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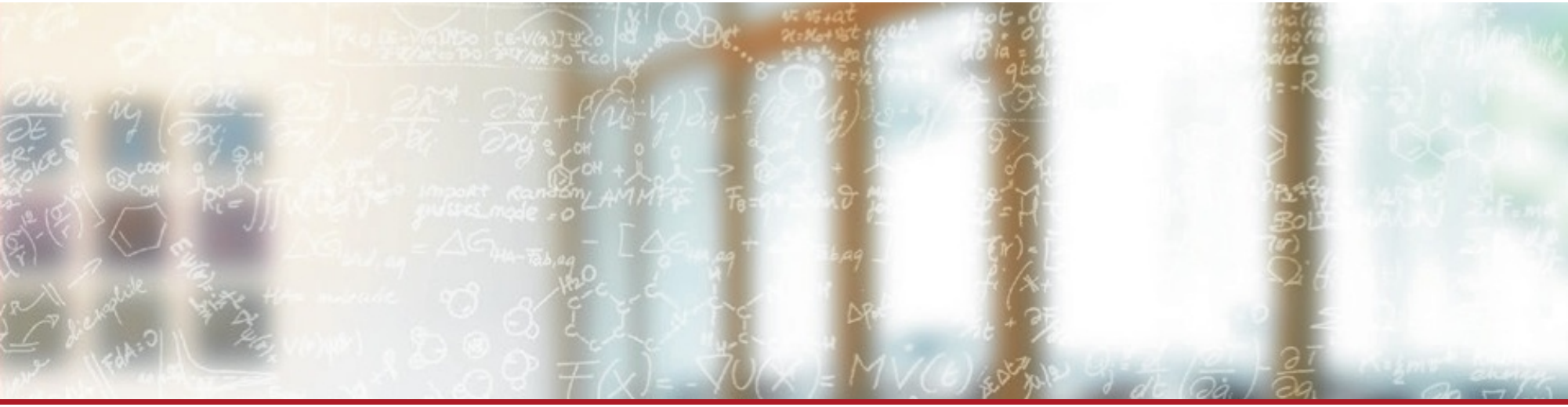


Message Passing Interface (MPI)

Summer School 2017 – Effective High Performance Computing

Tim Robinson, CSCS

July 19–20, 2017

Why MPI?

- Distributed memory - use more nodes and cores
- Industry standards endorsed by HPC community
- Several implementations exist:
  - MPICH, OpenMPI, IntelMPI, **CrayMPI**,. . .

Course prerequisites

- Basic C and/or Fortran knowledge
- Understand cluster architecture and tools
- Minimum understanding on Network metrics:
  - Bandwidth: ratio of message size / time (GB/s)
  - Latency: minimal time to send one bit (μs)
- To think parallel !

Course Objectives

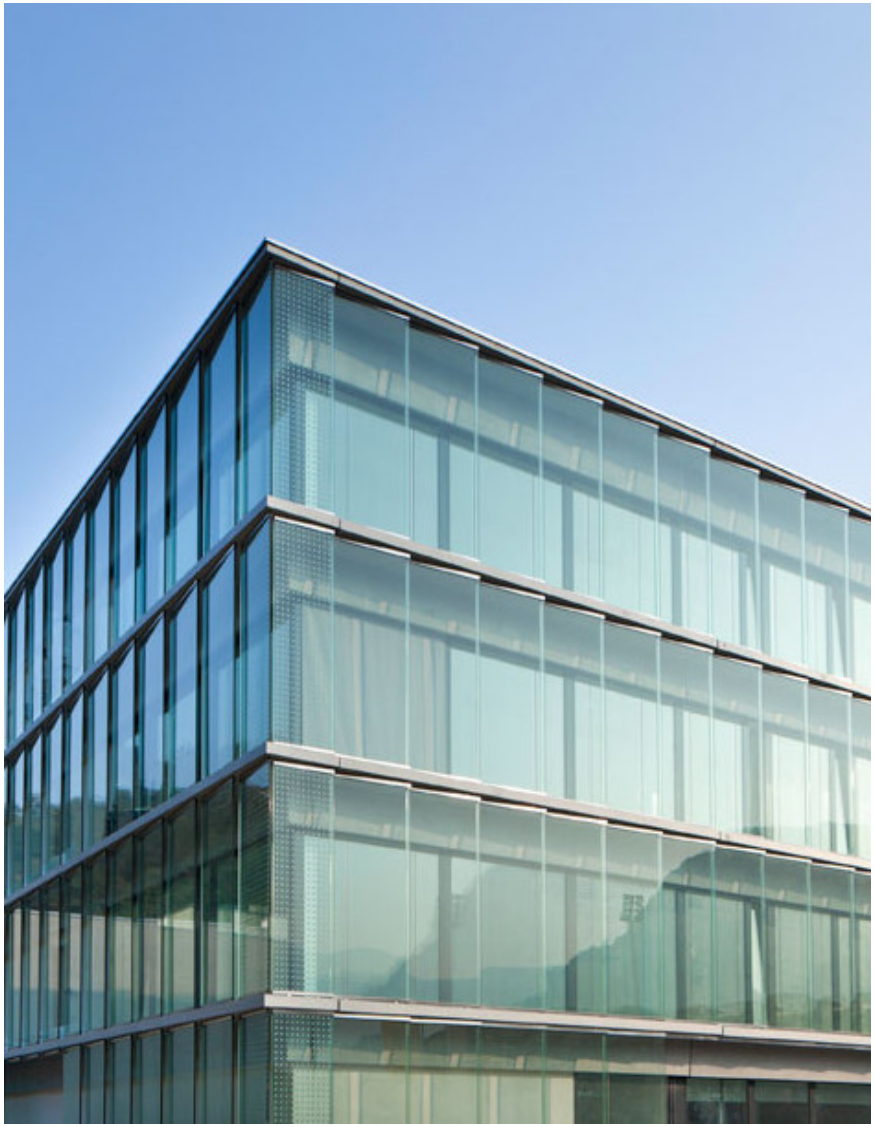
- The understanding of MPI's essential concepts
- Be able to use all basic features of MPI
- Be able to write highly parallel HPC code
- Knowing what advanced features exist in MPI
- The understanding of its pitfalls and tricky features

Behind the course

- Full standard:
  `http://www.mpi-forum.org`
- Tutorials:
  `https://computing.llnl.gov/tutorials/mpi/`
- Books:
  - Parallel Programming with MPI - Oct 96
  - MPI: The Complete Reference - Sept 98
  - Using MPI - 2nd Edition - Nov 99

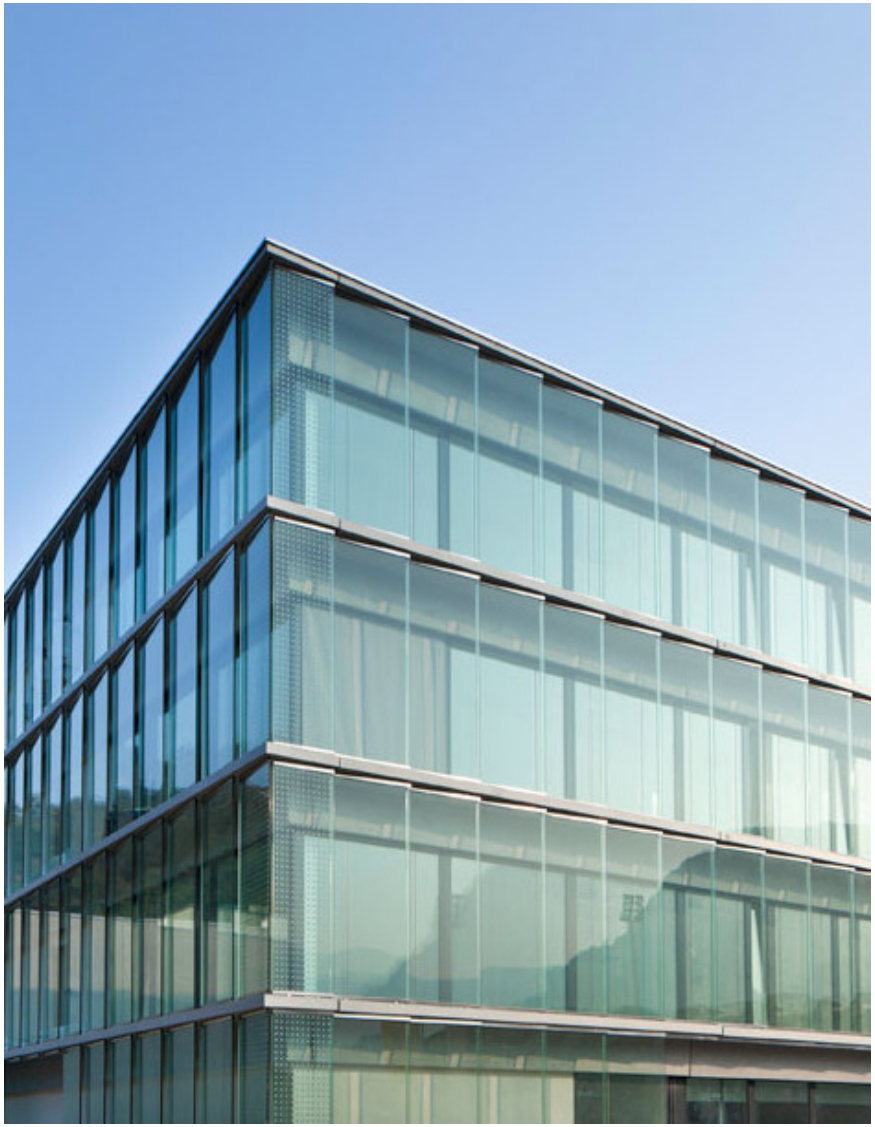
A lot of references and tutorials on Internet!

General Course Structure



- An introduction to MPI
- Point-to-point communications
- Collective communications
- Topology
- Datatypes

General Course Structure



- An introduction to MPI
  - MPI
  - Distributed memory
  - Using MPI in a program
  - MPI implementation insight
  - MPI features
  - Practicals
- Point-to-point communications
- Collective communications
- Topology
- Datatypes

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An introduction to MPI

Message Passing Interface

The Message Passing Interface (MPI) is a library specification for message-passing. It is a standard API (Application Programming Interface) that can be used to create parallel applications. The MPI standardization effort makes use of the most attractive features of a number of existing message passing systems, rather than selecting one of them and adopting it as the standard.

Key aspects

- A programming model NOT a programming language
- A set of functions to exchange messages between processes
- A standard that defines the behaviors of the MPI functions
- Bindings for C and Fortran

$\Rightarrow$ MPI is not a library, per se, rather a spec of what such a library should be

History

- Early 80's many communication libraries existed: PVM, LAM, P4,...
- 92: agreement to develop one generic library, MPI was born.
- Many companies helped finance the standard: IBM, Cray,...
- 94: First version of the standard was released, MPI-1
- 95: MPICH and LAM-MPI were the first implementations
- 98: Second version of the standard was released, MPI-2
- 02: MPI implementations were MPI-2 compliant
- 08: Third version of the standard was raised, MPI-3

MPI Standard

- This is a standard, not a user's guide
- It is designed to be unambiguous, not easy to follow.

MPI-1

- Basic facilities: pt2pt, collective, topology, datatypes,...
- Most people use only a small fraction of it!

MPI-2

- Parallel I/O, dynamic process management, remote memory operations

MPI-3

- Fortran 2008 bindings, removes deprecated C++ bindings

Message Passing Paradigm

- Resources are Local (differently from shared memory model)
- Each process runs in a “isolated” environment. Interactions require exchange of messages
- Messages can be: instructions, data, synchronization
- Message Passing works also in a Shared Memory system
- Time to exchange messages is much larger than accessing local memory

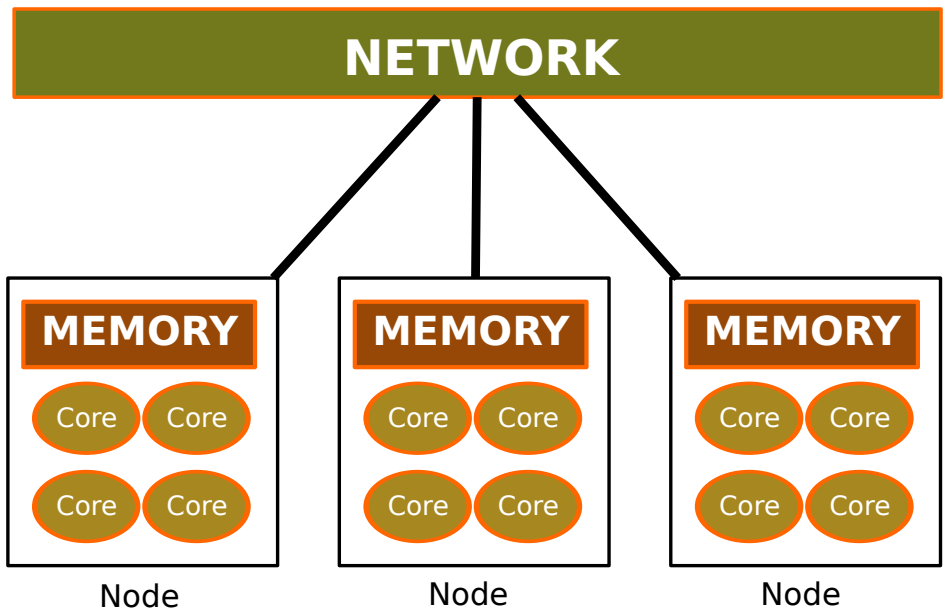
Message Passing is a **COOPERATIVE** approach,
based on **THREE** basic operations:

- SEND (a message)
- RECEIVE (a message)
- SYNCHRONIZE

Distributed memory

Distributed Memory

- A program is run as separate, independent processes
- Independent processes do not share data
- Processes interact only by message passing



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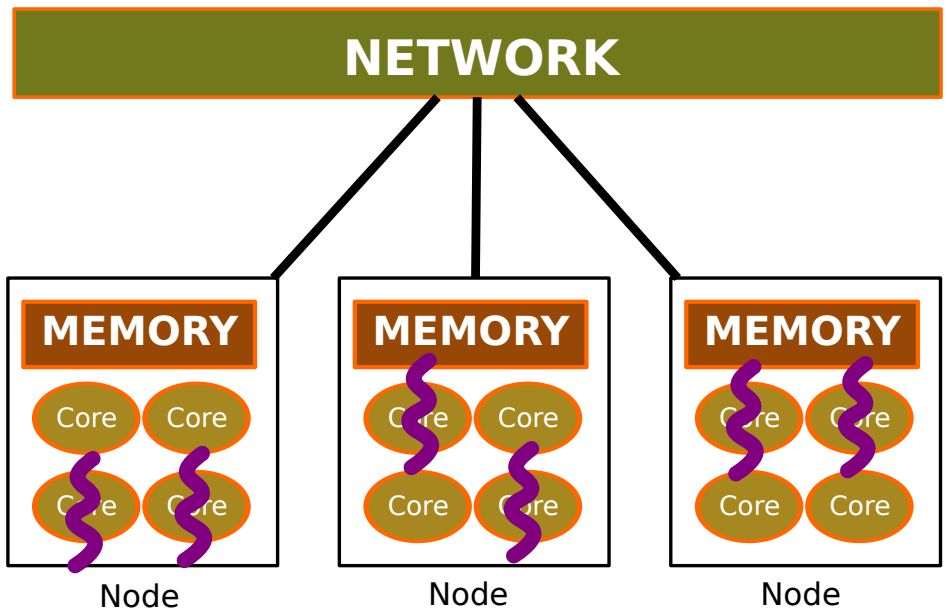

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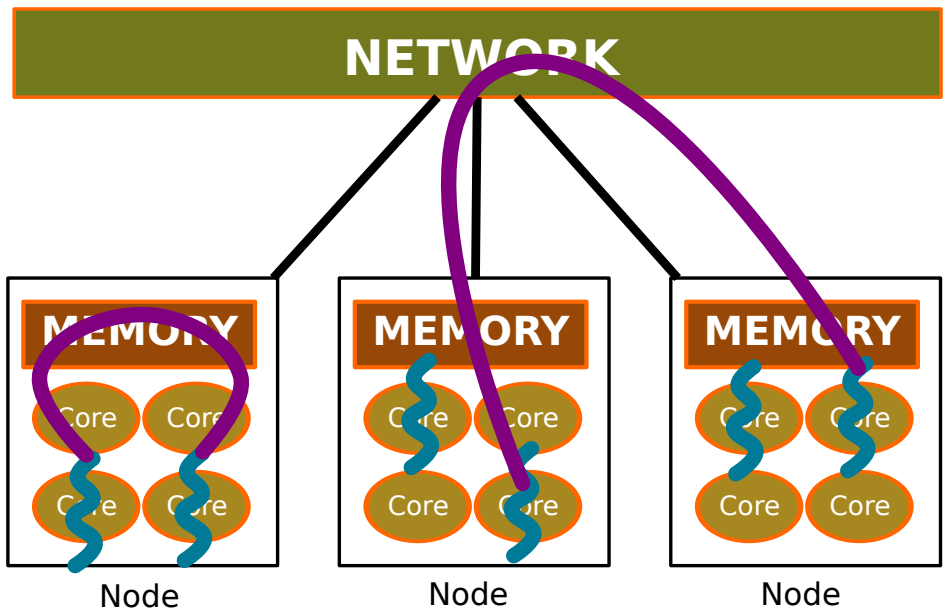
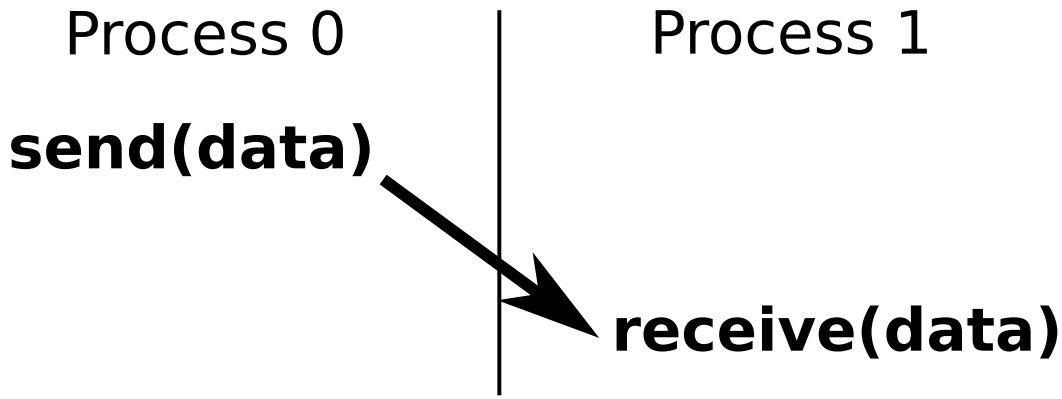


Send/Recv



- description of data?
- process identification?
- when has the operation completed?
  - synchronous send: sender will always stall until receieve has posted
  - regular send: returns when buffer can be reused – *may* be before receiver has actually posted the receive

Using MPI in a program

- Header files
- Initialize and finalize MPI
- Process identification
- Simple communication model
- Example of a simple source code

Header files

All Subprogram that contains calls to MPI subroutine must include the MPI header file.

Pseudo-code

```
#include <mpi.h>
```

Fortran 77

```
include 'mpif.h'
```

Fortran 90

```
USE MPI
```

The header file contains definitions of MPI constants, types and functions

MPI initialize and finalize

- Every MPI program starts by calling MPI_Init:

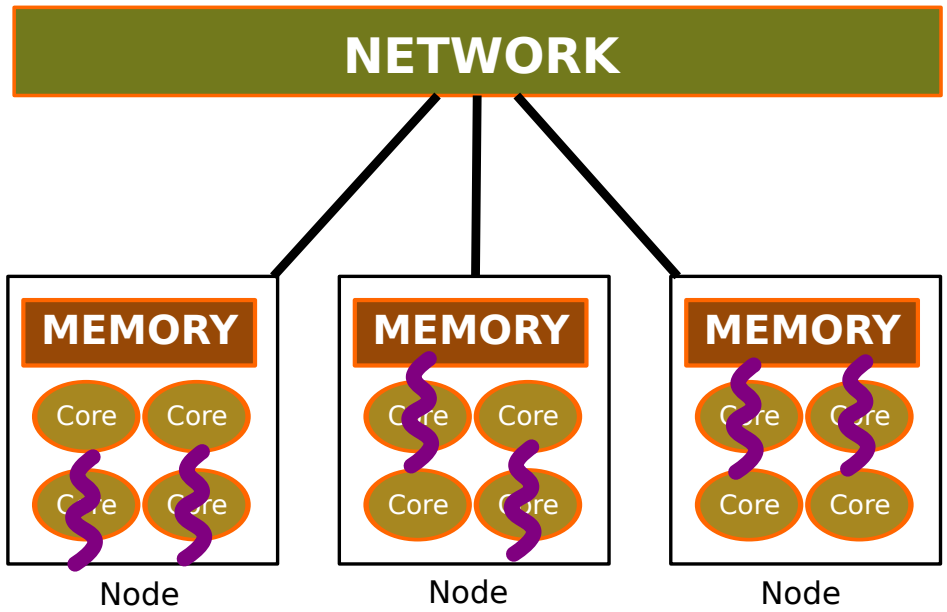
```
Pseudo-code
MPI_Init(argc, argv)
```

- Every MPI program ends by calling MPI_Finalize

```
Pseudo-code
MPI_Finalize()
```

MPI communicators and ranks

- Every process has an MPI rank and belongs to an MPI communicator



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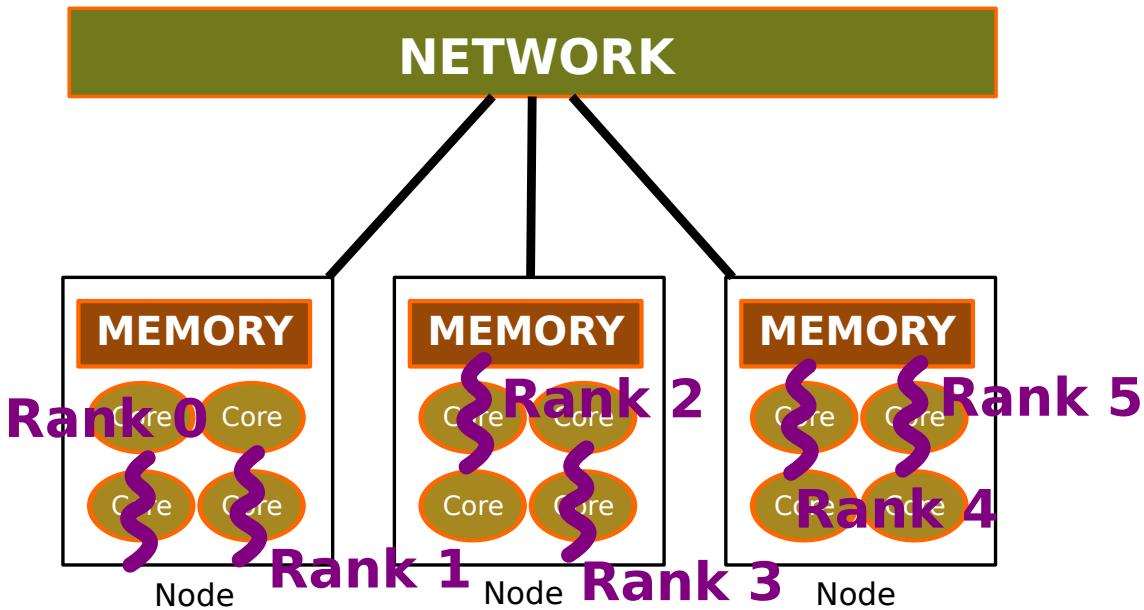

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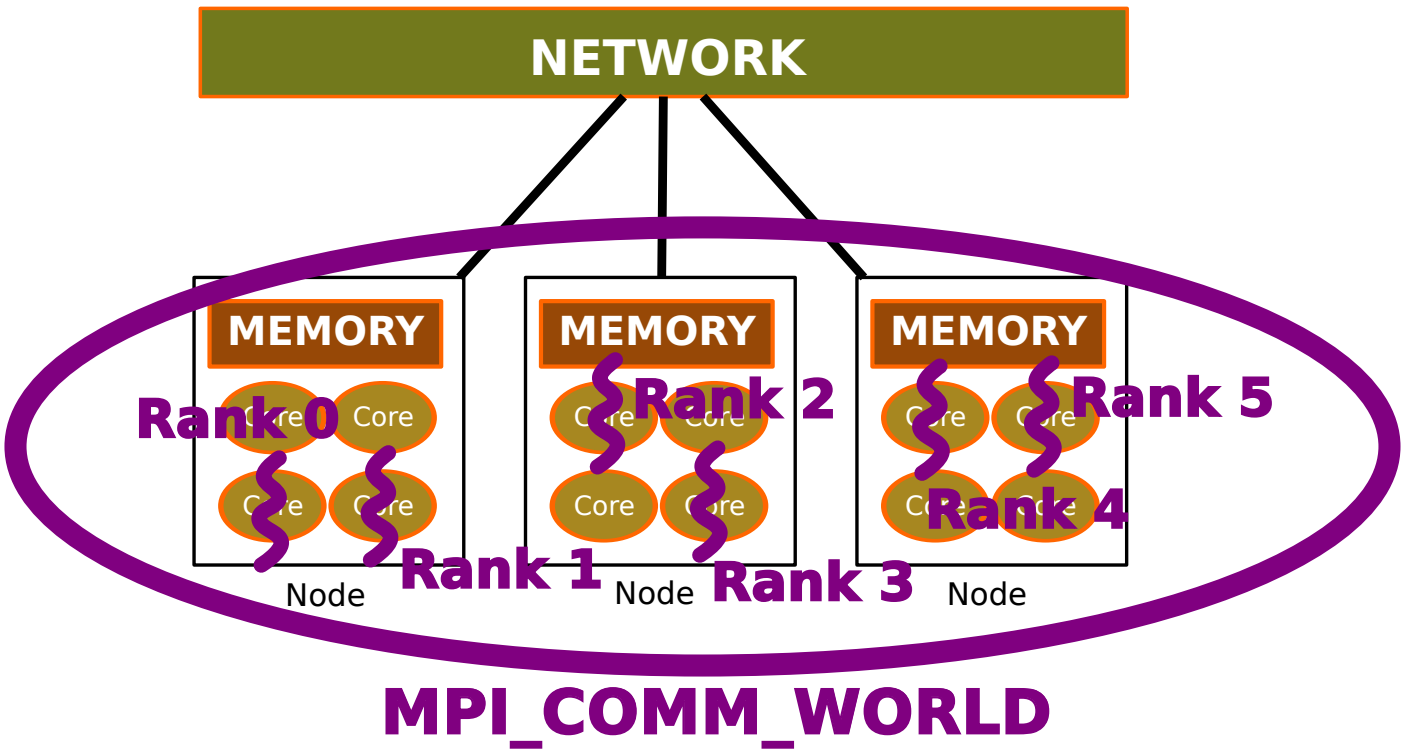

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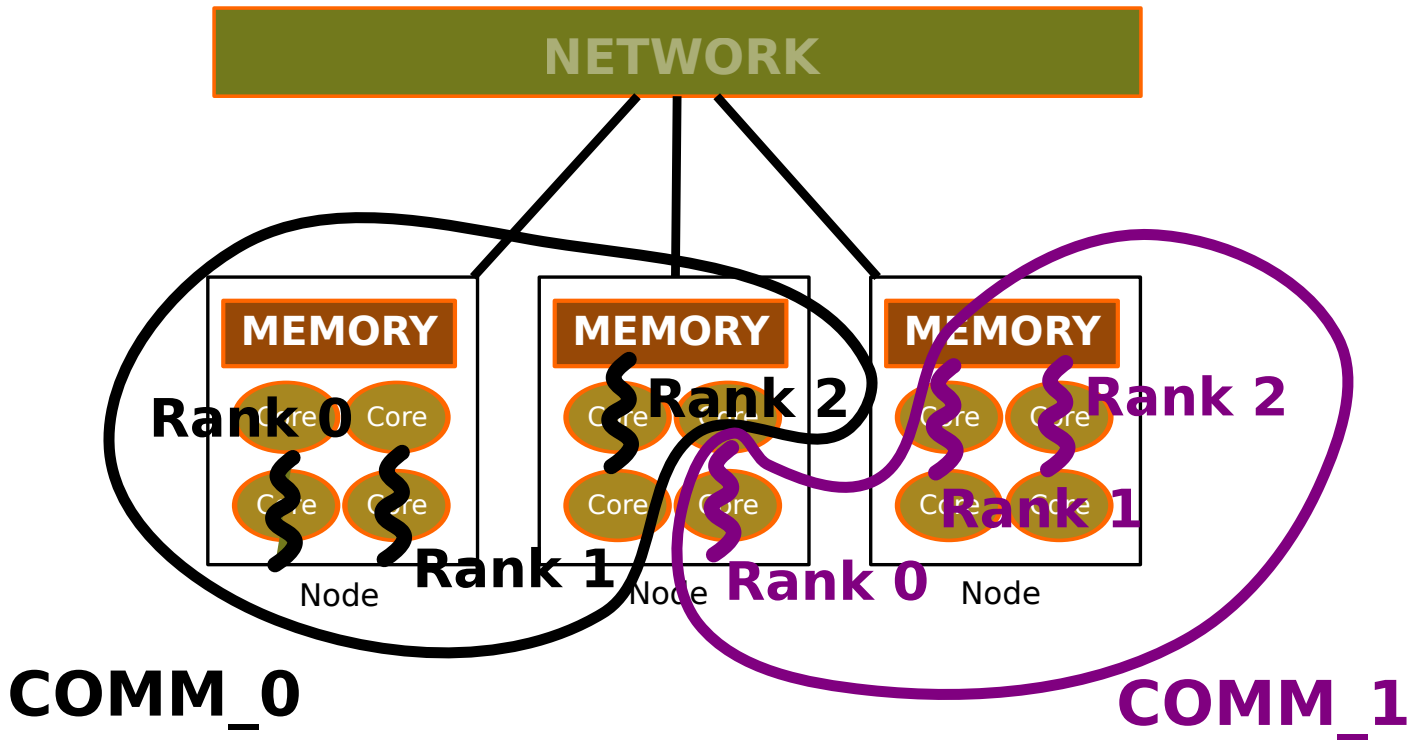
- An MPI communicator is a set of MPI ranks
- Ranks are numbered locally to communicator



Process identification

- How many processes are associated with a communicator?

```
Pseudo-code
MPI_Comm_size(MPI_Comm comm, size)
```

- How to get the rank of a process?

```
Pseudo-code
MPI_Comm_rank(MPI_Comm comm, rank)
```

Simple MPI communication model

Process with rank 1 sends to process with rank 2

```
Pseudo-code
Rank 1: MPI_Send(<send data buffer>, 2, MyCommunicator)
Rank 2: MPI_Recv(<recv data buffer>, 1, MyCommunicator)
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- same communicator: MyCommunicator
- send and recv buffer should be compatible:
  - receive buffer should be large enough
  - data type should match

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- send and recv buffer should be compatible:
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- Rank 2 is prepared to receive data from Rank 1
  - `MPI_Recv` is called in “the right order” (avoid deadlock)
  - Rank 2 knows the maximum bound on the buffer size

⇒ **Parallel!**

Example of MPI source code

C/C++

```c
#include<mpi.h>
#include<assert.h>
int main(int argc, char *argv[]){
    int data[64];
    int nranks, my_rank;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nranks);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
    assert(nranks % 2 == 0);// if not?

    if (my_rank % 2 == 0) {
        MPI_Send(data, 64, MPI_INT, my_rank+1, 0,
            MPI_COMM_WORLD);
    } else {
        MPI_Recv(data, 64, MPI_INT, my_rank-1, 0,
            MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    }
    MPI_Finalize();
}
```

MPI implementation insight

⇒ **Implementation dependent!**

Launcher: mpirun/srun

- Starts all process on all compute nodes (ssh)
- Attributes rank numbers
- Applies specific options like process pinning

Library functions

- Setup process (rank, size) from launcher
- Setup underlying network library (TCP, RDMA, . . .)
- Process event coming from the application
  - send, receive, wait, test, cancel,. . .

MPI features

- Different flavours of point-to-point communications
  - Blocking, non-blocking, synchronous, ...
- Collective operations among ranks
  - Broadcast, scatter, gather, reduce, alltoall, ...
- Topology for managing rank numbering
  - Cartesian topology, graph topology, ...
- User specific data type (like C structure)
- Parallel I/O
  - read and write files in parallel

Practicals

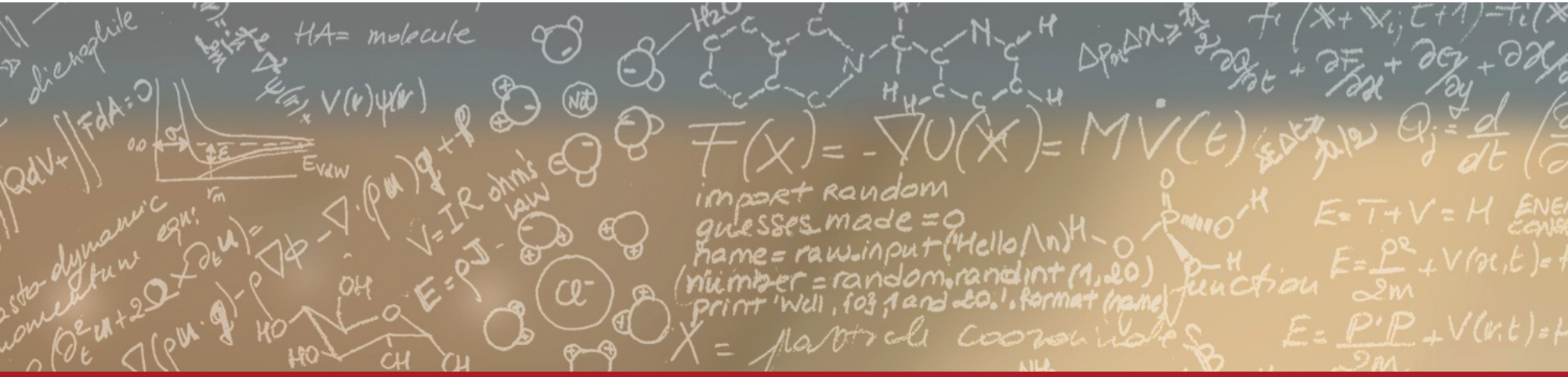
Exercises: 01.MPI_Intro

1. Hello World!
2. Hello World! with rank number

Reminder

```
srun -n 2 ./my_application my_args
```

Starts with 2 MPI ranks.



Thank you for your attention.