90}` add a new function/subroutine `dot_parallel(x, y[, n])` that uses multiple threads to perform the dot product. Do not use the `reduction` clause. Modify the main part of the program to have your function/subroutine tested.

Hint:

- Decomposition of the work load should be similar to the last exercise
- Partial results of different threads should be combined in a shared variable
- Use a suitable synchronization mechanism to coordinate access

Bonus

Use the `reduction` clause to simplify your program.

PART XIII

WORKSHARING

71 INTRODUCTION

WORKSHARING CONSTRUCTS

- Decompose work for concurrent execution by multiple threads
- Used inside `parallel` regions
- Available worksharing constructs:
  - `single` and `sections` construct
  - loop construct
  - `workshare` construct
  - `task` worksharing

72 THE SINGLE CONSTRUCT

THE SINGLE CONSTRUCT [OpenMP-5.1, 11.1]

```
#pragma omp single [clause[[,] clause]...]
  structured-block
```
C

```
!$omp single [clause[[,] clause]...]
  structured-block
!$omp end single [end_clause[[,] end_clause]...]
```
F08

- The *structured block* is executed by a single thread in the encountering team.
- Permissible clauses are `firstprivate`, `private`, `copyprivate` and `nowait`.
- `nowait` and `copyprivate` are end_clauses in Fortran.

73 SINGLE CLAUSES

IMPLICIT BARRIERS & THE NOWAIT CLAUSE [OpenMP-5.1, 15.3.2, 15.6]

- Worksharing constructs (and the `parallel` construct) contain an implied barrier at their exit.
- The `nowait` clause can be used on worksharing constructs to disable this implicit barrier.

THE COPYPRIVATE CLAUSE [OpenMP-5.1, 5.7.2]

```
*  copyprivate(list)
```

- *list* contains variables that are `private` in the enclosing parallel region.
- At the end of the `single` construct, the values of all *list* items on the single thread are copied to all other threads.
- E.g. serial initialization
- `copyprivate` cannot be combined with `nowait`.

74 THE LOOP CONSTRUCT

WORKSHARING-LOOP CONSTRUCT [OpenMP-5.1, 11.5]

```C
#pragma omp for [clause[[,] clause]...]
  for-loops
```

```F08
!$omp do [clause[[,] clause]...]
  do-loops
[!$omp end do [nowait]]
```

Declares the iterations of a loop to be suitable for concurrent execution on multiple threads.

Data-environment clauses

- `private`
- `firstprivate`
- `lastprivate`
- `reduction`

Worksharing-Loop-specific clauses

- `schedule`
- `collapse`

CANONICAL NEST LOOP FORM [OpenMP-5.1, 4.4.1]

In C and C++ the `for-loops` must have the following form:

```C
for ([type] var = lb; var relational-op b; incr-expr)
↪ structured-block
```

```C++
for (range-decl: range-expr) structured-block
```

- `var` can be an integer, a pointer, or a random access iterator
- `incr-expr` increments (or decrements) `var`, e.g. `var = var + incr`
- The increment `incr` must not change during execution of the loop
- For nested loops, the bounds of an inner loop (b and `lb`) may depend at most linearly on the iteration variable of an outer loop, i.e. `a0 + a1 * var-outer`
- `var` must not be modified by the loop body
- The beginning of the range has to be a random access iterator
- The number of iterations of the loop must be known beforehand

In Fortran the `do-loops` must have the following form:

```F08
do [label] var = lb, b[, incr]
```

- `var` must be of integer type
- `incr` must be invariant with respect to the outermost loop
- The loop bounds b and `lb` of an inner loop may depend at most linearly on the iteration variable of an outer loop, i.e. `a0 + a1 * var-outer`
- The number of iterations of the loop must be known beforehand

75 LOOP CLAUSES

THE COLLAPSE CLAUSE [OpenMP-5.1, 4.4.3]

```
*  collapse(n)
```

- The `loop` directive applies to the outermost loop of a set of nested loops, by default
- `collapse(n)` extends the scope of the `loop` directive to the n outer loops
- All associated loops must be perfectly nested, i.e.:

```
for (int i = 0; i < N; ++i) {
  for (int j = 0; j < M; ++j) {
    // ...
  }
}
```

THE SCHEDULE CLAUSE [OpenMP-5.1, 11.5.3]

```
schedule(kind[, chunk_size])
```

Determines how the iteration space is divided into chunks and how these chunks are distributed among threads.

`static` Divide iteration space into chunks of `chunk_size` iterations and distribute them in a round-robin fashion among threads. If `chunk_size` is not specified, chunk size is chosen such that each thread gets at most one chunk.

`dynamic` Divide into chunks of size `chunk_size` (defaults to 1). When a thread is done processing a chunk it acquires a new one.

`guided` Like dynamic but chunk size is adjusted, starting with large sizes for the first chunks and decreasing to `chunk_size` (default 1).

`auto` Let the compiler and runtime decide.

`runtime` Schedule is chosen based on ICV *run-sched-var*.

If no `schedule` clause is present, the default schedule is implementation defined.

76 EXERCISES

Exercise 13 – Loop Worksharing
13.1 Generalized Vector Addition (`axpy`)

In the file `axpy.{c|c++|f90}` add a new function/subroutine `axpy_parallel_for(a, x, y, z[, n])` that uses loop worksharing to perform the generalised vector addition.

13.2 Dot Product

In the file `dot.{c|c++|f90}` add a new function/subroutine `dot_parallel_for(x, y[, n])` that uses loop worksharing to perform the dot product.

Caveat: Make sure to correctly synchronize access to the accumulator variable.

77 WORKSHARE CONSTRUCT

WORKSHARE (FORTRAN ONLY) [OpenMP-5.1, 11.4]

```
!$omp workshare
  structured-block
!$omp end workshare [nowait]
```

F08

The structured block may contain:

- array assignments
- scalar assignments
- **`forall`** constructs
- **`where`** statements and constructs
- `atomic`, `critical` and `parallel` constructs

Where possible, these are decomposed into independent units of work and executed in parallel.

78 EXERCISES

Exercise 14 – `workshare` Construct
14.1 Generalized Vector Addition (`axpy`)

In the file `axpy.f90` add a new subroutine `axpy_parallel_workshare(a, x, y, z)` that uses the `workshare` construct to perform the generalized vector addition.

14.2 Dot Product

In the file `dot.f90` add a new function `dot_parallel_workshare(x, y)` that uses the `workshare` construct to perform the dot product.

Caveat: Make sure to correctly synchronize access to the accumulator variable.

79 COMBINED CONSTRUCTS

COMBINED CONSTRUCTS [OpenMP-5.1, 17]

Some constructs that often appear as nested pairs can be combined into one construct, e.g.

```
#pragma omp parallel
#pragma omp for
for (...; ...; ...) {
  ...
}
```

can be turned into

```
#pragma omp parallel for
for (...; ...; ...) {
  ...
}
```

Similarly, `parallel` and `workshare` can be combined.

Combined constructs usually accept the clauses of either of the base constructs.

PART XIV

TASK WORKSHARING

80 INTRODUCTION

TASK TERMINOLOGY

Terminology: Task

A specific instance of executable code and its *data environment*, generated when a *thread* encounters a `task`, `taskloop`, `parallel`, `target` or `teams` *construct*.

Terminology: Child Task

A *task* is a *child task* of its generating *task region*. A *child task region* is not part of its generating *task region*.

Terminology: Descendent Task

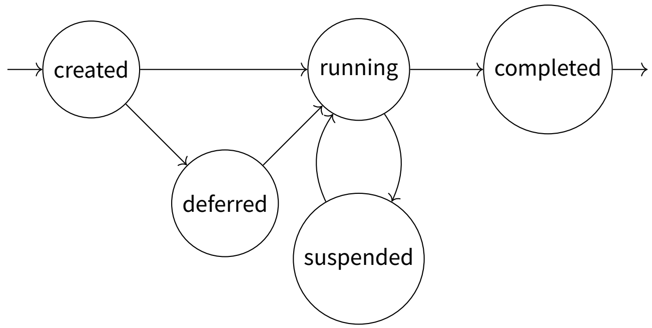
A *task* that is the *child task* of a *task region* or of one of its *descendent task regions*.

Terminology: Sibling Task

Tasks that are *child tasks* of the same *task region*.

TASK LIFE-CYCLE

- Execution of tasks can be *deferred* and *suspended*
- Scheduling is done by the OpenMP runtime system at *scheduling points*
- Scheduling decisions can be influenced by e.g. *task dependencies* and *task priorities*



81 THE TASK CONSTRUCT

THE TASK CONSTRUCT [OpenMP-5.1, 12.5]

```
#pragma omp task [clause[[,] clause]...]
  structured-block
```

```
!$omp task [clause[[,] clause]...]
  structured-block
!$omp end task
```

Creates a task. Execution of the task may commence immediately or be deferred.

Data-environment clauses

- `private`
- `firstprivate`
- `shared`

Task-specific clauses

- `if`
- `final`
- `untied`
- `mergeable`
- `depend`
- `priority`

TASK DATA-ENVIRONMENT [OpenMP-5.1, 5.1.1]

The rules for implicitly determined data-sharing attributes of variables referenced in task generating constructs are slightly different from other constructs:

If no `default` clause is present and

- the variable is `shared` by all implicit tasks in the enclosing context, it is also `shared` by the generated task,
- otherwise, the variable is `firstprivate`.

82 TASK CLAUSES

THE IF CLAUSE [OpenMP-5.1, 3.4, 12.5]

```
* if([task: ] scalar-expression)
```

If the scalar expression evaluates to *false*:

- Execution of the current task
  - is suspended and
  - may only be resumed once the generated task is complete
- Execution of the generated task may commence immediately

Terminology: Undeferred Task

A *task* for which execution is not deferred with respect to its generating *task region*. That is, its generating *task region* is suspended until execution of the *undeferred task* is completed.

THE FINAL CLAUSE [OpenMP-5.1, 12.3]

```
* final(scalar-expression)
```

If the scalar expression evaluates to *true* all *descendent tasks* of the generated task are

- *undeferred* and
- executed immediately.

Terminology: Final Task

A *task* that forces all of its *child tasks* to become *final* and *included tasks*.

Terminology: Included Task

A *task* for which execution is sequentially included in the generating *task region*. That is, an *included task* is *undeferred* and executed immediately by the *encountering thread*.

THE UNTIED CLAUSE [OpenMP-5.1, 12.1]

```
* untied
```

- The generated task is *untied* meaning it can be suspended by one thread and resume execution on another.
- By default, tasks are generated as *tied* tasks.

Terminology: Untied Task

A *task* that, when its *task region* is suspended, can be resumed by any *thread* in the team. That is, the *task* is not tied to any *thread*.

Terminology: Tied Task

A *task* that, when its *task region* is suspended, can be resumed only by the same *thread* that suspended it. That is, the *task* is tied to that *thread*.

THE PRIORITY CLAUSE [OpenMP-5.1, 12.4]

```
* priority(priority-value)
```

- *priority-value* is a scalar non-negative numerical value
- Priority influences the order of task execution
- Among tasks that are ready for execution, those with a higher priority are more likely to be executed next

THE DEPEND CLAUSE [OpenMP-5.1, 15.9.5]

```
  depend(in: list)
  depend(out: list)
* depend(inout: list)
```

- *list* contains storage locations
- A task with a dependence on *x*, `depend(in: x)`, has to wait for completion of previously generated *sibling tasks* with `depend(out: x)` or `depend(inout: x)`

- A task with a dependence `depend(out: x)` or `depend(inout: x)` has to wait for completion of previously generated *sibling tasks* with any kind of dependence on *x*
- `in`, `out` and `inout` correspond to intended read and/or write operations to the listed variables.

Terminology: Dependent Task

A *task* that because of a *task dependence* cannot be executed until its *predecessor tasks* have completed.

83 TASK SCHEDULING

TASK SCHEDULING POLICY [OpenMP-5.1, 12.9]

The task scheduler of the OpenMP runtime environment becomes active at *task scheduling points*. It may then

- begin execution of a task or
- resume execution of untied tasks or tasks tied to the current thread.

Task scheduling points

- generation of an explicit task
- task completion
- `taskyield` regions
- `taskwait` regions
- the end of `taskgroup` regions
- implicit and explicit `barrier` regions

THE TASKYIELD CONSTRUCT [OpenMP-5.1, 12.7]

C
```
#pragma omp taskyield
```

F08
```
!$omp taskyield
```

- Notifies the scheduler that execution of the current task may be suspended at this point in favor of another task
- Inserts an explicit scheduling point

84 TASK SYNCHRONIZATION

THE TASKWAIT & TASKGROUP CONSTRUCTS [OpenMP-5.1, 15.4, 15.5]

C
```
#pragma omp taskwait
```

F08
```
!$omp taskwait
```

Suspends the current task until all *child tasks* are completed.

C
```
#pragma omp taskgroup
  structured-block
```

F08
```
!$omp taskgroup
  structured-block
!$omp end taskgroup
```

The current task is suspended at the end of the `taskgroup` region until all *descendent tasks* generated within the region are completed.

85 EXERCISES

Exercise 15 – Task worksharing

15.1 Generalized Vector Addition (axpy)

In the file `axpy.{c|c++|f90}` add a new function/subroutine `axpy_parallel_task(a, x, y, z[, n])` that uses task worksharing to perform the generalized vector addition.

15.2 Dot Product

In the file `dot.{c|c++|f90}` add a new function/subroutine `dot_parallel_task(x, y[, n])` that uses task worksharing to perform the dot product.

Caveat: Make sure to correctly synchronize access to the accumulator variable.

15.3 Bitonic Sort

The file `bsort.{c|c++|f90}` contains a serial implementation of the bitonic sort algorithm. Use OpenMP task worksharing to parallelize it.

PART XV

WRAP-UP

ALTERNATIVES

Horizontal Alternatives

Parallel languages Fortran Coarrays, UPC; Chapel, X10

Parallel frameworks Charm++, HPX, StarPU

Shared memory tasking Cilk, TBB

Accelerators CUDA, OpenCL, OpenACC, SYCL

Platform solutions PLINQ, GCD, `java.util.concurrent`

Vertical Alternatives

Applications Gromacs, CP2K, ANSYS, OpenFOAM

Numerics libraries PETSc, Trilinos, DUNE, FEniCS

Machine Learning Tensorflow, Keras, PyTorch

JSC COURSE PROGRAMME

- Directive-based GPU programming with OpenACC, **27 – 29 October**
- Introduction to the usage and programming of supercomputer resources in Jülich, **22 – 25 November**
- (Using the supercomputers at JSC – a hands-on tutorial)
- Advanced Parallel Programming with MPI and OpenMP, **29 November – 01 December**
- And more, see `https://www.fz-juelich.de/ias/jsc/courses`

PART XVI

TUTORIAL

N-BODY SIMULATIONS

Dynamics of the N-body problem:

$$\mathbf{a}_{i,j} = \frac{q_i q_j}{\sqrt{\left(\mathbf{x}_i - \mathbf{x}_j\right) \cdot \left(\mathbf{x}_i - \mathbf{x}_j\right)}^3} \left(\mathbf{x}_i - \mathbf{x}_j\right)$$

$$\ddot{\mathbf{x}}_i = \mathbf{a}_i = \sum_{j \neq i} \mathbf{a}_{i,j}$$

Velocity Verlet integration:

$$\mathbf{v}^*\left(t + \frac{\Delta t}{2}\right) = \mathbf{v}\left(t\right) + \frac{\Delta t}{2}\mathbf{a}\left(t\right)$$

$$\mathbf{x}\left(t + \Delta t\right) = \mathbf{x}(t) + \mathbf{v}^*\left(t + \frac{\Delta t}{2}\right)\Delta t$$

$$\mathbf{v}\left(t + \Delta t\right) = \mathbf{v}^*\left(t + \frac{\Delta t}{2}\right) + \frac{\Delta t}{2}\mathbf{a}\left(t + \Delta t\right)$$

Program structure:

```
  read initial state from file
  calculate accelerations
  for number of time steps:
    write state to file
    calculate helper velocities v*
    calculate new positions
    calculate new accelerations
    calculate new velocities
* write final state to file
```

A SERIAL N-BODY SIMULATION PROGRAM

Compiling nbody

```
$ cmake -B build
$ cmake --build build
...
```

Invoking nbody

```
$ ./build/nbody
Usage: nbody <input file>
$ ./build/nbody ../input/kaplan_10000.bin
Working on step 1...
```

Visualizing the results

```
$ paraview --state=kaplan.pvsm
```

Initial conditions based on: A. E. Kaplan, B. Y. Dubetsky, and P. L. Shkolnikov. “Shock Shells in Coulomb Explosions of Nanoclusters.” In: *Physical Review Letters* 91 (14 Oct. 3, 2003), p. 143401. DOI: 10.1103/PhysRevLett.91.143401

SOME SUGGESTIONS

Distribution of work
Look for loops with a number of iterations that scales with the problem size N. If the individual loop iterations are independent, they can be run in parallel. Try to distribute iterations evenly among the threads / processes.

Distribution of data
What data needs to be available to which process at what time? Having the entire problem in the memory of every process will not scale. Think of particles as having two roles: targets (i index) that experience acceleration due to sources (j index). Make every process responsible for a group of either target particles or source particles and communicate the same particles in the other role to other processes. What particle properties are important for targets and sources?

Input / Output
You have heard about different I/O strategies during the MPI I/O part of the course. Possible solutions include:

- Funneled I/O: one process reads then scatters or gathers then writes
- MPI I/O: every process reads or writes the particles it is responsible for

Scalability
Keep an eye on resource consumption. Ideally, the time it takes for your program to finish should be inversely proportional to the number of threads or processes running it $O(N^2/p)$. Similarly, the amount of memory consumed by your program should be independent of the number of processes $O(N)$.

EXERCISES

Exercise 16 – N-body simulation program
16.1 OpenMP parallel version

Write a version of nbody that is parallelized using OpenMP. Look for suitable parts of the program to annotate with OpenMP directives.

16.2 MPI parallel version

Write a version of nbody that is parallelized using MPI. The distribution of work might be similar to the previous exercise. Ideally, the entire system state is not stored on every process, thus particle data has to be communicated. Communication could be point-to-point or collective. Input and output functions might have to be adapted as well.

16.3 Hybrid parallel version

Write a version of nbody that is parallelized using both MPI and OpenMP. This might just be a combination of the previous two versions.

Bonus

A clever solution is described in: M. Driscoll et al. “A Communication-Optimal N-Body Algorithm for Direct Interactions.” In: *2013 IEEE 27th International Symposium on Parallel and Distributed Processing*. 2013, pp. 1075–1084. DOI: 10.1109/IPDPS.2013.108. Implement Algorithm 1 from the paper.

COLOPHON

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