MPI Basics

Chris Kauffman

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Logistics

Reading: Grama Ch 6 + 4

- Ch 6: MPI basics
- Ch 4: Communication patterns
- Zaratan Setup Link on Schedule (Week 1)

Assignments

- A1 Due Soon
  - On-time by Thu 12-Feb
  - Late through Sat 14-Feb
- **Questions?**
- A2 up next week: MPI Programming

Today

- Primitives for Distributed Memory Computing
- MPI Programming

Next Week

- Communication Patterns
- Thu 19-Feb: Mini-Exam 1

Announcements

Assignment Clarifications

Several clarifications regarding Assignment 1 discussed on Piazza posts, some of which are added to the assignment.

- Network embedding: Mesh into Ring example from last week
- Speedup definition
- Assumptions about perfect trees in networks
- Meaning of times

Coding Environment Setup

Zaratan Setup added to schedule in Week 1
https://www.cs.umd.edu/~profk/416/setup-guide.html

- Good idea to code your K-Means solution there to get acquainted as later codes MUST run there
- Provided test cases / `testy` run on Zaratan and most Linuxes, likely not on other platforms

Generic Send and Receive

- Distributed memory machines require explicit sharing of data
- Minimum required functionality is:

```
    send(void *sendbuf, int nelems, int dst_proc);
receive(void *recvbuf, int nelems, int src_proc);
```

- Referred to as a "point-to-point" communication
- **Sample Use**

```
1  // P0 runs                  // P1 runs
2  a = 100;                   receive(&a, 1, 0)
3  send(&a, 1, 1);            printf("%d\n", a);
4  a=50;
```

- Proc 0 sends a single integer to Proc 1
- Proc 0 then changes that integer
- Proc 1 receives and prints the integer

Programmatic Send/Receive

- Typically write this as a single program which every processor runs: Single Program, Multiple Data (SPMD)
- Assume availability of a function giving logical Proc Number
- Branching on proc number to take different actions

```
1  void exchange(){
2    int a = -1;
3    int my_proc = get_processor_number();
4    if(my_proc == 0){
5      a = 100;
6      send(&a, 1, 1);      // send data 100 to Proc 1
7      a=50;
8    }
9    else if(my_proc == 1){
10     receive(&a, 1, 0);  // receive data from Proc 0
11     printf("%d\n", a);
12   }
13   printf("my_proc: %d  a: %d\n",my_proc,a);
14 }
```

Flavors of Send/Receive

- Hardware+OS may support copying message into a "buffer" space which allows sending program to proceed faster: copy to buffer, OS/Hardware handles the rest
- Functions usually available to do both Blocking `send()` and Nonblocking "immediate" `isend()` BUT without OS/Hardware support they are the same

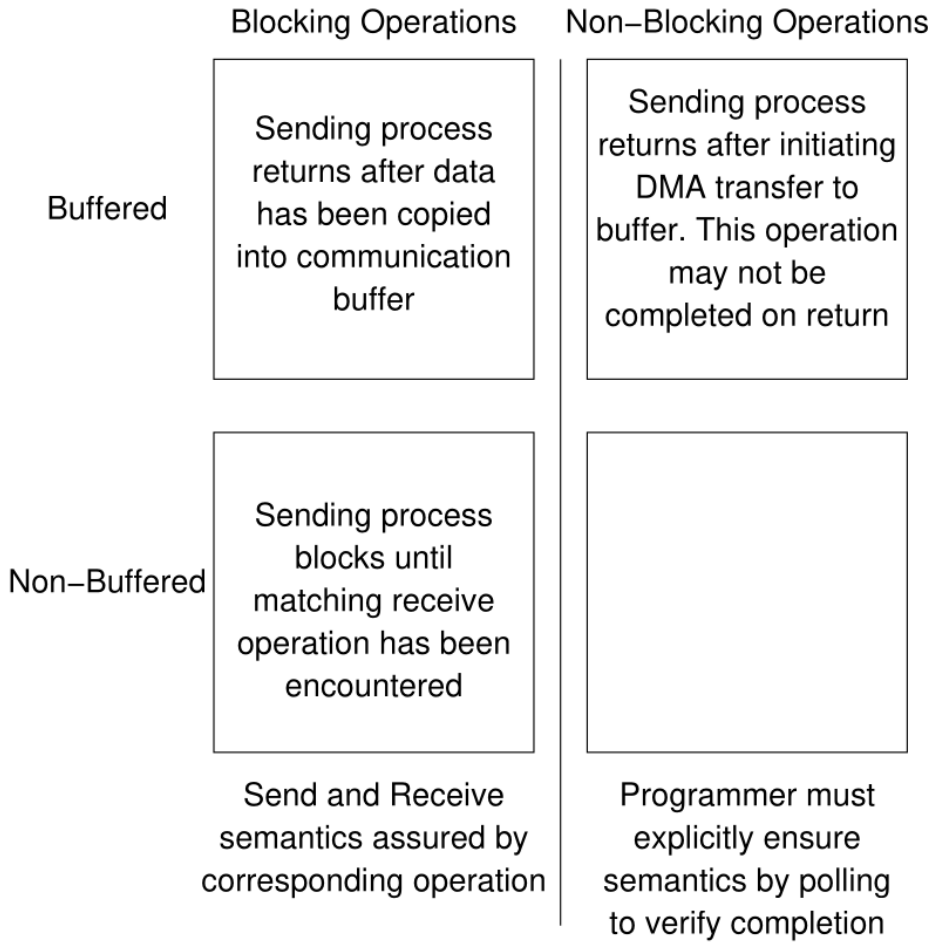


Figure 6.3 Space of possible protocols for send and receive operations.

Blocking + Unbuffered Send/Receive

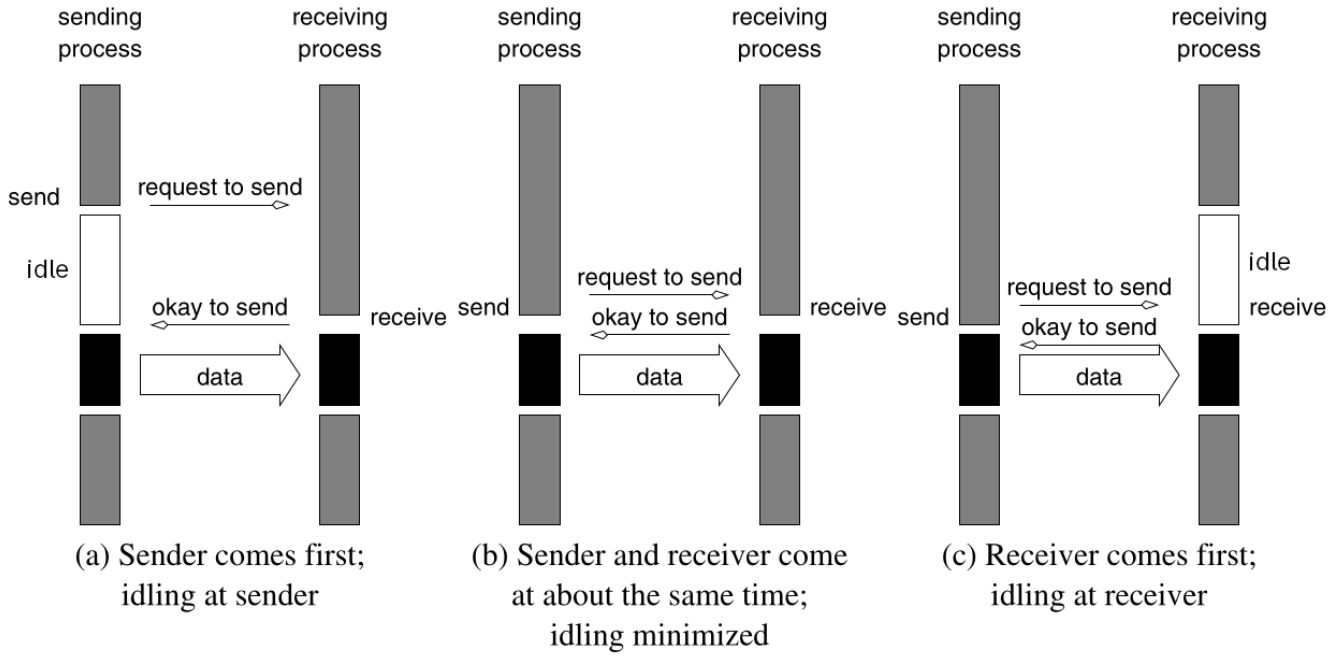


Figure 6.1 Handshake for a blocking non-buffered send/receive operation. It is easy to see that in cases where sender and receiver do not reach communication point at similar times, there can be considerable idling overheads.

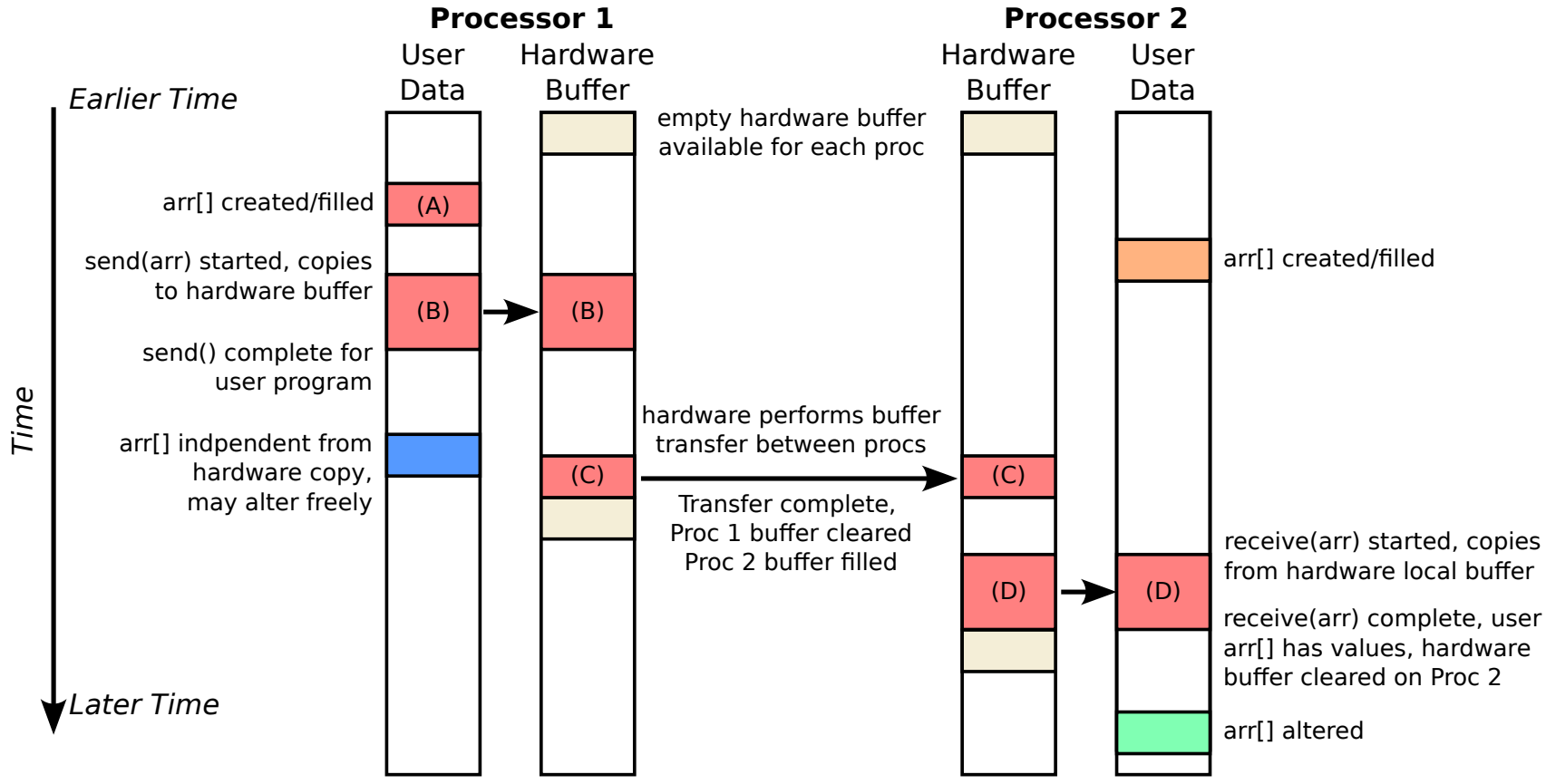
Blocking/Unbuffered: no extra buffer available to hold pending sends/receives so must wait until message is sent to proceed
Blocked processors are idle, do no work, which cuts into speedup

Improper Send/Receive Order May Deadlock

```
1 // P0                          // P1
2 send(&a, 1, 1);               send(&a, 1, 0);  // both blocked
3 receive(&b, 1, 1);            receive(&b, 1, 0);
```

- Above ordering is a bug: both processors block until the other receives a message
- They may both wait forever, a form of Deadlock
- On some platforms for some message sizes, the above may NOT produce deadlock due to `send()` being **buffered** by OS/Hardware

Blocking + Buffered Send/Receive



Blocking + Buffered Send/Receive

Commonly finite-sized hardware communications buffers are available that offload data transfer work from the main processor; decouples `send()`/`receive()` operations on processors

Buffers are no Panacea: Deadlocks Still Possible

Receive always Blocks

```
1  // P0                    // P1
3  receive(&a, 1, 1);      receive(&a, 1, 0);
3  send(&b, 1, 1);         send(&b, 1, 0);
```

- `receive()` always blocks until message is obtained
- Does the above code work even in the buffered setting?

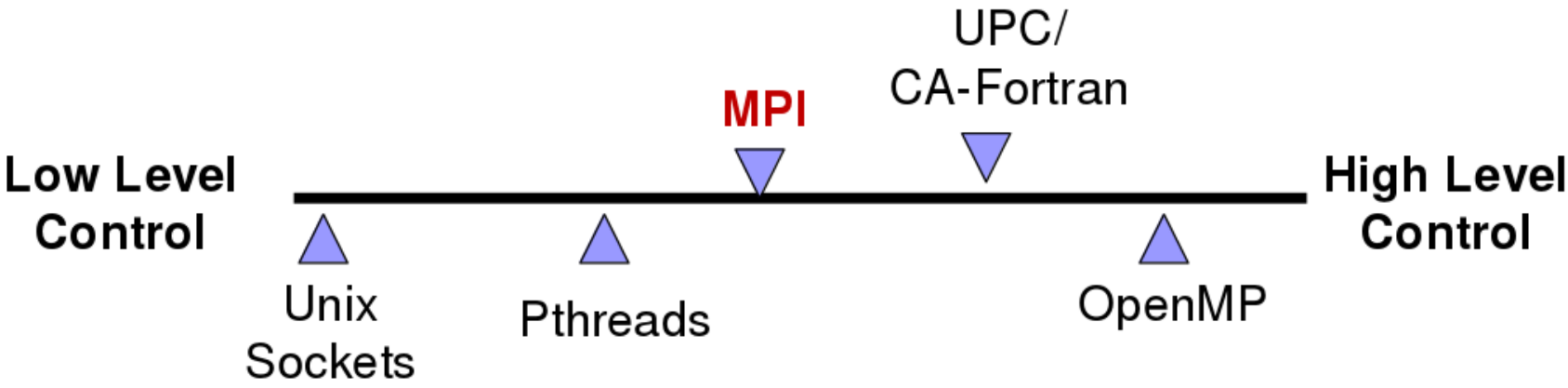
Finite Buffer Sizes

```
1 // P0                     // P1
2 send(&a, N, 1);           send(&a, N, 0);
3 receive(&b, N, 1);        receive(&b, N, 0);
```

- For small `N`, does not deadlock due to buffers
- For large `N`, does deadlock due to finite buffer size

MPI: Message Passing Interface

- Standardized library of functions for C/C++/Fortran
- Communicate between processors in a distributed memory machine
- First appearing around 1992
- MPI Version 1.x universally deployed, Version 2.x less so
- Open Source Versions: MPICH, Open MPI
- Proprietary Versions: Intel, Platform, IBM, Platform, Cray
- Typically vendor configures MPI for particular architecture / network of a large-scale machine



MPI In a Nutshell: 6 Essential Functions

```
// Initialize and Terminate MPI
int MPI_Init(int *argc, char ***argv);
int MPI_Finalize();

// Get total number of processors
int MPI_Comm_size(MPI_Comm comm, int *size);

// Get logical proc number of calling process
int MPI_Comm_rank(MPI_Comm comm, int *rank);

// Send a message to dest processor
int MPI_Send(void *buf, int count, MPI_Datatype datatype,
             int dst_proc, int tag, MPI_Comm comm);

// Receive a message from source processor
int MPI_Recv(void *buf, int count, MPI_Datatype datatype,
             int src_proc, int tag, MPI_Comm comm,
             MPI_Status *status);
```

MPI Hello World

```c
// mpi_hello.c: C Example of hello world with MPI.  Compile and run as
// > mpicc -o mpi_hello mpi_hello.c
// > mpirun ./mpi_hello      # use number of processors equal to total machine
// > mpirun -np 2 mpi_hello  # use 2 processors
// > mpirun -np 8 mpi_hello  # use 8 processors

#include <stdio.h>
#include <mpi.h>

int main (int argc, char *argv[]){
  int rank;                       // the id of this processor
  int size;                       // the number of processors being used

  MPI_Init (&argc, &argv);                  // starts MPI
  MPI_Comm_rank (MPI_COMM_WORLD, &rank); // get current process id
  MPI_Comm_size (MPI_COMM_WORLD, &size); // get number of processes

  // Say hello from this proc
  printf( "Proc %d of %d says 'Hello world'\n", rank, size );

  MPI_Finalize();
  return 0;
}
```

Compiling and Running

- Demo using openmpi implementation
- `mpirun` for interactive running
- `mpirun -np 4 progr` sets number of "processors" to 4

```
>> cd 04-mpi-code/
>> mpicc -o mpi_hello mpi_hello.c
>> ./mpi_hello
...
Proc 0 of 1 says 'Hello world'

>> mpirun -np 2 mpi_hello
...
Proc 0 of 2 says 'Hello world'
Proc 1 of 2 says 'Hello world'

>> mpirun mpi_hello
...
Proc 2 of 4 says 'Hello world'
Proc 0 of 4 says 'Hello world'
Proc 1 of 4 says 'Hello world'
Proc 3 of 4 says 'Hello world'
```

MPI Implementations and OpenMPI Warnings

- Several Implementations of MPI:
  - OpenMPI and MPICH are free, open source, widely available
  - HPC Vendors like IBM and Cray provide their own tailored MPI versions
- Recent Versions of OpenMPI can complain a LOT about various items missing; usually options / environment vars exist to suppress these warnings
  - Example: `--mca btl_base_warn_component_unused 0` to warn about missing HPC network components during `mpirun`
  - Example: `--mca opal_warn_on_missing_libcuda 0` if not intending to use GPU libraries
- Exact nature of warnings/errors varies a lot, look at messages which often dictate how to disable them
- Zaratan does not warn a lot as it seems configured well but course staff may provide specific instructions if warnings emerge

Warning Suppression in OpenMPI

```
>> mpicc mpi_hello_plus.c

# On the below machine, warnings abound
>> mpirun -np 2 a.out
--------------------------------------------------------------------------
The library attempted to open the following supporting CUDA libraries,
but each of them failed.  CUDA-aware support is disabled.
libcuda.so.1: cannot open shared object file: No such file or directory
libcuda.dylib: cannot open shared object file: No such file or directory
/usr/lib64/libcuda.so.1: cannot open shared object file: No such file or directory
/usr/lib64/libcuda.dylib: cannot open shared object file: No such file or directory
If you are not interested in CUDA-aware support, then run with
--mca opal_warn_on_missing_libcuda 0 to suppress this message.  If you are interested
in CUDA-aware support, then try setting LD_LIBRARY_PATH to the location
of libcuda.so.1 to get passed this issue.
--------------------------------------------------------------------------
P0000 [val]: Hello world from process    0 of 2
P0001 [val]: Hello world from process    1 of 2
[val:558294] 1 more process has sent help message help-mpi-common-cuda.txt / dlopen failed
[val:558294] Set MCA parameter "orte_base_help_aggregate" to 0 to see all help / error messages

# in BASH, sourcing provided script sets some environment variables to quiet things down
>> source mpiopts.sh

>> mpirun $MPIOPTS -np 2 a.out
P0001 [val]: Hello world from process    1 of 2
P0000 [val]: Hello world from process    0 of 2
```

MPI Oversubscribing

Default OpenMPI config uses all processors on a single machine, fails for larger requests unless using option `--oversubscribe`

```
>> mpirun -np 2 a.out
...
P0001 [val]: Hello world from process    1 of 2
P0000 [val]: Hello world from process    0 of 2

>> mpirun -np 16 a.out
--------------------------------------------------------------------------
There are not enough slots available in the system to satisfy the 16
slots that were requested by the application:

  a.out

Either request fewer slots for your application, or make more slots
available for use.
...
Alternatively, you can use the --oversubscribe option to ignore the
number of available slots when deciding the number of processes to
launch.
--------------------------------------------------------------------------

>> mpirun  --oversubscribe -np 16 a.out
P0009 [val]: Hello world from process    9 of 16
...
P0014 [val]: Hello world from process   14 of 16
P0012 [val]: Hello world from process   12 of 16

# Newer MPI versions prefer `--map-by :OVERSUBSCRIBE` to `--oversubscribe`
```

Hostfiles

- For laptop/desktop MPI or on Zaratan, system config establishes the nodes with processors
- Some clusters instead use a **hostfile** in `mpirun` to indicate host names of other machines in cluster
- Simplest form of hostfile is a list of symbolic or IP addresses for machines to recruit for the run

```
myclust>> cat hostfile.txt
node01.mycluster.umd.edu
node02.mycluster.umd.edu
node03.mycluster.umd.edu
node04.mycluster.umd.edu
node05.mycluster.umd.edu

myclust>> mpirun -hostfile hostfile.txt -np 100 ./a.out
...
P0003 [node01]: Hello world from process    3 of 100
...
P0089 [node02]: Hello world from process   39 of 100
...
P0190 [node05]: Hello world from process   89 of 100
```

- Again, **we won't need hostfiles as Zaratan is already configured for MPI**

MPI On Zaratan

- UMD's HPC cluster is Zaratan, access via

  ```
  >> ssh MYID@login.zaratan.umd.edu
  ```

- **Login Nodes** are `login-1 login-2 login-3` and are meant for development, compilation, data manipulation, short (<= 1min) tests
- Most nodes (including login) have 128 cores on them but are shared among all logged in useres
- Keep code runs on `login` short and sweet
- When experimenting with MPI, limit procs requested to **no more than 16**

```
profk@login-1 [04-mpi-code]% mpicc -o mpi_hello_plus mpi_hello_plus.c
profk@login-1 [04-mpi-code]% mpirun -np 16 mpi_hello_plus
P0011 [login-1.zaratan.umd.edu]: Hello world from process   11 of 16
P0013 [login-1.zaratan.umd.edu]: Hello world from process   13 of 16
P0014 [login-1.zaratan.umd.edu]: Hello world from process   14 of 16
...
```

- To request longer jobs and more processors, use the **SLURM Scheduler** discussed in more detail later

MPI Hello On Zaratan

```
# assumes correct environment configuration on Zaratan,
# that ~/.bashrc has lines below for mpicc / mpirun
#   source ~profk/bin/cmsc216-env
#   source ~profk/bin/cmsc416-env

>> ssh profk@login.zaratan.umd.edu
...
Last login: Thu Jan 29 17:18:51 2026
profk@login-1 [04-mpi-code]% cd 416/04-mpi-code/
profk@login-1 [04-mpi-code]% mpicc -o mpi_hello_plus mpi_hello_plus.c

profk@login-1 [04-mpi-code]% mpirun -np 16 mpi_hello_plus
P0011 [login-1.zaratan.umd.edu]: Hello world from process  11 of 16
P0013 [login-1.zaratan.umd.edu]: Hello world from process  13 of 16
P0014 [login-1.zaratan.umd.edu]: Hello world from process  14 of 16
P0010 [login-1.zaratan.umd.edu]: Hello world from process  10 of 16
P0000 [login-1.zaratan.umd.edu]: Hello world from process   0 of 16
P0002 [login-1.zaratan.umd.edu]: Hello world from process   2 of 16
P0004 [login-1.zaratan.umd.edu]: Hello world from process   4 of 16
P0005 [login-1.zaratan.umd.edu]: Hello world from process   5 of 16
P0006 [login-1.zaratan.umd.edu]: Hello world from process   6 of 16
P0007 [login-1.zaratan.umd.edu]: Hello world from process   7 of 16
P0009 [login-1.zaratan.umd.edu]: Hello world from process   9 of 16
P0012 [login-1.zaratan.umd.edu]: Hello world from process  12 of 16
P0015 [login-1.zaratan.umd.edu]: Hello world from process  15 of 16
P0001 [login-1.zaratan.umd.edu]: Hello world from process   1 of 16
P0003 [login-1.zaratan.umd.edu]: Hello world from process   3 of 16
P0008 [login-1.zaratan.umd.edu]: Hello world from process   8 of 16
```

MPI Send and Recieve

MPI's most basic functionality is point-to-point message transfer via `MPI_Send()` / `MPI_Recv()`

```
1  {
2    int count = 5;
3    int a[count]={10,20,30,40,50};
4    int b[count];
5    int partner = 1;
6    int tag = 1;
7
8    // Send contents of a to partner proc with tag=1
9    MPI_Send(a, count, MPI_INT, partner, tag, MPI_COMM_WORLD);
10
11   // Receive message into b from partner proc
12   MPI_Recv(b, count, MPI_INT, partner, tag, MPI_COMM_WORLD,
13            MPI_STATUS_IGNORE);  // ignore status of receipt
14 }
```

- Analyze the codepack program `send_recv_demo.c`
  - Study code then try several runs
  - Pick a number of procs that will cause it problems
- Compare with `send_recv_bugs.c`
  - Vary the `ss` and `rr` param to demo stalls
  - Vary the size of buffers sent to check implementation
  - Note Laptop vs Zaratan buffer sizes differ

Tags Make Messages Unique

```
int a[10], b[10], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
  ////////////////////////  V : TAG to send
  MPI_Send(a, 10, MPI_INT, 1, 123, MPI_COMM_WORLD);
  MPI_Send(b, 10, MPI_INT, 1, 456, MPI_COMM_WORLD);
}
else if (myrank == 1) {
  ////////////////////////  V : TAG to receive
  MPI_Recv(b, 10, MPI_INT, 0, 456, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
  MPI_Recv(a, 10, MPI_INT, 0, 123, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

- Send/Recv have an integer Tag parameter which must match between sender and receiver
- Above code may deadlock if not buffered due to the misordering of Tags
- Mostly we will use `tag=1` for simplicity
- Alternatively `MPI_ANY_TAG` works for `MPI_Recv()`
- Receiver can capture the received status (last param) and query what tag was received (we won't bother with this)

MPI Data Types Supported

```
// Sends a message.
int MPI_Send(void *buf, int count, MPI_Datatype datatype,
             int dst_proc, int tag, MPI_Comm comm);

// Receives a message.
int MPI_Recv(void *buf, int count, MPI_Datatype datatype,
             int src_proc, int tag, MPI_Comm comm,
             MPI_Status *status);
```

- Buffer is always untyped (`void* buf`)
- To strive for slightly better safety, MPI has standard datatypes

`MPI_CHAR`	signed char
`MPI_INT`	signed int
`MPI_LONG`	signed long int
`MPI_FLOAT`	float
`MPI_DOUBLE`	double
`MPI_BYTE`	Last two used for sending
`MPI_PACKED`	structure arrays

Unsigned types also available

Sending Structs

Sending structs can be done via the `MPI_BYTE` type

```
{                                          // from send_structs.c
  typedef struct {
    double x;
    int a, b;
  } dint_t;
  dint_t mine[10] = { {.x=1.23, .a=5, .b=7}, {.x=...}, ...}
  ...;
  // calculate data sizes "manually" just as is done in a malloc()
  MPI_Send(mine,  10*sizeof(dint_t), MPI_BYTE,
           partner, 1, MPI_COMM_WORLD);
}
```

- Simple and effective if all compute nodes **use the same binary layout** (the typical case)
- MPI also provides a (complex) method for situations where struct layout differs between nodes
- Must Dictate # of struct fields, types, and ordering into a `MPI_Datatype` and use `MPI_Type_create_struct()`
- Likely hurts performance if struct layout differs so will not discuss in detail

Exercise: Heat Transfer in MPI

- Discuss conversion of the following A1 code to an MPI version
- How is data in `H[][]` divided up?
- Is communication required?
- How would one arrange `MPI_Send()` / `MPI_Recv()` calls?
- How much data needs to be transferred and between who?
- When the computation is finished, how can all data be printed / displayed / saved?

```
// Simulate the temperature changes for internal cells
for(t=0; t<max_time-1; t++){
  for(p=1; p<width-1; p++){
    double left_diff  = H[t][p] - H[t][p-1];
    double right_diff = H[t][p] - H[t][p+1];
    double delta = -k*( left_diff + right_diff );
    H[t+1][p] = H[t][p] + delta;
  }
}
```

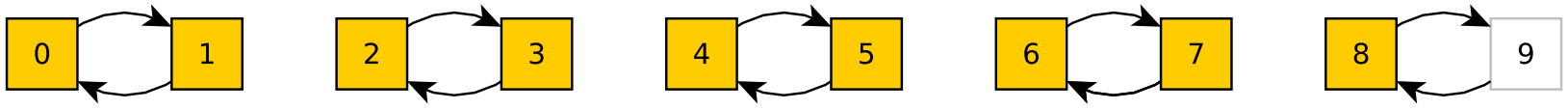
Some Patterns that occur in the problem

- Pair exchange of items: made easier with `MPI_Sendrecv()`
- Collecting final output for display: `MPI_Gather()`
  - Previewed here
  - Discussed in following lectures

Exchange: Sendrecv() for exchanging data between pairs

```
{
  double send[10], recv[10]; int partner;
  if(procid % 2 == 1 ){ // odd procs send left, receive left
    partner = procid-1;
    MPI_Send(send, 10, MPI_DOUBLE, partner, 1, MPI_COMM_WORLD);
    MPI_Recv(recv, 10, MPI_DOUBLE, partner, 1, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
  }
  else{                    // even procs receive right, send right
    partner = procid+1;
    MPI_Recv(recv, 10, MPI_DOUBLE, partner, 1, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
    MPI_Send(send, 10, MPI_DOUBLE, partner, 1, MPI_COMM_WORLD);
  }
}
{ // Sendrecv simplifies this pattern
  double send[10], recv[10]; int partner;
  partner = (procid % 2 == 1) ? procid-1 : procid+1;
  MPI_Sendrecv(send, 10, MPI_DOUBLE, partner, 1,
               recv, 10, MPI_DOUBLE, partner, 1,
               MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

Take Care: Pair exchange can hang

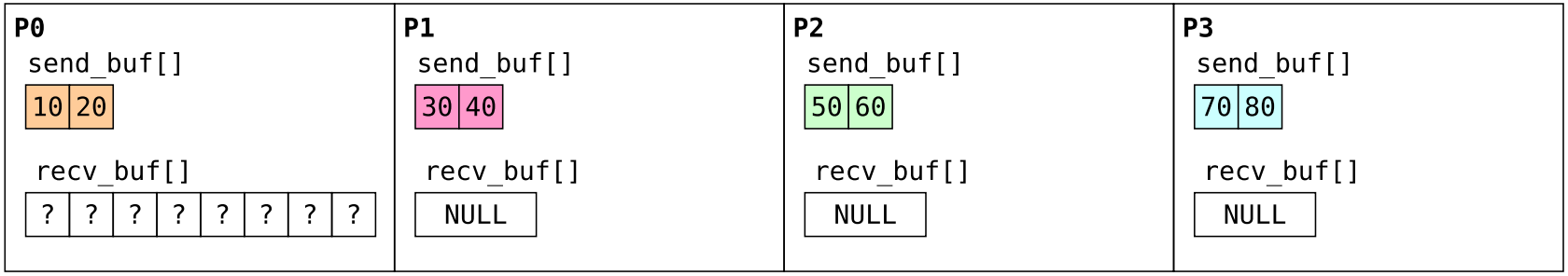



```
{
  double send[10], recv[10]; int partner;
  partner = (procid % 2 == 1) ? procid-1 : procid+1;
  MPI_Sendrecv(send, 10, MPI_DOUBLE, partner, 1,
               recv, 10, MPI_DOUBLE, partner, 1,
               MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
```

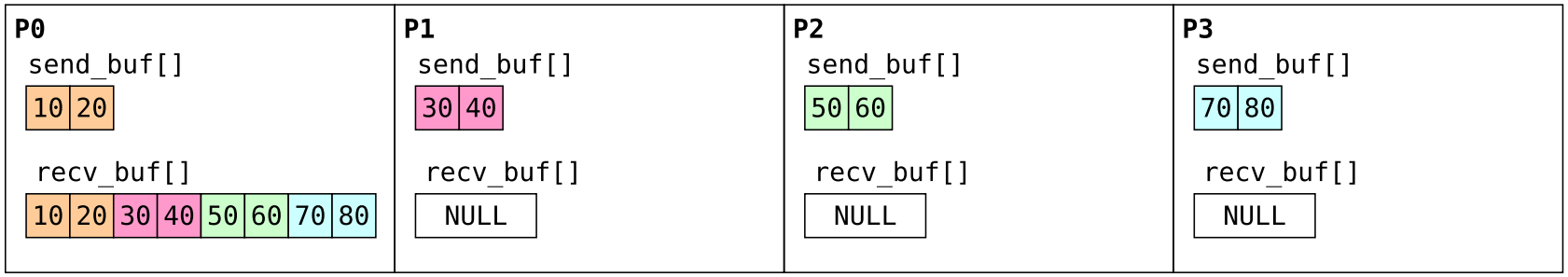
- With 9 processors, logic is broken
- Proc 8 will wait to communicate with absent partner
- Program never terminates
- Special checks for `procid == (nprocs-1)` can surmount this
- Heat problem is interesting as it involves communicating with a Left AND Right partner, yet more complex and part of A2...

Getting Answers to Root Proc: Gather

Before Call Begins



`MPI_Gather(send_buf,2,MPI_INT, recv_buf,2,MPI_INT, 0,MPI_COMM_WORLD);`



After Call Completes

- At the end of Heat, every processor has computed some columns
- One processor needs to gather all of the data for printing / saving, usually "root" processor with ID/rank 0
- Everyone calls `MPI_Gather()` to get data to root proc

MPI_Gather Sample

Use of Gather

```
// Preamble for any code
MPI_Comm comm = MPI_COMM_WORLD;
int sendarray[100];
int procid, total_procs, *rbuf;
...;
// Only proc 0 needs space for to
// receive entirety of data
if(procid == 0) {
  rbuf = malloc(total_procs*100*
                sizeof(int));
}

// Everyone calls gather
// proc 0 gets all data eventually
MPI_Gather(sendarray, 100, MPI_INT,
           rbuf, 100, MPI_INT,
           0, comm);
```

Equivalent Non-Gather Code

```
if(rank == 0){
  for(i=0; i<100; i++){
    rbuf[i] = sendarray[i];
  }
  for(i=1; i<total_procs; i++){
    int *rloc = &rbuf[i*100];
    MPI_Recv(rloc, 100,
             MPI_INT, i,
             tag, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
  }
}
else{
  MPI_Send(sendarray, 100,
           MPI_INT, 0,
           tag, MPI_COMM_WORLD);
}
```

Collective Communication Patterns Next

- `gather` is an example of a **Collective Communication Pattern**
- Will study more of these in subsequent lectures
- Using built-in collective comm. patterns simplifies programs
  - Without Collective Comm: hand-code proc I sends to proc I/2 who receives, then to proc I/4, then to...
  - With Collective Comm: `MPI_Reduce()`
- MPI implementation typically uses the most efficient underlying communications for a particular network

Non-Blocking Communication: "Immediate" Operations

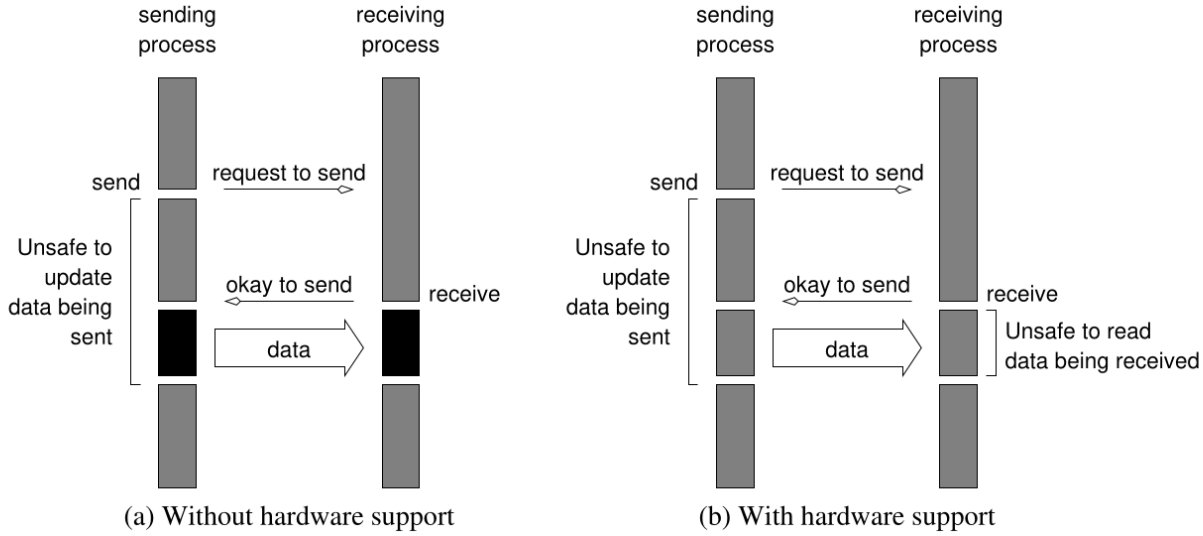


Figure 6.4 Non-blocking non-buffered send and receive operations (a) in absence of communication hardware; (b) in presence of communication hardware.

- Non-Blocking calls return immediately
  - `isend(data,dest,request)`: send w/o waiting
  - `ireceive(data,dest,request)`: receive w/o waiting
- `wait(request)`: block until requested send/receive finishes, required to avoid race conditions
- Will revisit later if time permits:
  More Control = More Potential Speedup + More Potential Bugs

Non-Blocking Send / Receive in MPI

Effect	**Blocking**	**Non-Blocking**
Send	`MPI_Send(...)`	`MPI_Isend(..., &request)`
Receive	`MPI_Recv(...)`	`MPI_Irecv(..., &request)`
Sync	Automatic	`MPI_Wait(&request, ...)`

- Non-blocking calls trigger send/receive to be initiated but do not block process(or) to completion
- `MPI_Request` struct tracks whether operation has completed
- Block via `MPI_wait()` until send/recv completes
- Prior to blocking, unsafe to alter/use data in buffers
- Can pair `MPI_ISend()` / `MPI_Recv()` and vice versa
- Allows for more overlap of computation and communication at the cost of more complexity

Faux Example of MPI_Isend() / MPI_IRecv()

```
1  int data_a[100] = {...};
2  int data_b[100] = {...};
3  int partner = ...;
4  int tag = ...;
5
6  ...; // compute data_a[]
7
8  MPI_Request request;
9  MPI_Isend(data_a, 100, MPI_INT, partner, tag, MPI_COMM_WORLD, &request);
10
11 ...; // unsafe to alter data_a[] so compute data_b[]
12
13 MPI_Wait(&request, MPI_STATUS_IGNORE); // block until data_a[] has been sent
14                                        // now safe to alter data_a[]
15 for(int i=0; i<100; i++){             // more computations on data_a[]
16   data_a[i]++;
17 }
18 ...;
19 MPI_Irecv(data_a, 100, MPI_INT, partner, tag, MPI_COMM_WORLD, &request);
20
21 ...; // unsafe to do anything with data_a[], compute on data_b[]
22
23 MPI_Wait(&request, MPI_STATUS_IGNORE); // block until data_a[] has been sent
24                                        // now safe to alter data_a[]
25 for(int i=0; i<100; i++){             // more computations on data_a[]
26   data_a[i]++;
27 }
```

Actual code example in `send_recv_immediate.c`