COMP 364 / 464
High Performance Computing

Distributed Memory Parallelism:

Message Passing Interface (MPI)

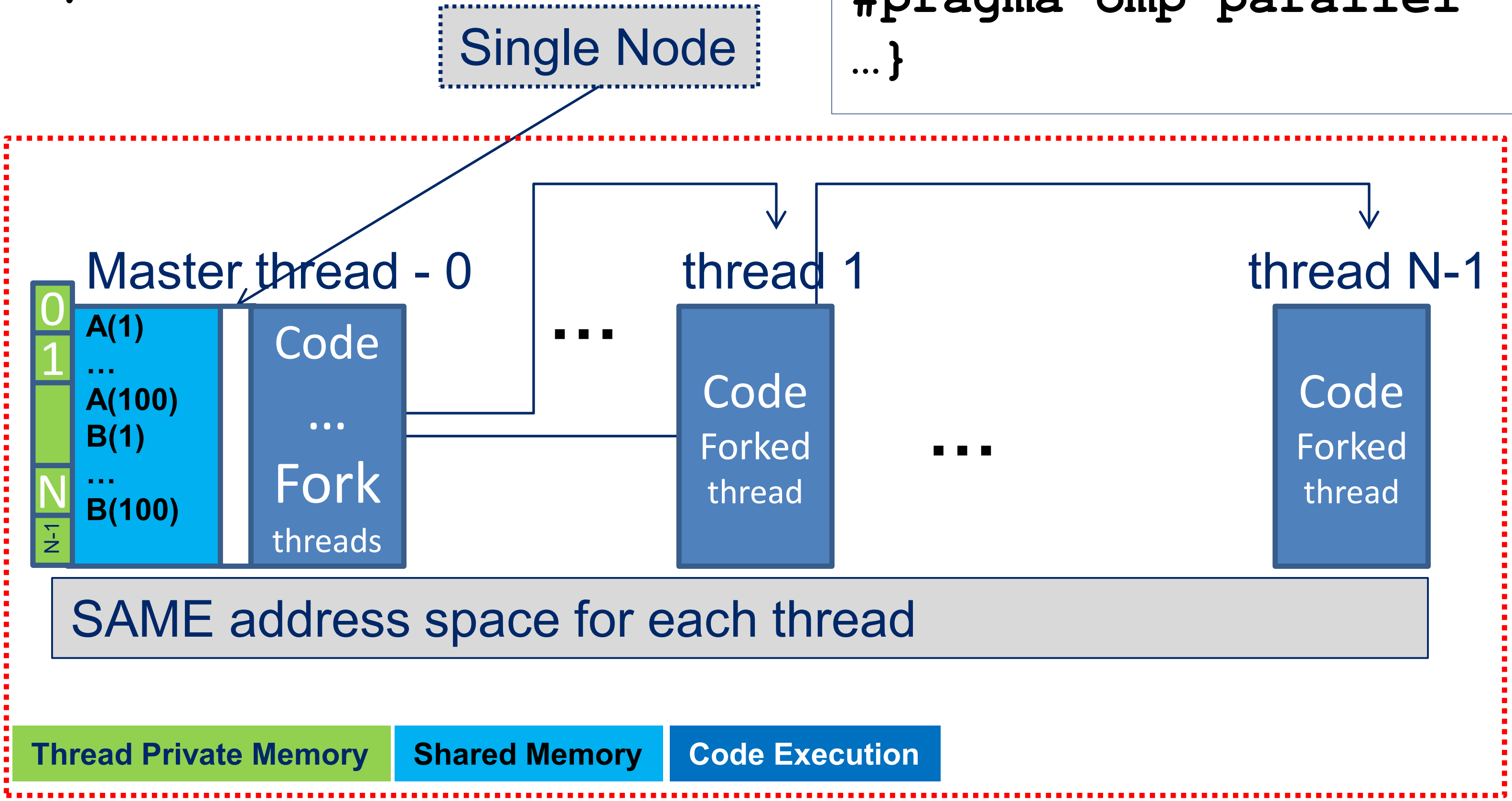
OpenMP (shared memory)

Compile→ **`a.out`**

Set `OMP_NUM_THREADS` to `N`

`./a.out`

```
int main () {
double a(100), b(100);
    …
#pragma omp parallel
…}
```



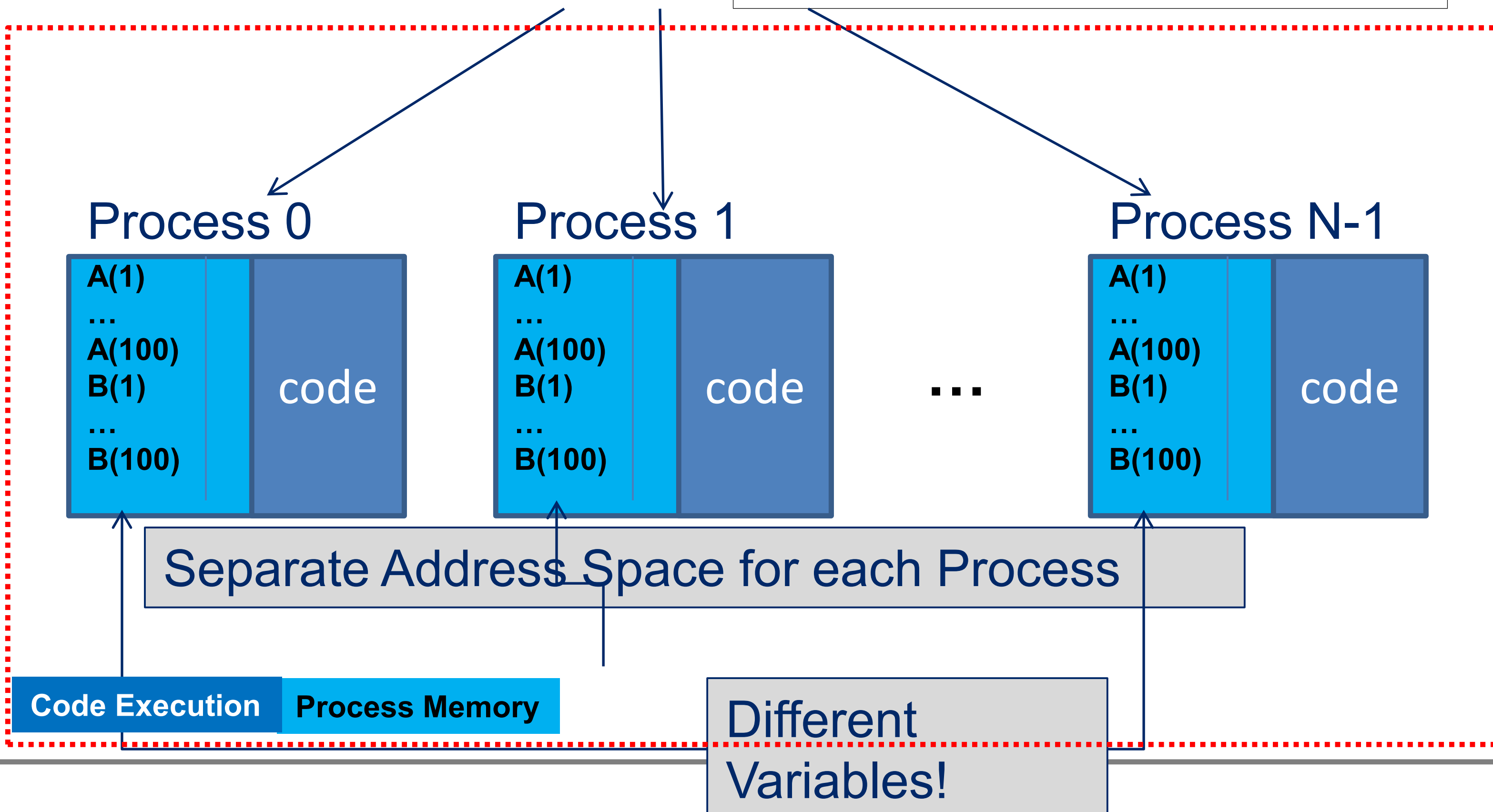
MPI (distributed memory)

Compile→ `a.out`

`Launch` on **`N`** cores

```
mpirun –n N ./a.out
```

```
int main () {
double a(100), b(100);
    …
}
```



Message Passing Paradigm

- A Parallel MPI Program is launched as separate processes, each with their own address space.
  - Requires partitioning data across tasks.
- Data is explicitly moved from process to process
  - A process accesses the data of another process through a transaction called "message passing" in which a copy of the data (message) is transferred (passed) from one process to another.
- There are two classes of message passing (transfers)
  - Point-to-Point messages involve only two processes
  - Collective messages involve a set of processes
- P2P transfers use synchronous or asynchronous protocols
- Messaging can be arranged into efficient topologies

Key Concepts-- Summary

- Used to create parallel SPMD programs on distributed-memory machines with explicit message passing
- Routines available for
  - Point-to-Point Communication
  - Collective Communication
    - 1-to-many (broadcast / scatter)
    - many-to-1 (reduce / gather)
    - many-to-many (gather + scatter)
  - Data Types
  - Synchronization (barriers, blocking v. non-blocking messages)
  - Parallel IO
  - Topologies

Advantages of Message Passing

- Universality
  - Message passing model works on separate processors connected by any network (and even on shared memory systems)
  - Matches the hardware of most of today's parallel supercomputers as well as ad hoc networks of computers
- Performance/Scalability
  - Scalability is the most compelling reason why message passing will remain a permanent component of HPC. Unlimited scalability!
  - As modern systems increase core counts, management of the memory hierarchy (including distributed memory) is key to extracting the highest performance
  - Each message passing process only directly uses its local data, avoiding complexities of process-shared data, and allowing compilers and cache management hardware to function without contention.

MPI-1

- MPI-1 - Message Passing Interface (v. 1.2)
  - Library
  - Specification: defined by committee of vendors, implementers, and parallel programmers
  - Designed with SPMD (single program, multiple data) technique in mind.
- Available on almost all parallel machines in C/C++ and Fortran
- About 125 routines
  - 6 basic routines
    - Send/Recv/Broadcast/Scatter/Gather/Reduce
  - The rest are extensions that can simplify algorithm implementation and optimize performance

MPI-2

- Includes features left out of MPI-1
  - One-sided communications
  - Dynamic process control
  - More complicated collectives
  - MPI-IO
- Implementations
  - Not quickly undertaken after the standard document was released (in 1997)
  - Now OpenMPI, MPICH2 (and its descendants), and the vendor implementations are complete

MPI-3

- Includes features left out of MPI-1 and MPI-2 and tries to fix many problems with MPI-2 (e.g., 1-sided comm)
  - Better one-sided communications
  - Nonblocking collective operations
  - Neighborhood collectives (down in the weeds)
  - Memory hierarchy (node-level shared memory)
  - Dropped the C++ bindings … just use the C bindings for C++ now.

Compiling MPI Programs

- Generally use a special compiler or compiler wrapper script
  - not defined by the standard
  - consult your implementation
  - handles correct include path, library path, and libraries
- MPICH-style (the most common)
  - C:
    ```
    mpicc  -o myc.exe mycode.c
    ```
  - C++:
    ```
    mpicxx  -o myc++.exe mycode.cxx
    mpiCC   -o myc++.exe mycode.cc
    ```
  - Fortran:
    ```
    mpif90 -o myf.exe mycode.f
    ```

Running MPI Programs

- MPI programs require some help to get started
  - what computers should I run on?
  - how do I access them?
- MPICH or OpenMPI … the two most common open-source libraries.

```
mpirun -np 10 ./a.out
mpiexec -n 10 ./a.out
```

- When batch systems are involved, all bets are off.

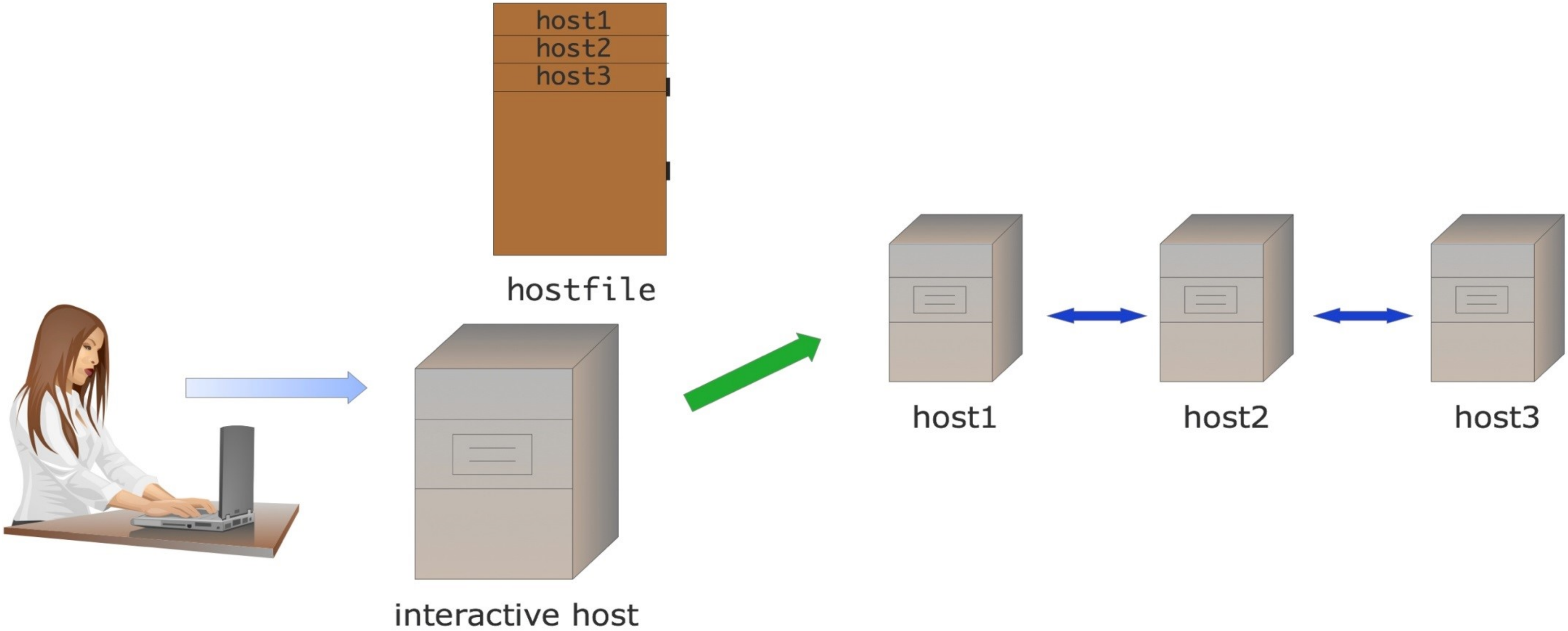
The Parallel Code

- Parallel executables are nothing more than independent processes (tasks) launched by ssh commands:

  ssh <nodename> <environment> *executable.*

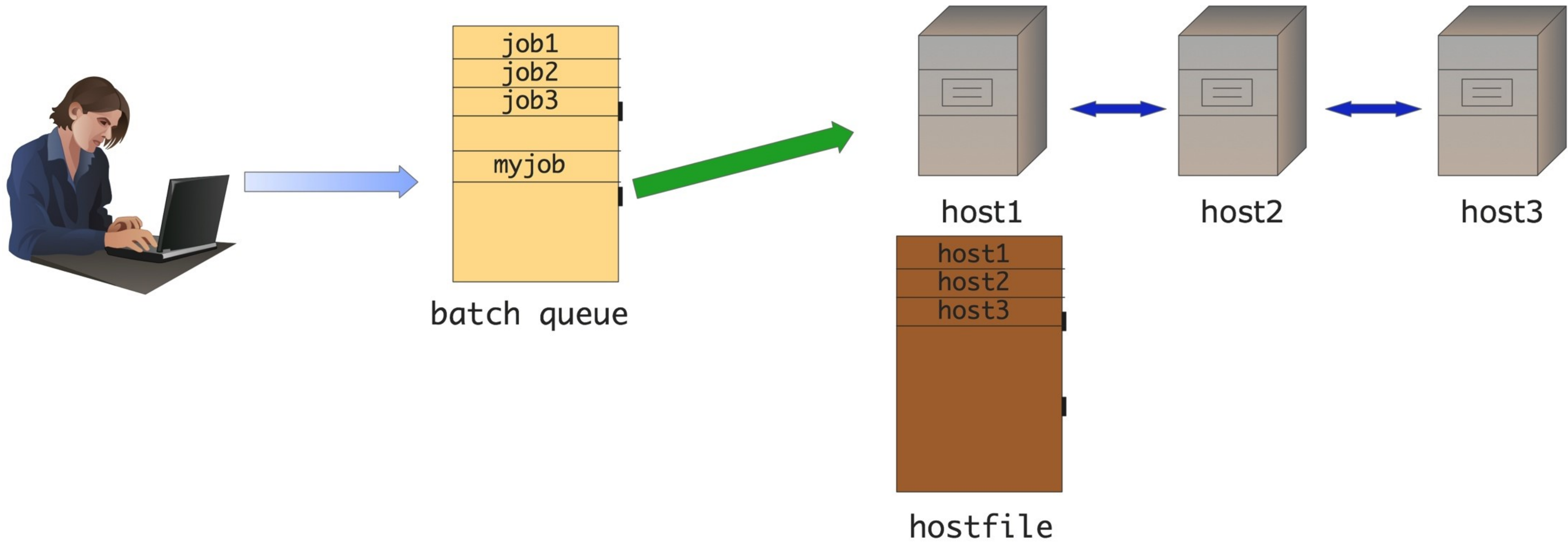
  - Executables need organization info (initialize).
  - Executables needs to synchronize.
  - Each task needs to know its id (rank) and # of execs.
  - Executables need to clean up at end.

Interactive Scenario



mpirun -np 5 -h host1,host2,host3 ./prgram <arguments>

Batch Scenario



- User submits batch job to queue, executed later by scheduler

Minimal MPI program

- Every MPI program needs these…

```
#include <mpi.h>
int main(int argc, char* argv[])
{
  ierr = MPI_Init(&argc, &argv);
  ierr = MPI_Comm_size(MPI_COMM_WORLD, &numRanks);
  ierr = MPI_Comm_rank(MPI_COMM_WORLD, &myRank);
  ...
  MPI_Finalize();
  return 0;
}
```

- In C MPI routines are functions which return the error value

MPI Initialization & Termination

- All processes must initialize and finalize MPI (each is a **`collective call*`**).
  - *Collective* means all tasks must execute this call – not necessarily at the same time (but ideally very soon together).
  - **`MPI_Init`**: starts up the MPI runtime environment
  - **`MPI_Finalize`**: shuts down the MPI runtime environment
- Must include header files – provides basic MPI function definitions, operators and datatypes.

Header File: **`#include <mpi.h>`**

Format of MPI calls: **`int ierr = MPI_Xyyy (parameters…)`**

Run Parameters

- **`MPI_Comm_size(MPI_Comm comm, int *size)`**
  - Gets the number of processes in a run with **`MPI_Comm = MPI_COMM_WORLD`**
  - Result is an integer (typically called just after **`MPI_Init`**).
- **`MPI_Comm_rank(MPI_Comm comm, int *rank)`**
  - Gets the process ID (rank) of the current process
  - Results is an integer between 0 and *NP*-1 inclusive (typically called just after **`MPI_Init`**).

Communicators

- Communicators
  - MPI uses a communicator object (and groups) to identify a set of processes which communicate only within their subset.
  - **`MPI_COMM_WORLD`** is defined in the MPI include file as the collection of all processes (i.e., ranks) associated with your job
  - Required parameter for most MPI calls
  - You can create subset communicators of **`MPI_COMM_WORLD`**
- Rank
  - Unique *process ID* within a communicator
  - Assigned by the system when the process initializes (for **`MPI_COMM_WORLD`**)
  - Processors within a communicator are assigned numbers 0 to n-1
  - Used to specify sources and destinations of messages, process specific indexing and operations.

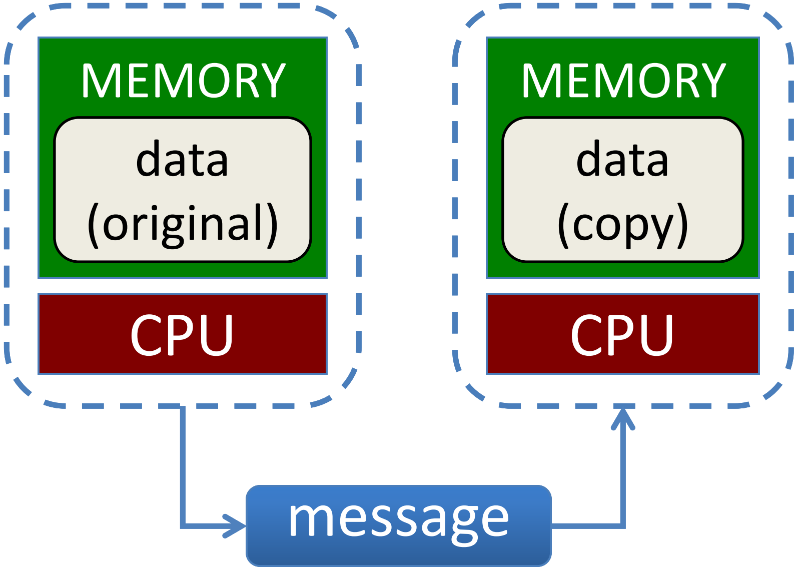
Include files

- The MPI include file: `mpi.h`
  - Defines many constants used within MPI programs
  - In C/C++, defines the interfaces for the functions

- MPI-aware compilers know where to find the include files
  - regular compilers are usually called through mpicc/mpiCC/mpic++/mpicxx wrapper scripts or the equivalent

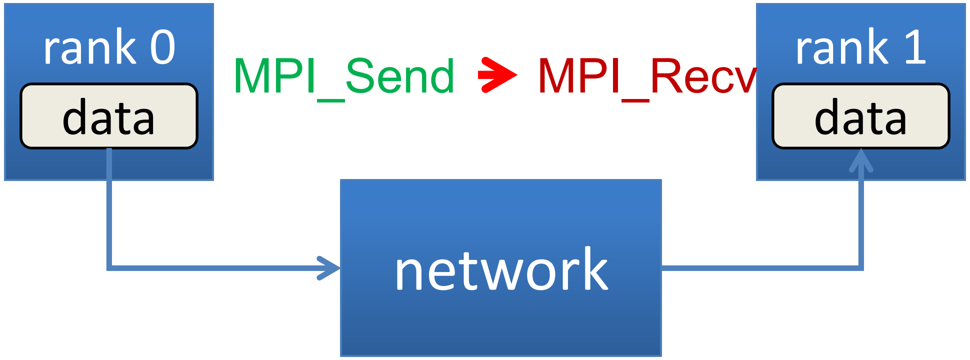
Parallel Code

- The programmer is responsible for determining all parallelism
  - Data Partitioning
  - Deriving Parallel Algorithms
  - Moving Data between Processes
- Ranks (independent processes executing anywhere) send and receive “messages” to exchange data
- Data transfer requires cooperation between two (or more) processes.
  - Fundamental communication is point-to-point between two processes.



Point-to-Point Communication

- Sending data from one point (process) to another point (process)
- One process sends while another receives
- Various synchronization options available. Both ends handshake.



Basic Communications in MPI

- Standard **`MPI_Send/MPI_Recv`** routines
  - Blocking calls used for basic P2P messaging

Point-to-Point (P2P) Modes of Operation

- Blocking
  - Call does not return until the received data is safe to use and the send data is safe to free/overwrite
- Non-blocking
  - Initiates send or receive operation, returns immediately
  - Can check or wait for completion of the operation
  - Data is not safe for use until completion is confirmed.
- Synchronous and Buffered (later)

Data Types (basics)

- Data types (more of a mapping than a declaration)
  - Specifies the data type and element size in MPI routines
  - Predefined MPI types correspond to language types

Representation	MPI Type C	C
32-bit floating point	`MPI_FLOAT`	`float`
64-bit floating point	`MPI_DOUBLE`	`double`
32-bit integer	`MPI_INT`	`int`
8-bit character	`MPI_CHAR`	`char`

- Methods exists for creating user-defined types
  - Simple (just combinations of normal data types)
  - Advanced (a map of data to be send)

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