Introduction to MPI and OpenMP (with Labs)

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Based on materials developed by Kent Milfeld at TACC, Steve Lantz at CAC, and Brandon Barker at CAC

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Components

- OpenMP (***shared memory***)
  - Parallel programming on a single node
- MPI (***distributed memory***)
  - Parallel computing running on multiple nodes
- OpenMP + MPI (***hybrid computing***)
  - Combine to maximize use of HPC systems

What is OpenMP?

- OpenMP is an acronym for Open Multi-Processing
- An Application Programming Interface (API) for developing parallel programs in shared-memory architectures
- Three primary components of the API are:
  - Compiler Directives
  - Runtime Library Routines
  - Environment Variables
- De facto standard -- specified for C, C++, and FORTRAN
- http://www.openmp.org/ has the specification, examples, tutorials and documentation
- OpenMP 4.5 specified November 2015

OpenMP = Multithreading

- All about executing concurrent work (tasks)
  - Tasks execute as independent *threads*
  - Threads access the same *shared memory* (no message passing!)
  - Threads synchronize only at *barriers*
- Simplest way to do multithreading – run tasks on multiple cores/units
  - Insert OpenMP *parallel directives* to create tasks for concurrent threads
  - So, shared-memory parallel programming is super-easy with OpenMP?
  - Nope! Updates to a shared variable, e.g., need special treatment…

```
// repetitive work: OK
#pragma omp parallel for
for (i=0; i<N; i++)
     a[i] = b[i] + c[i];
```

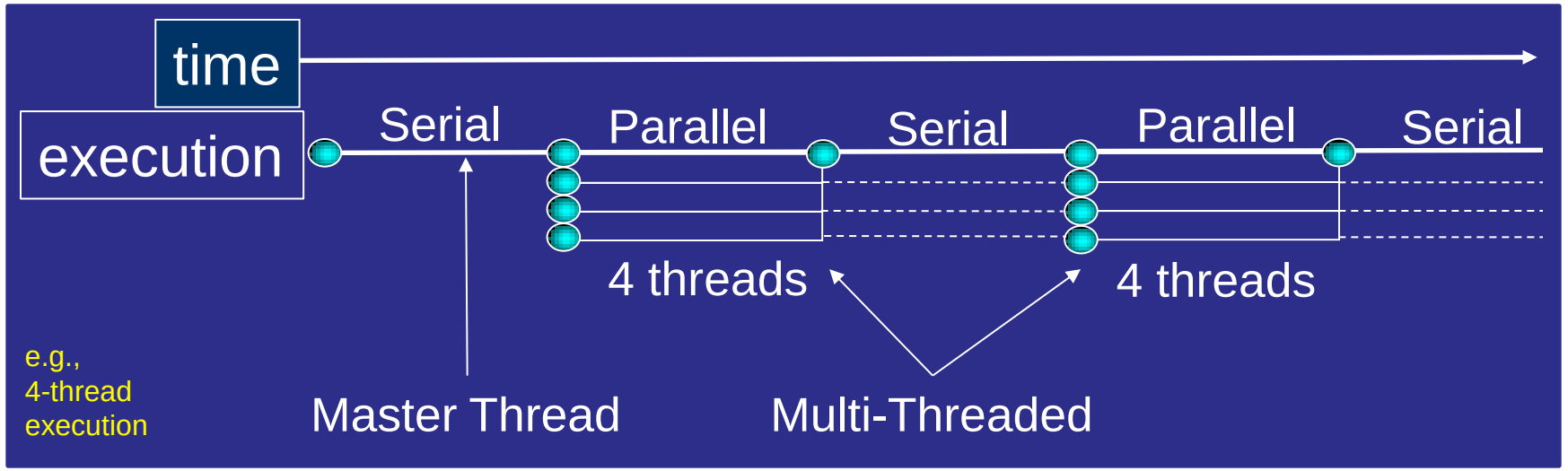
```
// repetitive updates: oops
#pragma omp parallel for
for (i=0; i<N; i++)
     sum = sum + b[i]*c[i];
```

Role of the Compiler

- OpenMP relies on the compiler to do the multithreading
  - Compiler recognizes OpenMP directives, builds in appropriate code
- A special flag is generally required to enable OpenMP
  - GNU: `gcc -fopenmp`
  - Intel: `icc -openmp`
- On the Stampede 2 login node, extra flags may be required for KNL
  - Tell the Intel compiler to use MIC-only instructions: `-xMIC-AVX512`
  - Putting it all together, e.g.: `icc -openmp -xMIC-AVX512`
  - Must do multithreading to make full use of the Xeon Phi!

OpenMP Fork-Join Parallelism

- Programs begin as a single process: master thread
- Master thread executes until a parallel region is encountered
  - Master thread creates (forks) a team of parallel threads
  - Threads in team simultaneously execute tasks in the parallel region
  - Team threads synchronize and sleep (join); master continues



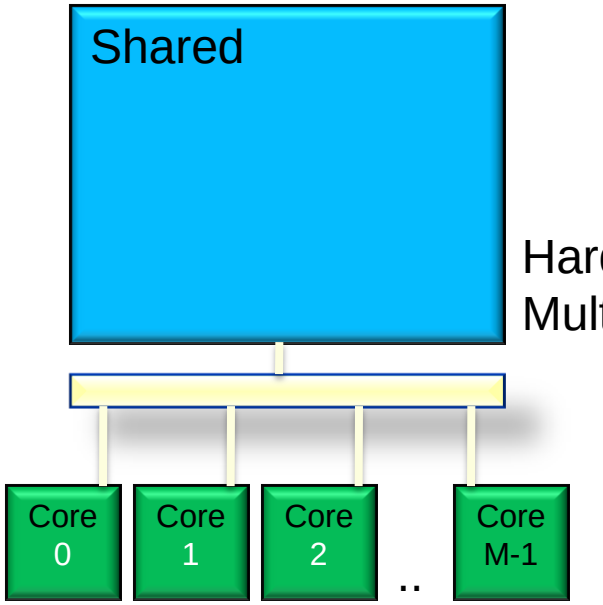
Parallel Region: C/C++

LAB: OMP Hello World
(saw already in intro lab)

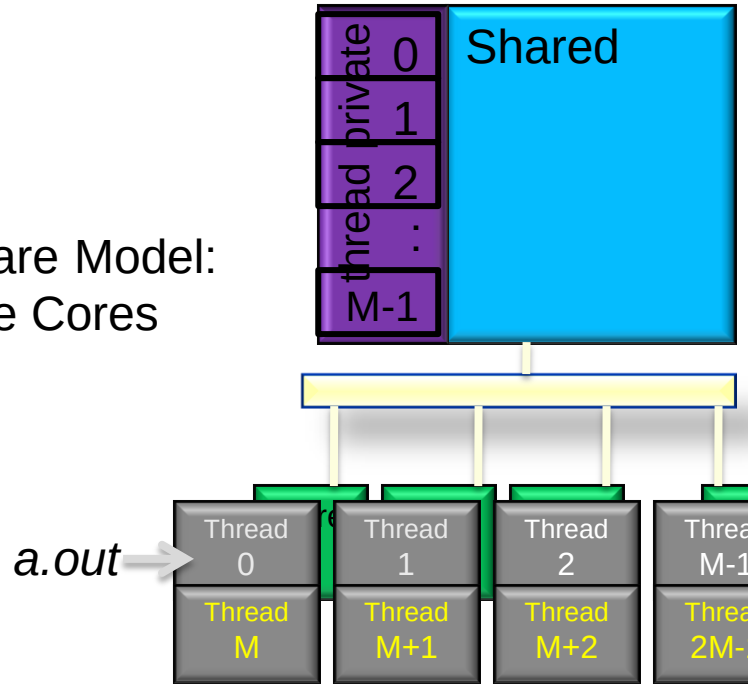
```
1  #pragma omp parallel
2   { code block
3     a = work(...);
4   }
```

Line 1	Team of threads is formed at parallel region
Lines 2–3	Each thread executes code block and subroutine call, no branching into or out of a parallel region
Line 4	All threads synchronize at end of parallel region (implied barrier)

OpenMP on Shared Memory Systems



Hardware Model:
Multiple Cores



Software Model:
Threads in
Parallel Region

Shared = accessible by all threads

x = private memory for thread x

M threads are usually mapped to M cores.

For KNL cores, 2-4 SW threads are mapped to 4 HW threads on each core.

OpenMP Directives

- OpenMP directives are comments in source code that specify parallelism for shared-memory parallel (SMP) machines
- FORTRAN compiler directives begin with one of the sentinels `!$OMP`, `C$OMP`, or `*$OMP` – use `!$OMP` for free-format F90
- C/C++ compiler directives begin with the sentinel `#pragma omp`

Fortran 90

```
!$OMP parallel
  ...
!$OMP end parallel

!$OMP parallel do
  DO ...
!$OMP end parallel do
```

C/C++

```
#pragma omp parallel
    {...
    }

#pragma omp parallel for
    for(...){...
    }
```

OpenMP Syntax

- OpenMP Directives: Sentinel, construct, and clauses

  #pragma omp construct [clause [[,]clause]…] C

- Example

  #pragma omp parallel private(i) reduction(+:sum) C

- Most OpenMP constructs apply to a “structured block”, that is, a block of one or more statements with one point of entry at the top and one point of exit at the bottom.

Worksharing Loop: C/C++

```
1  #pragma omp parallel for
2   for (i=0; i<N; i++)
3   {
4     a[i] = b[i] + c[i];
5   }
6
```

General form:

```
#pragma omp parallel
{
   #pragma omp for
   for (i=0; i<N; i++)
   {a[i] = b[i] + c[i];}
}
```

Line 1 Team of threads formed (parallel region).

Lines 2–6 Loop iterations are split among threads.
Implied barrier at end of block(s) {}.

Each loop iteration must be independent of other iterations

(at a minimum, compiler will complain and your loop won't be parallelized).

OpenMP Clauses

- *Directives* dictate what the OpenMP thread team will do
  - *Parallel regions* are marked by the **`parallel`** directive
  - *Worksharing loops* are marked by **`do`**, **`for`** directives (Fortran, C/C++)
- *Clauses* control the behavior of any particular OpenMP directive
  1. Scoping of variables: **`private`**, **`shared`**, **`default`**
  2. Initialization of variables: **`copyin`**, **`firstprivate`**
  3. Scheduling: **`static`**, **`dynamic`**, **`guided`**
  4. Conditional application: **`if`**
  5. Number of threads in team: **`num_threads`**

Illustration of a Race Condition

Intended

Thread 0		Thread 1		Value
read	←			0
increment				0
write	→			1
		read	←	1
		increment		1
		write	→	2

Possible…

Thread 0		Thread 1		Value
				0
read	←			0
increment		read	←	0
write	→	increment		1
		write	→	1
				1

- In a critical section, need *mutual exclusion* (mutex) to get intended result
  - Only use when needed; incurs a performance penalty due to serial execution
- The following OpenMP directives prevent this race condition:

#pragma omp critical – for a code block (C/C++)
#pragma omp atomic – for single statements

OpenMP Reduction

- Recall previous example of parallel dot product
  - Simple parallel-for doesn't work due to race condition on shared **sum**
  - Best solution is to apply OpenMP's reduction clause
  - Doing private partial sums is fine too; add a critical section for **sum** of **ps**

```
// repetitive updates: oops
#pragma omp parallel for
for (i=0; i<N; i++)
     sum = sum + b[i]*c[i];
```

```
// repetitive reduction: OK
#pragma omp parallel for \
     reduction(+:sum)
for (i=0; i<N; i++)
     sum = sum + b[i]*c[i];
```

```
// repetitive updates: OK
int ps = 0;
#pragma omp parallel \
      firstprivate(ps)
{
#pragma omp for
   for (i=0; i<N; i++)
      ps = ps + b[i]*c[i];
#pragma omp critical
   sum = sum + ps; }
```

Runtime Library Functions

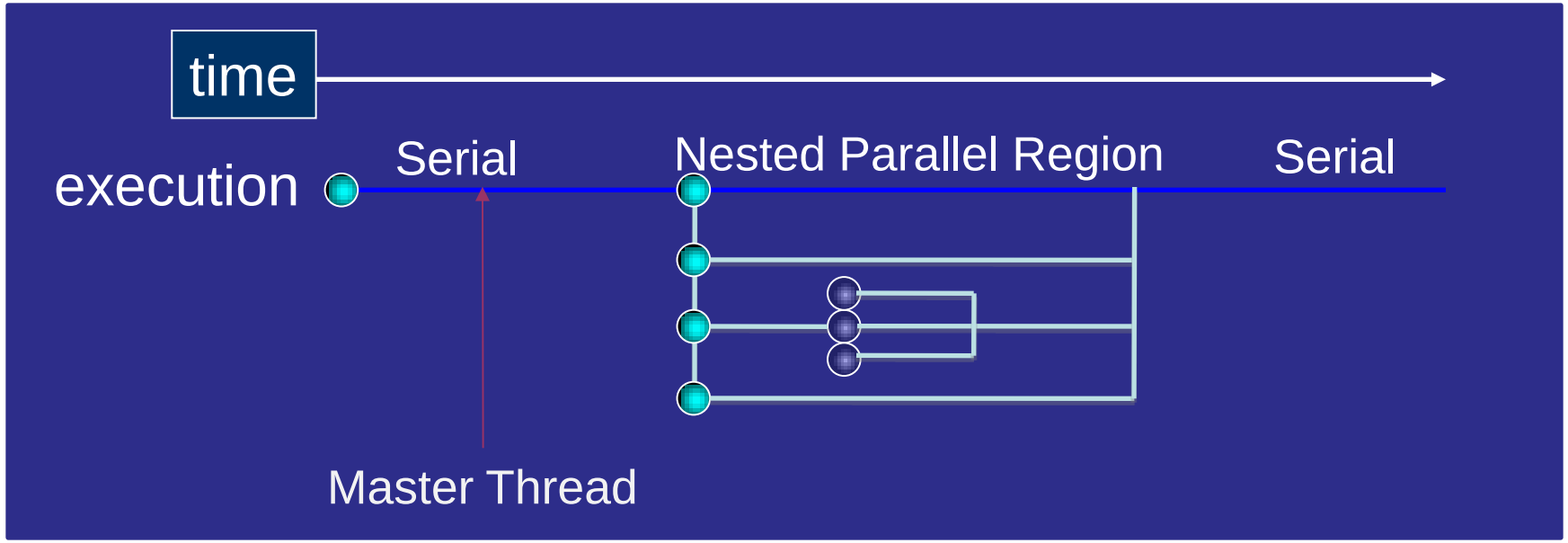
`omp_get_num_threads()`	Number of threads in current team
`omp_get_thread_num()`	Thread ID, {0: N-1}
`omp_get_max_threads()`	Number of threads in environment, **`OMP_NUM_THREADS`**
`omp_get_num_procs()`	Number of machine CPUs
`omp_in_parallel()`	True if in parallel region & multiple threads are executing
`omp_set_num_threads(#)`	Changes number of threads for parallel region, if dynamic threading is enabled

Environment Variables, More Functions

- To control the OpenMP runtime environment

`OMP_NUM_THREADS`	Set to permitted number of threads: this is the value returned by **`omp_get_max_threads()`**
`OMP_DYNAMIC`	TRUE/FALSE for enable/disable dynamic threading by calling **`omp_set_num_threads`** (can also use a function to do this).

Loop Nesting in 3.0



- OpenMP 3.0 supports nested parallelism, older implementations may ignore the nesting and serialize inner parallel regions.
- A nested parallel region can specify any number of threads to be used for the thread team, new id's are assigned.

MPI: Message Passing

- Overview
- Basics
  - Hello World in MPI
  - Compiling and running MPI programs (LAB)
- MPI messages
- Point-to-point communication
  - Deadlock and how to avoid it (LAB)
- Collective communication

Overview Introduction

- What is message passing?
  - Sending and receiving messages between *tasks* or *processes*
  - Includes performing operations on data in transit and synchronizing tasks
- Why send messages?
  - Clusters have distributed memory, i.e. each process has its own address space and no way to get at another's
- How do you send messages?
  - Programmer makes use of an Application Programming *Interface* (API)
    - In this case, MPI.
  - MPI specifies the functionality of high-level communication routines
  - MPI's functions give access to a low-level *implementation* that takes care of sockets, buffering, data copying, message routing, etc.

Overview API for Distributed Memory Parallelism

- Assumption: processes do not see each other's memory
  - Some systems overcome this assumption
    - GAS (Global Address Space) abstraction and variants
- Communication speed is determined by some kind of network
  - Typical network = switch + cables + adapters + software stack…
- Key: the *implementation* of MPI (or any message passing API) can be optimized for any given network
  - Expert-level performance
  - No code changes required
  - Works in shared memory, too

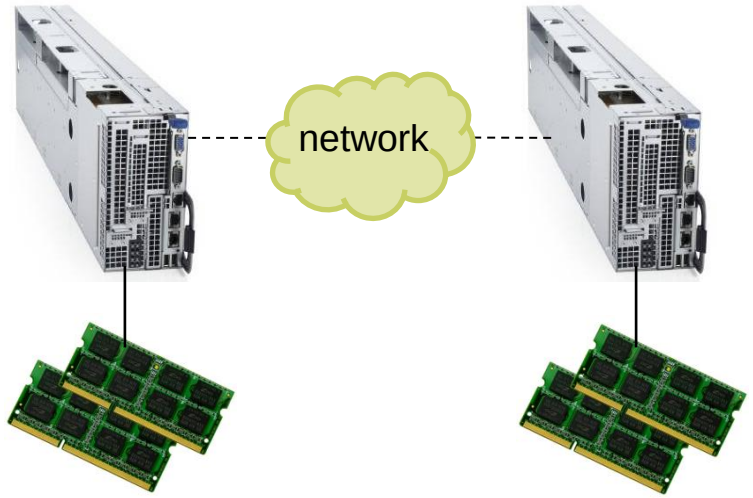


Image of Dell PowerEdge C8220X: http://www.theregister.co.uk/2012/09/19/dell_zeus_c8000_hyperscale_server/

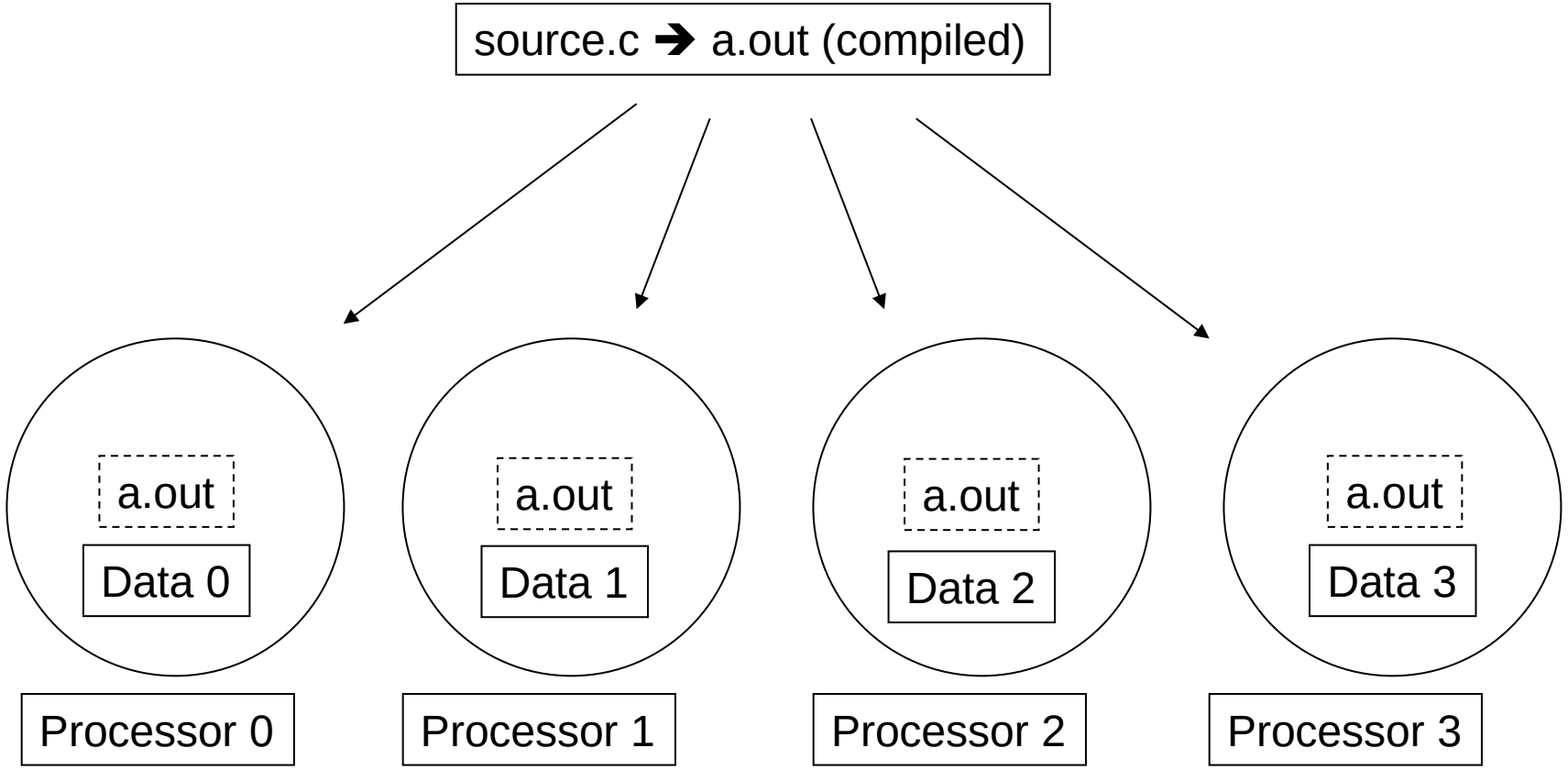
Overview Why Use MPI?

- MPI is a de facto standard for distributed memory computing
  - Public domain versions are easy to install
  - Vendor-optimized version are available on most hardware
- MPI is “tried and true”
  - MPI-1 was released in 1994, MPI-2 in 1996, and MPI-3 in 2012.
- MPI applications can be fairly portable
- MPI is a good way to learn parallel programming
- MPI is expressive: it can be used for many different models of computation, therefore can be used with many different applications
- MPI code is efficient (though some think of it as the “assembly language of parallel processing”)
- MPI has freely available implementations (e.g., MPICH, OpenMPI)

MPI and Single Program, Multiple Data (SPMD)

- One source code is written
- Same program runs multiple times, but each time with different data
- With MPI
  - Code can have conditional execution based on which processor is executing the copy: choose data
  - All copies of code are started simultaneously and may communicate and sync with each other periodically
  - Conclusion: MPI allows more SPMD programs than embarrassingly parallel applications

SPMD Programming Model



Basics Simple MPI

Here is the basic outline of a simple MPI program :

- Include the implementation-specific header file –

  #**include <mpi.h>** inserts basic definitions and types
- Initialize communications –

  MPI_Init initializes the MPI environment
  MPI_Comm_size returns the number of processes
  MPI_Comm_rank returns this process's number (rank)
- Communicate to share data between processes –

  MPI_Send sends a message
  MPI_Recv receives a message
- Exit from the message-passing system –

  MPI_Finalize

Basics Minimal Code Example: hello_mpi.c

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>
main(int argc, char **argv)
{
   char message[20];
   int i, rank, size, tag = 99;
   MPI_Status status;
   MPI_Init(&argc, &argv);
   MPI_Comm_size(MPI_COMM_WORLD, &size);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   if (rank == 0) {
      strcpy(message, "Hello, world!");
      for (i = 1; i < size; i++)
         MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);
   } else {
      MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);
   }
   printf("Message from process %d : %.13s\n", rank, message);
   MPI_Finalize();
}
```

Basics Initialize and Close Environment

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>
main(int argc, char **argv)
{
  char message[20];
  int i, rank, size, tag = 99;
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  if (rank == 0) {
    strcpy(message, "Hello, world!");
    for (i = 1; i < size; i++)
      MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);
  } else
    MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);
  printf("Message from process %d : %.13s\n", rank, message);
  MPI_Finalize();
}
```

Initialize MPI environment

An implementation may also use this call as a mechanism for making the usual argc and argv command-line arguments from “main” available to all tasks (C language only).

Close MPI environment

Basics Query Environment

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>
main(int argc, char **argv)
{
  char message[20];
  int i, rank, size, tag = 99;
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  if (rank == 0) {
    strcpy(message, "Hello, world!");
    for (i = 1; i < size; i++)
      MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);
  } else
    MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);
  printf("Message from process %d : %.13s\n", rank, message);
  MPI_Finalize();
}
```

Returns number of processes
This, like nearly all other MPI functions, must be called after MPI_Init and before MPI_Finalize. Input is the name of a communicator (MPI_COMM_WORLD is the global communicator) and output is the size of that communicator.

Returns this process' number, or rank
Input is again the name of a communicator and the output is the rank of this process in that communicator.

Basics Pass Messages

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>
main(int argc, char **argv)
{
   char message[20];
   int i, rank, size, tag = 99;
   MPI_Status status;
   MPI_Init(&argc, &argv);
   MPI_Comm_size(MPI_COMM_WORLD, &size);
   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
   if (rank == 0) {
      strcpy(message, "Hello, world!");
      for (i = 1; i < size; i++)
         MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);
   } else
      MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);
   printf("Message from process %d : %.13s\n", rank, message);
   MPI_Finalize();
}
```

Send a message
Blocking send of data in the buffer.

Receive a message
Blocking receive of data into the buffer.

Basics Compiling MPI Programs

- Generally, one uses a special compiler or wrapper script
  - Not defined by the standard
  - Consult your implementation
  - Correctly handles include path, library path, and libraries
- On Stampede 2, use MPICH-style wrappers (the most common)

```
mpicc -o foo foo.c
mpicxx -o foo foo.cc
mpif90 -o foo foo.f
```
(also mpif77)

  - Choose compiler+MPI with “module load” (default, Intel17+Intel MPI)

Basics Running MPI Programs

- To run a simple MPI program, use MPICH-style commands

  (Can't do this on login nodes!)

  `mpirun -n 4 ./foo` (usually mpirun is just a soft link to…)

  `mpiexec -n 4 ./foo`

- Some options for running

  `-n` -- states the number of MPI processes to launch

  `-wdir <dirname>` -- starts in the given working directory

  `--help` -- shows all options for *mpirun*

- To run over Stampede 2's Omni-Path (as part of a batch script)

  `ibrun ./foo` (Can't do this on login nodes either!)

  `ibrun –help ### This is OK!`

  – The scheduler handles the rest

- Note: *mpirun*, *mpiexec*, and compiler wrappers are not part of MPI, but they can be found in nearly all implementations

Basics Creating an MPI Batch Script

- To submit a job to the compute nodes on Stampede, you must first create a SLURM batch script with the commands you want to run.

```
#!/bin/bash
#SBATCH -J myMPI            # job name
#SBATCH -o myMPI.o%j        # output file (%j = jobID)
#SBATCH -e myMPI.err%j      # Direct error to the error file
#SBATCH -N 1                # number of nodes requested
#SBATCH -n 16               # number of MPI (total) tasks requested
#SBATCH -p normal           # queue (partition)
#SBATCH -t 00:01:00         # run time (hh:mm:ss)
#SBATCH -A TG-TRA140011     # account number

echo 2000 > input
ibrun ./myprog < input      # run MPI executable "myprog"
```

Basics LAB: Submitting MPI Programs

- Obtain the **hello_mpi.c** source code:

```
cd IntroMPI_lab/hello
```

- Compile the code using **mpicc** to output the executable **hello_mpi**
- Modify the **myMPI.sh** batch script to run **hello_mpi**
  - Do you really need the “echo” command, e.g.?
  - (see myMPI_solution.sh for corrections)
- Submit the batch script to SLURM, the batch scheduler
  - Check on progress until the job completes
  - Examine the output file

```
sbatch --reservation=CAC2 -p normal myMPI.sh
# see myMPI_solution.sh for hints
squeue -u <my_username>
less myMPI.o*
```

Messages Three Parameters Describe the Data

MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);

MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);

Type of data, should be same for send and receive
MPI_Datatype type

Number of elements (items, not bytes)
Recv number should be greater than or equal to amount sent
int count

Address where the data start
void data*

Messages Three Parameters Specify Routing

MPI_Send(message, 13, MPI_CHAR, i, tag, MPI_COMM_WORLD);

MPI_Recv(message, 20, MPI_CHAR, 0, tag, MPI_COMM_WORLD, &status);

Identify process you're communicating with by rank number
int dest/src

Arbitrary tag number, must match up (receiver can specify MPI_ANY_TAG to indicate that any tag is acceptable)
int tag

Communicator specified for send and receive must match, no wildcards
MPI_Comm comm

Returns information on received message
MPI_Status status*

Messages Fortran Notes

```
mpi_send (data, count, type, dest, tag, comm, ierr)
mpi_recv (data, count, type, src,  tag, comm, status, ierr)
```

- A few Fortran particulars
  - All Fortran arguments are passed by reference
  - *INTEGER ierr:* variable to store the error code (in C/C++ this is the return value of the function call)

- Wildcards are allowed in C and Fortran
  - *src* can be the wildcard MPI_ANY_SOURCE
  - *tag* can be the wildcard MPI_ANY_TAG
  - *status* returns information on the source and tag
  - Receiver might check *status* when wildcards are used, e.g., to check sender rank

Point to Point Topics

- MPI_Send and MPI_Recv: how simple are they really?
- Blocking vs. non-blocking send and receive
- Ways to specify synchronous or asynchronous communication
- Reducing overhead: ready mode, standard mode
- Combined send/receive
- Deadlock, and how to avoid it

Point to Point Blocking vs. Non-Blocking

MPI_Send, MPI_Recv

A ***blocking*** call suspends execution of the process until the message buffer being sent/received is safe to use.

MPI_Isend, MPI_Irecv

A ***non-blocking*** call just initiates communication; the status of data transfer and the success of the communication must be verified later by the programmer (MPI_Wait or MPI_Test).

Point to Point Send and Recv: So Many Choices

The communication mode indicates how the message should be *sent*.

Communication Mode	Blocking Routines	Non-Blocking Routines
Synchronous	MPI_Ssend	MPI_Issend
Ready	MPI_Rsend	MPI_Irsend
Buffered	MPI_Bsend	MPI_Ibsend
Standard	MPI_Send	MPI_Isend
	MPI_Recv	MPI_Irecv
	MPI_Sendrecv	
	MPI_Sendrecv_replace	

Note: the receive routine does not specify the communication mode -- it is simply blocking or non-blocking.

Point to Point MPI_Sendrecv

```
MPI_Sendrecv(sendbuf,sendcount,sendtype,dest,sendtag,
             recvbuf,recvcount,recvtype,source,recvtag,
             comm,status)
```

- Good for two-way communication between a pair of nodes, in which each one sends and receives a message
- However, destination and source need not be the same (ring, e.g.)
- Equivalent to blocking send + blocking receive
- Send and receive use the same communicator but have distinct tags

Point to Point Two-Way Communication: Deadlock!

- **Deadlock 1**

```
IF (rank==0) THEN
  CALL MPI_RECV (recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ie)
  CALL MPI_SEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
ELSEIF (rank==1) THEN
  CALL MPI_RECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ie)
  CALL MPI_SEND (sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,ie)
ENDIF
```

- **Deadlock 2**

```
IF (rank==0) THEN
  CALL MPI_SSEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
  CALL MPI_RECV (recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ie)
ELSEIF (rank==1) THEN
  CALL MPI_SSEND (sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,ie)
  CALL MPI_RECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ie)
ENDIF
```

  - MPI_Send has same problem for count*MPI_REAL > 12K (the MVAPICH2 “eager threshold”; it’s 256K for Intel MPI)

Basics LAB: Deadlock

- cd to **IntroMPI_lab/deadlock**
- Compile the C or Fortran code to output the executable **deadlock**
- Create a batch script including no #SBATCH parameters:

```
cat > sr.sh
#!/bin/sh
ibrun ./deadlock
```
[ctrl-D to exit cat]

- Submit the job, specifying parameters on the command line

```
sbatch -N 1 -n 8 --reservation=CAC2 -p normal -t 00:00:30 -A TG-TRA140011 sr.sh
```

- Check job progress with **squeue**; check output with **less**.
- The program will not end normally. Edit the source code to eliminate deadlock (e.g., use **sendrecv**) and resubmit until the output is good.

Point to Point Deadlock Solutions

- Solution 1

```
IF (rank==0) THEN
  CALL MPI_SEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
  CALL MPI_RECV (recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ie)
ELSEIF (rank==1) THEN
  CALL MPI_RECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ie)
  CALL MPI_SEND (sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,ie)
ENDIF
```

- Solution 2

```
IF (rank==0) THEN
  CALL MPI_SENDRECV (sendbuf,count,MPI_REAL,1,tag, &
                     recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ie)
ELSEIF (rank==1) THEN
  CALL MPI_SENDRECV (sendbuf,count,MPI_REAL,0,tag, &
                     recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ie)
ENDIF
```

Point to Point More Deadlock Solutions

- Solution 3

```
IF (rank==0)    THEN
  CALL MPI_IRECV (recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,req,ie)
  CALL MPI_SEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
ELSEIF (rank==1) THEN
  CALL MPI_IRECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,req,ie)
  CALL MPI_SEND (sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,ie)
ENDIF
CALL MPI_WAIT (req,status)
```

- Solution 4

```
IF (rank==0) THEN
  CALL MPI_BSEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
  CALL MPI_RECV (recvbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,status,ie)
ELSEIF (rank==1) THEN
  CALL MPI_BSEND (sendbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,ie)
  CALL MPI_RECV(recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,status,ie)
ENDIF
```

Point to Point Two-way Communications: Summary

	Task 0	Task 1
Deadlock 1	Recv/Send	Recv/Send
Deadlock 2	Send/Recv	Send/Recv
Solution 1	Send/Recv	Recv/Send
Solution 2	Sendrecv	Sendrecv
Solution 3	Irecv/Send, Wait	(I)recv/Send, (Wait)
Solution 4	Bsend/Recv	(B)send/Recv

Collective Motivation

- What if one task wants to send to *everyone*?

```
if (mytid == 0) {
  for (tid=1; tid<ntids; tid++) {
    MPI_Send( (void*)a, /* target= */ tid, … );
  }
} else {
  MPI_Recv( (void*)a, 0, … );
}
```

- Implements a very naive, serial broadcast
- Too primitive
  - Leaves no room for the OS / switch to optimize
  - Leaves no room for more efficient algorithms
- Too slow

Collective Overview

- Collective calls involve ALL processes within a communicator
- There are 3 basic types of collective communications:
  - Synchronization (MPI_Barrier)
  - Data movement (MPI_Bcast/Scatter/Gather/Allgather/Alltoall)
  - Collective computation/reduction (MPI_Reduce/Allreduce/Scan)
- Programming considerations & restrictions
  - Blocking operation (also non-blocking in MPI-3)
  - No use of message tag argument
  - Collective operations within subsets of processes require separate grouping and new communicator

Collective Barrier Synchronization, Broadcast

- *Barrier* blocks until all processes in comm have called it
  - Useful when measuring communication/computation time

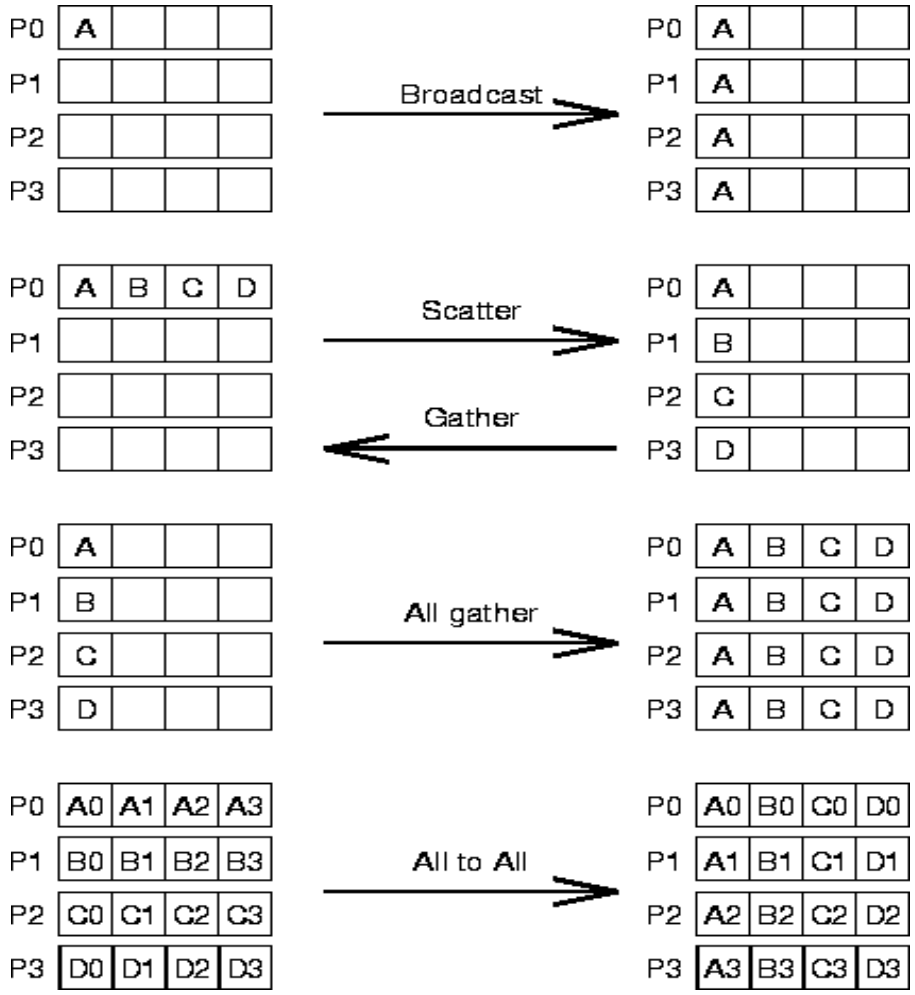
```
mpi_barrier(comm, ierr)
MPI_Barrier(comm)
```

- *Broadcast* sends data from root to all processes in comm
  - Again, blocks until all tasks have called it

```
mpi_bcast(data, count, type, root, comm, ierr)
MPI_Bcast(data, count, type, root, comm)
```

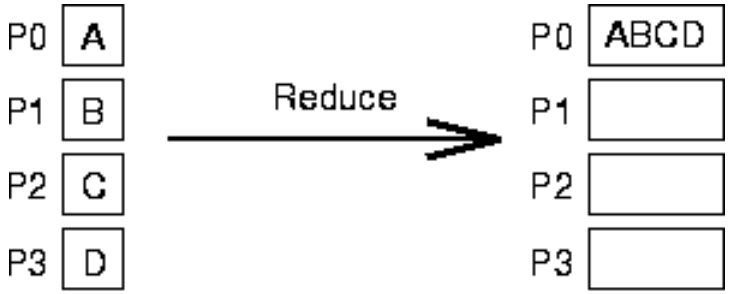
Collective Data Movement

- Broadcast
- Scatter/Gather
- Allgather
- Alltoall

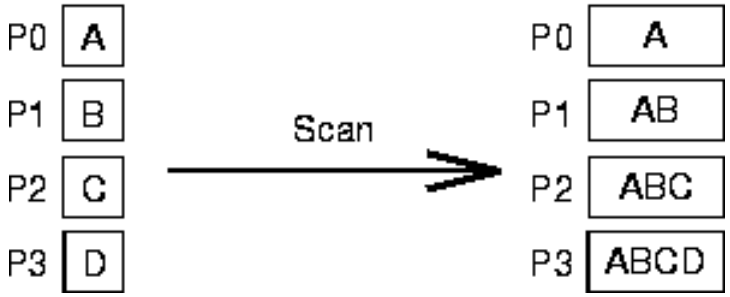


Collective Reduction Operations

- Reduce



- Scan (Prefix)



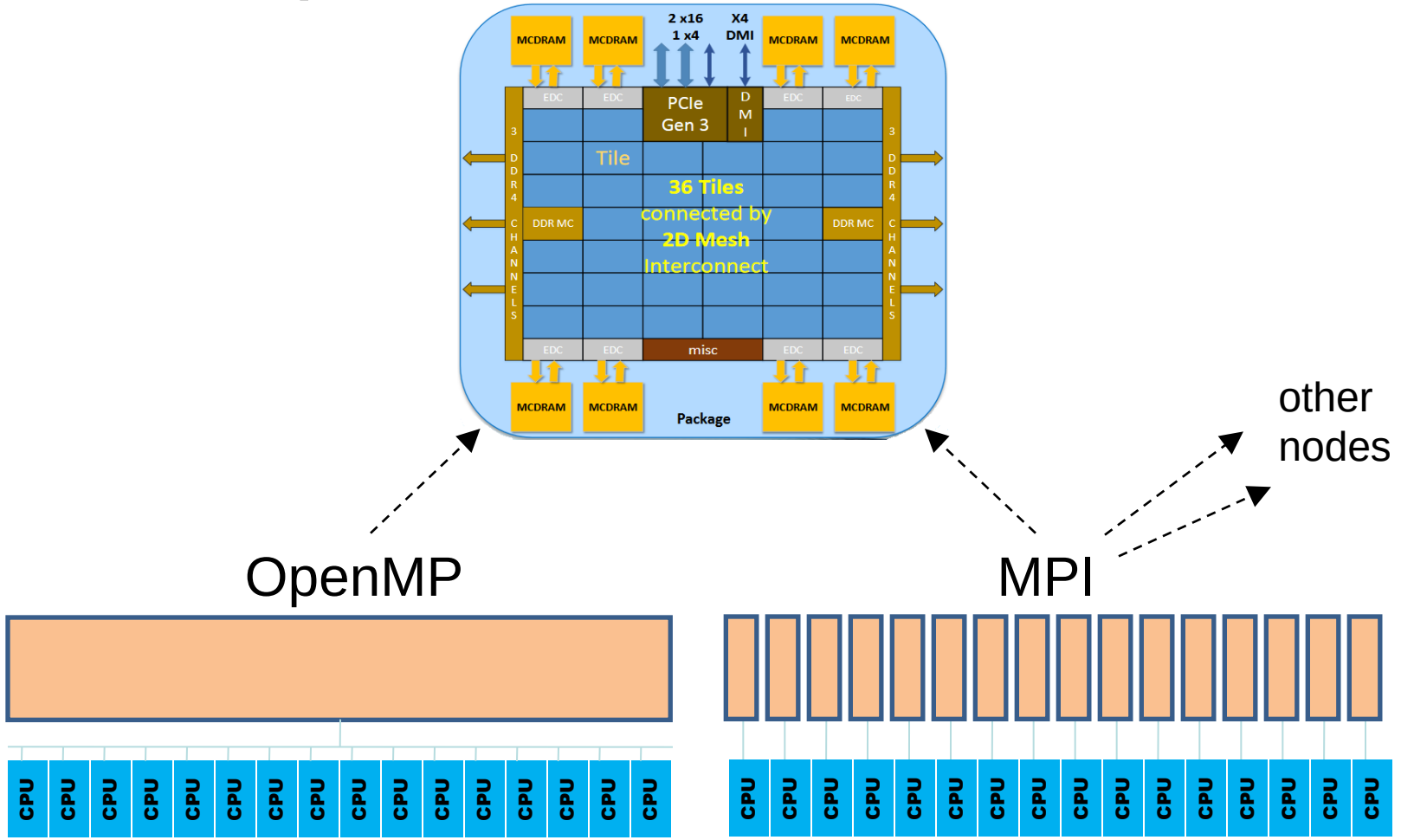
Collective Reduction Operations

Name	Meaning
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical and
MPI_BAND	Bit-wise and
MPI_LOR	Logical or
MPI_BOR	Bit-wise or
MPI_LXOR	Logical xor
MPI_BXOR	Logical xor
MPI_MAXLOC	Max value and location
MPI_MINLOC	Min value and location

Hybrid Why use OpenMP and MPI?

- Try to exploit the whole shared/distributed memory hierarchy
- Memory is insufficient within one node
  - ***Essential concept for KNL, need to take advantage of shared data within process***
  - ***Note:*** Each of Stampede 2's KNL nodes has 96GB of main memory
    - Remember, MCDRAM (16GB) is used as cache by default.
  - To run 1 process (rank) per node, have **`sbatch -N x -n y,`** with x == y, e.g.:
  - **`#SBATCH -N 64`** **`# number of nodes requested`**
  - **`#SBATCH -n 64`** **`# number of MPI (total) tasks requested`**

Two Views of a Stampede 2 Node



Threading Example: One MPI, Many OpenMP

C

```
#include <mpi.h>
int main(int argc,
  char **argv) {
int rank, size, ie, i;
ie= MPI_Init(&argc,&argv[]);
ie= MPI_Comm_rank(...&rank);
ie= MPI_Comm_size(...&size);
//Setup shared mem, comp/comm

#pragma omp parallel for
  for(i=0; i<n; i++){
    <work>
  }

// compute & communicate
ie= MPI_Finalize();
}
```

Some Programming Models for Intel MIC

- **OpenMP**
  - On Stampede 2, TACC expects that this is the most approachable programming model for HPC users
- Intel Threading Building Blocks (TBB)
  - For C++ programmers
- Intel Cilk Plus
  - Task-oriented add-ons for OpenMP
  - Currently for C++ programmers, may become available for Fortran
- Intel Math Kernel Library (MKL)
  - MKL is inherently parallelized with OpenMP
- CAF (Actor model) library
  - Lightweight message passing
    - (actors per thread instead of threads per task, as in Hybrid OpenMP+MPI)
  - One API for distributed and shared memory programming
  - Partially fault-tolerant (compare to MPI)

References

- Standards
  - OpenMP: http://www.openmp.org/specifications/
    - All of v4 and most of v4.5 supported by Intel Compiler 17: https://software.intel.com/en-us/node/684308
  - MPI: http://mpi-forum.org/docs/mpi-3.1/index.htm (Supported by Intel '17)
- CAC Virtual workshop: https://cvw.cac.cornell.edu/topics
  - Covers MPI and OpenMP in more detail
  - Corresponding Fortran examples
  - More references!

The End

OpenMP Worksharing

Use OpenMP directives to specify worksharing in a parallel region, as well as synchronization

```
#pragma omp parallel
{
        #pragma omp
} // end parallel
```

Code block	*Thread action*
`for`	Worksharing
`sections`	Worksharing
`single`	One thread
`master`	One thread
`critical`	One thread at a time

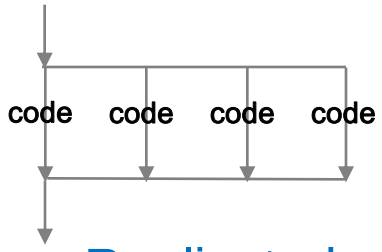
```
parallel do/for
parallel sections
```

Directives can be combined, if a parallel region has just one worksharing construct.

OpenMP Parallel Directives

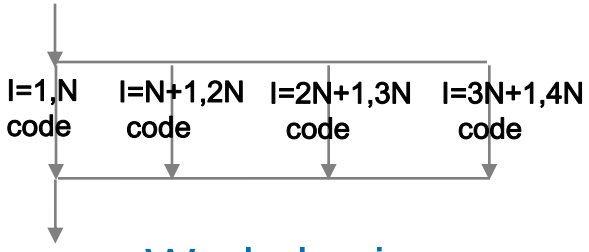
- Replicated – executed by all threads
- Worksharing – divided among threads

```
PARALLEL
  {code}
END PARALLEL
```



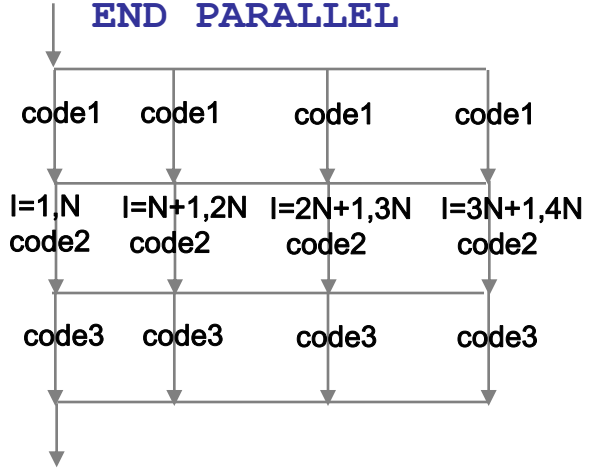
Replicated

```
PARALLEL DO
  do I = 1,N*4
    {code}
  end do
END PARALLEL DO
```



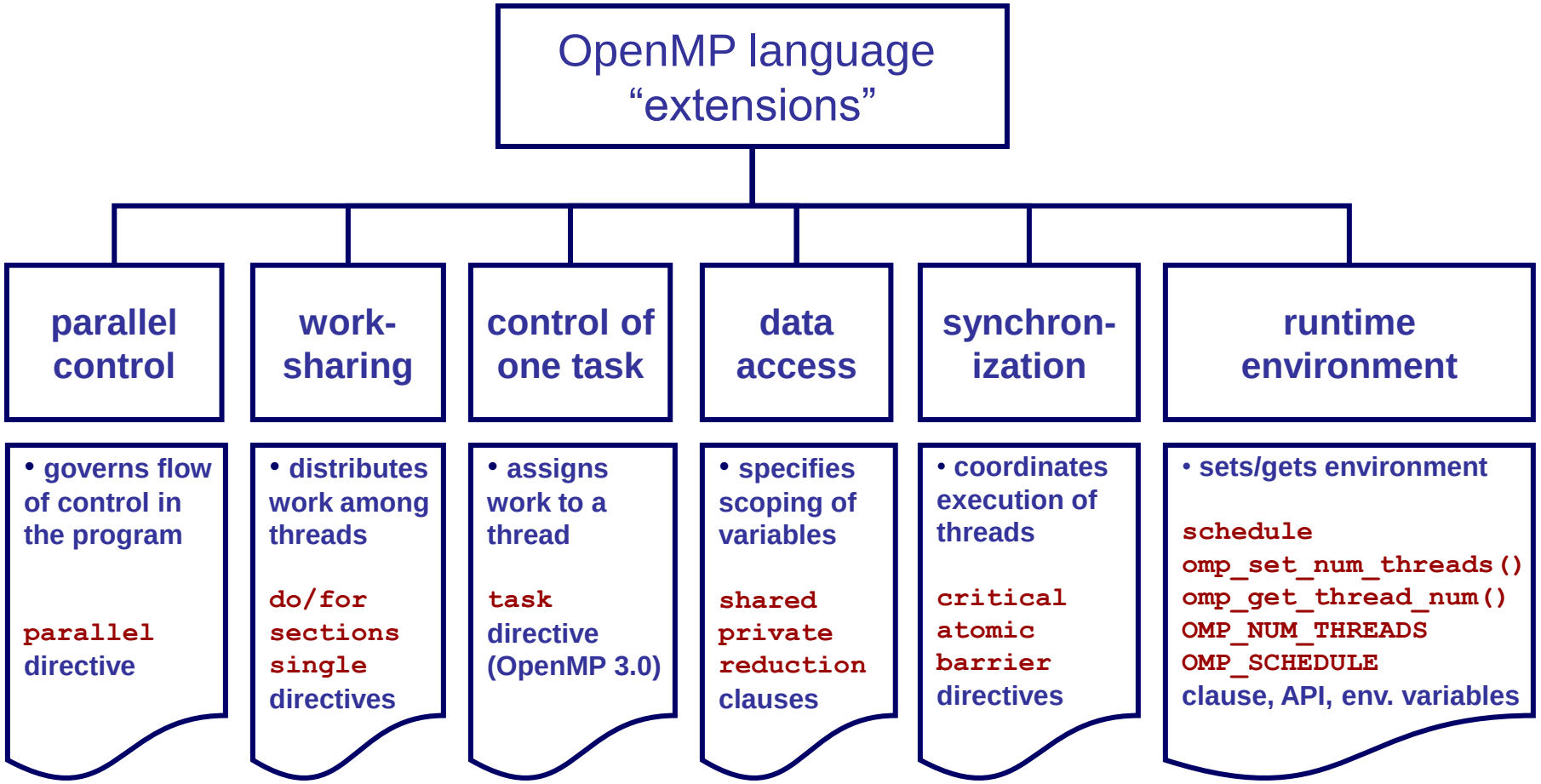
Worksharing

```
PARALLEL
    {code1}
DO
  do I = 1,N*4
    {code2}
  end do
    {code3}
END PARALLEL
```



Combined

OpenMP Constructs



Private, Shared Clauses

- In the following loop, each thread needs a private copy of temp
  - The result would be unpredictable if temp were shared, because each processor would be writing and reading to/from the same location

```
!$omp parallel do private(temp,i) shared(A,B,C)
      do i=1,N
         temp = A(i)/B(i)
         C(i) = temp + cos(temp)
      enddo
!$omp end parallel do
```

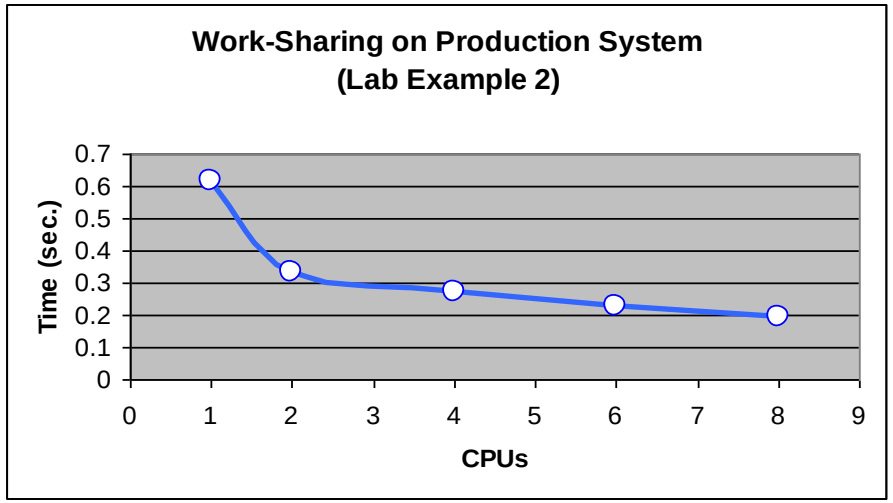
  - A “lastprivate(temp)” clause will copy the last loop (stack) value of temp to the (global) temp storage when the parallel DO is complete
  - A “firstprivate(temp)” initializes each thread’s temp to the global value

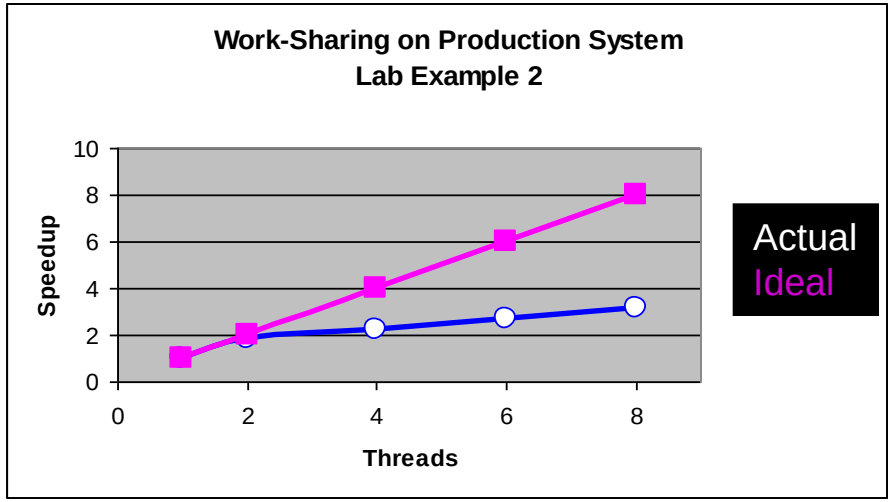
Worksharing Results

Speedup =
cputime(1) / cputime(N)

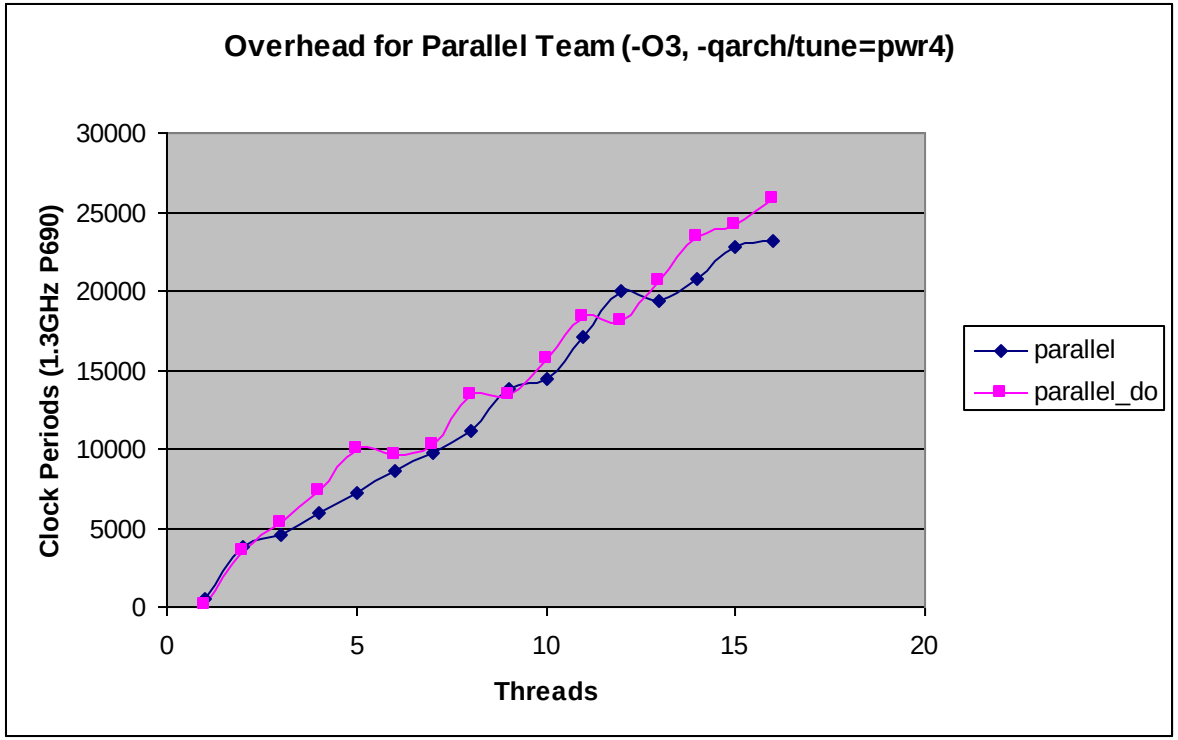
If work is completely parallel, scaling is linear.

Scheduling, memory contention and overhead can impact speedup and Gflop/s rate.





Overhead to Fork a Thread Team



- Increases roughly linearly with number of threads

Additional Topics to Explore…

- Schedule clause: specify how to divide work among threads

  `schedule(static)` `schedule(dynamic,M)`

- Reduction clause: perform collective operations on shared variables

  `reduction(+:asum)` `reduction(*:aprod)`

- Nowait clause: remove the barrier at the end of a parallel section

  `for ... nowait` `end do nowait`

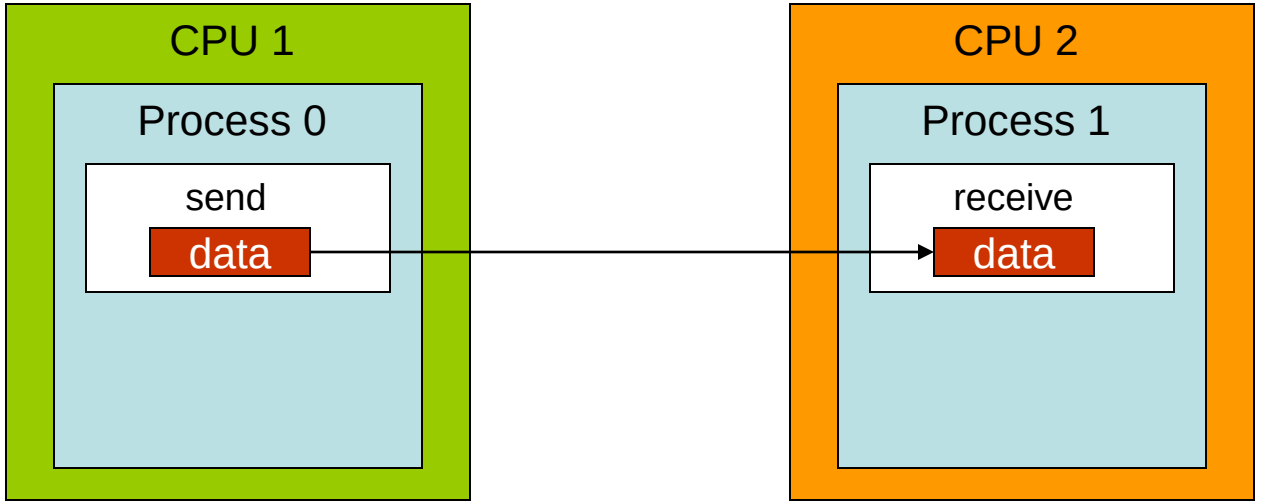
- Lock routines: make mutual exclusion more lightweight and flexible

  `omp_init_lock(var)` `omp_set_lock(var)`

- Rectangular loop parallelization made simple

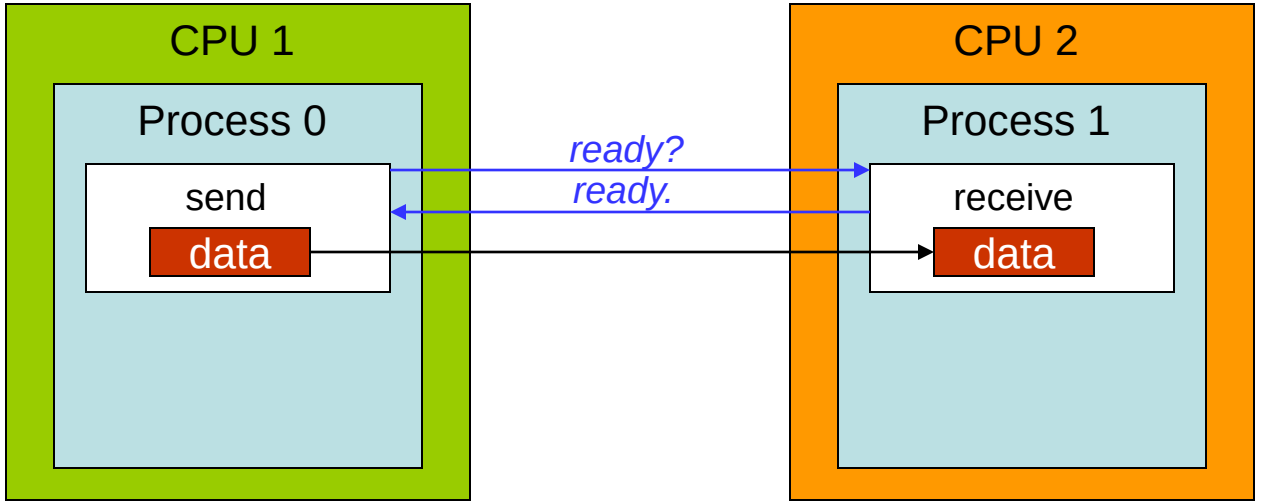
  `collapse(n)`

Point to Point Send and Recv: Simple?



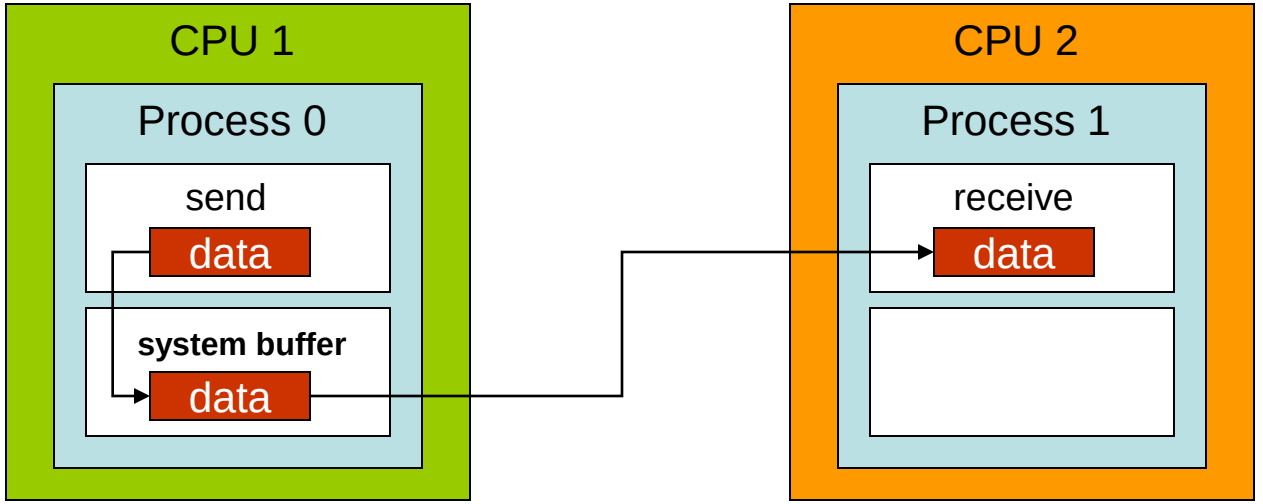
- Sending data ***from*** one point (process/task)
  to another point (process/task)
- One task sends while another receives
- But what if process 1 isn't **ready** for the message from process 0?…
- MPI provides different communication modes in order to help

Point to Point Synchronous Send, MPI_Ssend



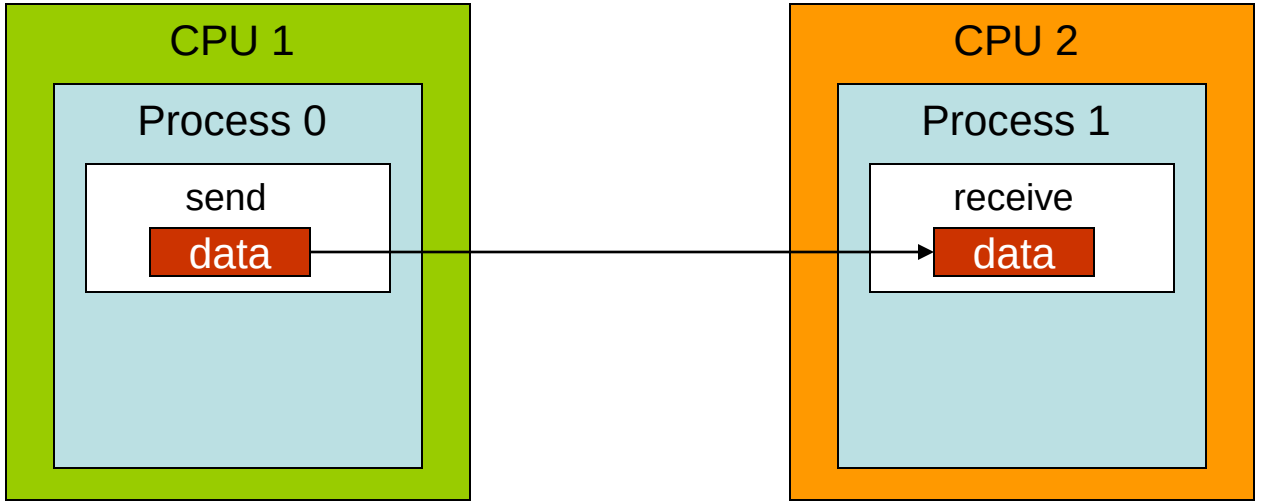
- Handshake procedure ensures both processes are ready
- It's likely that one of the processes will end up waiting
  - If the *send* call occurs first: sender waits
  - If the *receive* call occurs first: receiver waits
- Waiting and an extra handshake? – this could be slow

Point to Point Buffered Send, MPI_Bsend



- Message data are copied to a system-controlled block of memory
- Process 0 continues executing other tasks without waiting
- When process 1 is ready, it fetches the message from the remote system buffer and stores it in the appropriate memory location
- Must be preceded with a call to MPI_Buffer_attach

Point to Point Ready Send, MPI_Rsend

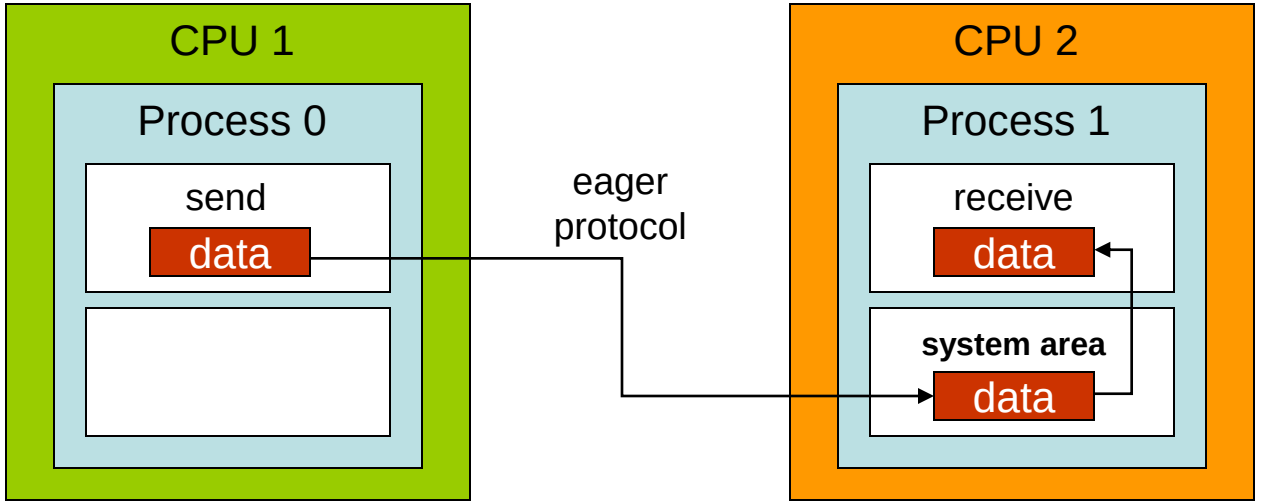


- Process 0 just assumes process 1 is ready! The message is sent!
- Truly simple communication, no extra handshake or copying
- But an error is generated if process 1 is unable to receive
- Only useful when logic dictates that the receiver *must* be ready

Point to Point Overhead

- **System overhead**
  Buffered send has more system overhead due to the extra copy operation.
- **Synchronization overhead**
  Synchronous send has no extra copying but more waiting, because a handshake must arrive before the send can occur.
- **MPI_Send**
  Standard mode tries to trade off between the types of overhead.
  - Large messages use the "rendezvous protocol" to avoid extra copying: a handshake procedure establishes direct communication.
  - Small messages use the "eager protocol" to avoid synchronization cost: the message is quickly copied to a small system buffer on the receiver.

Point to Point Standard Send, Eager Protocol



- Message goes a system-controlled area of memory *on the receiver*
- Process 0 continues executing other tasks; when process 1 is ready to receive, the system simply copies the message from the system buffer into the appropriate memory location controlled by process
- *Does not* need to be preceded with a call to MPI_Buffer_attach

Point to Point One-Way Blocking/Non-Blocking

- Blocking send, non-blocking recv

```
IF (rank==0) THEN
  ! Do my work, then send to rank 1
  CALL MPI_SEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,ie)
ELSEIF (rank==1) THEN
  CALL MPI_IRECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,req,ie)
  ! Do stuff that doesn't yet need recvbuf from rank 0
  CALL MPI_WAIT (req,status,ie)
  ! Do stuff with recvbuf
ENDIF
```

- Non-blocking send, non-blocking recv

```
IF (rank==0) THEN
  ! Get sendbuf ready as soon as possible
  CALL MPI_ISEND (sendbuf,count,MPI_REAL,1,tag,MPI_COMM_WORLD,req,ie)
  ! Do other stuff that doesn't involve sendbuf
ELSEIF (rank==1) THEN
  CALL MPI_IRECV (recvbuf,count,MPI_REAL,0,tag,MPI_COMM_WORLD,req,ie)
ENDIF
CALL MPI_WAIT (req,status,ie)
```

Basics LAB: Allreduce

- cd to `IntroMPI_lab/allreduce`
- In the call to MPI_Allreduce, the reduction operation is wrong!
  - Modify the C or Fortran source to use the correct operation
- Compile the C or Fortran code to output the executable **allreduce**
- Submit the **myall.sh** batch script to SLURM, the batch scheduler
  - Check on progress until the job completes
  - Examine the output file

```
sbatch myall.sh
squeue -u <my_username>
less myall.o*
```

- Verify that you got the expected answer

MPI-1

- MPI-1 - Message Passing Interface (v. 1.2)
  - Library standard defined by committee of vendors, implementers, and parallel programmers
  - Used to create parallel SPMD codes based on explicit message passing
- Available on almost all parallel machines with C/C++ and Fortran bindings (and occasionally with other bindings)
- About 125 routines, total
  - 6 basic routines
  - The rest include routines of increasing generality and specificity
- This presentation has primarily covered MPI-1 routines

MPI-2

- MPI-2 includes features left out of MPI-1
  - One-sided communications
  - Dynamic process control
  - More complicated collectives
  - Parallel I/O (MPI-IO)
- Implementations of MPI-2 came along only gradually
  - Not quickly undertaken after the reference document was released (in 1997)
  - Now OpenMPI, MPICH2 (and its descendants), and the vendor implementations are nearly complete or fully complete
- Most applications still rely on MPI-1, plus maybe MPI-IO

MPI-3

- MPI-3 is largely but not strictly compatible with MPI-2
  - One-sided communication
    - Improved support for shared memory models
  - Collective communication
    - Added nonblocking functions
    - Added neighborhood collectives for specifying process topology
  - Added Fortran 2008 bindings
  - Removed C++ bindings; use C bindings from C++ instead
  - MPIT Tool Interface - allows inspection of MPI internal variables
- Not the default implementation on Stampede, but can be used, e.g:
  - `module swap mvapich2/1.9a2 mvapich2-x/2.0b`
  - Some implementations may not be MPI-3 complete.

MPI_COMM MPI Communicators

- Communicators
  - Collections of processes that can communicate with each other
  - Most MPI routines require a communicator as an argument
  - Predefined communicator MPI_COMM_WORLD encompasses all tasks
  - New communicators can be defined; any number can co-exist
- Each communicator must be able to answer two questions
  - *How many processes exist in this communicator?*
  - MPI_Comm_size returns the answer, say, N_p
  - *Of these processes, which process (numerical rank) am I?*
  - MPI_Comm_rank returns the rank of the current process within the communicator, an integer between 0 and N_p-1 inclusive
  - Typically these functions are called just after MPI_Init

MPI_COMM C Example: param.c

```
#include <mpi.h>
main(int argc, char **argv){
   int np, mype, ierr;

   ierr = MPI_Init(&argc, &argv);
   ierr = MPI_Comm_size(MPI_COMM_WORLD, &np);
   ierr = MPI_Comm_rank(MPI_COMM_WORLD, &mype);
            :
   MPI_Finalize();
}
```

MPI_COMM C++ Example: param.cc

```
#include "mpif.h"
[other includes]
int main(int argc, char *argv[]){
   int np,  mype,  ierr;
 [other declarations]
                :
          MPI::Init(argc, argv);
   np   = MPI::COMM_WORLD.Get_size();
   mype = MPI::COMM_WORLD.Get_rank();
                :
         [actual work goes here]
                :
          MPI::Finalize();
}
```

MPI_COMM Fortran Example: param.f90

```
program param
  include 'mpif.h'
  integer ierr, np, mype

  call mpi_init(ierr)
  call mpi_comm_size(MPI_COMM_WORLD, np   , ierr)
  call mpi_comm_rank(MPI_COMM_WORLD, mype, ierr)
            :
  call mpi_finalize(ierr)
end program
```

Point to Point Communication Modes

Mode	Pros	Cons
Synchronous – sending and receiving tasks must 'handshake'.	- Safest, therefore most portable - No need for extra buffer space - SEND/RECV order not critical	Synchronization overhead
Ready- assumes that a 'ready to receive' message has already been received.	- Lowest total overhead - No need for extra buffer space - Handshake not required	RECV *must* precede SEND
Buffered – move data to a buffer so process does not wait.	- Decouples SEND from RECV - No sync overhead on SEND - Programmer controls buffer size	Buffer copy overhead
Standard – defined by the implementer; meant to take advantage of the local system.	- Good for many cases - Small messages go right away - Large messages must sync - Compromise position	Your program may not be suitable

Point to Point C Example: oneway.c

```
#include "mpi.h"
main(int argc, char **argv){
  int ierr, mype, myworld; double a[2];
  MPI_Status status;
  MPI_Comm icomm = MPI_COMM_WORLD;
  ierr = MPI_Init(&argc, &argv);
  ierr = MPI_Comm_rank(icomm, &mype);
  ierr = MPI_Comm_size(icomm, &myworld);
  if(mype == 0){
    a[0] = mype; a[1] = mype+1;
    ierr = MPI_Ssend(a,2,MPI_DOUBLE,1,9,icomm);
  }
  else if (mype == 1){
    ierr = MPI_Recv(a,2,MPI_DOUBLE,0,9,icomm,&status);
    printf("PE %d, A array= %f %f\n",mype,a[0],a[1]);
  }
  MPI_Finalize();
}
```

Point to Point Fortran Example: oneway.f90

```
program oneway
  include "mpif.h"
  real*8,  dimension(2)                  :: A
  integer, dimension(MPI_STATUS_SIZE) :: istat
  icomm = MPI_COMM_WORLD
  call mpi_init(ierr)
  call mpi_comm_rank(icomm,mype,ierr)
  call mpi_comm_size(icomm,np  ,ierr);

  if (mype.eq.0) then
    a(1) = dble(mype); a(2) = dble(mype+1)
    call mpi_send(A,2,MPI_REAL8,1,9,icomm,ierr)
  else if (mype.eq.1) then
    call mpi_recv(A,2,MPI_REAL8,0,9,icomm,istat,ierr)
    print '("PE",i2," received A array =",2f8.4)',mype,A
  endif
  call mpi_finalize(ierr)
end program
```

Collective C Example: allreduce.c

```
#include <mpi.h>
#define WCOMM MPI_COMM_WORLD
main(int argc, char **argv){
  int npes, mype, ierr;
  double sum, val; int calc, knt=1;
  ierr = MPI_Init(&argc, &argv);
  ierr = MPI_Comm_size(WCOMM, &npes);
  ierr = MPI_Comm_rank(WCOMM, &mype);

  val  = (double)mype;
  ierr = MPI_Allreduce(
           &val, &sum, knt, MPI_DOUBLE, MPI_SUM, WCOMM);

  calc = (npes-1 +npes%2)*(npes/2);
  printf(" PE: %d sum=%5.0f calc=%d\n",mype,sum,calc);
  ierr = MPI_Finalize();
}
```

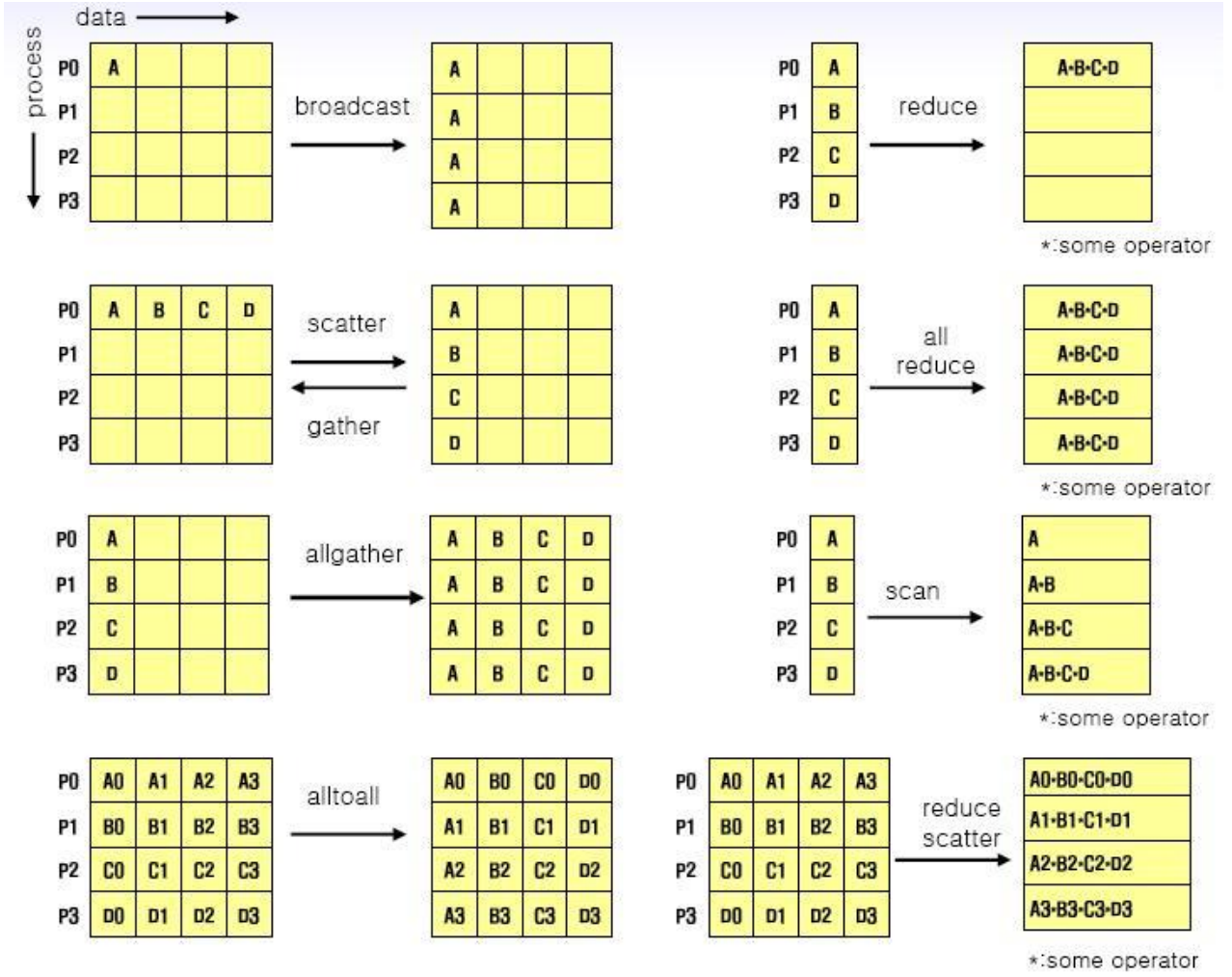
Collective Fortran Example: allreduce.f90

```
program allreduce
  include 'mpif.h'
  double precision :: val, sum
  icomm = MPI_COMM_WORLD
  knt = 1
  call mpi_init(ierr)
  call mpi_comm_rank(icomm,mype,ierr)
  call mpi_comm_size(icomm,npes,ierr)

  val = dble(mype)
  call mpi_allreduce(val,sum,knt,MPI_REAL8,MPI_SUM,icomm,ierr)

  ncalc = (npes-1 + mod(npes,2))*(npes/2)
  print '(" pe#",i5," sum =",f5.0, " calc. sum =",i5)', &
          mype, sum, ncalc
  call mpi_finalize(ierr)
end program
```

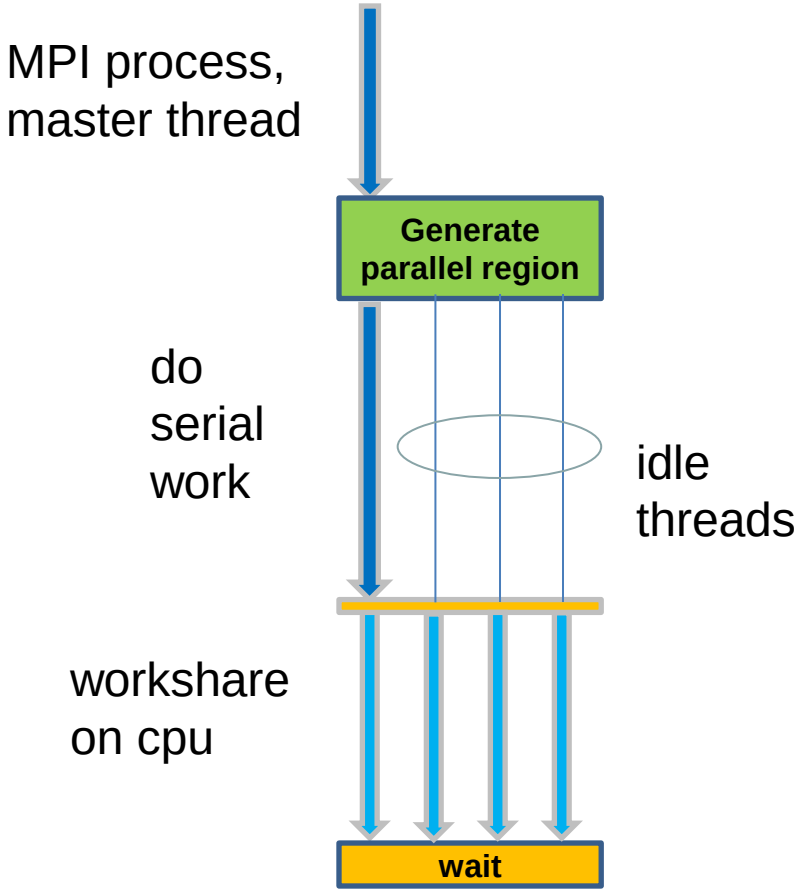
Collective The Collective Collection!



References

- MPI standards
  - http://www.mpi-forum.org/docs/
  - Documents with marked-up changes available
  - Latest version: http://mpi-forum.org/docs/mpi-3.1/index.htm
  - Other mirror sites: http://www.mcs.anl.gov/mpi/
  - Freely available implementations
    - MPICH, http://www.mcs.anl.gov/mpi/mpich
    - Open MPI, http://www.open-mpi.org
- CAC Virtual workshop: https://cvw.cac.cornell.edu/topics
- Books
  - *Using MPI*, by Gropp, Lusk, and Skjellum
  - *MPI Annotated Reference Manual,* by Marc Snir, *et al*
  - *Parallel Programming with MPI*, by Peter Pacheco
  - *Using MPI-2*, by Gropp, Lusk and Thakur

Heterogeneous Threading, Sequential

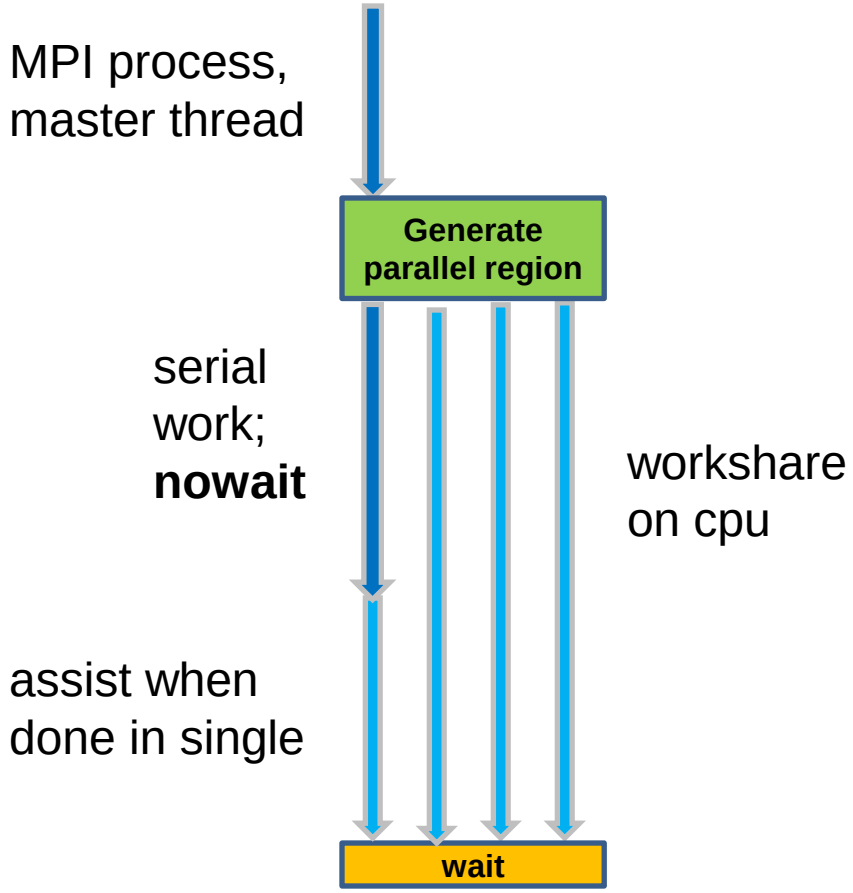


C/C++

```
#pragma omp parallel
 {
#pragma omp single
   { serialWork(); }

#pragma omp for
   for(i=0; i<N; i++){...}
 }
```

Heterogeneous Threading, Concurrent



C/C++

```
#pragma omp parallel
 {
#pragma omp single nowait
   { serialWork(); }

#pragma omp for schedule(dynamic)
   for(i=0; i<N; i++){...}
 }
```