## Overview: Message Passing

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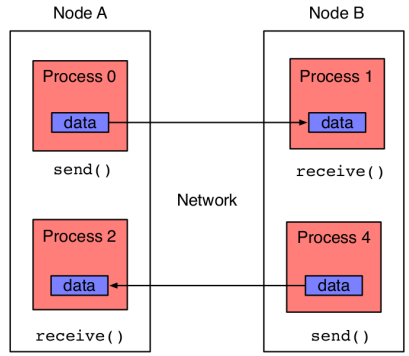
## Message Passing in a Nutshell

- parallelism realized by multiple processes (aka tasks) each with their own local memory address space
- data is moved from address space of one process to that of another by sending/receiving messages
- processes may run on separate compute nodes, different cores within a node, or even on same processor core
- all variables in a process are local to this process. No concept of shared-memory
- strictly required if target parallel computer is distributed-memory.
- “de facto” standard is MPI






## A bit of history (the advent of MPI-1)

- parallel computer vendors initially developed own message-passing APIs
  - e.g. Fujitsu’s APLib for the AP1000 series (1991–1998)
  - big issue: portability across machines was difficult (if not impossible)
  - one typically ended with a different version of the parallel code for each different machine vendor !!!
- early work on a standard started in 1992 at Oak Ridge National Lab and Rice Uni
- at that stage, there was a plethora of different message passing environments
- target was C and FORTRAN applications
- MPI-1 released in May 94 (over 40 academic and government participants)
  - contains: point-to-point communications, collective operations, process topologies
- minor clarifications: MPI 1.1 (June 95), MPI 1.2 (July 97)



## What is MPI?

The Message Passing Interface (MPI) is a standardized specification of a set of library subroutines for the portable and flexible development of efficient message-passing parallel programs

- MPI Forum in charge of standardization (40 participating organizations, including vendors, researchers, software library developers, and users)
- revised several times, with the most recent being MPI-4. Actual implementations differ in the version/features of the standard they support
- supported on virtually all HPC platforms. Several free (e.g., OpenMPI, MPICH) and commercial implementations (Intel MPI) available
- provides FORTRAN, C (this course), and C++ bindings
- very broad standard with a huge # of library subroutines (over 440 in MPI-3). Fortunately, most applications merely require less than a dozen of those
- documentation for all versions of the MPI standard available here

## How does MPI work?

MPI conforms with the following rules:

- Single Program Multiple Data (SPMD) model: the same program runs on all processes. All processes taking part in a parallel calculation can be distinguished by a unique identifier called rank
- The program is written in a sequential language like Fortran, C, or C++. Data exchange is carried out via calls to MPI library subroutines
- All variables in a process are local to this process. There is no concept of shared-memory



## "Hello world" MPI program (I)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char** argv) {
  int np, me, ierr;
  ierr=MPI_Init(&argc, &argv);
  ierr=MPI_Comm_size(MPI_COMM_WORLD, &np);
  ierr=MPI_Comm_rank(MPI_COMM_WORLD, &me);
  printf("Hello world I am %d out of %d\n", me, np);
  ierr=MPI_Finalize();
}
```

- All MPI calls return an error code (here `ierr`) which tells the user program whether MPI operation succeeded or not (`MPI_SUCCESS` means no error)
- `MPI_Init` initializes parallel environment. MUST precede any other MPI library call
- Upon initialization, MPI sets up the world communicator (`MPI_COMM_WORLD`)
  → A communicator defines a group of processes referred to by a handler
  → `MPI_COMM_WORLD` handler describes all processes started with parallel program
  → If required, other communicators can be defined as subsets of `MPI_COMM_WORLD`
  → Almost all MPI calls require a communicator handler as an argument



## "Hello world" MPI program (II)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char** argv) {
  int np, me, ierr;
  ierr=MPI_Init(&argc, &argv);
  ierr=MPI_Comm_size(MPI_COMM_WORLD, &np);
  ierr=MPI_Comm_rank(MPI_COMM_WORLD, &me);
  printf("Hello World, I am %d out of %d\n", me, np);
  ierr=MPI_Finalize();
}
```

- The calls to `MPI_Comm_size` and `MPI_Comm_rank` determine the number of processes running the parallel code, and the unique identifier (called *rank*) of the calling process, respectively
  → The ranks in a communicator are consecutive, starting from zero
- The call to `MPI_Finalize` shuts down the parallel program
  → No process except 0 is guaranteed to execute any code after `MPI_Finalize`



## Code compilation and execution

The way MPI programs are compiled and started is NOT fixed by the standard

- Compiler and linker need special options that specify where modules and libraries, resp., can be found. Considerable variation in those locations among installations
- Most MPI implementations provide compiler wrapper scripts (e.g., `mpicc`) that automatically supply the required options to the underlying native compiler
- Typically a script called `mpirun` is provided to start a message-passing program
  → Processor cores may have to be allocated from batch system in advance
  → How exactly processes are created is entirely up to the implementation
  → Typically `mpirun` uses the batch system's infrastructure to launch processes
- For our example, a "common" implementation may require the following steps:

```
$ mpicc -O3  hello.c -o hello
$ mpirun -np 4 ./hello
Hello World, I am 0 out of 4
Hello World, I am 2 out of 4
Hello World, I am 1 out of 4
Hello World, I am 3 out of 4
```

## MPI messages

- A MPI message is defined as a 1D array of elements of a particular MPI data type
- MPI data types can be either basic (see table below) or derived

| MPI data type | C data type |
|---|---|
| MPI_CHAR | char |
| MPI_INT | int |
| MPI_FLOAT | float |
| MPI_DOUBLE | double |
| MPI_BYTE | unsigned char |
| ⋮ | ⋮ |

- MPI derived types created by calling appropriate MPI calls (later in the lecture)
- MPI needs to know the data type of messages as it supports heterogeneous environments where it may be necessary to perform on-the-fly data conversions
- MPI data types on sender and receiver MUST MATCH for messages to proceed



## Point-to-point communication (I)

- data exchange that involves exactly one sender and one receiver
- both ends are identified uniquely by their ranks
- each message carries an extra integer, called tag, that MUST MATCH on both ends
- tag is programmer-defined and can be used to create classes of messages; may just be set to some constant value if not needed
- the basic (but not unique!) call to send data from one process to another is `MPI_Send`:

```
int MPI_Send(void *buf,              // message buffer
             int count,              // # of items
             MPI_Datatype datatype,  // MPI data type
             int dest,               // destination rank
             int tag,                // message tag
             MPI_Comm comm);         // MPI communicator handler
```



## Point-to-point communication (II)

- the basic (but not unique!) call to receive a message is `MPI_Recv`:

```
int MPI_Recv(void *buf,              // message buffer
             int count,              // maximum # of items
             MPI_Datatype datatype,// MPI data type
             int source,             // source rank
             int tag,                // message tag
             MPI_Comm comm,          // MPI communicator handler
             MPI_Status *status);    // pointer to status object
```

- `status` is an output argument which may be used to guess parameters that have not been fixed by the `MPI_Recv` arguments. In particular:
  - Actual message size (`count` is only a maximum value at receiver side)
  - Sender's rank if receive not tailored to particular sender (source=`MPI_ANY_SOURCE`)
  - Message tag if receive not tailored to particular tag (tag=`MPI_ANY_TAG`)



## Blocking semantics (crucial slide)

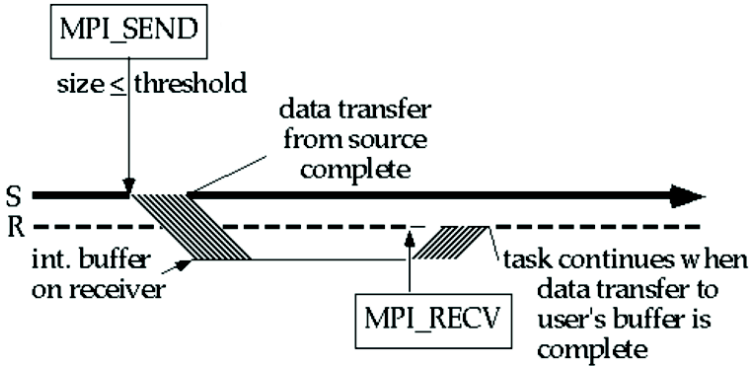
`MPI_Send` and `MPI_Recv` have blocking semantics, meaning that:

1. buffer can safely be written upon `MPI_Send` return without altering on-going comm
2. one can be sure that the message has been received upon `MPI_Recv` return

- this provides high freedom in the actual implementation of `MPI_Send`, i.e., it JUST specifies that it MUST comply with blocking semantics
- internally, it may work synchronously (e.g., it may return once message transfer has at least started after a handshake with the receiver process)
- however, it may also copy the message to an internal buffer and return immediately, allowing handshake and transmission progress to occur in the background
- it may even switch its behaviour depending on any explicit or hidden parameters
- e.g., most MPI implementations provide a (small) internal buffer for short messages, and switch to synchronous mode when internal buffer is full or too small
- this has to be taken into account when writing parallel programs to avoid so-called deadlocks

## Possible implementation of `MPI_Send`

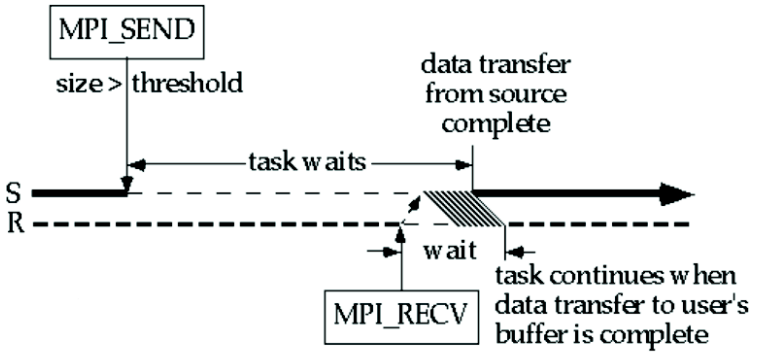
One possible implementation of `MPI_Send` with "small" message sizes






## Another possible implementation of `MPI_Send`

Another possible implementation of `MPI_Send` with "large" message sizes






## Let us think ...

Consider the execution of the following MPI program on two processes, attempting to send each other's `a` array:

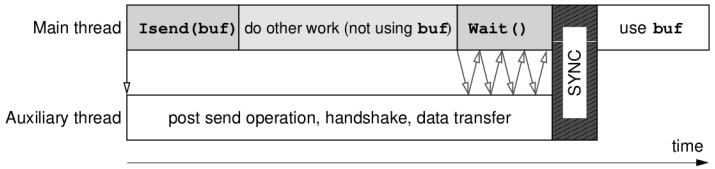
```
char a[N]; int rank;
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
// code to initialize a goes here ...
MPI_Send(a, N, MPI_CHAR, 1-rank, 0, MPI_COMM_WORLD);
MPI_Recv(a, N, MPI_CHAR, 1-rank, 0, MPI_COMM_WORLD,
         MPI_STATUS_IGNORE);
```

Do you anticipate any issue with this MPI program? If yes, how would you solve it?



## Non-blocking point-to-point communication (concept)

- MPI has support for non-blocking sends (`MPI_Isend`) and receives (`MPI_Irecv`)
- Merely initiate message transmission and return **very quickly** to the user code
- The message buffer must not be used as long as user code has not been notified that it is safe to do so
- **If MPI implemented efficiently**, sync and data transfer can occur in the **background**, leaving CPU free for useful computations (**comm/comp overlap**)




- Many non-blocking sends/receives can be pending at any time on a given process
- Non-blocking/blocking calls are **mutually compatible**
  → `MPI_Send` matches `MPI_Irecv`, `MPI_Isend` matches `MPI_Recv`, ...

## Non-blocking point-to-point communication (`Isend` and `Irecv`)

- `MPI_Isend` initiates a non-blocking send

```
int MPI_Isend(const void *buf,        // message buffer
              int count,              // # of items
              MPI_Datatype datatype, // MPI data type
              int dest,               // destination rank
              int tag,                // message tag
              MPI_Comm comm,          // MPI communicator
              MPI_Request *request)   // request handle
```

- Compared to `MPI_Send`, and additional output argument, *request handle*
- Serves as an identifier to later refer to "pending" communication request
- Correspondingly, `MPI_Irecv` initiates a non-blocking receive

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

- Compared to `MPI_Recv`, no `status` provided as output
- No actual communication has taken place when the call returns to user code!



## Non-blocking point-to-point communication (`Test` or `Wait`)

- Check a pending comm for completion can be done with `MPI_Test` or `MPI_Wait`:

```
int MPI_Test(MPI_Request *request, // pending request
             int *flag,            // true if request complete
             MPI_Status *status)   // status object

int MPI_Wait(MPI_Request *request, // pending request
             MPI_Status *status)   // status object
```

- `MPI_Test` tests for completion, returns true if buffer can be safely used
- `MPI_Wait` **blocks** until message buffer can be safely used
- `status` only contains useful information only if pending communication is a completed receive (i.e., `flag` must be true in case of `MPI_Test`)
- Checking multiple pending comms for completion can be done with `MPI_Waitall` (homework: to investigate this function)



## MPI Collective Operations (brief coverage)

- barrier: synchronizes all members in a communicator
  - it should not be used in general, only for debugging or profiling purposes
- broadcast: send same message to many processors
  - must define processors in the group (specified by a communicator)
  - must define who sends and who receives information
  - has blocking semantics; may or may not synchronize processors (implementation dependent)

  e.g. `MPI_Bcast(A, n, MPI_DOUBLE, 0/*root*/, MPI_COMM_WORLD);`
- scatter: 1 process sends unique data to every other in group
- gather: reverse of above
- reduction: gather + an arithmetic/logical operation
  - result goes to just one process, or goes to all processes (`All` variants)

All the above can be constructed from simple sends and receives ... BUT MPI provides (usually highly optimized, underlying network tailored) calls to perform all of these. Use them!



## MPI Derived Datatypes

- often, we want to send or receive $m$ items of data with a stride $s > 1$ (e.g. a column in a row-major matrix)
- e.g. for double precision, if $s$ represents the number of elements between the start of each block, we can create a datatype with an implicit stride:

```
MPI_Datatype sVec;
MPI_Type_vector(1 /*number of blocks*/, 1 /*block length*/, s,
                MPI_DOUBLE, &sVec);
MPI_Type_commit(&sVec);
...
MPI_Send(A, m, sVec, ...)
```

- alternatively, we could do:

```
MPI_Type_vector(m, 1, s, MPI_DOUBLE, &matCol);
MPI_Type_commit(&matCol);
..
MPI_Send(A, 1, matCol, ...);
```

- this allows MPI to handle the allocation, copying to/from and de-allocation of temporary buffers

## A note of communicators

- MPI allows to create new communicators by duplicating or splitting other communicators (e.g., `MPI_COMM_WORLD`)
- using `MPI_COMM_WORLD` all the way through in MPI programs is in general dangerous, as there might be message mismatches among those that are internally generated by a library and those generated by the application program
- Solution: define a different communicator for user application program and library: