Programming with MPI

Parallel Programming for Engineers

2026-06-08

Prof. Dr. Michael Kuhn
michael.kuhn@ovgu.de

Parallel Computing and I/O
Institute for Intelligent Cooperating Systems
Faculty of Computer Science
Otto von Guericke University Magdeburg
https://parcio.ovgu.de

Outline

- What is the difference between kernel mode and user mode?
  1. Kernel mode can only execute instructions from the kernel binary
  2. Kernel mode has unrestricted access to the hardware
  3. Kernel mode is slower than user mode due to overhead

- What is the difference between kernel mode and user mode?
  1. Kernel mode can only execute instructions from the kernel binary
  2. Kernel mode has unrestricted access to the hardware ✔
  3. Kernel mode is slower than user mode due to overhead

- Why should system calls be avoided in HPC applications?
  1. System calls are a legacy approach
  2. Interrupts are better suited for HPC applications
  3. System calls can cause the application to lose their processor allocation
  4. System calls are slow due to management overhead

- Why should system calls be avoided in HPC applications?
  1. System calls are a legacy approach
  2. Interrupts are better suited for HPC applications
  3. System calls can cause the application to lose their processor allocation ✔
  4. System calls are slow due to management overhead ✔

- How are thread-safety and reentrancy related?
  1. Both describe the same concept
  2. Thread-safety implies reentrancy
  3. Reentrancy implies thread-safety
  4. Neither implies the other

- How are thread-safety and reentrancy related?
  1. Both describe the same concept
  2. Thread-safety implies reentrancy
  3. Reentrancy implies thread-safety
  4. Neither implies the other ✔

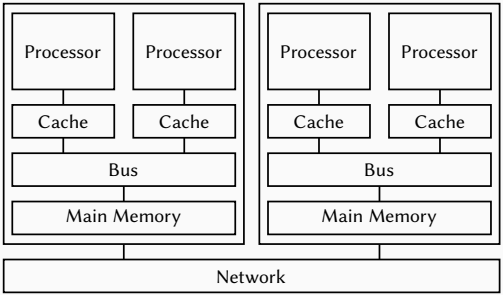
- Which function allows starting threads?
  1. `fork`
  2. `exec`
  3. `clone`
  4. `open`

- Which function allows starting threads?
  1. `fork`
  2. `exec`
  3. `clone` ✔
  4. `open`

Outline

Motivation

- Shared memory systems have limited scalability
  - Two to four processors with a few hundred cores
- Complex problems require more nodes
  - Distributed memory can be scaled arbitrarily
- Nodes are connected via a network
  - Determines scalability and performance
- Different network technologies and topologies
  - Major competitors: Ethernet and InfiniBand



Motivation...

- OpenMP is a convenient and high-level programming concept
  - It is limited to shared memory systems
- Parallel applications across multiple nodes require message passing
  - Message Passing Interface (MPI) provides necessary functionality
- MPI supports basic and complex operations
  - Sending, receiving, reduction etc.
  - Process groups and synchronization
  - Point-to-point, collective or one-sided communication
- MPI also offers parallel I/O
  - Concurrent access to shared files

- MPI is a standard by the MPI Forum
  - Over 40 participating organizations
  - First standardized and vendor-independent API
  - MPI is not a library but a specification of one
- There are multiple implementations of the standard
  - MPICH, MVAPICH, OpenMPI, Intel MPI etc.
  - Vendors often provide their own implementations

Message Passing Interface...

- MPI implementations are not necessarily binary-compatible
  - They have the same API but different ABIs
  - Compiling an application works with any implementation
- Running compiled application requires original implementation
  - Different implementations might have different constants etc.
  - Way to start processes on different nodes might differ
- Some implementations promise ABI compatibility
  - MPICH ABI Compatibility Initiative for MPICH, Intel MPI, Cray MPT, MVAPICH2, Parastation MPI and RIKEN MPI [MPICH Collaborators, 2026]

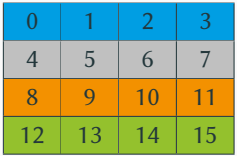
Challenges

- Parallel applications now run as independent processes
  - Processes can only access their own data, no shared memory
  - No risk of overwriting other processes' data accidentally
  - Results have to be communicated between processes
- Application code is typically still contained in one file
  - MPI allows us to write a generic version of the application
  - We can determine our rank and the number of processes

Challenges...

- MPI applications often use SPMD
  - All tasks execute same application but at different points
  - Tasks use different data (domain decomposition)
  - Additional logic to execute only parts of the application
- Decomposition is critical for achievable performance
  - Rows might be faster than columns depending on memory layout
  - Size of sub-domains determines load of each task
- Distribution also determines communication schema
  - Communication might have to be performed at boundaries

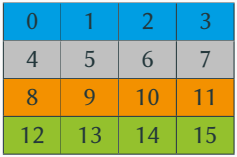
Challenges...



- MPI applications often use SPMD
  - All tasks execute same application but at different points
  - Tasks use different data (domain decomposition)
  - Additional logic to execute only parts of the application
- Decomposition is critical for achievable performance
  - Rows might be faster than columns depending on memory layout
  - Size of sub-domains determines load of each task
- Distribution also determines communication schema
  - Communication might have to be performed at boundaries

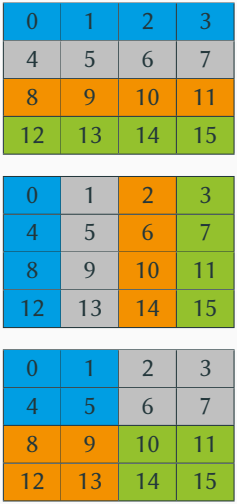
Challenges...

- MPI applications often use SPMD
  - All tasks execute same application but at different points
  - Tasks use different data (domain decomposition)
  - Additional logic to execute only parts of the application
- Decomposition is critical for achievable performance
  - Rows might be faster than columns depending on memory layout
  - Size of sub-domains determines load of each task
- Distribution also determines communication schema
  - Communication might have to be performed at boundaries



Challenges...

- MPI applications often use SPMD
  - All tasks execute same application but at different points
  - Tasks use different data (domain decomposition)
  - Additional logic to execute only parts of the application
- Decomposition is critical for achievable performance
  - Rows might be faster than columns depending on memory layout
  - Size of sub-domains determines load of each task
- Distribution also determines communication schema
  - Communication might have to be performed at boundaries



Challenges...

- Application has to be made available on multiple nodes
  - This is normally achieved by using a common file system on all nodes
  - For instance, an NFS file system can be mounted everywhere
- Processes have to be started on participating nodes
  - Many implementations include support for spawning processes via SSH
  - The batch scheduler can also take care of it, requires coordination
- Processes have to locate each other and coordinate
  - Similar to previous point, implementation often takes care of both
  - If the scheduler is involved, it has to pass information to the implementation
  - Process Management Interface (PMI) is typically used to connect components

Outline

- MPI is the current de-facto standard in HPC
  - Previously, Parallel Virtual Machine (PVM) was widely used
- MPI is developed by the MPI Forum, started in 1992
  - MPI-1.0 in 1995: Basic features, communication only
  - MPI-2.0 in 1997: Additional features, including I/O
  - MPI-3.0 in 2012: Better support for one-sided communication
  - MPI-4.0 in 2021: Large-count routines, persistent collectives
  - MPI-5.0 in 2025: Standardized Application Binary Interface (ABI)
- Standard is important for portability across different systems
  - MPI also offers high performance and convenience

- MPI standard defines an API for C and Fortran
  - C++ used to be available but has been deprecated
  - Bindings are also available for Python, Java etc.
- Abstraction to support efficient communication and I/O
  - Functions have to be high-level enough to be able to apply optimizations
- Standard allows thread-safe implementations but does not require them
  - MPI implementations are typically thread-unsafe by default
  - Thread-safety does have a performance impact due to locking etc.

Interface...

- MPI defines syntax and semantics
  - Syntax determines arguments, semantics how a function behaves
- Example: Function for sending data
  - Standard includes description of behavior and rationale
    - "The send call [...] is blocking: it does not return until the message data and envelope have been safely stored away so that the sender is free to modify the send buffer." [Message Passing Interface Forum, 2015]
  - Abstract: `MPI_SEND(buf, count, datatype, dest, tag, comm)`
    - Arguments are annotated as IN/OUT/INOUT and described
  - C: `int MPI_Send(const void* buf, ...)`
    - Return value via normal method
  - Fortran: `MPI_Send(buf, ..., ierror)`
    - Return value via extra argument (`ierror`)

Interface...

- Non-blocking
  - Call returns before operation has been completed
  - User might not be allowed to reuse specified resources (for example, buffers)
- Blocking
  - User is allowed to reuse resources
- Local
  - Completion of a call depends only on the local process
- Non-local
  - Completion of a call might depend on remote processes
  - Communication might be required to happen before completion
- Collective
  - All processes in a communicator have to be involved in a call

History

- 1992: “Standards for Message Passing in a Distributed Memory Environment”
  - Working group established and prepares draft for MPI-1
  - Group consists of 175 people from 40 organizations
- 1994: MPI-1.0 is released
  - MPI-1.1 in 1995, MPI-1.2 in 1997 and MPI-1.3 in 2008
  - Point-to-point and collective communication
  - Groups, communicators and topologies
  - Environment checks
  - Profiling interface

History...

- 1998: MPI-2.0 is released
  - MPI-2.1 in 2008 and MPI-2.2 in 2009
  - One-sided communication
  - Dynamic process management
  - Parallel I/O
- 2012: MPI-3.0 is released
  - MPI-3.1 in 2015
  - Improved one-sided communication
  - Non-blocking collectives

History...

- 2021: MPI-4.0 is released
  - MPI-4.1 in 2023
  - Large-count versions of many routines
  - Persistent collectives
  - Partitioned communication
- 2025: MPI-5.0 is released
  - Standardized Application Binary Interface (ABI)

Compiler Support

- MPI implementations consist of headers and libraries
  - Main header (`mpi.h`) has to be included
  - Applications have to be linked to MPI libraries
- MPI provides own compilers for convenience
  - `mpicc` for C and `mpifort` for Fortran
  - These are usually compiler wrappers around the underlying compiler
- Compiler wrappers take care of linking etc.
  - Compiler flags can usually be extracted if linking should be done manually

Outline

Initialization

- MPI needs to be initialized and finalized
  - Has to be done manually
  - Do as little as possible before and after
- `MPI_Init` expects application's arguments
  - MPI might parse certain arguments
  - It is possible to pass `NULL` to ignore
- `MPI_Finalize`
  - Only rank 0 is guaranteed to continue
  - Any other rank is not required to return from the call (but could)

```
1  int main(void) {
2      MPI_Init(NULL, NULL);
3      hello();
4      MPI_Finalize();
5
6      return 0;
7  }
```

Initialization

- MPI uses communicators
  - Basically a group of processes
- We can determine our rank
  - Similar to OpenMP's thread ID
- We can query the communicator's size
  - This is the total amount of processes

```
1  void hello(void) {
2      int rank;
3      int size;
4
5      MPI_Comm_rank(MPI_COMM_WORLD,
6                    &rank);
7      MPI_Comm_size(MPI_COMM_WORLD,
8                    &size);
9
10     printf("Hello from %d/%d.\n",
11            rank, size);
12 }
```

- We can start the application directly
  - It will usually start with one process
- `mpiexec` allows spawning more processes
  - Optional and specified by the standard
  - There is also often `mpirun`
- The `-n` argument is standardized
  - Implementations provide additional ones

```
$ ./hello
Hello from 0/1.

$ mpiexec -n 1 ./hello
Hello from 0/1.

$ mpiexec -n 4 ./hello
Hello from 0/4.
Hello from 3/4.
Hello from 1/4.
Hello from 2/4.
```

Multi-Threaded Initialization

- MPI_Init only allows serial processes
  - That is, no threads are allowed to run
- Thread-safety requires locks
  - MPI is tuned for high performance
  - Locking overhead should be avoided
- MPI_Init_thread allows requesting a thread-safety level
  - Implementations may not support all

```
1  int main(void) {
2      int thread_level;
3
4      MPI_Init_thread(NULL, NULL,
5          MPI_THREAD_MULTIPLE,
6          &thread_level);
7
8      printf("thread_level=%d\n",
9          thread_level);
10
11     MPI_Finalize();
12     return 0;
13 }
```

Multi-Threaded Initialization

- MPI_THREAD_SINGLE
  - Only one thread will run
- MPI_THREAD_FUNNELED
  - Process can be multi-threaded but only the main thread will make MPI calls
- MPI_THREAD_SERIALIZED
  - All threads can make MPI calls but not at the same time
- MPI_THREAD_MULTIPLE
  - Threads can make MPI calls in parallel

```
1  int main(void) {
2      int thread_level;
3
4      MPI_Init_thread(NULL, NULL,
5          MPI_THREAD_MULTIPLE,
6          &thread_level);
7
8      printf("thread_level=%d\n",
9          thread_level);
10
11     MPI_Finalize();
12     return 0;
13 }
```

Multi-Threaded Initialization

- MPI_THREAD_SINGLE
  - Only one thread will run
- MPI_THREAD_FUNNELED
  - Process can be multi-threaded but only the main thread will make MPI calls
- MPI_THREAD_SERIALIZED
  - All threads can make MPI calls but not at the same time
- MPI_THREAD_MULTIPLE
  - Threads can make MPI calls in parallel

```
$ ./init_thread
thread_level=3

$ mpiexec -n 4 ./init_thread
thread_level=3
thread_level=3
thread_level=3
thread_level=3
```

- `MPI_Get_processor_name`
  - Returns an implementation-defined processor name
  - This typically returns the hostname of the current node
- `MPI_Initialized`
  - Checks whether MPI has been initialized
  - Useful if libraries want to check for MPI support
- `MPI_Wtime`
  - Returns wall-clock time for time measurements
- `MPI_Wtick`
  - Returns resolution of `MPI_Wtime`

Rationale

- Communicators allow separating different sets of processes
  - Groups contain processes
  - Communicators are based on groups
- All processes are available by default (`MPI_COMM_WORLD`)
  - Ranks are numbered from 0 to n-1
- Communicators can be used to define independent contexts
  - For instance, MPI-aware library should not interfere with application
- Some operations should only be performed by the local process
  - If they require a communicator, `MPI_COMM_SELF` can be used

Communicators

- Chicken and egg problem
  - Creating new communicator requires an existing communicator
  - MPI_COMM_WORLD can be used
- Processes can have multiple ranks
  - Rank only valid in a communicator
  - Processes can belong to multiple groups and communicators

```
1  void comm(void) {
2      MPI_Comm new_comm;
3      MPI_Group new_group;
4      MPI_Group world_group;
5
6      MPI_Comm_group(MPI_COMM_WORLD,
7          &world_group);
8      MPI_Group_incl(world_group,
9          size, reverse_ranks,
10         &new_group);
11     MPI_Comm_create(MPI_COMM_WORLD,
12         new_group, &new_comm);
13
14     print_rank(new_comm);
15 }
```

Communicators

- Chicken and egg problem
  - Creating new communicator requires an existing communicator
  - `MPI_COMM_WORLD` can be used
- Processes can have multiple ranks
  - Rank only valid in a communicator
  - Processes can belong to multiple groups and communicators

```
1 void print_rank(MPI_Comm comm) {
2     int new_rank;
3
4     MPI_Comm_rank(comm, &new_rank);
5     printf("rank=%d (world=%d)\n",
6         new_rank, rank);
7 }
```

```
$ mpiexec -n 4 ./comm
rank=3 (world=0)
rank=2 (world=1)
rank=1 (world=2)
rank=0 (world=3)
```

Outline

Guarantees

- Message order is guaranteed
  - If a process sends two messages, the first one will be received first
  - If a process posts two receives, the first one will get the message
- Rules do not apply when multi-threaded
  - If two threads send one message each, their order is undefined
  - Would require coordinating threads, that is, introduce overhead
- There are no fairness guarantees
  - A message might never be received because of other matching messages

Sending and Receiving

- Point-to-point between two processes
- Sending
  - Buffer: Data to send
  - Count: Number of elements
  - Datatype: Type of elements
  - Destination: Target rank
  - Tag: Distinguish messages
  - Communicator: Process mapping

```
1  void mysend(void) {
2      char str[100];
3      snprintf(str, 100,
4          "Hello from %d\n", rank);
5
6      MPI_Send(str, 100, MPI_CHAR,
7          (rank + 1) % size,
8          0, MPI_COMM_WORLD);
9      MPI_Recv(str, 100, MPI_CHAR,
10         (size + rank - 1) % size,
11         0, MPI_COMM_WORLD,
12         MPI_STATUS_IGNORE);
13
14     printf("%d: %s", rank, str);
15 }
```

Sending and Receiving

- Point-to-point between two processes
- Receiving
  - Buffer: Where to receive data
  - Count: Number of elements
  - Datatype: Type of elements
  - Source: Source rank
  - Tag: Distinguish messages
  - Communicator: Process mapping
  - Status: Query information

```
1  void mysend(void) {
2      char str[100];
3      snprintf(str, 100,
4          "Hello from %d\n", rank);
5
6      MPI_Send(str, 100, MPI_CHAR,
7          (rank + 1) % size,
8          0, MPI_COMM_WORLD);
9      MPI_Recv(str, 100, MPI_CHAR,
10         (size + rank - 1) % size,
11         0, MPI_COMM_WORLD,
12         MPI_STATUS_IGNORE);
13
14     printf("%d: %s", rank, str);
15 }
```

Sending and Receiving

- Point-to-point between two processes
- Ring communication
  - Send to next process
  - Receive from previous process
  - Output order might be mixed

```
$ mpiexec -n 4 ./send
1: Hello from 0
0: Hello from 3
3: Hello from 2
2: Hello from 1
```

Sending and Receiving...

- Might not be clear from which process to receive
  - Functions require specifying a source rank and tag
- Wildcards allow matching any source or any tag
  - `MPI_ANY_SOURCE` instead of actual source rank
  - `MPI_ANY_TAG` instead of actual source tag
- We still might be interested to know which rank and tag a message came from
  - Can be queried via `MPI_Status`'s `MPI_SOURCE` and `MPI_TAG` members
- `MPI_Get_count` returns the number of received elements

- What happens if we send 100,000 bytes?
  1. The same as with 100
  2. Application deadlocks
  3. Crash due to stack overflow
  4. MPI warns about too many elements

```c
void mysend(void) {
    char str[100];
    snprintf(str, 100,
        "Hello from %d\n", rank);

    MPI_Send(str, 100, MPI_CHAR,
        (rank + 1) % size,
        0, MPI_COMM_WORLD);
    MPI_Recv(str, 100, MPI_CHAR,
        (size + rank - 1) % size,
        0, MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);

    printf("%d: %s", rank, str);
}
```

- What happens if we send 100,000 bytes?
  1. The same as with 100
  2. Application deadlocks ✔
  3. Crash due to stack overflow
  4. MPI warns about too many elements

```c
void mysend(void) {
    char str[100];
    snprintf(str, 100,
        "Hello from %d\n", rank);

    MPI_Send(str, 100, MPI_CHAR,
        (rank + 1) % size,
        0, MPI_COMM_WORLD);
    MPI_Recv(str, 100, MPI_CHAR,
        (size + rank - 1) % size,
        0, MPI_COMM_WORLD,
        MPI_STATUS_IGNORE);

    printf("%d: %s", rank, str);
}
```

Blocking Send

- `MPI_Send` is the default blocking send function
  - Standard allows using a buffer but does not mandate it
  - "The send call [...] uses the standard communication mode. In this mode, **it is up to MPI to decide whether outgoing messages will be buffered**. [...] In such a case, the send call may complete before a matching receive is invoked. On the other hand, [...] MPI may choose not to buffer outgoing messages, for performance reasons. In this case, the send call will not complete until a matching receive has been posted, and the data has been moved to the receiver. [...] The standard mode send is non-local: successful completion of the send operation may depend on the occurrence of a matching receive." [Message Passing Interface Forum, 2015]
- Buffering is typically only used for small messages
  - Larger messages make the send operation synchronous

Blocking Send...

- There are a number of different send/receive variants
  - Synchronous send (`MPI_Ssend`)
    - Blocks until the destination process has started to receive the message
    - Behaves like `MPI_Send` for large messages
  - Blocking and non-blocking (`MPI_Send` and `MPI_Isend`)
    - Blocking behavior specifies when calls return and buffers can be reused
    - Non-blocking allows overlapping communication with computation
  - Buffered (`MPI_Bsend`)
    - Data is explicitly buffered, buffers have to be provided manually
    - Behaves like `MPI_Send` for small messages
  - Ready send (`MPI_Rsend`)
    - Requires matching receive operation to be started already, otherwise undefined
  - Combined blocking send and receive (`MPI_Sendrecv`)
    - Avoids deadlocks due to blocking sends waiting for receives to be posted

Non-Blocking Send

- Non-blocking send does not deadlock
  - `I` stands for immediate
- `MPI_Wait` blocks until completion
  - Functions to wait for multiple requests (all, any or some)
  - It is an error not to wait or access the buffer before the send has finished
- Alternatively, `MPI_Test` or `MPI_Probe`

```
1  void mysend(char* str, char* buf) {
2      MPI_Request req;
3
4      MPI_Isend(str, 100000, MPI_CHAR,
5          (rank + 1) % size,
6          0, MPI_COMM_WORLD, &req);
7      MPI_Recv(buf, 100000, MPI_CHAR,
8          (size + rank - 1) % size,
9          0, MPI_COMM_WORLD,
10         MPI_STATUS_IGNORE);
11     MPI_Wait(&req,
12         MPI_STATUS_IGNORE);
13
14     printf("%d: %s", rank, buf);
15 }
```

Non-Blocking Send

- Non-blocking send does not deadlock
  - I stands for immediate
- MPI_Wait blocks until completion
  - Functions to wait for multiple requests (all, any or some)
  - It is an error not to wait or access the buffer before the send has finished
- Alternatively, MPI_Test or MPI_Probe

```
$ mpiexec -n 4 ./isend
2: Hello from 1.
0: Hello from 3.
1: Hello from 0.
3: Hello from 2.
```

Combined Send and Receive

- Combined blocking send and receive
  - Still blocking but avoids deadlock
- Abstraction to achieve typical use case
  - For example, send to and receive from neighboring processes
  - Implementation can handle this specific use case efficiently and correctly

```
1  void mysend(void) {
2      char str[100000];
3      char buf[100000];
4      snprintf(str, 100000,
5          "Hello from %d.\n", rank);
6
7      MPI_Sendrecv(str, 100000,
8          MPI_CHAR, (rank + 1) % size,
9          0, buf, 100000, MPI_CHAR,
10         (size + rank - 1) % size,
11         0, MPI_COMM_WORLD,
12         MPI_STATUS_IGNORE);
13
14     printf("%d: %s", rank, buf);
15 }
```

Combined Send and Receive

- Combined blocking send and receive
  - Still blocking but avoids deadlock
- Abstraction to achieve typical use case
  - For example, send to and receive from neighboring processes
  - Implementation can handle this specific use case efficiently and correctly

```
$ mpiexec -n 4 ./sendrecv
0: Hello from 3.
3: Hello from 2.
1: Hello from 0.
2: Hello from 1.
```

<table>
<tr><th></th><th>Send</th><th>Receive</th><th>Testing</th></tr>
<tr><td rowspan="2">Blocking</td><td>MPI_Send
MPI_Ssend
MPI_Rsend
MPI_Bsend</td><td>MPI_Recv</td><td rowspan="2">MPI_Probe
MPI_Wait</td></tr>
<tr><td colspan="2">MPI_Sendrecv</td></tr>
<tr><td rowspan="2">Non-blocking</td><td>MPI_Isend
MPI_Issend
MPI_Irsend
MPI_Ibsend</td><td>MPI_Irecv</td><td rowspan="2">MPI_Iprobe
MPI_Test</td></tr>
<tr><td colspan="2">MPI_Isendrecv</td></tr>
</table>

- Blocking is easier to use, non-blocking can be more efficient

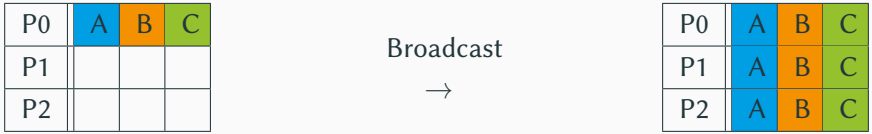
Outline

Overview

- Point-to-point communication happens between two ranks
  - Collective communication happens between all ranks
- Which ranks are involved depends on communicator
  - By default, we only have `MPI_COMM_WORLD` and `MPI_COMM_SELF`
- MPI contains a wide range of collective communication functions
  - Broadcast
  - Barrier
  - Distributing or collecting data
- One collective call is often more efficient than many point-to-point calls
  - InfiniBand hardware typically has support for efficient collectives

- 1:1 communication
  - Traditional point-to-point communication such as send and receive
- 1:n communication
  - Collective communication such as broadcast
- n:1 communication
  - Collective communication such as reduction
- n:n communication
  - Collective communication such as reduction to all

Overview...



Overview...


P0
A
B
C
P1
P2
Broadcast
→
P0
A
B
C
P1
A
B
C
P2
A
B
C
P0
A
B
C
P1
P2
Scatter
→
P0
A
B
C
P1
B
P2
C

Overview...


P0 A B C
P1
P2
Broadcast
→
P0 A B C
P1 A B C
P2 A B C
P0 A B C
P1
P2
Scatter
→
P0 A B C
P1 B
P2 C
P0 A
P1 B
P2 C
Gather
→
P0 A B C
P1 B
P2 C

Reduction

- Reducing
  - Send buffer: Data to reduce
  - Receive buffer: Root needs separate buffer
  - Count: Number of elements
  - Datatype: Type of elements
  - Operation: Reduction to perform
  - Root: Rank to reduce at
  - Communicator: Process mapping
- Reduction operations known from OpenMP
  - Apply a given function to multiple buffers, reducing it to one buffer
- Ordering is arbitrary, might influence result

```
1 void reduce(void) {
2     int buf = 42;
3
4     MPI_Reduce(&rank, &buf, 1,
5         MPI_INT, MPI_MAX,
6         0, MPI_COMM_WORLD);
7
8     printf("%d: %d\n", rank, buf);
9 }
```

Reduction

- Reducing
  - Send buffer: Data to reduce
  - Receive buffer: Root needs separate buffer
  - Count: Number of elements
  - Datatype: Type of elements
  - Operation: Reduction to perform
  - Root: Rank to reduce at
  - Communicator: Process mapping
- Reduction operations known from OpenMP
  - Apply a given function to multiple buffers, reducing it to one buffer
- Ordering is arbitrary, might influence result

```
$ mpiexec -n 4 ./reduce
0: 3
1: 42
2: 42
3: 42
```

Reduction to All

- Reducing to all
  - Send buffer: Data to reduce
  - Receive buffer: Needs separate buffer
  - Count: Number of elements
  - Datatype: Type of elements
  - Operation: Reduction to perform
  - Communicator: Process mapping
- No root rank specified anymore
  - Reduced buffer is available for all ranks

```
1  void reduce(void) {
2      int buf = 42;
3
4      MPI_Allreduce(&rank, &buf, 1,
5          MPI_INT, MPI_MAX,
6          MPI_COMM_WORLD);
7
8      printf("%d: %d\n", rank, buf);
9  }
```

Reduction to All

- Reducing to all
  - Send buffer: Data to reduce
  - Receive buffer: Needs separate buffer
  - Count: Number of elements
  - Datatype: Type of elements
  - Operation: Reduction to perform
  - Communicator: Process mapping
- No root rank specified anymore
  - Reduced buffer is available for all ranks

```
$ mpiexec -n 4 ./allreduce
0: 3
1: 3
2: 3
3: 3
```

- Why not use `MPI_Reduce` followed by `MPI_Broadcast`?
  1. More optimization potential
  2. Two collectives could deadlock
  3. Data could be broadcasted before reduction is finished

```c
void reduce(void) {
    int buf = 42;

    MPI_Allreduce(&rank, &buf, 1,
        MPI_INT, MPI_MAX,
        MPI_COMM_WORLD);

    printf("%d: %d\n", rank, buf);
}
```

- Why not use `MPI_Reduce` followed by `MPI_Broadcast`?
  1. More optimization potential ✔
  2. Two collectives could deadlock
  3. Data could be broadcasted before reduction is finished

```
1  void reduce(void) {
2      int buf = 42;
3
4      MPI_Allreduce(&rank, &buf, 1,
5          MPI_INT, MPI_MAX,
6          MPI_COMM_WORLD);
7
8      printf("%d: %d\n", rank, buf);
9  }
```

Barrier

- Barrier
  - Communicator: Process mapping
- Waits for all processes
  - Can cause significant overhead
  - Often not necessary due to implicit synchronization via messages

```c
void barrier(void) {
    printf("%d: before barrier\n",
        rank);

    MPI_Barrier(MPI_COMM_WORLD);

    printf("%d: after barrier\n",
        rank);
}
```

Barrier

- Barrier
  - Communicator: Process mapping
- Waits for all processes
  - Can cause significant overhead
  - Often not necessary due to implicit synchronization via messages
- Does not work for everything
  - Terminal output might be buffered
  - Output has to be collected from nodes

```
$ mpiexec -n 4 ./barrier
1: before barrier
0: before barrier
2: before barrier
2: after barrier
3: before barrier
3: after barrier
0: after barrier
1: after barrier
```

Outline

- MPI supports most basic data types out of the box
  - `char`, `int`, `long`, `float`, `double` etc.
- Applications often use their own data types
  - For instance, structures containing multiple values
- MPI allows handling these data types directly
  - Developers have to replicate the data types for MPI
  - MPI might be able to handle them more efficiently then
- Data types can then be specified like normal ones
  - Every function that accepts a data type also accepts derived ones

Non-Contiguous Data Types

- Example: Diagonal of a 3×3 matrix
  - For instance, within a function doing parallel matrix calculations

Non-Contiguous Data Types

- Example: Diagonal of a 3×3 matrix
  - For instance, within a function doing parallel matrix calculations
- MPI supports a vector data type
  - Count: Number of blocks
  - Block length: Elements per block
  - Stride: Elements between blocks
  - Old type: Old data type
  - New type: New data type

```
1 int MPI_Type_vector (
2     int count,
3     int blocklength,
4     int stride,
5     MPI_Datatype oldtype,
6     MPI_Datatype* newtype)
```

Non-Contiguous Data Types

- Example: Diagonal of a 3×3 matrix
  - For instance, within a function doing parallel matrix calculations
- MPI supports a vector data type
  - Count: Number of blocks
  - Block length: Elements per block
  - Stride: Elements between blocks
  - Old type: Old data type
  - New type: New data type

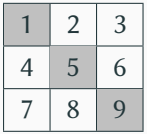
```
int MPI_Type_vector (
    int count,
    int blocklength,
    int stride,
    MPI_Datatype oldtype,
    MPI_Datatype* newtype)
```

```
MPI_Type_vector(3, 1, 4,
    MPI_DOUBLE, &newtype);
MPI_Type_commit(&newtype);
MPI_Send(matrix, 1, newtype,
    rank, 0, MPI_COMM_WORLD);
```

Non-Contiguous Data Types

- Matrix is stored in row- or column-major order
  - 3×3 matrix has three diagonal elements
  - Each diagonal element is a double value
  - Diagonal elements are four values apart
- Can be generalized for arbitrary dimensions
  - Sender and receiver have to agree on data type
- There are many more data type constructors
  - Interactive tools can help create own derived data types [RookieHPC, 2026]

```
1 MPI_Type_vector(3, 1, 4,
2     MPI_DOUBLE, &newtype);
```



Outline

Summary

- MPI is a standard for parallel programming on distributed memory systems
  - It supports communication, synchronization, I/O and much more
- Groups of processes can be assigned to communicators
  - Allows separating different parts of an application or library
- Point-to-point communication allows sending messages between two processes
  - There are various versions of basic send and receive functions
- Collective communication involves all processes in a communicator
  - This includes actual communication as well as synchronization functionality
- Derived data types allow MPI to handle application-specific data types directly
  - Allows the MPI implementation to make access more convenient and efficient

References

[Barney, 2026] Barney, B. (2026). **Message Passing Interface (MPI).** https://hpc-tutorials.llnl.gov/mpi/.

[Message Passing Interface Forum, 2015] Message Passing Interface Forum (2015). **MPI: A Message-Passing Interface Standard Version 3.1.** https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report/mpi31-report.htm.

[MPICH Collaborators, 2026] MPICH Collaborators (2026). **MPICH ABI Compatibility Initiative.** https://www.mpich.org/abi/.

[RookieHPC, 2026] RookieHPC (2026). **MPI datatype creator.** https://rookiehpc.org/mpi/tools/datatype_creator/.