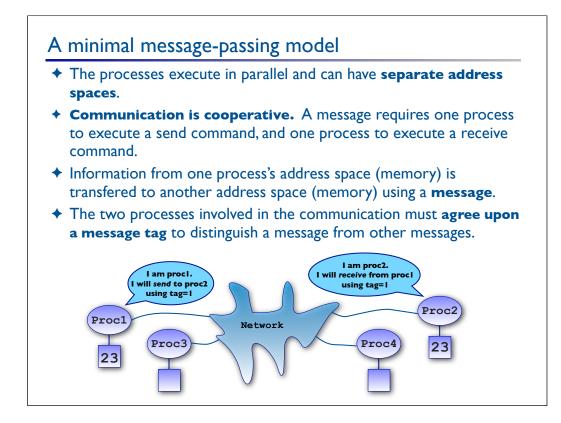
MPI Part I

✦ References:

Using MPI. Gropp, Lusk Skjellum

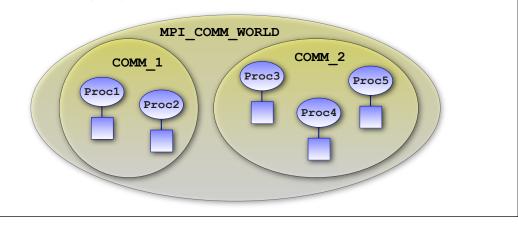
http://www.mpi-forum.org/docs/mpi-11-html/node182.html

- ✦ What is MPI?
 - I. MPI allows a collection of processes to communicate with messages.
 - 2. MPI is a **library** of subroutines called from Fortran, C and C++. Programs are compiler with ordinary compilers and linked with the MPI library.
 - 3. MPI is a **specification** which is independent from particular implementations. An MPI program should be portable to any vendors hardware that supports MPI.



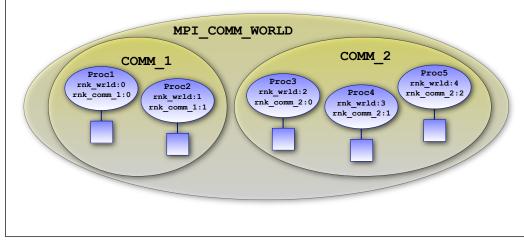
Communicators

- + Groups of processes are called communicators.
 - The default communicator is called MPI_COMM_WORLD. This communicator contains all the processes in the current MPI universe.
 - MPI allows for the formation of communicators within the global communicator.
 - Message tags are defined within the context of a communicator.



Rank

- + Processes are identified within a communicator by their rank
 - Rank is an integer
 - Rank defined within the context of a communicator.
 - If a communicator contains n processes, then the ranks are integers from 0 to n-1.



The "hello world" Program

- Important features of the hello_world program
 - I. Use the mpi module, or include the include file called mpif.h
 - 2. Initialize the MPI environment.
 - 3. Determine how many processes are in the current MPI environment.
 - 4. Determine rank within the MPI_COMM_WORLD communicator
 - 5. Terminate the MPI environment

PROGRAM hello_world USE mpi	
<pre>IMPLICIT NONE INTEGER :: npe_wrld, &! number of process</pre>	
CALL MPI_INIT (ierr) CALL MPI_COMM_SIZE (MPI_COMM_WORLD,npe_wr CALL MPI_COMM_RANK (MPI_COMM_WORLD,rnk_wr	
PRINT "(A19,I3,A4,I4)"," hello from proc	= ",rnk_wrld," of ",npe_wrld
CALL MPI_FINALIZE (ierr)	! terminate MPI environment
END PROGRAM hello_world	

PROGRAM hello_world JSE mpi	
/	er of processes within the world communicator of process within the world communicator
	! initialize MPI environment WORLD,npe_wrld,ierr) ! determine world size
PRINT "(A19,I3,A4,I4)"," hel	[_WORLD,rnk_wrld,ierr) ! determine rank within world lo from proc = ",rnk_wrld," of ",npe_wrld ! terminate MPI environment
	<pre>lo from proc = ",rnk_wrld," of ",npe_wrld</pre>
RINT "(A19,I3,A4,I4)"," hel	lo from proc = ",rnk_wrld," of ",npe_wrld ! terminate MPI environment
PRINT "(A19,I3,A4,I4)"," hel CALL MPI_FINALIZE (ierr) CND PROGRAM hello_world	<pre>lo from proc = ",rnk_wrld," of ",npe_wrld</pre>
PRINT "(A19,13,A4,14)"," hel CALL MPI_FINALIZE (ierr) CND PROGRAM hello_world TO run the code use mpirun. The -np	<pre>lo from proc = ",rnk_wrld," of ",npe_wrld</pre>
PRINT "(A19,I3,A4,I4)"," hel CALL MPI_FINALIZE (ierr) CND PROGRAM hello_world To run the code use	<pre>lo from proc = ",rnk_wrld," of ",npe_wrld</pre>

The slightly modified "hello world" Program

- Important features of the slightly modified hello_world program
 - I. Use the mpi commands MPI_GET_PROCESSOR_NAME to determine where a processes is actually running.
 - 2. Use the mpi commands MPI_WTICK and MPI_WTIME to time code
 - 3. Use the mpi commands MPI_BARRIER write output in order.

PROGRAM hello_world_2 USE mpi IMPLICIT NONE
<pre>INTEGER :: npe_wrld, &! number of processes within the world communicator</pre>
CHARACTER (LEN=128) :: proc_name
CALL MPI_INIT (ierr)
CALL MPI_COMM_SIZE (MPI_COMM_WORLD,npe_wrld,ierr) CALL MPI_COMM_RANK (MPI_COMM_WORLD,rnk_wrld,ierr)

The slightly modified "hello world" Program

Code (continued) for the slightly modified hello_world program

```
CALL MPI_GET_PROCESSOR_NAME (proc_name,name_len,ierr)
  wall tick = MPI WTICK () ! wall clock timer increment in seconds
  IF (rnk_wrld == 0) PRINT "(A13,F12.8)"," wall_tick = ",wall_tick
 do some useless work
1
  time_start = MPI_WTIME () ! wall clock timer start
  x = \overline{0}.08
  DO j = 1,5000
     DO i = 1,5000
       x = x + SIN (x+FLOAT (rnk_wrld))
     ENDDO
  ENDDO
  time end = MPI WTIME () ! wall clock timer stop
! write the results
  DO n = 0, npe wrld-1
     IF (rnk_wrld == n) THEN
        PRINT "(A19, I3, A4, I4, A12, A16, A10, F8.5, A10, F12.8)", &
                             " hello from proc = ",rnk wrld," of ",npe wrld, &
                             " running on ", TRIM (proc_name), &
                             " time = ",time_end-time_start," answer = ",x
     ENDIF
      CALL MPI_BARRIER (MPI_COMM_WORLD,ierr)
  ENDDO
  CALL MPI FINALIZE (ierr)
  END PROGRAM hello_world_2
```

Collective Communication

 Transfer information for one process to many (scatter) or collect information from many processes to one (gather)

Collective Communication: Scatter

♦ MPI_BCAST broadcasts a message from the process with rank ROOT to all processes of the communicator group COMM, itself included. It is called by all members of group using the same arguments. On return, the contents of root's send buffer has been copied to the receive buffer on all processes.

MPI_BCAST (buffer,data_count,data_type,root,comm)

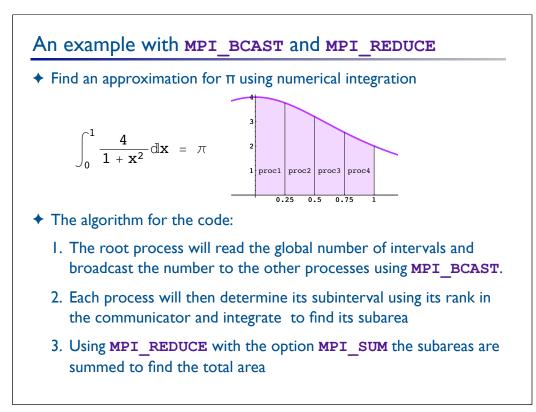
Collective Communication: Gather

MPI_GATHER: Each process (root process included) sends the contents of its send buffer to the root process. The root process receives the messages into the receive buffer and stores them in rank order.

MPI_GATHER(send_buffer,send_count,send_type, recv_buffer,recv_count,recv_type,root,comm,ierr)

MPI_REDUCE: Combines the elements in the send buffer of each process in the communicator group comm, using the operation op, and returns the combined value in the receive buffer of the process with rank root.

where **op** can be several things including **MPI_MAX(MPI_MIN)** for maximum(minimum), **MPI_SUM** for summation.



Code the Pi example

PROGRAM pi USE mpi IMPLICIT NONE INTEGER :: npe_wrld,rnk_wrld,n,i,ierr REAL (KIND=SELECTED_REAL_KIND (12)) :: & del_x,x_left,pi_piece,pi_approx,time_start,time_end,x ! setup MPI CALL MPI_INIT (ierr) CALL MPI_INIT (ierr) CALL MPI_COMM_SIZE (MPI_COMM_WORLD,npe_wrld,ierr) CALL MPI_COMM_RANK (MPI_COMM_WORLD,rnk_wrld,ierr)

Code the Pi example, continued

```
! read and broadcast total number of intervals
  IF (rnk wrld==0) THEN
     PRINT *, 'Enter the total number of intervals '
     READ (*,*) n
  ENDIF
  CALL MPI_BCAST (n,1,MPI_INTEGER,0,MPI_COMM_WORLD,ierr)
  time_start = MPI_WTIME () ! wall clock timer start
! integrate subinterval
  del_x = 1.0_8/DBLE (n); x_left = DBLE (rnk_wrld)/DBLE (npe_wrld);
  pi_{piece} = \overline{0.08}
  DO i = 1,n/npe_wrld
     x = x left + del x*(DBLE(i)-0.5 8)
     pi_piece = pi_piece + del_x*(4.0_8/(1.0_8 + x**2))
  ENDDO
! gather the pieces of the pi
  CALL MPI REDUCE (pi piece, pi approx, 1, MPI DOUBLE PRECISION, MPI SUM, 0, &
                                                        MPI_COMM_WORLD, ierr)
  time_end = MPI_WTIME () ! wall clock timer stop
! print the approximate value
  IF (rnk_wrld==0) THEN
    PRINT "(A12,F22.20)","pi_approx = ",pi_approx
  ENDIF
  CALL MPI BARRIER (MPI COMM WORLD, ierr)
  PRINT "(A12,F14.10)", "time"
                                  = ",time_end-time_start
  CALL MPI_FINALIZE (ierr)
  END PROGRAM pi
```

Point-to-point communication

- + Here we send messages directly form one process to another.
- ♦ MPI_SEND:
 - This is a **blocking** send. Control does not return until the message data has been safely stored away so that the sender is free to overwrite the send buffer.
 - The syntax of the blocking send operation is given below:

MPI_SEND (BUFFER, DATA_COUNT, DATA_TYPE, DEST, TAG, COMM, IERR)

where

DEST is the rank of destination (integer) within COMM TAG is the message tag (integer)

Point-to-point communication

♦ MPI RECV:

- This is a blocking receive. Control returns only after the receive buffer contains the newly received message.
- The syntax of the blocking send operation is given below:

MPI_RECV (BUFFER, DATA_COUNT, DATA_TYPE, SOUR, TAG, COMM, STATUS, IERR)

where

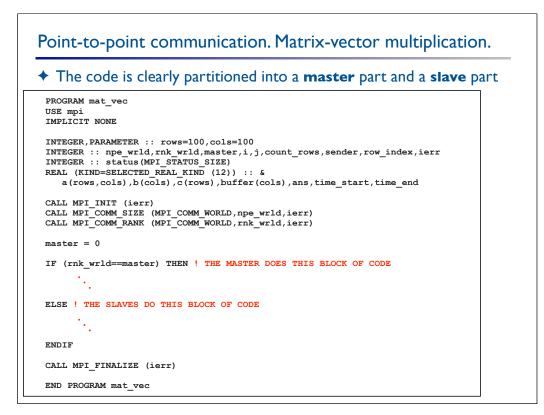
SOUR is the rank of source (integer) within COMM. The source can also be specified as MPI_ANY_SOURCE TAG is the message tag (integer). The tag can also be specified as MPI_ANY_TAG

Point-to-point communication. Matrix-vector multiplication

- This is a "master-slave" algorithm. One process (the master) is responsible for the coordinating the work of the others (the slaves).
- ◆ We wish to perform a matrix-vector multiply in parallel.

Ab=c

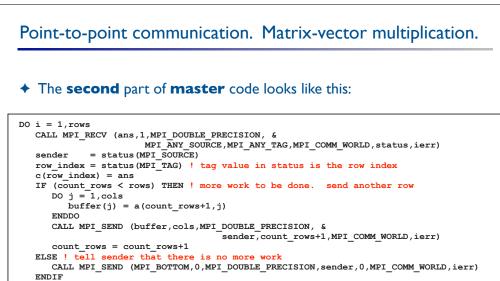
- The master algorithm for the code:
 - I. The master will broadcast the vector b to all the slaves.
 - 2. The master will send one row of the matrix $oldsymbol{A}$ to each slave.
 - 3. The master then waits for the slave to perform the dot product and return the element of c. At this time the master sends that slave a new row of A. Continue until all rows are processed.
- The slave algorithm for the code:
 - I. The slaves receive vector \boldsymbol{b} from master.
 - 2. Perform dot-products of \boldsymbol{b} and rows of \boldsymbol{A} . Send result to master



Point-to-point communication. Matrix-vector multiplication.

+ The **first** part of **master** code looks like this:

```
D0 j = 1,cols ! make an arbitrary matrix a and vector b
    b(j) = 1.0_8
    D0 i = 1,rows
        a(i,j) = DBLE (i+j)
    ENDDO
    CALL MPI_BCAST (b,cols,MPI_DOUBLE_PRECISION,master,MPI_COMM_WORLD,ierr)
    count_rows = 0
    D0 i = 1,npe_wrld-1
    D0 j = 1,cols
        buffer(j) = a(i,j)
    ENDDO
    CALL MPI_SEND (buffer,cols,MPI_DOUBLE_PRECISION,i,i,MPI_COMM_WORLD,ierr)
    count_rows = count_rows+1
    ENDDO
```





Point-to-point communication. Matrix-vector multiplication.

✦ The slave code looks like this:

```
CALL MPI_BCAST (b,cols,MPI_DOUBLE_PRECISION,master,MPI_COMM_WORLD,ierr)

DO

CALL MPI_RECV (buffer,cols,MPI_DOUBLE_PRECISION,master, &

    MPI_ANY_TAG,MPI_COMM_WORLD,status,ierr)

IF (status(MPI_TAG)==0) EXIT ! there is no more work

row_index = status(MPI_TAG) ! tag value status is the row index

ans = 0.0_8

DO i = 1,cols

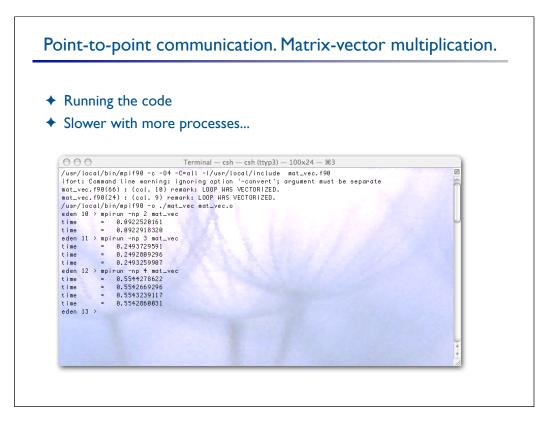
    ans = ans + buffer(i)*b(i)

ENDDO

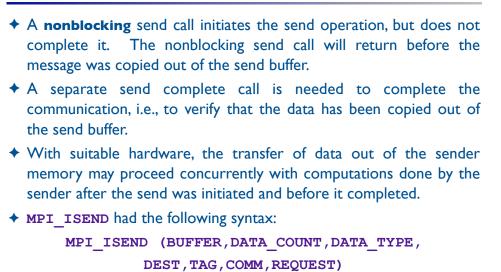
CALL MPI_SEND (ans,1,MPI_DOUBLE_PRECISION, &

    master,row_index,MPI_COMM_WORLD,ierr)

ENDDO
```



Nonblocking Send



where the **REQUEST** argument determines if the operation has completed.

Nonblocking Receive

- A nonblocking receive call initiates the receive operation, but does not complete it. The call will return before a message is stored into the receive buffer.
- A separate receive complete call is needed to complete the receive operation and verify that the data has been received into the receive buffer.
- With suitable hardware, the transfer of data into the receiver memory may proceed concurrently with computations done after the receive was initiated and before it completed.
- MPI_IRECV had the following syntax:

```
MPI_IRECV (BUFFER, DATA_COUNT, DATA_TYPE, SOUR, TAG, COMM, REQUEST)
```

where the **REQUEST** argument determines if the operation has completed.

Completion of Nonblocking Send and Receive

- The call MPI_WAITALL blocks until all communication operations associated with active handles in the list are completed, and returns the status of all these operations.
- MPI_WAITALL had the following syntax:

where the **REQUEST** argument determines if the operation has completed.

Domain decomposition

- Here we will demonstrate the method of parallelization called domain decomposition. We will partition the physical domain into pieces and assign each piece to a process. Each process will communicate with it neighboring domain using message passing.
- ✤ We will numerically solve the Poisson equation.
- The continuous form of the problem:

 $abla^2 \alpha = \beta(x, y)$ on the interior of the unit square $\begin{bmatrix} 0, 1 \end{bmatrix} \times \begin{bmatrix} 0, 1 \end{bmatrix}$ $\alpha(x, y) = \gamma(x, y)$ on the boundary

 This simple PDE can be used as a template for more complicated problems. The communication patterns here are the same as more complex problems.

Discrete Poisson problem: The grid

- The solution is approximated at discrete points. These points called a grid.
- The positions of the grid points (x_i, y_j) are given by:

$$x_i = \frac{i}{n+1}, i = 0, \dots, n+1$$
 $y_j = \frac{j}{n+1}, j = 0, \dots, n+1$

- + The notation $\alpha_{i,j}$ refers to approximation of α at (x_i, y_j)
- The distance between grid points is given by

$$h = \frac{1}{n+1}$$

Discrete Poisson problem: The discrete equation

✦ The continuous equation

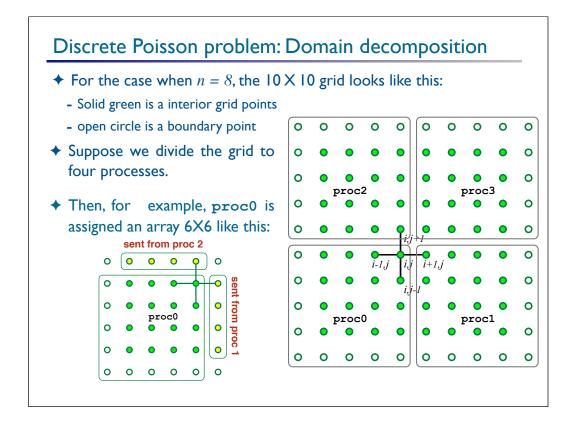
$$\frac{\partial^2 \alpha}{\partial x^2} + \frac{\partial^2 \alpha}{\partial y^2} = \beta$$

✦ The discrete equation

$$\frac{\alpha_{i-1,j} - 2\alpha_{i,j} + \alpha_{i+1,j}}{h^2} + \frac{\alpha_{i,j-1} - 2\alpha_{i,j} + \alpha_{i,j+1}}{h^2} = \beta_{i,j}$$

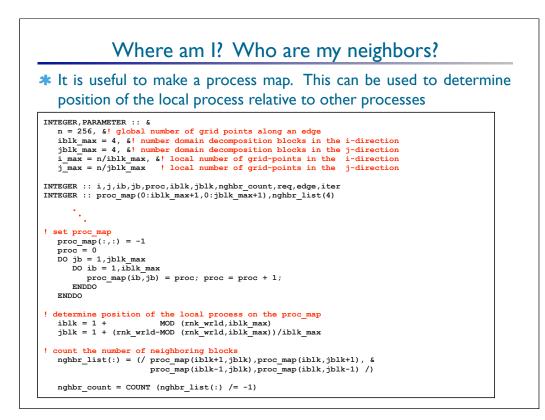
+ Solve for $\pmb{lpha}_{i,j}$ gives the Jacobi iteration

$$\alpha_{i,j}^{(k+1)} = \frac{1}{4} \Big(\alpha_{i-1,j}^{(k)} + \alpha_{i+1,j}^{(k)} + \alpha_{i,j-1}^{(k)} + \alpha_{i,j+1}^{(k)} - h^2 \beta_{i,j}^{(k)} \Big)$$

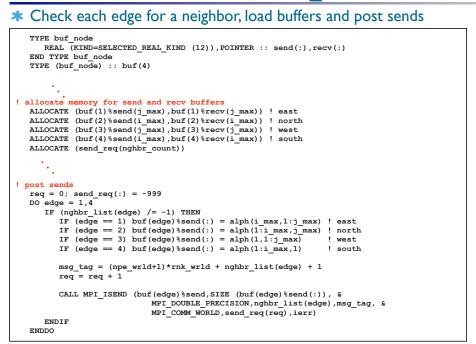


Discrete Poisson problem: Algorithm

- The algorithm for the Jacobi iteration is given by:
 - I. Communicate information to fill ghost cells
 - a. Initiate nonblocking sends
 - b. Initiate nonblocking receives
 - c. Wait for message to be completed
 - 2. Perform one sweep of the Jacobi iteration
 - 3. GOTO I.



Initiate sends with MPI_ISEND



Initiate receives with MPI_IRECV

* Check each edge for a neighbor, clear buffers and post receives

```
! post receives
req = 0; recv_req(:) = -999
D0 edge = 1,4
IF (nghbr_list(edge) /= -1) THEN
buf(edge)%recv(:) = 0.0
msg_tag = (npe_wrld+1)*nghbr_list(edge) + rnk_wrld + 1
req = req + 1
CALL MPI_IRECV (buf(edge)%recv,SIZE (buf(edge)%recv(:)), &
MPI_DOUBLE_PRECISION,nghbr_list(edge),msg_tag, &
MPI_COMM_WORLD,recv_req(req),ierr)
ENDIF
ENDDO
```



* Check each edge for a neighbor, clear buffers and post receives

! allocate send_req, recv_req, send_status, recv_status ALLOCATE (send_req(nghbr_count)) ALLOCATE (recv_req(nghbr_count)) ALLOCATE (send_status(MPI_STATUS_SIZE,nghbr_count)) ALLOCATE (recv_status(MPI_STATUS_SIZE,nghbr_count))

! wait for messages to complete send_status(:,:) = -999; recv_status(:,:) = -999; CALL MPI_WAITALL (nghbr_count,send_req,send_status,ierr) CALL MPI_WAITALL (nghbr_count,recv_req,recv_status,ierr)

۰.

