The MPI Message-passing Standard Practical use and implementation (I)

SPD Course

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Massimo Coppola

References

- Standard MPI 5.0
  - Only those parts that we will cover during the lessons
  - They will be specified in the slides/web site.
  - Available online :
    - https://www.mpi-forum.org/docs/
- B. Wilkinson, M. Allen Parallel Programming, 2nd edition. 2005, Prentice-Hall.
  - This book will be also used; the 1st edition can as well do, and it is available in the University Library of the Science Faculty, [C.1.2 w74 INF]

What is MPI

- MPI: Message Passing Interface
  - a standard defining a *communication library* that allows message passing applications, languages and tools to be written in a portable way
- MPI 1.0 released in 1994
- Standard by the MPI Forum
  - aims at wide adoption
- Goals
  - Portability of programs, flexibility, portability and efficiency of the MPI library implementation
  - Enable portable exploitation of shortcuts and hardware acceleration
- Approach
  - Implemented as a library, static linking
- Intended use of the implemented standard
  - Support **Parallel Programming Languages** and **Application-specific Libraries**, not only parallel programs

Standard history

- 1994 - 1.0 core MPI
  - 40 organizations aim at a widely used standard
- 1995 - 1.1 corrections & clarifications
- 1997 - 1.2 minor changes
  - small changes to 1.1 that allow extensions to MPI 2.0
- 1997 - 2.0 – large additions
  - process creation/management,
  - one-sided communications,
  - extended collective communications,
  - external interfaces,
  - parallel I/O
- 2008 - 1.3 – streamlining
  - combines MPI 1.1 and 1.2 + errata
- 2008 - 2.1 – streamlining
  - merges 1.3 and 2.0 + errata
- 2009 - 2.2 – maintenance
  - few extensions to 2.1 + errata
- 2012 - 3.0
  - Nonblocking collectives,
  - more one-side comm.s,
  - language bindings
- 2015 - 3.1 corrections &clarifications
  - Improvements for portability, I/O and nonblocking
- 2021 - 4.0 – major update
  - large-count protos,
  - persistent collectives,
  - partitioned communications,
  - alternative init, assertions, error handling
- 2023 - 4.1 – corrections & clarifications
- 2025 - 5.0 – new functionalities
  - standard ABI for interoperability

What do we mean with message passing?

An MPI program is composed of multiple processes with **separate memory spaces & environments**

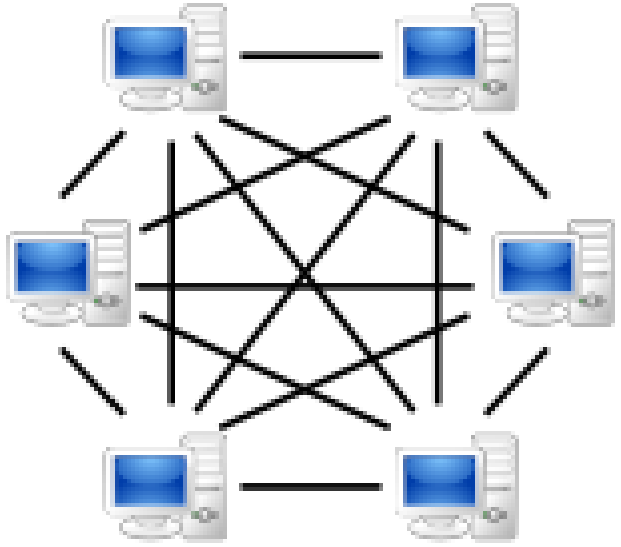
Processes are possibly on separate computing resources

Interaction happens via **explicit message exchanges**

Support code provides primitives for communication and synchronization

The MPI primitives and the overall communication structure they provide do constrain the way application are expressed

Different implementation levels will be involved in managing the MPI support



SPMD: single-program multiple-data

1. A *basic* MPI program is a **single executable** that is started in multiple parallel instances (possibly on separate hardware resources)
2. As already stated, an MPI program is composed of multiple processes with **separate memory spaces & environments**
3. Each process has **its own** execution environment, status and **control-flow**
4. In SPMD C/C++/Fortran programs, sequential data types are likely common to all process instances
5. However, variable and buffer **allocation** as well as **MPI runtime** status (e.g. MPI data types, buffers) are entirely **local**
6. Understanding (and debugging) the interaction of multiple program flows within the same code requires proper program structuring
7. Changes were introduced with MPI2.0 and over, with dynamic process spawn allowing a full MPMD (multiple-program, multiple data) execution model

On the meaning of Portability

- Preserve software *functional* behaviour across systems :
  - (recompiled) programs return correct results
- Preserve *non-functional* behaviour :
  - You expect also performance, efficiency, robustness and other features to be preserved

In the "parallel world", the big issue is to safeguard parallel performance and scalability

- Performance Tuning
  - Fiddling with program and deployment parameters to enhance performance
- Performance Debugging
  - Correct results, but awful performance: what happened?
  - Mismatched assumptions among SW/HW layers

What do we do with MPI?

MPI is a tool to develop:

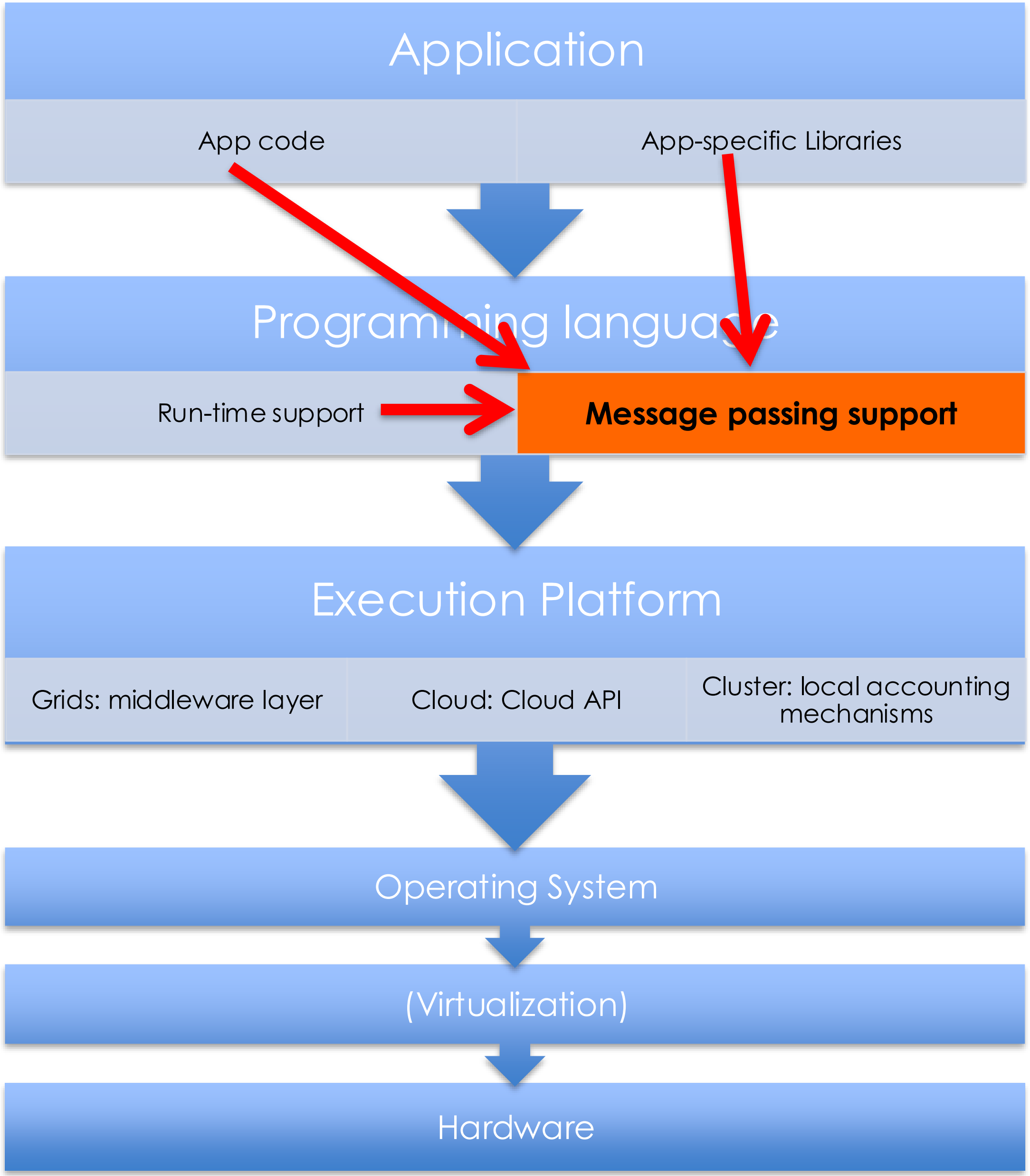
- Applications
- Programming Languages
- Libraries

Interoperation of Programming languages (Fortran, C, C++ …)

Heterogeneous resources

Big/little endianness

FP formats



MPI functionalities

- MPI lets **processes** in a **distributed/parallel** execution environment **coordinate** and **communicate**
  - Possibly processes on different machines
  - We won't care about threads
    - MPI implementations can be compatible with threads, but you program the threads using some other shared-memory mechanism: pthreads, OpenMP …
- Same MPI library instance can be called by multiple high-level languages
  - Interoperability, multiple language bindings
  - impact on standard definition and its implementation
  - The MPI Library is eventually linked to the program, its support libraries and its language runtime
  - Some functionalities essential for programming language development

Key MPI Concepts

- Communicators
- Point to point communication
- Collective Communication
- Data Types

Key MPI Concepts: Communicators

- Communicators
  - Process groups + communication state
  - Inter-communicators vs Intra-communicators
  - Rank of a process

- Point to point communication

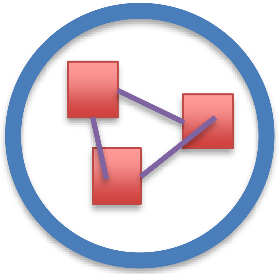
- Collective Communication

- Data Types

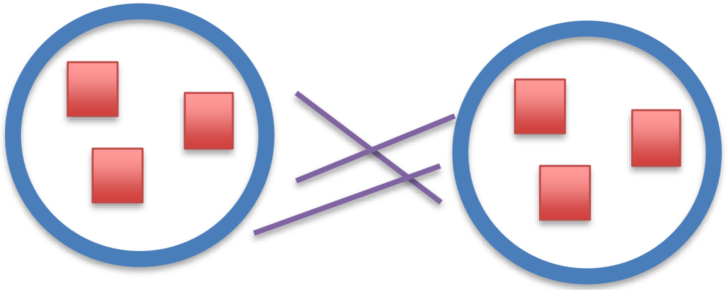
Communicators

- Specify the communication context
  - Each communicator is a separate “universe”, no message interaction between different communicators
- A group of processes AND a global communication state
  - Forming a communicator implies some agreement among the communication support of the composing processes
  - A few essential communicators are created by the MPI initialization routine (e.g. MPI_COMM_WORLD)
  - More communicator features later in the course

Types of communicators



- Intracommunicator
  - Formed by a single group of processes
  - Allows message passing interaction among the processes within the communicator



- Intercommunicators
  - Formed by two groups A, B of processes
  - Allows message passing between pairs of processes of the two different groups (x,y) can communicate *if-and-only-if*
    x belongs to group A and y belongs to B

Communicators and Ranks

- No absolute process identifiers in MPI
- The **Rank** of a process is always relative to a specific communicator
- In a group or communicator with N processes, ranks are consecutive integers 0…N-1
- No process is guaranteed to have the same rank in different communicators,
  - unless the communicator is specially built by the user

Key MPI Concepts : point to point

- Communicators
- Point to point communication
  - Envelope
  - **Local** vs **global completion**
  - **Blocking** vs **non-blocking** communication
  - Communication **modes**
- Collective Communication
- Data Types

Envelopes

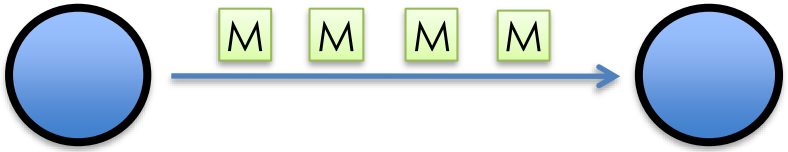
Envelope =

(source, destination, TAG, communicator)

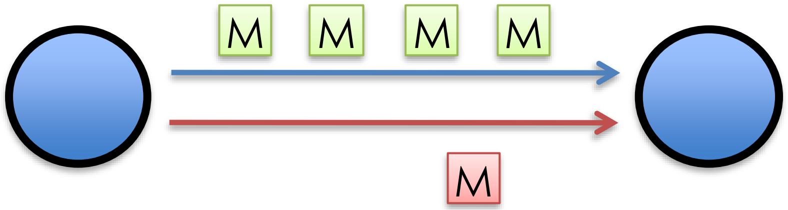
- Qualifies all point-to-point communications
- Source and dest are ***related*** to the communicator
- Two point-to-point operations (send+receive) match iff their envelopes match **exactly**
- **TAG** meaning is user-defined → play with tags to assign semantics to a communication
  - TAG provide communication insulation within a communicator, for semantic purposes
  - Allow any two processes to establish multiple communication *"Channels" (in a non-technical meaning)*

Envelopes and comunication semantics

- Messages with the same envelope never overtake each other



- No guarantee on messages with different envelope!



- E.g. : different tags

A first look at the SEND primitive

MPI_SEND(buf, count, datatype, dest, tag, comm)

- IN buf — initial address of send buffer
- IN count — number of elements in send buffer (non-negative integer, **in datatypes**)
- IN datatype — datatype of each send buffer element (handle)
- IN dest — rank of destination
- IN tag — message tag
- IN comm — communicator (handle)

Local and global completion

- **Local completion** : a primitive does not need to interact with other processes to complete
  - Forming a group of processes
  - Asynchronous send of a message while ignoring the communication status
- **Global completion** : interaction with other processes is needed to complete the primitive
  - Turning a group into a communicator
  - Synchronous send/receive : semantics mandates that parties interact before communication happens

Blocking vs non-blocking operations

- Blocking operation
  - The call returns only once the operation is complete
  - No special treatment is needed, only error checking

- Non-blocking operation
  - The call returns as soon as possible
  - Operation may be in progress or haven't started yet
  - Resources required by the operation cannot be reused (e.g. message buffer is not to be modified)
  - User need to subsequently check the operation completion and its results

- Tricky question: do we mean local or global completion?

Communication MODES

- Synchronous
  - Follows the common definition of synchronous communication, first process waits for the second one to reach the matching send/receive
- Buffered
  - Communication happens through a buffer, operation completes as soon as the data is in the buffer
  - Buffer allocation is onto the user AND the MPI implementation
- Ready
  - Assumes that the other side is already waiting (can be used if we know the communication party already issued a matching send/receive)
- **Standard**
  - The most common, and less informative
  - MPI implementation is free to use any available mode, i.e. almost always Synchronous or Buffered

Example: portability and modes

- Standard sends are implementer's choice
  - Choice is never said to remain constant…
- A user program exploit standard sends, implicitly relying on *buffered* sends
  - Implementation actually chooses them, so program works
- What if
  - Implementation has to momentarily switch to synchronous sends due to insufficient buffer space?
  - Program is recompiled on a different MPI implementation, which does not use buffered mode by default?

Combining concepts

- Point to point concepts of ***communication mode*** and ***non-blocking*** are completely orthogonal : you can have all combinations

- local / global completion depends on
  - The primitive (some inherently local/global)
  - The combination of mode and blocking behavior
  - The MPI implementation and the hardware always have the last word

- We will be back to this later on in the course

Key MPI Concepts : Collective operations

- Communicators
- Point to point communication
- Collective Communication (old-style)
  - A **whole** communicator is involved
  - Always locally blocking *
    - *Only true for blocking collectives since MPI 3.0, but we will disregard non-blocking collectives for now*
  - No modes: collectives in a same communicator are **serialized**
- Data Types

Collective operations - I

- Basically, a different model of parallelism in the same library
- Collectives act on a **whole** communicator
  - All processes in the communicator must call the collective operation
  - With compatible parameters
  - *Locally the collectives are always blocking*
    (no longer true since MPI 3, there are two separate kinds of collective op.s)
- Collective operations are **serialized** within a communicator
  - By contrast, point to point message passing is intrinsically concurrent
  - No communication modes or non-blocking behaviour apply to collective operations

Collective operations - II

- Much detail is left to the implementation
  - The standards makes minimal assumptions
  - Leaves room for machine specific optimization
- Still **No guarantee** that all processes are actually within the collective at the same time
  - Freedom for MPI developers to choose the implementation algorithms: collective may start or complete at different moments for different processes
  - MPI_Barrier is of course an exception

Key MPI Concepts : Datatypes

- Communicators
- Point to point communication
- Collective Communication
- Data Types
  - A particular kind of **Opaque objects**
  - MPI **primitive** datatypes
  - MPI **derived** datatypes

Opaque objects

- Data structures whose exact definition is hidden
  - Obj. internals depend on the MPI implementation
  - Some fields may be explicitly documented and made accessible to the MPI programmer
  - Other fields are only accessed through dedicated MPI primitives and object **handles**
  - Allocated and freed (directly or indirectly) only by the MPI library code
    - If the user is required to do so, it has to call an MPI function which is specific to the kind of opaque object
  - Example:
    Communicators and datatypes are Opaque Obj.

Primitive Datatypes

- MPI Datatypes are needed to let the MPI implementation know how to handle data
  - Data conversion
  - Packing data into buffers for communication, and unpacking afterwards
  - Also used for MPI I/O functionalities
- Primitive datatypes
  - Correspond to basic types of most programming languages: integers, floats, chars…
  - Have bindings for MPI supported languages
  - Enough for simple communication

MPI derived datatypes

- Derivate datatypes correspond to composite types of modern programming languages
  - Set of MPI constructors corresponding to various kinds of arrays, structures, unions
  - Memory organization of the data is highly relevant, and can be explicitly considered
  - Derived datatypes can automate packing and unpacking of complex data structures for communications, and allow semantically correct parallel operation on partitioned data structures

FILLING IN THE GAPS

Beware

- MPI uses a different abstraction than physical / logic channels, the one you know from previous courses
- When we speak of "channels" in MPI we mean the set of messages sharing the same envelope and some ordering constraint
- There is not such thing as an implementation of the channel defined or referenced in the MPI standard
- The two abstractions have different goals, but the implementation issues are the same: HW features, coprocessors, zero copy…
- You are expected to understand both and not confuse them

From Send and Recv to programs

- Simplest programs do not need much beyond Send and Recv
- Keep in mind that each process lives in a separate memory space
  - Need to initialize all your data structures
  - Need to initialize your instance of the MPI library
  - Should you make assumptions on process number?
  - How portable will your program be?

Running, Initializing the runtime

- Basic process spawning is done by the MPI launcher:
  `mpirun` [*mpi options*] <**`program _name`**>[*arguments*]
  - Check the mpirun man page of your MPI implementation

Each MPI process calls AT LEAST

- MPI_Init(int *argc, char ***argv)
  - Shall be called before using any MPI calls (very few exceptions)
  - Initializes the MPI runtime for all processes in the running program, some kind of handshaking implied
    - e.g. creates **MPI_COMM_WORLD**
- MPI_Finalize()
  - Frees all MPI resources and cleans up the MPI runtime, taking care of any operation pending
  - Any further call to MPI is forbidden
  - some runtime errors can be detected at finalize
    - e.g. calling finalize with communications still pending and unmatched

References

- MPI 5.0 standard (see http://www.mpi-forum.org/)
  - Only some parts
- Parallel Programming, B. Wilkinson & M. Allen. Prentice-Hall (2nd ed., 2005)
  - Only some references, 1st edition is ok too.

- Relevant Material for 1st lesson, MPI standard
  - Chapter 1: have a look at it.
  - Chapter 2: defines many concepts and terms used in the standard
    sec 2.1 – 2.5 check defined terms as needed
    sec 2.7, 2.8
  - Chapter 3:
    sec. 3.1, 3.2.3, 3.2.4, 3.4, 3.5, 3.7