Programming with MPI

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- Which aspect is not part of the POSIX Threads standard?
	- 1. Thread management
	- 2. Mutexes
	- 3. Semaphores
	- 4. Condition variables
	- 5. Synchronization
- Which thread-to-task mapping does Linux use?
	- 1. 1:1 mapping (each thread is mapped to a kernel task)
	- 2. n:1 mapping (all threads are mapped to one kernel task)
	- 3. m:n mapping (multiple threads are mapped to multiple kernel tasks)
- What happens if a thread is not joined after termination?
	- 1. The process can crash
	- 2. Zombie threads remain
	- 3. Stack memory can overflow
- When will a thread be canceled by pthread_cancel?
	- 1. Before the next function call
	- 2. After the next function call
	- 3. After a timeout of 100 ms
	- 4. After an I/O operation such as printf
	- 5. When a cancellation point function is called

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- Shared memory systems have limited scalability
	- Two to four processors with a few dozen 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

- 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
- 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 [\[MPICH Collaborators, 2024\]](#page-72-0)
- 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
- 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
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8 9 10 11 12 13 14 15

Challenges. . . Introduction

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- 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

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- 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
- 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... History

- 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." [\[Message Passing Interface Forum, 2015\]](#page-72-1)
	- 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... History

- 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
- 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
- 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
- 2021: MPI-4.0 is released
	- MPI-4.1 in 2023
	- Large-count versions of many routines
	- Persistent collectives
	- Partitioned communication
- 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

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- 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

```
1 int main (void) {
2 MPI_Init ( NULL , NULL );
3 \mid hello();
4 MPI_Finalize () ;
5
6 return 0;
7 }
```
- MPI uses communicators
	- Basically a group of processes
- We can determine our rank
	- Same as OpemMP'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 8 rank );
7 MPI_Comm_size ( MPI_COMM_WORLD ,
8 \& size);
Q10 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.
```
- 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 }
```


- 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
- 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

- 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

```
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);
\overline{7}
```

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


```
1 void mysend (void) {
2 char str [100];
3 snprintf (str, 100,
4 WHello 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 }
```
- Point-to-point between two processes
- Ring communication
	- Send to next process
	- Receive from previous process
	- Output order might be mixed

- 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

- 1. The same as with 100
- 2. Application deadlocks
- 3. Crash due to stack overflow
- 4. MPI warns about too many elements

```
1 void mysend (void) {
2 char str [100];
3 \text{ s} snprintf (str, 100,
4 Whello 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 }
```
- 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." [\[Message Passing Interface Forum, 2015\]](#page-72-0)
- Buffering is typically only used for small messages
	- Larger messages make the send operation synchronous

- 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

- It is an error not to wait or access the buffer before the send has finished
- Alternatively, MPI_Test or MPI_Probe

```
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 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 Point-To-Point Communication

- 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 $_{11}$ use case efficiently and correctly

```
void mysend ( void ) {
2 char str [100000];
3 char buf [100000];
4 snprintf ( str , 100000 ,
5 "He1lo from %d.\n', rank);
7 MPI_Sendrecv ( str , 100000 ,
8 MPI_CHAR, (rank + 1) % size,
9 0, buf, 100000, MPI_CHAR,
10 ( size + rank - 1) % size ,
          0, MPI_COMM_WORLD,
12 MPI_STATUS_IGNORE);
14 printf ("%d: %s", rank, buf);
15 }
```
13

6

- 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.
```


- Most functions are available as blocking and non-blocking versions
	- There are also non-blocking synchronous functions
- Blocking is easier to use, non-blocking is more efficient

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- 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

Broadcast

$$
\rightarrow
$$

Broadcast

$$
\rightarrow
$$

Scatter \rightarrow

Broadcast

 \rightarrow

Scatter

 \rightarrow

Gather

 \rightarrow

- 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 9 }
- Ordering is arbitrary, might influence result

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- Send buffer: Data to reduce
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- No root rank specified anymore
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- Send buffer: Data to reduce
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- No root rank specified anymore
	- Reduced buffer is available for all ranks

- 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

- Communicator: Process mapping
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• 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

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

- Example: Diagonal of a 3×3 matrix
	- For instance, within a function doing parallel matrix calculations
- MPI supports a vector data type
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	- Old type: Old data type
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- 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 [\[RookieHPC, 2024\]](#page-72-1)

MPI_Type_vector (3, 1, 4,

```
2 MPI_DOUBLE , & newtype ) ;
```


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- 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
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