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Parallel Computing for Science and Engineering

MPI Introduction

Outline

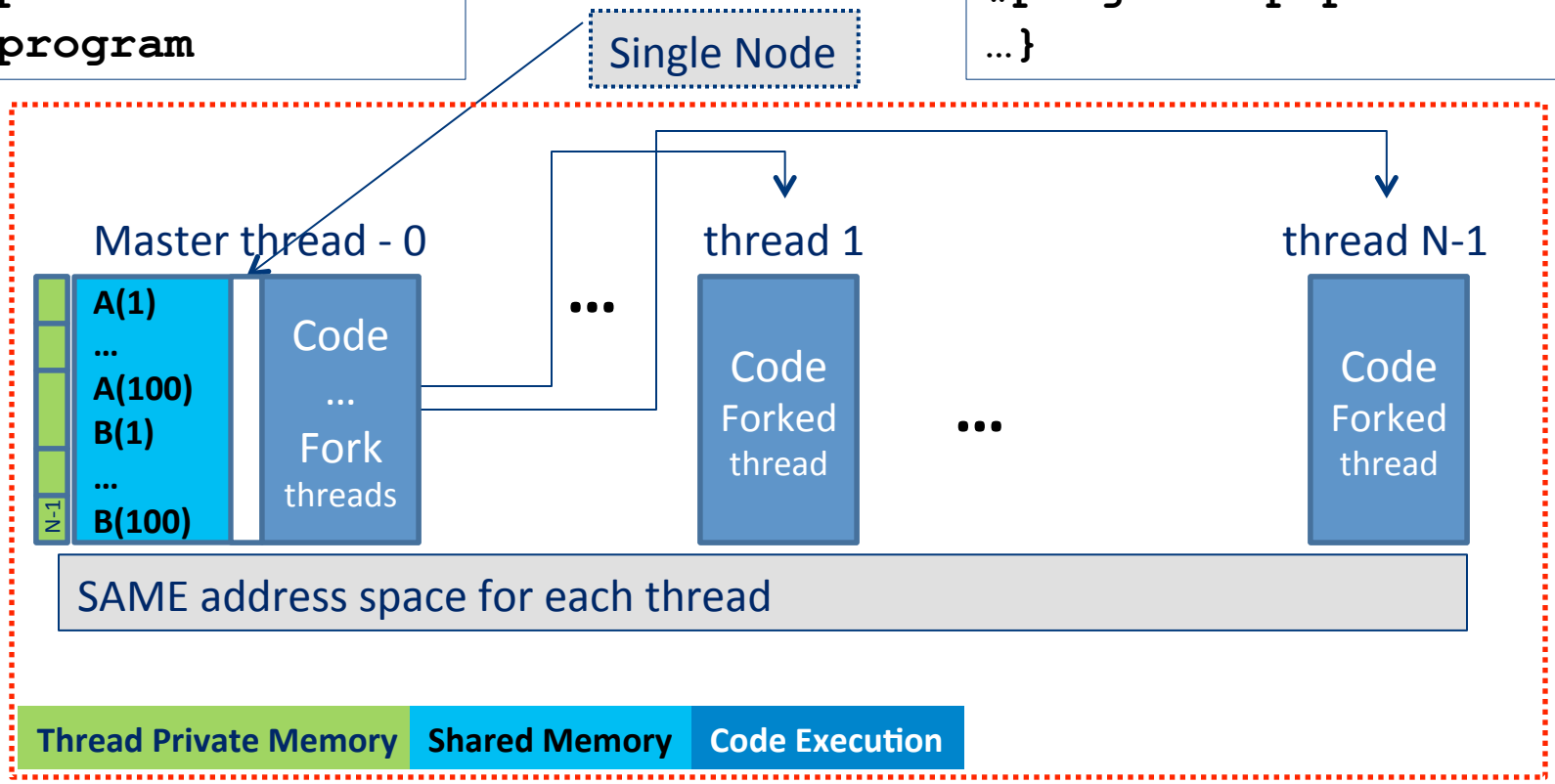
- Executing OpenMP and MPI
- Paradigm/Key Concepts/Advantages
- MPI History version 1 and 2, implementations
- Compiling, running
- MPI initialize, finalize, and task-id/task-count
- MPI communicators

OpenMP (shared memory)

```
program  myomp
real*8   a(100), b(100)
…
!$omp parallel
… end program
```

Compile→ `a.out`
Set `OMP_NUM_THREADS` to `N`
`./a.out`

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

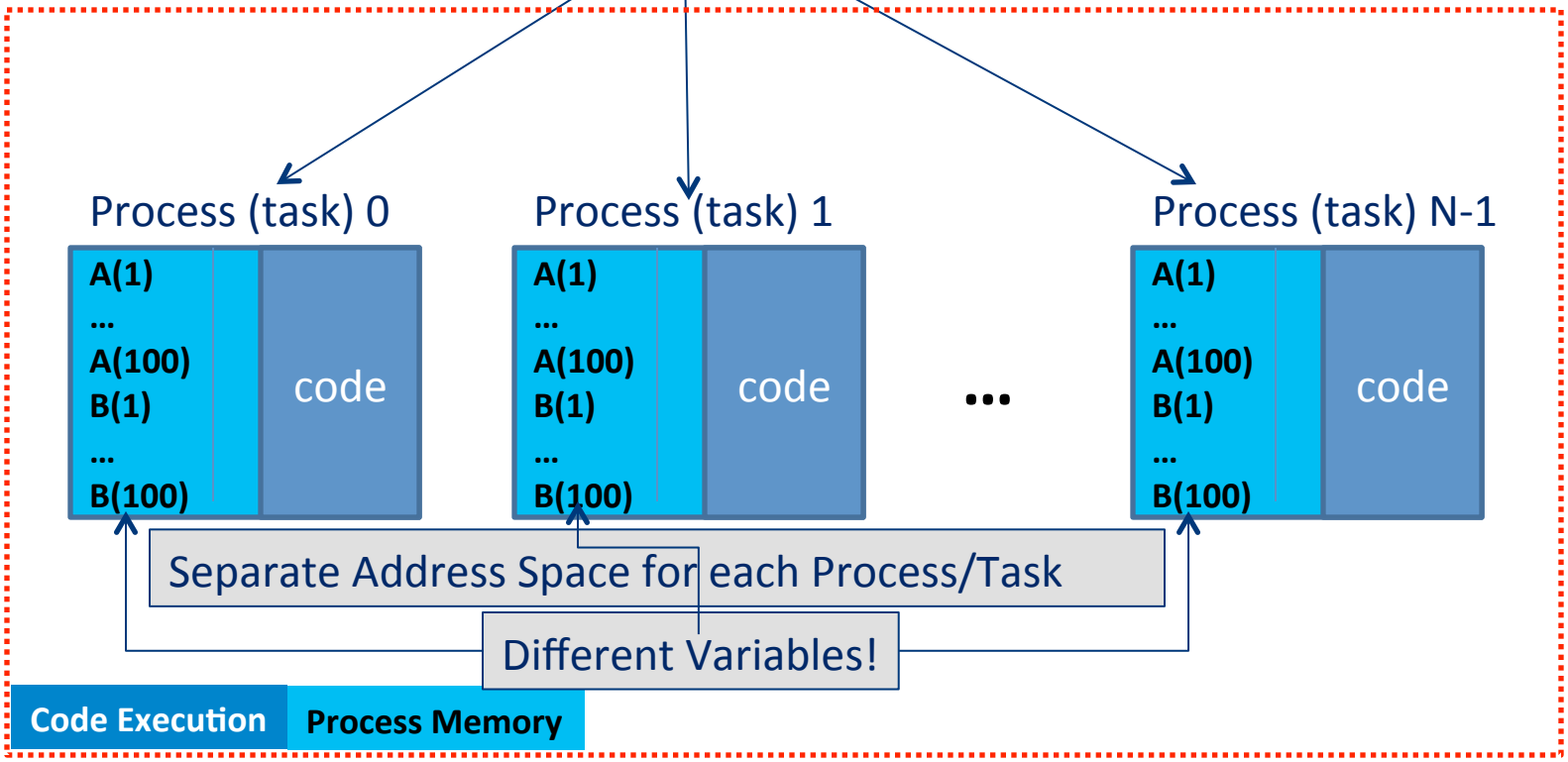


MPI (distributed memory)

```
program  mympi
real*8   a(100), b(100)
…
end program
```

Compile→ `a.out`
Launch on **N** cores
`ibrun ./a.out`

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



Message Passing Paradigm

- A Parallel MPI Program is launched as separate processes (tasks), each with their own address space.
  - Requires partitioning data across tasks.
- Data is explicitly moved from task to task
  - A task accesses the data of another task through a transaction called "message passing" in which a copy of the data (message) is transferred (passed) from one task to another.
- There are two classes of message passing (transfers)
  - Point-to-Point messages involve only two tasks
  - Collective messages involve a set of tasks
- Access to subsets of complex data structures is simplified
  - A data subset is described as a single Data Type entity
- 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
    - many-to-1
    - many-to-many
  - Data Types
  - Synchronization (barriers, non-blocking MP)
  - 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 (High Performance Computing)
  - As modern systems increase core counts, management of the memory hierarchy (including distributed memory) is the 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
  - The rest are extensions that can simplify algorithm implementation and optimize performance

MPI-1

Web

- www-unix.mcs.anl.gov/mpi/
- www.mcs.anl.gov/research/projects/mpich2/
- www.mpi-forum.org/

Books

- *Using MPI*, by Gropp, Lusk, and Skjellum
- *Using MPI-2*, by Gropp, Lusk and Thakur
- *MPI Annotated Reference Manual,* by Marc Snir, *et al*
- *Parallel Programming with MPI*, by Peter Pacheco

Getting Started

- www.mcs.anl.gov/research/projects/mpi/tutorial/gropp/talk.html
- http://ci-tutor.ncsa.illinois.edu/
- www.nersc.gov/nusers/help/tutorials/mpi/intro/ (simple, direct)
- https://computing.llnl.gov/?set=training&page=index
- Advanced: www.mcs.anl.gov/research/projects/mpi/tutorial/

Standard

- www.mpi-forum.org/docs/

MPI-1 Implementations

- Many parallel machine, HPC interconnect, and commercial software vendors have optimized versions
  - Hardware vendors: IBM, Sun, HP, Intel
  - Interconnect vendors: Myricomm, Quadrics, InfiniBand*
    * InfiniBand: open source drivers/university MPI collaboration
      http://www.openib.org/
      http://mvapich.cse.ohio-state.edu/
  - Software vendors: MPI/Pro, Platform MPI (was Scali MPI), etc.

- Others
  - MPICH www-unix.mcs.anl.gov/mpi/mpich/
  - MPICH-G2, Globus-based www3.niu.edu/mpi/
  - MPICH-VMI, Virtual Machine Interface http://vmi.ncsa.uiuc.edu/
  - MVAPICH http://mvapich.cse.ohio-state.edu/
  - OpenMPI (formerly LAM/MPI) http://www.open-mpi.org/

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 pretty complete or fully complete

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 mycexe mycode.c
```

  - Fortran:

```
mpif90 -o myfexe 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-style

```
mpirun -np 10 -machinefile mach ./a.out
```

- When batch systems are involved, all bets are off.
- For TACC systems (via a job script)…

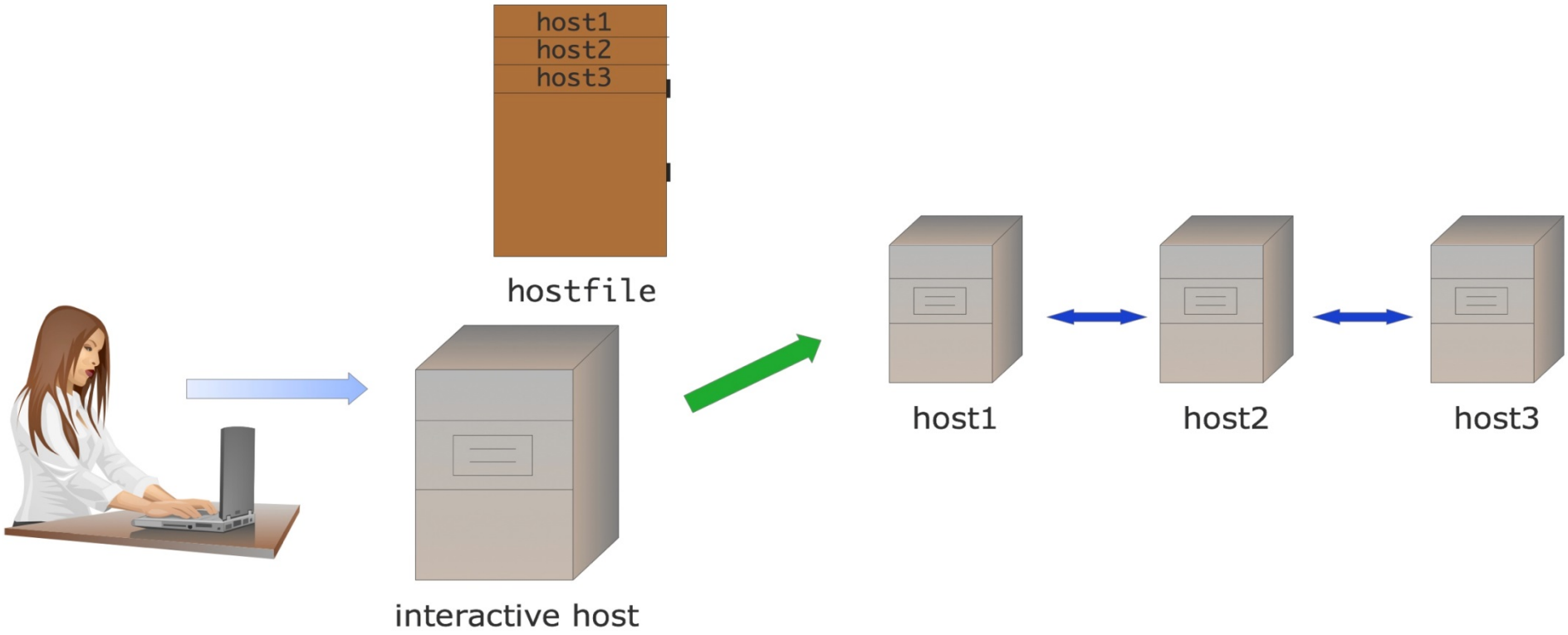
```
ibrun tacc_affinity ./a.out
```

  - Batch utility (SGE or slurm) handles the rest

The Parallel Code

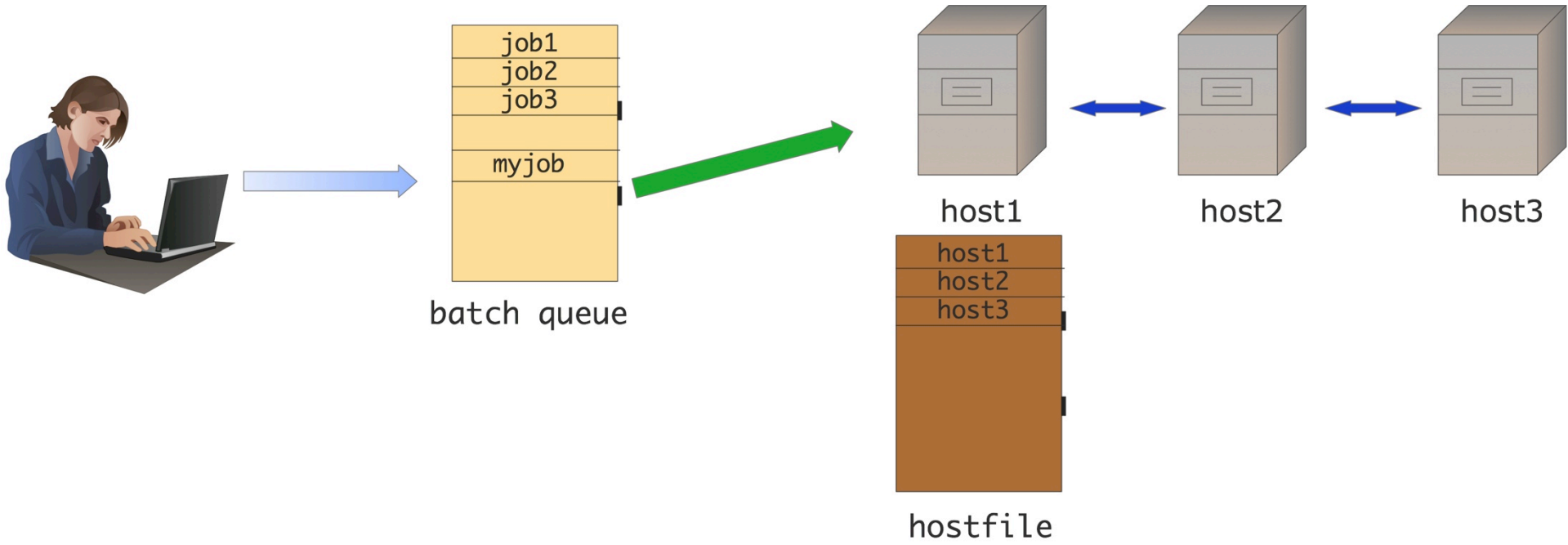
- Parallel executables are nothing more than independent processes (tasks) launched by ssh commands: ssh <nodename> <environment> *executable.*
  - Executables need organization info (initialize).
  - Executables needs to synchronize.
  - Each task needs to know its id (rank) and # of execs.
  - Executables need to clean up at end.

Interactive Scenario



User type: **`mpirun -np 5 hostfile ./myprogram arguments`**

Batch Scenario



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

Minimal MPI program

- Every MPI program needs these…
  - C version

```
#include <mpi.h>
  ...
ierr=MPI_Init(&argc, &argv);
ierr=MPI_Comm_size(MPI_COMM_WORLD, &npes);
ierr=MPI_Comm_rank(MPI_COMM_WORLD, &iam);
  ...
ierr=MPI_Finalize();
```

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

Minimal MPI program

- Every MPI program needs these…
  - Fortran version

```
include 'mpif.h' ! or "use mpi"
    ...
call MPI_Init(ierr)
call MPI_Comm_size(MPI_COMM_WORLD, npes, ierr)
call MPI_Comm_rank(MPI_COMM_WORLD, iam, ierr)
    ...
call MPI_Finalize(ierr)
```

- In Fortran, MPI routines are subroutines with the last parameter as the error value

MPI Initialization & Termination

- All processes must initialize and finalize MPI (each is a **collective call***).
  - **MPI_Init:** starts up the MPI runtime environment
  - **MPI_Finalize:** shuts down the MPI runtime environment
- Must include header files – provides basic MPI definitions and types.

Header File

Fortran 77	Fortran 90	C/C++
`include 'mpif.h'`	`use mpi`	`#include <mpi.h>`

Format of MPI calls

Fortran 77/90 binding (upper or lower case)	C/C++ binding
`CALL MPI_XYYY(parameters…, ierr)`	`ierr = MPI_Xyyy(parameters…)`

* Means the entire group of tasks must execute this call.

Run Parameters

- **`MPI_Comm_size`**
  - Gets the number of processes in a run
  - Result is an integer (typically called just after **`MPI_Init`**).
- **`MPI_Comm_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`**).

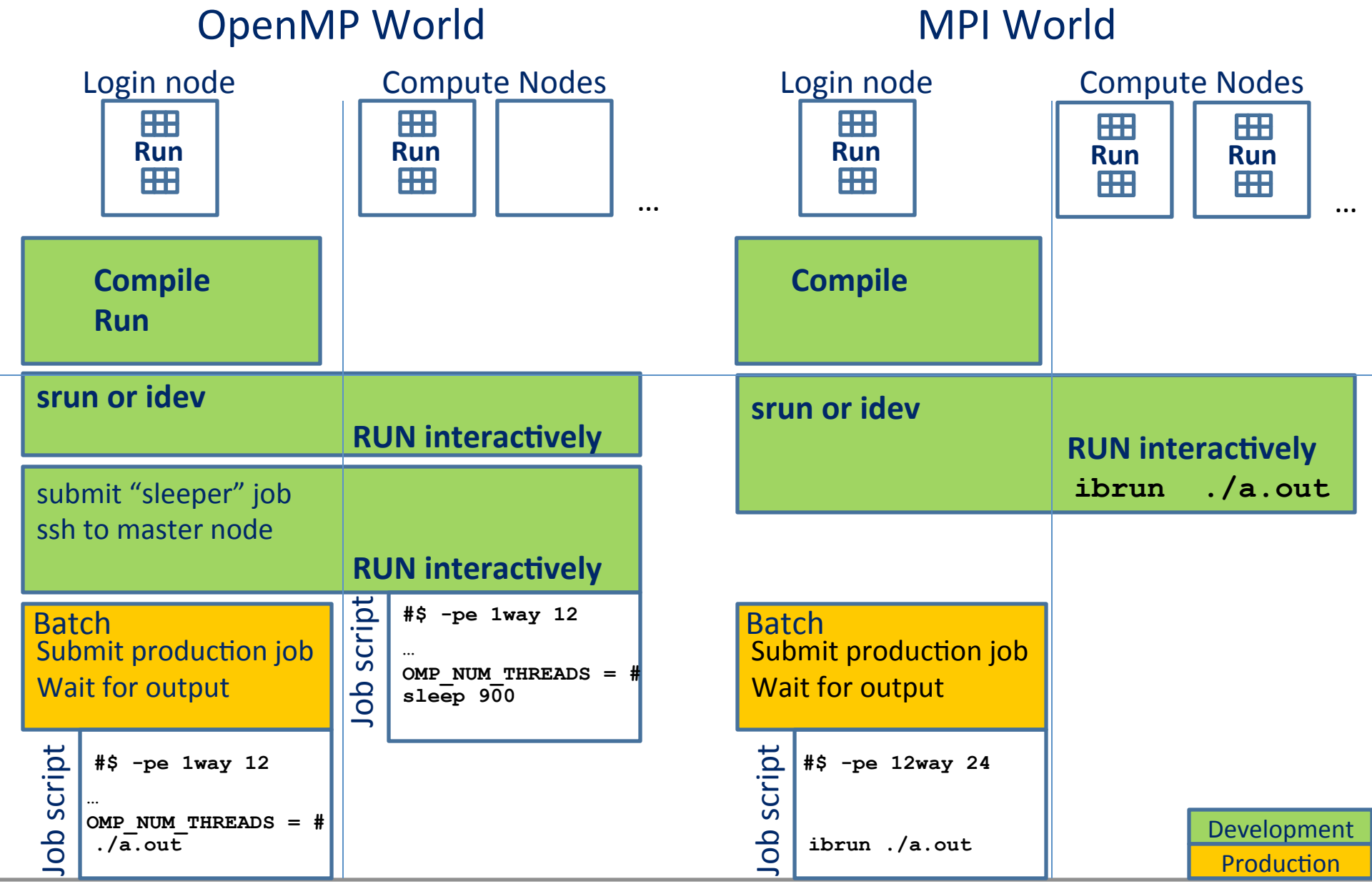
Communicators

- Communicators
  - MPI uses a communicator object (and groups) to identify a set of processes which communicate only within their set.
  - **`MPI_COMM_WORLD`** is defined in the MPI include file as the collection of all processes (tasks, ranks) associated with your job
  - Required parameter for most MPI calls
  - You can create subsets 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 (C/F90)
  - Used to specify sources and destinations of messages, process specific indexing and operations.

Include files

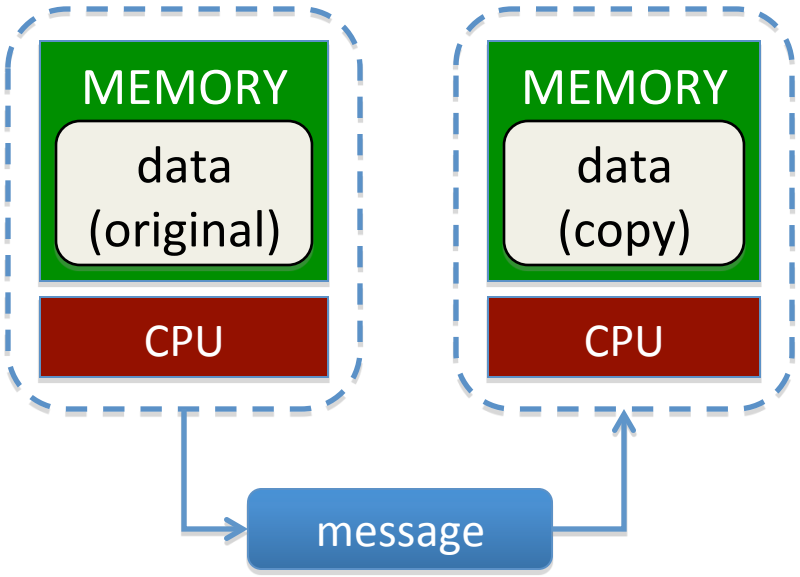
- The MPI include file
  - C: `mpi.h`
  - Fortran: `mpif.h`

    MPI module → use MPI
- Defines many constants used within MPI programs
  - In C, defines the interfaces for the functions
  - In C++, the interfaces are different, so be careful
  - In F90, module defines interface for subroutines
- MPI-aware compilers know where to find the include files
  - regular compilers are usually called through mpif90/mpicc wrapper scripts or the equivalent


OpenMP World
MPI World
Login node
Compute Nodes
Login node
Compute Nodes
Run
Run
Run
Run
Run
...
...
Compile
Run
Compile
srun or idev
RUN interactively
srun or idev
RUN interactively
ibrun ./a.out
submit "sleeper" job
ssh to master node
RUN interactively
Batch
Submit production job
Wait for output
Job script
#$ -pe 1way 12
...
OMP_NUM_THREADS = #
sleep 900
Batch
Submit production job
Wait for output
Job script
#$ -pe 1way 12
...
OMP_NUM_THREADS = #
./a.out
Job script
#$ -pe 12way 24
ibrun ./a.out
Development
Production

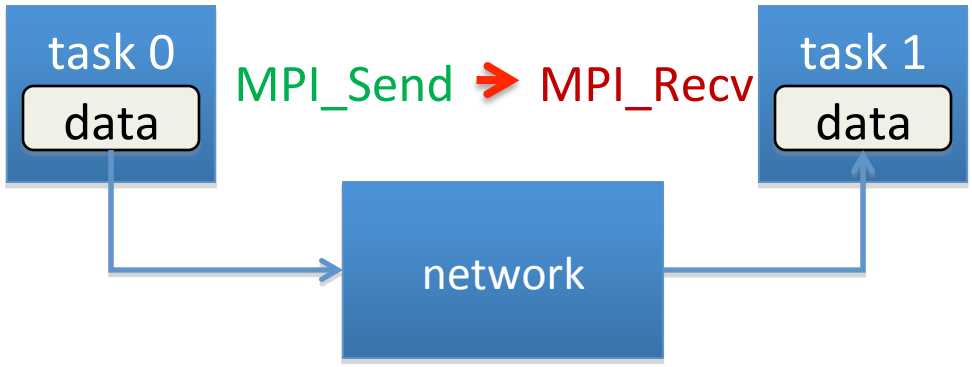
Parallel Code

- The programmer is responsible for determining all parallelism
  - Data Partitioning
  - Deriving Parallel Algorithms
  - Moving Data between Processes
- Tasks (independent processes executing anywhere) send and receive "messages" to exchange data
- Data transfer requires cooperative operation to be performed by each process (point to point communications)
- Message Passing Interface (MPI) was released in 1994. (MPI-2 in 1996) Now the de facto standard for message passing
- http://www-unix.mcs.anl.gov/mpi/



Point-to-Point Communication

- Sending data from one point (process/task) to another point (process/task)
- One task sends while another receives



Basic Communications in MPI

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

Point-to-Point Modes of Operation

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

Data Types (basics)

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

Representation	MPI Type Fortran	Fortran	MPI Type C	C
32-bit floating point	`MPI_REAL`	`REAL`	`MPI_FLOAT`	`float`
64-bit floating point	`MPI_DOUBLE_PRECISION`	`DOUBLE_PRECISION`	`MPI_DOUBLE`	`double`
32-bit integer	`MPI_INTEGER`	`INTEGER`	`MPI_INT`	`int`

- 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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