CSC367 Parallel computing

Lecture 14: Distributed Memory Architectures and their Parallel Programming Model-Cont.

The Message Passing Interface (MPI)

MPI standard

- Standard library for message passing
 - Write portable message passing algorithms, mostly using C or Fortran
 - Rich API (over 100 routines, but only a handful are fundamental)
 - Must install OpenMPI or MPICH2, etc.
 - Include mpi.h header
- Example run command: mpirun -np 8 ./myapp arg1 arg2
- Basic routines:

MPI_Init: initialize MPI environment

MPI_Finalize: terminate the MPI environment

MPI_Comm_size: get number of processes

MPI_Comm_rank: get the process ID of the caller

MPI_Send: send message

MPI_Recv: receive message

MPI basics

- MPI_Init: only called once at start by one thread, to initialize the MPI environment
 - int MPI_init(int *argc, char ***argv);
 - Extracts and removes the MPI parts of the command line (e.g., mpirun –np 8) from argv
 - Process your application's command line arguments only after the MPI_Init
 - On success => MPI_SUCCESS, otherwise error code

- MPI_Finalize: called at the end, to do cleanup and terminate the MPI environment
 - int MPI_Finalize();
 - On success => MPI_SUCCESS, otherwise error code
 - No MPI calls allowed after this, not even a new MPI_init!

 These calls are made by all participating processes, otherwise results in undefined behaviour

MPI Communication domains

- MPI communication domain = set of processes which are allowed to communicate with each other
- Communicators (MPI_Comm variables) store info about communication domains
- Common case: all processes need to communicate to all other processes
 - Default communicator: MPI COMM WORLD includes all processes
- In special cases, we may want to perform tasks in separate (or overlapping)
 groups of processes => define custom communicators
 - No messages for a given group will be received by processes in other groups
- Communicator size and id of current process can be retrieved with:

```
int MPI_Comm_size(MPI_Comm comm, int *size);int MPI_Comm_rank(MPI_Comm comm, int *rank);
```

The process calling these routines must be in the communicator comm

Hello (C)

```
#include "mpi.h"
#include <stdio.h>
int main( int argc, char *argv[] )
   int rank, size;
  MPI_Init( &argc, &argv );
   MPI_Comm_rank( MPI_COMM_WORLD, &rank );
   MPI_Comm_size( MPI_COMM_WORLD, &size );
   printf( "I am %d of %d\n", rank, size );
   MPI_Finalize();
   return 0;
```

Timing measurements

- Can use MPI_Wtime()
- Example:

```
double t1, t2;
t1 = MPI_Wtime();
...
t2 = MPI_Wtime();
printf("Elapsed time: %f\n", t2 - t1);
```

MPI data types

Equivalent to built-in C types, except for MPI_BYTE and MPI_PACKED

MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_BYTE	N/A
MPI_PACKED	N/A

Flavors of communication in MPI

- Collective operations: All processes in the communicator or group have to participate!
 - Barrier, Broadcast, Reduction, Prefix sum, Scatter / Gather, All-to-all, etc.

 Point-to-point operations: A processor explicitly communicants with another processor with send and receive messages

Point-to-point communication

Blocking sends and receives

Non-blocking sends and receives

Sending and receiving messages

- Each message has a tag associated to distinguish it from other messages
- The source and tag can be MPI_ANY_SOURCE/MPI_ANY_TAG
- The status can be used to get info about the MPI recv operation:

```
typedef struct MPI_Status {
   int MPI_SOURCE; // source of the received message
   int MPI_TAG; // tag of the received message
   int MPI_ERROR; // a potential error code
};
```

• The length of the received message can be retrieved using:

```
int MPI_Get_count(MPI_Status *status, MPI_Datatype datatype, int *count)
```

Implementations of MPI_Recv and MPI_Send

- MPI_Recv is blocking
 - It returns only after message is received and copied into the buffer!
 - Buffer can be safely reused right after MPI_Recv
- MPI_Send can be implemented with two options:
 - Option 1: returns only after the matching MPI_Recv is executed and the message was sent
 - Option 2: copy msg into buf and returns, without waiting for MPI_Recv
 - In both, the buffer can be safely reused right after MPI_Send

- Restrictions on MPI_Send/MPI_Recv, in order to avoid deadlocks
- Example: behaviour is MPI_Send implementation-dependent

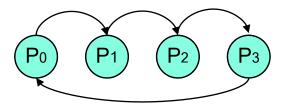
```
int a[20], b[20], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
    MPI_Send(a, 20, MPI_INT, 1, 1, MPI_COMM_WORLD);
    MPI_Send(b, 20, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
    MPI_Recv(b, 20, MPI_INT, 0, 2, MPI_COMM_WORLD, &status);
    MPI_Recv(a, 20, MPI_INT, 0, 1, MPI_COMM_WORLD, &status);
}
...
```

- If MPI-send is option 1 then deadlock, option 2 leads to no deadlock!
- Fix by matching the order of the send and recv operations
- We want to write "safe" programs which are not implementation dependent!

Another example: Circular chain of send/recv operation:

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
```

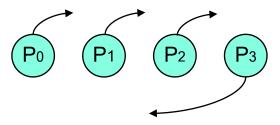
Works fine if send proceeds after copying to data



Another example: Circular chain of send/recv operation:

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
```

 Works fine if send proceeds after copying to data, but deadlocks if send has to wait for the receive.



Must rewrite the code to make it safe:

Sends are waiting for receive: deadlock!

Another example: Circular chain of send/recv operation:

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
```

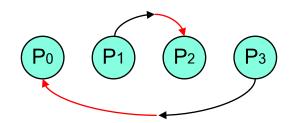
Must rewrite the code to make it safe:

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank % 2 == 1) {
    MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
}
else if (myrank % 2 == 0) {
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
    MPI_Send(a,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
    MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
}
```

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank % 2 == 1) {
    MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
}
else if (myrank % 2 == 0) {
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes)%np, 1, MPI_COMM_WORLD,&status);
    MPI_Send(a,20, MPI_INT, (myrank+1)%np, 1, MPI_COMM_WORLD);
}
```

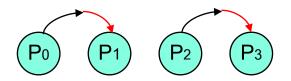
 The above code resolves the deadlock problem and is safe independent of the send implementation.

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank % 2 == 1) {
    MPI_Send(a,20, MPI_INT, (myrank+1) %np, 1, MPI_COMM_WORLD);
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes) %np, 1, MPI_COMM_WORLD, &status)
}
else if (myrank % 2 == 0) {
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes) %np, 1, MPI_COMM_WORLD, &status)
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes) %np, 1, MPI_COMM_WORLD, &status)
    MPI_Send(a,20, MPI_INT, (myrank+1) %np, 1, MPI_COMM_WORLD);
}
```



Odd-numbered processors send while even-numbers processors receive

```
int a[20], b[20], myrank, np;
MPI_Status status;
MPI_Comm_size(MPI_COMM_WORLD, &np);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank % 2 == 1) {
    MPI_Send(a,20, MPI_INT, (myrank+1) %np, 1, MPI_COMM_WORLD);
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes) %np, 1, MPI_COMM_WORLD, &status)
}
else if (myrank % 2 == 0) {
    MPI_Recv(b,20, MPI_INT, (myrank-1+npes) %np, 1, MPI_COMM_WORLD, &status)
    MPI_Send(a,20, MPI_INT, (myrank+1) %np, 1, MPI_COMM_WORLD);
}
```



Now even-numbered processors send while odd-numbers processors receive

Send/recv simultaneously

Previous example is a common pattern

Previous program becomes easier to write:

• Restriction: send and receive buffers must be disjoint, otherwise use:

Overlap communication with computation

- MPI provides non-blocking primitives
 - MPI_Isend starts a send operation, and returns before the data is copied out of the buffer
 - MPI_Irecv starts a recv operation, and returns before the data is received into the buffer

- Allocate a request object and return a pointer to it in the request argument (details later)
- Non-blocking operation can be matched with a corresponding blocking operation

Overlap communication with computation

- Problems with using these non-blocking primitives
 - At some point, we need the data to be guaranteed to have been sent/received, otherwise violates correctness

- Use MPI_Test and/or MPI_Wait to determine whether a non-blocking operation has finished, and/or to wait (block) until the non-blocking operation is completed
 - Use the request object provided by MPI_Isend/ MPI_Irecv to test/wait on the completion
 int MPI_Test(MPI_Request *request, int *flag, MPI_Status *status)
 - Returns non-zero if completed (if so, request is deallocated, set to MPI_REQUEST_NULL)
 int MPI_Wait(MPI_Request *request, MPI_Status *status)
 - Blocks until request completes, then deallocates request and sets it to MPI_REQUEST_NULL
 - Status is similar to the one for the blocking Send/Recv

Avoiding deadlocks

- Recall deadlock example for blocking operations
 - Implementation dependent may cause deadlocks

```
int a[20], b[20], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
    MPI_Send(a, 20, MPI_INT, 1, 1, MPI_COMM_WORLD);
    MPI_Send(b, 20, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
    MPI_Recv(b, 20, MPI_INT, 0, 2, MPI_COMM_WORLD, &status);
    MPI_Recv(a, 20, MPI_INT, 0, 1, MPI_COMM_WORLD, &status);
}
```

Avoiding deadlocks

- Recall deadlock example for blocking operations
 - Implementation dependent may cause deadlocks

```
int a[20], b[20], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
    MPI_Send(a, 20, MPI_INT, 1, 1, MPI_COMM_WORLD);
    MPI_Send(b, 20, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
    MPI_Irecv(b, 20, MPI_INT, 0, 2, &requests[0], MPI_COMM_WORLD);
    MPI_Irecv(a, 20, MPI_INT, 0, 1, &requests[1], MPI_COMM_WORLD);
}
```

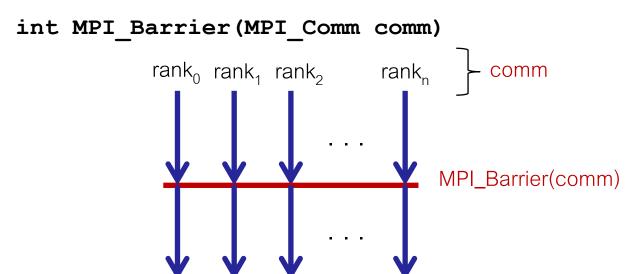
 If we replace either MPI_Send or MPI_Recv operations with non-blocking versions, the code will be safe, regardless of MPI implementation.

Collective communication / computation

- Common collective operations
 - Barrier
 - Broadcast
 - Reduction
 - Prefix sum
 - Scatter / Gather
 - All-to-all
- All processes in the communicator or group have to participate!

Barrier

Blocks until all processes in the given communicator hit the barrier

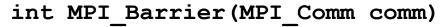


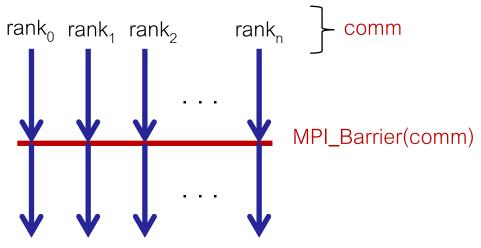
Warning1: Careful with potential deadlocks!

```
if(my_rank % 2 == 0) {
    // do stuff
    MPI_Barrier(MPI_COMM_WORLD);
}
```

Barrier

Blocks until all processes in the given communicator hit the barrier

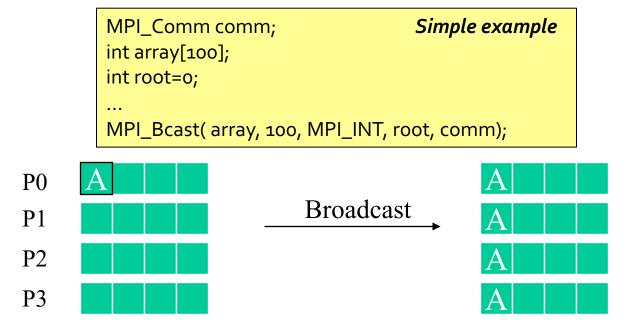




- Warning2: Barrier does not magically wait for pending non-blocking operations!
 - If you are using nonblocking sends/receives and want the guarantee that the processes sent/received all data after the MPI_Barrier you should use MPI_Wait.

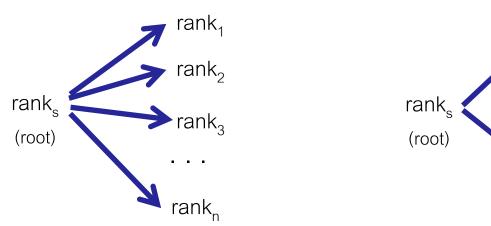
Broadcast

- Common misconception: receiver processes have to do an MPI_Recv
- MPI_Bcast blocks until all processes make a matching MPI_Bcast call: It is not required to block on all processes until the operation fully completes though

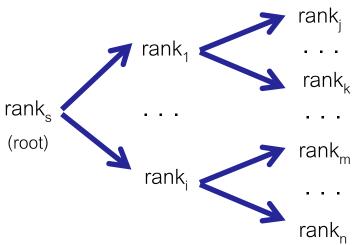


Broadcast vs. Send/Recv

- Why not implement this using Send/Recv pairs? Is MPI_Bcast just a fancy wrapper?
- Bcast communication pattern is optimized internally by the MPI library: In a Send/Recv implementation one processors send to all while Bcast uses a treebased hierarchy to broadcast, removing contention from the root!



loop over all other ranks and issue Send/Recv

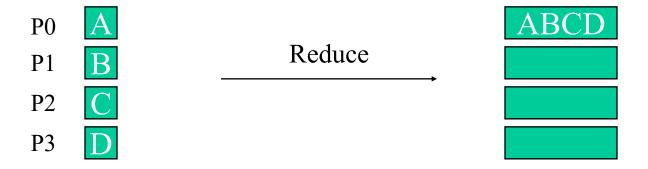


broadcast carried out hierarchically

Reduction

 Reduce: combines the elements from buffer of each process in the group and stores result in recybuf at the target receiver

- All processes must provide send and recv buffers of the same size and data type
- Built-in operations: MPI_SUM, MPI_MAX, MPI_MIN, MPI_PROD, etc. (see docs!)
 - Allows user-defined operations as well (see MPI documentation)



Reduction to all ranks

- If all processes need the reduction result: MPI_Allreduce
- No target necessary, all processes get the result in their own recybuf
- Example: calculate standard deviation
 - calculate average
 - calculate sums of all the squared differences from the mean
 - square root the average of the sums to get the standard deviation
- Use MPI_Reduce and MPI_Allreduce to implement this

```
rand nums = create rand nums(num elements per proc);
// Sum the numbers locally
float local sum = 0; int i;
for (i = 0; i < num elements per proc; i++) { local sum += rand nums[i]; }
// Reduce all of the local sums into the global sum in order to // calculate the mean
float global sum;
MPI Allreduce(&local sum, &global sum, 1, MPI FLOAT, MPI SUM, MPI COMM WORLD);
float mean = global sum / (num elements per proc * world size);
// Compute the local sum of the squared differences from the mean
float local sq diff = 0;
for (i = 0; i < num elements per proc; i++)
{ local sq diff += (rand nums[i] - mean) * (rand nums[i] - mean); }
// Reduce the global sum of the squared differences to the root process and print off the answer
float global sq diff;
MPI Reduce(&local sq diff, &global sq diff, 1, MPI FLOAT, MPI SUM, 0, MPI COMM WORLD);
// The standard deviation is the square root of the mean of the // squared differences.
if (world rank == 0)
     { float stddev = sqrt(global sq diff / (num elements per proc * world size));
printf("Mean - %f, Standard deviation = %f\n", mean, stddev); }
```

```
s = \int_{1}^{\infty} \frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N}
// Reduce all of the local sums into the global sum in order to // calculate the mean
float global sum;
MPI Allreduce(&local sum, &global sum, 1, MPI FLOAT, MPI SUM, MPI COMM WORLD);
float mean = global sum / (num elements per proc * world size);
```

// Reduce the global sum of the squared differences to the root process and print off the answer float global sq diff;

MPI_Reduce(&local_sq_diff; &global_sq_diff, 1, MPI_FLOAT, MPI_SUM, 0, MPI_COMM_WORLD);

// The standard deviation is the square root of the mean of the // squared differences. If (world, rook \Rightarrow 0)

{ float stddev = sqrt(global_sq_diff / (num_elements_per_proc * world_size))

printf("Mean - %f. Standard deviation = %f\n", mean; stddev); i

```
s = \sqrt{\frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N}}
// Compute the local sum of the squared differences from the mean
float local sq diff = 0;
for (i = 0; i < num elements per proc; i++)
{ local sq diff += (rand nums[i] - mean) * (rand nums[i] - mean); }
```

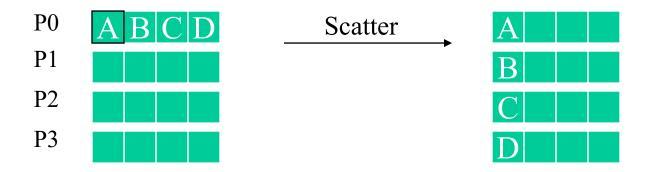
```
S = \sum_{i=1}^{N} \frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N}
// Reduce the global sum of the squared differences to the root process and print off the answer
float global sq diff;
MPI Reduce(&local sq diff, &global sq diff, 1, MPI FLOAT, MPI SUM, 0, MPI COMM WORLD);
```

```
// The standard deviation is the square root of the mean of the // squared differences.
if (world rank == 0)
     { float stddev = sqrt(global sq diff / (num elements per proc * world size));
printf("Mean - %f, Standard deviation = %f\n", mean, stddev); }
```

Scatter

• The source process sends a different part of sendbuf to all others (including itself)

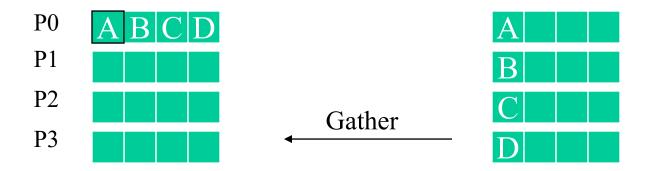
- Send recvcount contiguous elements to each process (all of them receive the same amount)
- sendcount is the number of elements sent to each individual process
- Send-related args are only applicable to the source, and are ignored for all others
- MPI_Scatterv variant allows a different number of items to be sent to each of the receivers,
 see MPI manual (might help for project!)



Gather

Each process (including target) send their sendbuf data to the target process

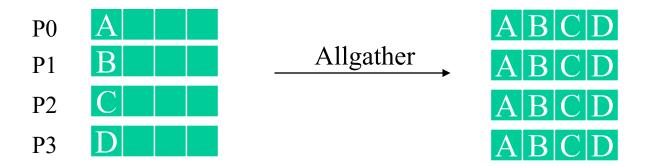
- The sent data must be of the same size and type at all processes
- Recv-related args are only applicable to the target, and are ignored for all others
- recvcount is the count received per process, not the total sum of counts from all processes
- See also: MPI_Gatherv variant, , see MPI manual (might help for project!)



All-Gather

Same as Gather, but data is gathered to all the processes, not just one target

Unlike Gather, all processes must provide a valid recybuf to store incoming data



All-to-all

Each process sends a different portion of sendbuf (sendcount contiguous items)
 to each other process (in order or rank), including itself

Also, vector variant MPI_Alltoallv (see MPI documentation for further details)

