Message Passing with MPI

PPCES 2018

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IT Center / JARA-HPC

Slides by Hristo Iliev
Agenda

- **Motivation**
- **Part 1**
  - Concepts
  - Point-to-point communication
  - Non-blocking operations
- **Part 2**
  - Collective operations
  - Communicators
  - User datatypes
- **Part 3**
  - Hybrid parallelisation
  - Common parallel patterns
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- Motivation

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- Part 3
  - Hybrid parallelisation
  - Common parallel patterns
Parallel Architectures

- **Clusters**
  - HPC market is at large dominated by distributed memory *multicomputers*: clusters and specialised *supercomputers*
  - Nodes have no direct access to other nodes’ memory and run a separate copy of the (possibly stripped down) OS
Parallel Architectures

- **Shared Memory**

  → All processing elements (P) have direct access to the main memory block (M)
Parallel Architectures

- **Shared Memory**

  - All processing elements (P) have direct access to the main memory block (M)

  ![Diagram of shared memory](image)

  - Data exchange is achieved through read/write operations on shared variables located in the global address space
Parallel Architectures

- **Shared Memory – Pros**
  - All processing elements (P) have direct access to the main memory (M)
  - Single System Image
  - One single OS instance – easier to install and manage
  - Execution streams typically implemented as a set of OS entities that share a single (virtual) address space – *threads* within a single *process*

  - Data exchange is achieved through the means of read/write operations in the global address space
    - Easy to conceptualise and program:
      
      thread 1: \( a = \text{produce\_value}() \);
      thread 2: \( \text{compute}(a) \);
Parallel Architectures

● Shared Memory – Cons

→ Requires complex hardware
  → Memory usually divided into regions (NUMA) to reduce complexity

→ Processing elements typically have caches
  → Maintaining cache coherence is very expensive
  → Non-cache-coherent systems are harder to program

→ Data races
  → Synchronisation needed to enforce access order – barriers, locks, etc.
Parallel Architectures

- **Distributed Memory**

  → Each processing element (P) has its separate main memory block (M)

![Diagram showing distributed memory architecture]

Network
Parallel Architectures

**Distributed Memory**

→ Each processing element (P) has its separate main memory block (M)

→ Data exchange is achieved through message passing over the network
Distributed Memory

- Each processing element (P) has its separate main memory block (M)
- Data exchange is achieved through message passing over the network
- Message passing could be either explicit (MPI) or implicit (PGAS)
- Programs typically implemented as a set of OS entities with own (virtual) address spaces – processes
- No shared variables
  - No data races
  - Explicit synchronisation mostly unneeded
    - Results as side effect of the send-receive semantics
Processes

- **A process is a running in-memory instance of an executable file**
  - Executable code, e.g., binary machine instructions
  - One or more threads of execution sharing memory address space
  - Memory: data, heap, stack, processor state (CPU registers and flags)
  - Operating system context (e.g. signals, I/O handles, etc.)
  - PID

- **Isolation and protection**
  - A process cannot interoperate with other processes or access their context (even on the same node) without the help of the operating system
  - No direct inter-process data exchange (isolated/virtual address spaces)
  - No direct inter-process synchronisation
Inter-Process Communication

Interaction with other processes

→ Shared memory segments
  → Restricted to the same node

→ File system
  → Slow; shared file system required for internode data access

→ Networking (e.g. sockets, named pipes, etc.)
  → Coordination and addressing issues

→ Special libraries (middleware) make IPC transparent and more portable
  → **MPI**, PVM – tightly coupled
  → Globus Toolkit (GRID infrastructure) – loosely coupled
  → **BOINC** (SETI@home, Einstein@home, *@home) – decoupled
SPMD Model

- Abstractions make programming and understanding easier
- **Single Program Multiple Data**
  
  → Multiple instruction flows (instances) from a Single Program working on Multiple (different parts of) Data
  
  → Instances could be threads (OpenMP) and/or processes (MPI)
  
  → Each instance receives a unique ID – can be used for flow control

```c
if (myID == specificID)
{
    do_something();
}
else
{
    do_something_different();
}
```
SPMD Model

SPMD Program Lifecycle – multiple processes (e.g. MPI)

- Source Code
  - Compile & Link
  - Executable
  - SPMD Launch
  - Parallel Execution

SPMD Model Diagram:

- Data
  - OS Process
    - OS Process
    - OS Process
    - OS Process
  - Result
SPMD Environments

- Provide dynamic identification of all peers
  - Who else is also working on this problem?

- Provide robust mechanisms to exchange data
  - Whom to send data to / From whom to receive the data?
  - How much data?
  - What kind of data?
  - Has the data arrived?

- Provide synchronisation mechanisms
  - Have all processes reached same point in the program execution flow?

- Provide methods to launch and control a set of processes
  - How do we start multiple processes and get them to work together?

- Portability
IPC Example: Sockets

- Sockets API is straightforward but there are some major issues:
  - How to obtain the set of communicating partners?
  - Where and how can these partners be reached?
    - Write your own registry server or use broadcast/multicast groups
    - Worst case: AF_INET sockets with FQDN and TCP port number
      e.g. linuxbmc0064.rz.rwth-aachen.de:24892
  - How to coordinate the processes in the parallel job?
    - Does the user have to start each process in his parallel job by hand?
    - Executable distribution and remote launch
    - Integration with DRMs (batch queuing systems)
  - Redirection of standard I/O and handling of signals
Going Parallel

- **Define the problem**
  - problem space
  - methods

- **Solution:**
  - input domain
  - algorithm
  - output domain

- **Decomposition**
  - Split the input domain into (preferably non-interacting) regions
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Message Passing with MPI (PPCES 2018)
Joachim Protze / Marc-André Hermanns | IT Center der RWTH Aachen University
- **Message Passing Interface**
  - The de-facto standard API for explicit message passing nowadays
  - A moderately large standard (v3.1 is a 868 pages long)
  - Maintained by the non-profit Message Passing Interface Forum
- **Many concrete implementations of the MPI standard**
  - Open MPI, MPICH, Intel MPI, MVAPICH, MS-MPI, etc.
- **MPI is used to express the explicit interaction (communication) in programs for computers with distributed memory**
- **MPI provides source level portability of parallel applications between different implementations and hardware platforms**
A language-independent specification (LIS) of a set of communication and I/O operations

- Standard bindings for C and Fortran
- Concrete function prototypes / interfaces
- Non-standard bindings for other languages exist:
  - C++: Boost.MPI
  - Java: Open MPI, MPJ Express
  - Python: mpi4py

Unlike OpenMP and PGAS languages, MPI does not extend the base language, but provides a set of library functions (+ specialised runtime) and makes use of existing compilers.
MPI History

- **Version 1.0 (1994):** FORTRAN 77 and C bindings
- **Version 1.1 (1995):** Minor corrections and clarifications
- **Version 1.2 (1997):** Further corrections and clarifications
- **Version 2.0 (1997):** MPI-2 – Major extensions
  - One-sided communication
  - Parallel I/O
  - Dynamic process creation
  - Fortran 90 and C++ bindings
  - Language interoperability
- **Version 2.1 (2008):** Merger of MPI-1 and MPI-2
- **Version 2.2 (2009):** Minor corrections and clarifications
  - C++ bindings deprecated
- **Version 3.0 (2012):** Major enhancements
  - Non-blocking collective operations
  - Modern Fortran 2008 bindings
  - C++ deleted from the standard
- **Version 3.1 (2015):** Corrections and clarifications
  - Portable operation with address variables
  - Non-blocking collective I/O
More Information & Documentation

- The MPI Forum document archive (free standards for everyone!)
  → http://www.mpi-forum.org/docs/

- The MPI home page at Argonne National Lab
  → http://www-unix.mcs.anl.gov/mpi/

- Open MPI (default MPI implementation on the RWTH cluster)
  → http://www.open-mpi.org/

- Manual pages
  → man MPI
  → man MPI_Xxx_yyy_zzz (for all MPI calls)
Literature about MPI

- **MPI: The Complete Reference Vol. 1**
  **The MPI Core**
  
  by Marc Snir, Steve Otto, Steven Huss-Lederman, David Walker, Jack Dongarra
  

- **MPI: The Complete Reference Vol. 2**
  **The MPI Extensions**
  
  by William Gropp, Steven Huss-Lederman, Andrew Lumsdain, Ewing Lusk, Bill Nitzberg, William Saphir, Marc Snir
  
Literature about MPI

- **Using MPI**
  
  by William Gropp, Ewing Lusk, Anthony Skjellum  

- **Using MPI-2**
  
  by William Gropp, Ewing Lusk, Rajeev Thakur  

- **Parallel Programming with MPI**
  
  by Peter Pacheco  
  Morgan Kaufmann Publishers, 1996
MPI Basics – Agenda

- **MPI Basics**
  - Start-up, initialisation, finalisation, and shutdown

- **Point-to-Point Communication**
  - Send and receive
  - Basic MPI data types
  - Message envelope
  - Combined send and receive
  - Send modes
  - Non-blocking operations
  - Common pitfalls
General Structure of an MPI Program

Start-up, initialisation, finalisation, and shutdown – C

1. Inclusion of the MPI header file

2. Pre-initialisation mode: uncoordinated
   - No MPI function calls allowed with few exceptions
   - All program instances run exactly the same code

3. Initialisation of the MPI environment
   Implicit synchronisation

4. Parallel MPI code
   Typically computation and communication

5. Finalisation of the MPI environment
   Internal buffers are flushed

6. Post-finalisation mode: uncoordinated
   - No MPI function calls allowed with few exceptions

C

```c
#include <mpi.h>

int main(int argc, char **argv)
{
    ... some code ...
    MPI_Init(&argc, &argv);

    ... computation & communication ...

    MPI_Finalize();
    ... wrap-up ...
    return 0;
}
```
General Structure of an MPI Program

- **Start-up, initialisation, finalisation, and shutdown – Fortran**

  ```fortran
  PROGRAM example
    USE mpi_f08 ! USE mpi
    ... some code ...
    CALL MPI_Init(ierr)
    ... computation & communication ...
    CALL MPI_Finalize(ierr)
    ... wrap-up ...
  END
  ```

  ![Fortran Diagram]

  1. Inclusion of the MPI module
  2. Pre-initialisation mode: uncoordinated
     - No MPI function calls allowed with few exceptions
     - All program instances run exactly the same code
  3. Initialisation of the MPI environment
     Implicit synchronisation
  4. Parallel MPI code
     Typically computation and communication
  5. Finalisation of the MPI environment
     Internal buffers are flushed
  6. Post-finalisation mode: uncoordinated
     - No MPI function calls allowed with few exceptions

*Message Passing with MPI (PPCES 2018)*
Joachim Protze / Marc-André Hermanns | IT Center der RWTH Aachen University
General Structure of an MPI Program

- How many processes are there in total?
- Who am I?

```c
#include <mpi.h>

int main(int argc, char **argv)
{
    ... some code ... 
    int ierr = MPI_Init(&argc, &argv),
               numberOfProcs, rank;
    ... other code ...
    ierr = MPI_Comm_size(MPI_COMM_WORLD,
                         &numberOfProcs);
    ierr = MPI_Comm_rank(MPI_COMM_WORLD,
                         &rank);
    ... computation & communication ...
    ierr = MPI_Finalize();
    ... wrap-up ...
    return 0;
}
```

1. Obtains the number of processes (ranks) in the MPI program
   Example: if the job was started with 4 processes, then `numberOfProcs` will be set to 4 by the call

2. Obtains the identity of the calling process within the MPI program
   NB: MPI processes are numbered starting from 0
   Example: if there are 4 processes in the job, then `rank` receive value of 0 in the first process, 1 in the second process, and so on
General Structure of an MPI Program

- How many processes are there in total?
- Who am I?

```fortran
PROGRAM example
  USE mpi_f08 ! USE mpi
  INTEGER :: rank, numberOfProcs, ierr
  ... some code ...
  CALL MPI_Init(ierr)
  ... other code ...
  CALL MPI_Comm_size(MPI_COMM_WORLD,&
                    numberOfProcs, ierr)
  CALL MPI_Comm_rank(MPI_COMM_WORLD,&
                     rank, ierr)
  ... computation & communication ...
  CALL MPI_Finalize(ierr)
  ... wrap-up ...
END PROGRAM example
```

1. Obtains the number of processes (ranks) in the MPI program

   Example: if the job was started with 4 processes, then `numberOfProcs` will be set to 4 by the call

2. Obtains the identity of the calling process within the MPI program

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   Example: if there are 4 processes in the job, then `rank` receive value of 0 in the first process, 1 in the second process, and so on
The processes in any MPI program are initially indistinguishable

- MPI_Init assigns each process a unique identity – rank

---

Ranks

- The processes in any MPI program are initially indistinguishable
- MPI_Init assigns each process a unique identity – rank
Ranks

- The processes in any MPI program are initially indistinguishable
- MPI_Init assigns each process a unique identity – rank
  - Without personality, the started MPI processes cannot do coordinated parallel work in the pre-initialisation mode
  - Ranks range from 0 up to the total number of processes minus 1
- Ranks are associated with the so-called communicators
  - Logical contexts where communication takes place
  - Represent groups of MPI processes with some additional information
  - The most important one is the world communicator `MPI_COMM_WORLD`
    - Contains all processes launched *initially* as part of the MPI program
  - Ranks are always provided in MPI calls in combination with the corresponding communicator
Basic MPI Use

- **Initialisation:**

  ```c
  ierr = MPI_Init(&argc, &argv);
  ```

  ```fortran
  CALL MPI_Init(ierr)
  ```

  - Initialises the MPI library and makes the process member of the world communicator
  - [C] Modern MPI implementations allow both arguments to be NULL, otherwise they *must* point to the arguments of `main()`
  - May not be called more than once for the duration of the program execution
  - Error code as return value in [C] and additional parameter in [F]

- **Finalisation:**

  ```c
  ierr = MPI_Finalize();
  ```

  ```fortran
  CALL MPI_Finalize(ierr)
  ```

  - Cleans up the MPI library and prepares the process for termination
  - Must be called once before the process terminates
  - Having other code after the finalisation call is not recommended
Basic MPI Use

Number of processes in the MPI program:

- Obtains the number of processes initially started in the MPI program (the size of the world communicator)
- `size` is an integer variable
- `MPI_COMM_WORLD` is a predefined constant MPI handle that represents the world communicator

```c
ierr = MPI_Comm_size(MPI_COMM_WORLD, &size);
```

```fortran
CALL MPI_Comm_size(MPI_COMM_WORLD, size, ierr)
```

Process identification:

- Determines the rank (unique ID) of the process within the world communicator
- `rank` is an integer variable; receives value between 0 and #processes - 1

```c
ierr = MPI_Comm_rank(MPI_COMM_WORLD, &rank);
```

```fortran
CALL MPI_Comm_rank(MPI_COMM_WORLD, rank, ierr)
```
Basic MPI Use

- Most MPI calls in C return an integer error code:
  - `int MPI_Comm_size(...)`

- Most MPI calls are Fortran subroutines with an extra INTEGER output argument (always last one in the list) for the error code:
  - `SUBROUTINE MPI_Comm_size(..., ierr)`
  - The Fortran 2008 interface makes the error argument optional

- Fortran note
  - The `USE mpi` interface does not provide interfaces for all MPI routines
  - `USE mpi_f08` when possible
Basic MPI Use

- **Error codes indicate the success of the operation:**
  
  → Failure is indicated by error codes other than `MPI_SUCCESS`
  
  → C: `if (MPI_SUCCESS != MPI_Init(NULL, NULL)) ...`
  
  → Fortran: `CALL MPI_Init(ierr)`
  `IF (ierr /= MPI_SUCCESS) ...`

- **An MPI error handler is called first before the call returns**
  
  → The default error handler for non-I/O calls aborts the entire MPI program!
  
  → Error checking in simple programs is redundant

- **NB: Actual MPI error code values are implementation specific**
Basic MPI Use

- **MPI objects (e.g. communicators) are referenced via handles**
  - Opaque process-local values
  - Cannot be passed from one process to another

- **C (mpi.h)**
  - typedef’d handle types: MPI_Comm, MPI_Datatype, MPI_File, etc.

- **Fortran (USE mpi)**
  - All handles are INTEGER values
  - Easy to pass the wrong handle type

- **Fortran 2008 (USE mpi_f08)**
  - Wrapped INTEGER values: TYPE(MPI_Comm), TYPE(MPI_File), etc.
  - The INTEGER handle is still available: comm%MPI_VAL
MPI as an SPMD Environment

✓ Provide dynamic identification of all peers
  → Who am I and who else is also working on this problem?

■ Provide robust mechanisms to exchange data
  → Whom to send data to / From whom to receive the data?
  → How much data?
  → What kind of data?
  → Has the data arrived?

■ Provide synchronisation mechanisms
  → Have all processes reached same point in the program execution flow?

■ Provide methods to launch and control a set of processes
  → How do we start multiple processes and get them to work together?

■ Portability
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  - User datatypes
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  - Hybrid parallelisation
  - Common parallel patterns
Message Passing

- The goal is to enable communication between processes that share no memory space

Explicit message passing requires:

→ Send and receive primitives (operations)
→ Known addresses of both the sender and the receiver
→ Specification of what has to be sent/received
Sending Data

Sending a message:

```c
MPI_Send (void *data, int count, MPI_Datatype type,
          int dest, int tag, MPI_Comm comm)
```

- **data**: location in memory of the data to be sent
- **count**: number of data elements to be sent (MPI is array-oriented)
- **type**: Handle of the *MPI datatype* of the buffer content
- **dest**: rank of the receiver
- **tag**: additional identification of the message
  - ranges from 0 to UB (impl. dependant but not less than 32767)
- **comm**: communication context (communicator handle)

```fortran
MPI_Send (data, count, type, dest, tag, comm, ierr)
```
Receiving Data

Receiving a message:

MPI_Recv (void *data, int count, MPI_Datatype type, int source, int tag, MPI_Comm comm, MPI_Status *status)

→ data: location of the receive buffer
→ count: size of the receive buffer in data elements
→ type: Handle of the MPI datatype of the data elements
→ source: rank of the sender or MPI_ANY_SOURCE (wildcard)
→ tag: message tag or MPI_ANY_TAG (wildcard)
→ comm: communication context
→ status: status of the receive operation or MPI_STATUS_IGNORE

MPI_Recv (data, count, type, src, tag, comm, status, ierr)
MPI Datatypes

- MPI is a library – it cannot infer the type of elements in the supplied buffer at run time and that’s why it has to be told what it is.

- MPI datatypes tell MPI how to:
  - read binary values from the send buffer
  - write binary values into the receive buffer
  - correctly apply value alignments
  - convert between machine representations in heterogeneous environments

- MPI datatype **must** match the language type(s) in the data buffer
- MPI datatype **must** match between sender and receiver
- MPI datatypes are handles and cannot be used to declare variables
MPI Datatypes

- MPI provides many predefined datatypes for each language binding:

  > C

<table>
<thead>
<tr>
<th>MPI data type</th>
<th>C data type</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_CHAR</td>
<td>char</td>
</tr>
<tr>
<td>MPI_SHORT</td>
<td>short</td>
</tr>
<tr>
<td>MPI_INT</td>
<td>int</td>
</tr>
<tr>
<td>MPI_FLOAT</td>
<td>float</td>
</tr>
<tr>
<td>MPI_DOUBLE</td>
<td>double</td>
</tr>
<tr>
<td>MPI_UNSIGNED_INT</td>
<td>unsigned int</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>MPI_BYTE</td>
<td>-</td>
</tr>
</tbody>
</table>

8 binary digits
no conversion
used for binary data
MPI Datatypes

MPI provides many predefined datatypes for each language binding:

- C
- Fortran

<table>
<thead>
<tr>
<th>MPI data type</th>
<th>Fortran data type</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_INTEGER</td>
<td>INTEGER</td>
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<tr>
<td>MPI_REAL</td>
<td>REAL</td>
</tr>
<tr>
<td>MPI_REAL8</td>
<td>REAL(KIND=8)</td>
</tr>
<tr>
<td>MPI_DOUBLE_PRECISION</td>
<td>DOUBLE PRECISION</td>
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<tr>
<td>MPI_COMPLEX</td>
<td>COMPLEX</td>
</tr>
<tr>
<td>MPI_LOGICAL</td>
<td>LOGICAL</td>
</tr>
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<td>MPI_CHARACTER</td>
<td>CHARACTER(1)</td>
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<td>...</td>
<td>...</td>
</tr>
<tr>
<td>MPI_BYTE</td>
<td>-</td>
</tr>
</tbody>
</table>
Message Passing as Assignment

- Message passing in MPI is explicit:
  - The value of variable \( b \) in rank 1 is copied into variable \( a \) in rank 0
  - For now, assume that \( comm \) is always MPI_COMM_WORLD
    → We will talk about other communicators later on

```c
MPI_Send(&b, 1, MPI_INT, 0, 0, MPI_COMM_WORLD);
MPI_Recv(&a, 1, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);
a = b;
```
Message passing in MPI is explicit:

```c
if (rank == 0) {
    MPI_Recv(&a, 1, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);
} else if (rank == 1) {
    MPI_Send(&b, 1, MPI_INT, 0, 0, MPI_COMM_WORLD);
}
```

```c
a = b;
```
MPI as an SPMD Environment

- Provide dynamic identification of all peers
  → Who am I and who else is also working on this problem?

- Provide robust mechanisms to exchange data
  → Whom to send data to / From whom to receive the data?
  → How much data?
  → What kind of data?
  → Has the data arrived? (only the receiver knows)

- Provide synchronisation mechanisms
  → Have all processes reached same point in the program execution flow?

- Provide methods to launch and control a set of processes
  → How do we start multiple processes and get them to work together?

Portability
Complete MPI Example

#include <mpi.h>

int main(int argc, char **argv)
{
    int nprocs, rank, data;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    if (rank == 0)
        MPI_Recv(&data, 1, MPI_INT, 1, 0, MPI_COMM_WORLD, &status);
    else if (rank == 1)
        MPI_Send(&data, 1, MPI_INT, 0, 0, MPI_COMM_WORLD);
    MPI_Finalize();
    return 0;
}
### Compiling MPI Programs

- MPI is a typical library with C header files, Fortran modules, etc.
- Some MPI vendors provide convenience compiler wrappers:

<table>
<thead>
<tr>
<th>cc</th>
<th>mpicc</th>
</tr>
</thead>
<tbody>
<tr>
<td>c++</td>
<td>mpic++</td>
</tr>
<tr>
<td>f90</td>
<td>mpif90</td>
</tr>
</tbody>
</table>

- On RWTH Compute Cluster (depending on the loaded modules):

<table>
<thead>
<tr>
<th>$CC$</th>
<th>$MPICC$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CXX$</td>
<td>$MPICXX$</td>
</tr>
<tr>
<td>$FC$</td>
<td>$MPIFC$</td>
</tr>
</tbody>
</table>
Compiling MPI Programs

- MPI is a typical library with C header files, Fortran modules, etc.
- Some MPI vendors provide convenience compiler wrappers:

```bash
cluster:~[1]$ $MPICC --show
icc
-I/opt/MPI/openmpi-1.6.5/linux/intel/include
-I/opt/MPI/openmpi-1.6.5/linux/intel/include/openmpi
-fexceptions
-pthread
-I/opt/MPI/openmpi-1.6.5/linux/intel/lib
-Wl,-rpath,/opt/MPI/openmpi-1.6.5/linux/intel/lib
-I/opt/MPI/openmpi-1.6.5/linux/intel/lib
-L/opt/MPI/openmpi-1.6.5/linux/intel/lib
-lmpi
-lldl
-Wl,--export-dynamic
-ldl
-llutil
```
Executing MPI Programs

Most MPI implementations provide a special launcher program:

```
mpiexec -n nprocs ... program <arg1> <arg2> <arg3> ...
```

→ launches `nprocs` instances of `program` with command-line arguments `arg1`, `arg2`, ... and provides the MPI library with enough information in order to establish network connections between the processes

The standard specifies the `mpiexec` program but does not require it:

→ IBM BG/Q: `runjob --np 1024 ...`
→ SLURM resource manager: `srun ...`

On RWTH Compute Cluster:

→ interactive jobs

```
$MPIEXEC -n nprocs ... program <arg1> <arg2> <arg3> ...
```

→ batch jobs

```
$MPIEXEC $FLAGS_MPI_BATCH ... program <arg1> <arg2> <arg3> ...
```
Executing MPI Programs

- Most MPI implementations provide a special launcher program:

  \[ \text{mpiexec} \ -n \ \text{nprocs} \ \ldots \ \text{program} \ <\text{arg1}> \ <\text{arg2}> \ <\text{arg3}> \ \ldots \]

  \( \rightarrow \) launches \text{nprocs} instances of \text{program} with command-line arguments \text{arg1}, \text{arg2}, \ldots \ and provides the MPI library with enough information in order to establish network connections between the processes

  \( \rightarrow \) Sometimes called \text{mpirun}

- The launcher often performs more than simply launching processes:

  \( \rightarrow \) Helps MPI processes find each other and establish the world communicator

  \( \rightarrow \) Redirects the standard output of all ranks to the terminal

  \( \rightarrow \) Redirects the terminal input to the standard input of rank 0

  \( \rightarrow \) Forwards received signals (Unix-specific)
MPI as an SPMD Environment

- Provide dynamic identification of all peers
  - Who am I and who else is also working on this problem?

- Provide robust mechanisms to exchange data
  - Whom to send data to / From whom to receive the data?
  - How much data?
  - What kind of data?
  - Has the data arrived? (only the receiver knows)

- Provide synchronisation mechanisms
  - Have all processes reached same point in the program execution flow?

- Provide methods to launch and control a set of processes
  - How do we start multiple processes and get them to work together?

- Portability

Message Passing with MPI (PPCES 2018)
Joachim Protze / Marc-André Hermanns | IT Center der RWTH Aachen University
Compile and Run a Simple MPI Program

```
cluster:~[1]$ vim hello.c

cluster:~[2]$ MPICC -o hello.exe hello.c

cluster:~[3]$ MPIEXEC -n 4 hello.exe
Hello world from rank 2 of 4
Hello world from rank 0 of 4
Hello world from rank 1 of 4
Hello world from rank 3 of 4
```
Message Envelope and Matching

- Reception of MPI messages is done by matching their envelope
- Send operation

```
MPI_Send (void *data, int count, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
```

- Message Envelope:

<table>
<thead>
<tr>
<th></th>
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<th>Receiver</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source</td>
<td>Implicit</td>
<td>Explicit, wildcard possible</td>
</tr>
<tr>
<td>Destination</td>
<td>Explicit</td>
<td>Implicit</td>
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<tr>
<td>Tag</td>
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</tr>
<tr>
<td>Communicator</td>
<td>Explicit</td>
<td>Explicit</td>
</tr>
</tbody>
</table>

- Receive operation

```
MPI_Recv (void *data, int count, MPI_Datatype type, int source, int tag, MPI_Comm comm, MPI_Status *status)
```
Message Envelope and Matching

- Reception of MPI messages is also dependent on the data.
- Recall:

  ```
  MPI_Send (void *data, int count, MPI_Datatype type, int dest, int tag, MPI_Comm comm)
  ```

  ```
  MPI_Recv (void *data, int count, MPI_Datatype type, int source, int tag, MPI_Comm comm, MPI_Status *status)
  ```

- The standard expects datatypes at both ends to match
  → Not enforced by most implementations
- Matching sends and receives must always come in pairs

- NB: messages do not aggregate

  ```
  Rank 0:
  MPI_Send(myArr, 1, MPI_INT, 1, 0, MPI_COMM_WORLD)
  ... some code ...
  MPI_Send(myArr, 1, MPI_INT, 1, 0, MPI_COMM_WORLD)
  ```

  ```
  Rank 1:
  MPI_Recv(myArr, 2, MPI_INT, 0, 0, MPI_COMM_WORLD, &stat)
  ... some code ...
  ```

Unmatched
Message Reception and Status

- The receive buffer must be able to fit the entire message
  - send count ≤ receive count  \( \text{OK} \) (but check status)
  - send count > receive count  \( \text{ERROR} \) (message truncation)

- The MPI status object holds information about the received message

- C: `MPI_Status` status;
  - `status.MPI_SOURCE`  message source rank
  - `status.MPI_TAG`  message tag
  - `status.MPI_ERROR`  receive status code
Message Reception and Status

- The receive buffer must be able to fit the entire message
  - send count ≤ receive count  → OK (but check status)
  - send count > receive count → ERROR (message truncation)

- The MPI status object holds information about the received message

- Fortran: `INTEGER, DIMENSION(MPI_STATUS_SIZE) :: status`
  - status(MPI_SOURCE) → message source rank
  - status(MPI_TAG) → message tag
  - status(MPI_ERROR) → receive status code
Message Reception and Status

- The receive buffer must be able to fit the entire message
  - send count ≤ receive count \(\rightarrow\) **OK** (but check status)
  - send count > receive count \(\rightarrow\) **ERROR** (message truncation)

- The MPI status object holds information about the received message

- **Fortran 2008:**
  - \(\rightarrow\) `TYPE(MPI_Status) :: status`
  - `status%MPI_SOURCE` \(\rightarrow\) message source rank
  - `status%MPI_TAG` \(\rightarrow\) message tag
  - `status%MPI_ERROR` \(\rightarrow\) receive status code
Inquiry Operations

- **Blocks until a matching message appears:**

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

  - Message is not received, one must call `MPI_Recv` to receive it
  - Information about the message is stored in the status field

  ```
  MPI_Probe(MPI_ANY_SOURCE, MPI_ANY_TAG, comm, &status);
  ```

  - Checks for any message in the given communicator

- **Message size inquiry:**

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

  - Calculates how many integral `datatype` elements can be formed from the data in the message referenced by `status`
  - If the number is not integral, `count` is set to `MPI_UNDEFINED`
  - Can be used with the status from `MPI_Recv` too
Operation Completion

- MPI operations complete once the message buffer is no longer in use by the MPI library and is thus free for reuse

- Send operations complete:
  - once the message is constructed and
  - placed completely onto the network or
  - buffered completely (by MPI, the OS, the network, …)

- Receive operations complete:
  - once the entire message has arrived and has been placed into the buffer

- Blocking MPI calls only return once the operation has completed
  - MPI_Send and MPI_Recv are blocking
Blocking Calls

- **Blocking send (w/o buffering) and receive calls:**

 Sender

<table>
<thead>
<tr>
<th>Program</th>
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<tr>
<td>MPI_Send</td>
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<tr>
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</tr>
<tr>
<td>Send the envelope and wait</td>
</tr>
<tr>
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<tr>
<td>First message part</td>
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<tr>
<td>Last message part</td>
</tr>
<tr>
<td>MPI_Recv</td>
</tr>
<tr>
<td>Data must not be used</td>
</tr>
</tbody>
</table>

  Receiver
Deadlocks

Both MPI_Send and MPI_Recv calls are blocking:

→ The receive operation only returns after a matching message has arrived
→ The send operation *might* be buffered (*implementation-specific!!!*) and therefore return before the message is actually placed onto the network
→ Larger messages are usually sent only when both the send and the receive operations are active (synchronously)
→ *Never rely on any implementation-specific behaviour!!!*

Deadlock in a typical data exchange scenario:

Both ranks wait for Receive to get called
Deadlocks

- Both MPI_Send and MPI_Recv calls are blocking:
  - The receive operation only returns after a matching message has arrived
  - The send operation might be buffered (implementation-specific!!!) and therefore return before the message is actually placed onto the network
  - Larger messages are usually sent only when both the send and the receive operations are active (synchronously)
  - Never rely on any implementation-specific behaviour!!!

- Deadlock prevention in a typical data exchange scenario:
Combined Send and Receive

MPI_Sendrecv (void *senddata, int sendcount, MPI_Datatype sendtype, int dest, int sendtag, void *recvdata, int recvcount, MPI_Datatype recvtype, int source, int recvtag, MPI_Comm comm, MPI_Status *status)

- Combines message send and receive into a single call

<table>
<thead>
<tr>
<th></th>
<th>Send</th>
<th>Receive</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data</td>
<td>senddata</td>
<td>recvdata</td>
</tr>
<tr>
<td>Count</td>
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<td>recvcount</td>
</tr>
<tr>
<td>Type</td>
<td>sendtype</td>
<td>recvtype</td>
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<tr>
<td>Destination</td>
<td>dest</td>
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<tr>
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<td>-</td>
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</tr>
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</table>
Combined Send and Receive

**MPI_Sendrecv**

```c
MPI_Sendrecv (void *senddata, int sendcount, MPI_Datatype sendtype,
              int dest, int sendtag, void *recvdata, int recvcount,
              MPI_Datatype recvtype, int source, int recvtag,
              MPI_Comm comm, MPI_Status *status)
```

- Sends one message and receives one message (in any order) without deadlocking (unless unmatched)
- **Send and receive buffers must not overlap!**

**MPI_Sendrecv_replace**

```c
MPI_Sendrecv_replace (void *data, int count, MPI_Datatype datatype,
                      int dest, int sendtag, int source, int recvtag,
                      MPI_Comm comm, MPI_Status *status)
```

- First sends a message to *dest*, then receives a message from *source*, using the same memory location, elements count and datatype for both operations
- Usually slower than MPI_Sendrecv and might use more memory
Message Ordering

- **Order is preserved in a given communicator for point-to-point operations between any pair of processes**
  - Messages within some communicator to the same rank are non-overtaking
  - Probe/receive returns the earliest matching message

- **Order is not guaranteed for**
  - messages sent within different communicators
  - messages arriving from different senders

```c
MPI_Status status;

MPI_Probe(MPI_ANY_SOURCE, 0, MPI_COMM_WORLD, &status);
... allocate buffer based on message size ...
MPI_Recv(buffer, size, MPI_INT, MPI_ANY_SOURCE, 0,
         MPI_COMM_WORLD, &status);
```
Message Ordering

- Order is preserved in a given communicator for point-to-point operations between any pair of processes
  - Messages within some communicator to the same rank are non-overtaking
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```c
MPI_Status status;

MPI_Probe(MPI_ANY_SOURCE, 0, MPI_COMM_WORLD, &status);
... allocate buffer based on message size ...
MPI_Recv(buffer, size, MPI_INT, status.MPI_SOURCE, 0,
          MPI_COMM_WORLD, &status);
```

Also applies to sequences of wildcard receives
Agenda

- Motivation
- Part 1
  - Concepts
  - Point-to-point communication
  - Non-blocking operations
- Part 2
  - Collective operations
  - Communicators
  - User datatypes
- Part 3
  - Hybrid parallelisation
  - Common parallel patterns

Message Passing with MPI (PPCES 2018)
Joachim Protze / Marc-André Hermanns | IT Center der RWTH Aachen University
Blocking Calls

- Blocking send (w/o buffering) and receive calls:

 Sender

 Program

 MPI_Send

 Send the envelope and wait

 Acknowledge envelope match

 First message part

 Intermediate message part

 Intermediate message part

 Last message part

 Receiver

 Program

 MPI_Recv

 Data must remain constant

 Data must not be used

 Blocking send (w/o buffering) and receive calls:

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Non-Blocking Calls

- Non-blocking MPI calls return immediately while the communication operation continues asynchronously in the background.

- Each non-blocking operation is represented by a request handle:
  - C: `MPI_Request`
  - Fortran: `INTEGER`
  - Fortran 2008: `TYPE(MPI_Request)`

- Non-blocking operations are progressed by certain MPI calls but most notably by the `test` and `wait` MPI calls.

- Blocking MPI calls are equivalent to making a non-blocking call and waiting immediately afterwards for the operation to complete.

- Used to overlay communication and computation and to prevent possible deadlocks.
Non-Blocking Send and Receive

- **Initiation of non-blocking send and receive operations:**

  ```c
  MPI_Isend (void *data, int count, MPI_Datatype dataType,
             int dest, int tag, MPI_Comm comm,
             MPI_Request *request)
  ```

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

  → **request:** on success set to the handle of the non-blocking operation

- **Blocking wait for completion:**

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

  → **request:** handle for an active non-blocking operation freed and set to `MPI_REQUEST_NULL` upon successful return

  → **status:** status of the completed operation
Blocking send (w/o buffering) and receive calls:

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MPI_Send

First message part

Intermediate message part

Intermediate message part

Last message part

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Equivalent with non-blocking calls:

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Communication-Computation Overlay
Communication-Computation Overlay

- Other work can be done in between*:

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Non-blocking operations can be used to prevent deadlocks in symmetric code:

- That is how MPI_Sendrecv is usually implemented.
Non-Blocking Request Testing

Test if given operation has completed:

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

→ flag: true if the operation has completed, otherwise false
→ status: status of the completed operation, only set if flag is true

→ Can be (and usually is) called repeatedly inside a loop

→ Upon completion of the operation (i.e. when flag is true), the operation is freed and the request handle is set to MPI_REQUEST_NULL

If called with a null request (MPI_REQUEST_NULL):

→ MPI_Wait returns immediately with an empty status
→ MPI_Test sets flag to true and returns an empty status
Test and Wait on Many Requests

- **MPI_Waitany / MPI_Testany**
  - Wait for one of the specified requests to complete and free it
  - Test if one of the specified requests has completed and free it if it did

- **MPI_Waitall / MPI_Testall**
  - Wait for all the specified requests to complete and free them
  - Test if all of the specified requests have completed and free them if they have

- **MPI_Waitsome / MPI_Testsome**
  - Wait for any number of the specified requests to complete and free them
  - Test if any number of the specified requests have completed and free these that have

- To ignore the status from `-all/-some`, pass `MPI_STATUSES_IGNORE`
Communication Modes

- There are four send modes in MPI:
  - Standard
  - Synchronous
  - Buffered
  - Ready

- Send modes differ in the relation between the completion of the operation and the actual message transfer

- Single receive mode:
  - Synchronous
Send Modes

- **Standard mode**
  - The call blocks until the message has *either* been transferred *or* copied to an internal buffer for later delivery

- **Synchronous mode**
  - The call blocks until a matching receive has been posted and the message reception has started

- **Buffered mode**
  - The call blocks until the message has been copied to a user-supplied buffer. Actual transmission may happen at a later point

- **Ready mode (don’t use!)**
  - The operation succeeds *only if a matching receive has already been posted.* Behaves as standard send in every other aspect
Send Modes

- **Call names:**
  - `MPI_Send` blocking standard send
  - `MPI_Isend` non-blocking standard send
  - `MPI_Ssend` blocking synchronous send
  - `MPI_Issend` non-blocking synchronous send
  - `MPI_Bsend` blocking buffered send
  - `MPI_Ibsend` non-blocking buffered send
  - `MPI_Rsend` blocking ready-mode send
  - `MPI_Irsend` non-blocking ready-mode send

- **Buffered operations require an explicitly provided user buffer**
  - `MPI_Buffer_attach (void *buf, int size)`
  - `MPI_Buffer_detach (void *buf, int *size)`
  - Buffer size must account for the envelope size (`MPI_BSEND_OVERHEAD`)
Send Modes

- One rarely needs anything else except the standard send

- The synchronous send can be used to synchronise two ranks

- Simple correctness check
  - Replacing all blocking standard sends with blocking synchronous sends should not result in deadlock
  - If program deadlocks, you are relying on the buffering behaviour of the standard send → change your algorithm

- Buffered sends guarantee that messages are always buffered, but it is possible to run out of buffer space
  - No way to test if the buffer is still in use by MPI
Utility Calls

- **Attempt to abort all MPI processes in a given communicator:**

  
  
  ```c
  MPI_Abort (MPI_Comm comm, int errorcode)
  ```

  - `errorcode` is returned to the OS if supported by the implementation.
  - Note: Open MPI does not return the error code to the OS.

- **Portable timer function:**

  ```c
  double MPI_Wtime ()
  ```

  - Returns the wall-clock time that has elapsed since an unspecified (but fixed for successive invocations) point in the past

- **Obtain a string ID of the processor:**

  ```c
  MPI_Get_processor_name (char *name, int *resultlen)
  ```

  - `name`: buffer of at least `MPI_MAX_PROCESSOR_NAME` characters
  - `resultlen`: length of the returned processor ID (w/o the ‘\0’ terminator)
MPI Lifecycle Management

- **MPI can only be initialised once and finalised once** for the lifetime of each MPI process
  - Multiple calls to `MPI_Init` or `MPI_Finalize` result in error

- **Determine if MPI is already initialised:**
  ```c
  MPI_Initialized (int *flag)
  ```
  - `flag` set to **true** if `MPI_Init` was called

- **Determine if MPI is already finalised:**
  ```c
  MPI_Finalized (int *flag)
  ```
  - `flag` set to **true** if `MPI_Finalize` was called

- **Intended for use in parallel libraries built on top of MPI**
Common Pitfalls – C/C++

- Do not pass pointers to pointers in MPI calls

```c
int scalar;
MPI_Send(&scalar, MPI_INT, 1, …

int array[5];
MPI_Send(array, MPI_INT, 5, …
    … or …
MPI_Send(&array[0], MPI_INT, 5, …

int *pointer = new int[5];
MPI_Send(pointer, MPI_INT, 5, …
    … or …
MPI_Send(&pointer[0], MPI_INT, 5, …

// ERRONEOUS
MPI_Send(&pointer, MPI_INT, 5, …
```

- `&array` will work too, but is not recommended
- Will result in the value of the pointer itself (i.e. the memory address) being sent, possibly accessing past allocated memory
Common Pitfalls – C/C++

Do not pass pointers to pointers in MPI calls

```c
void func (int scalar)
{
    MPI_Send(&scalar, MPI_INT, 1, ...

void func (int& scalar)
{
    MPI_Send(&scalar, MPI_INT, 1, ...

void func (int *scalar)
{
    MPI_Send(scalar, MPI_INT, 1, ...

void func (int *array)
{
    MPI_Send(array, MPI_INT, 5, ...
    ... or ...  
    MPI_Send(&array[0], MPI_INT, 5, ...
```
Common Pitfalls – C/C++

- Use flat multidimensional arrays; arrays of pointers do not work

```c
// Static arrays are OK
int mat2d[10][10];
MPI_Send(&mat2d, MPI_INT, 10*10, ...

// Flat dynamic arrays are OK
int *flat2d = new int[10*10];
MPI_Send(flat2d, MPI_INT, 10*10, ...

// DOES NOT WORK
int **p2d[10] = new int*[10];
for (int i = 0; i < 10; i++)
    p2d[i] = new int[10];
MPI_Send(p2d, MPI_INT, 10*10, ...
... or ...
MPI_Send(&p2d[0][0], MPI_INT, 10*10, ...
```

MPI has no way to know that there is a hierarchy of pointers
Common Pitfalls – C/C++

- **Passing pointer values around makes little to no sense**
  - Pointer values are process-specific
  - No guarantee that memory allocations are made at the same addresses in different processes
    - Especially on heterogeneous architectures, e.g., host + co-processor
  - No guarantee that processes are laid out in memory the same way, even when they run on the same host
    - Address space layout randomisation
    - Stack and heap protection

- **Relative pointers could be passed around**
Non-contiguous array sections should not be passed to non-blocking MPI calls

```
INTEGER, DIMENSION(10,10) :: mat

! Probably OK
CALL MPI_Isend(mat(:,1:3), ...

! NOT OK
CALL MPI_Isend(mat(1:3,:), ...

! NOT OK
CALL MPI_Isend(mat(1:3,1:3), ...
```

A temporary contiguous array is created and passed to MPI. It might get destroyed on return from the call before the actual send is complete!

Solved in MPI-3.0 with the introduction of the new Fortran 2008 interface `mpi_f08`, which allows array sections to be passed