Parallel Programming Using MPI

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Thank you

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Outline

- General Comments
- Concepts
- Environment Management Routines
- Point-to-Point Communication Routines
- Collective Communication Routines
- Asynchronous Communication

General Comments

- Biggest hurdle to parallel computing is just getting started

- I will not cover all of the functionality of the MPI library
  - Focus on basic point-to-point and collective communications.

- You can do almost everything you ever need to do with just 8 commands.
  - Another 4 commands for collective communications are also useful.
  - Probably 95% of MPI users can get away with just these 12 commands, so I will focus on these commands here, and briefly mention a few others.

Concepts

- Communicators
- Point-to-point vs. collective communications
- Buffering of messages
- Issues of Synchronization and Determinism
  - Deadlocks and Race Conditions

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Environment Management Routines

Basic Requirements:

- Include Header File:

C	`#include "mpi.h"`
Fortran	`include 'mpif.h'`

- General Format of calls differs between C and Fortran

C	`rc = MPI_Bsend(&buf,count,type,dest,tag,comm)`
Fortran	`CALL MPI_BSEND(buf,count,type,dest,tag,comm,ierr)`

Initializing and Finalizing parallel tasks in MPI:

- Initialization

C	`MPI_Init (&argc,&argv)`
Fortran	`MPI_INIT (ierr)`

- Finalization

C	`MPI_Finalize ()`
Fortran	`MPI_FINALIZE (ierr)`

Environment Management Routines

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Size and Rank:

• Determine number of MPI tasks

C	`MPI_Comm_size (comm,&size)`
Fortran	`MPI_COMM_SIZE (comm,size,ierr)`

Arguments:

Intent	Argument	Type	Description
IN	`comm`	handle	Communicator
OUT	`size`	integer	Number of MPI tasks associated with `comm`

• Determine rank of this MPI task:

C	`MPI_Comm_rank (comm,&rank)`
Fortran	`MPI_COMM_RANK (comm,rank,ierr)`

-Rank is the Task ID

Example: Hello World

Serial Version:

```
!--------------------------------------------------
!          HELLO WORLD
!--------------------------------------------------
program helloworld_serial
  implicit none

  !Write out message to screen
  write(*,'(a)')'Hello World.'

end program helloworld_serial
```

Example: Hello World

Parallel Version:

```
!----------------------------------------------------
!          HELLO WORLD
!----------------------------------------------------
program helloworld
  implicit none
  include 'mpif.h'
  integer :: nproc  !Number of Processors
  integer :: iproc  !Number of local processors
  integer :: ierror !Integer error flag

  !Initialize MPI message passing
  call mpi_init (ierror)
  call mpi_comm_size (mpi_comm_world, nproc, ierror)
  call mpi_comm_rank (mpi_comm_world, iproc, ierror)

  !Write out message to screen
  write(*,'(a,i4,a,i4)')'Hello World. I am processor ',iproc, &
    ' of ',nproc

  !Finalize MPI message passing
  call mpi_finalize (ierror)

end program helloworld
```

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Point-to-Point Communication Routines

- Send a Message

C	`MPI_Send (&buf,count,datatype,dest,tag,comm)`
Fortran	`MPI_SEND (buf,count,datatype,dest,tag,comm,ierr)`

Arguments:

Intent	Argument	Type	Description
IN	`buf`	choice	Address of data array to send
IN	`count`	integer(≥ 0)	Number of array elements to send
IN	`datatype`	handle	Type of data to send
IN	`dest`	integer	Rank (task ID) of destination task
IN	`tag`	integer	Message tag
IN	`comm`	handle	Communicator

Point-to-Point Communication Routines

- Receive a Message

C	`MPI_Recv (&buf,count,datatype,source,tag,comm,&status)`
Fortran	`MPI_RECV (buf,count,datatype,source,tag,comm,status,ierr)`

Arguments:

Intent	Argument	Type	Description
OUT	`buf`	choice	Address of data array to receive
IN	`count`	integer(≥ 0)	Number of array elements to receive
IN	`datatype`	handle	Type of data to recv
IN	`source`	integer	Rank (task ID) of source task
IN	`tag`	integer	Message tag
IN	`comm`	handle	Communicator
OUT	`status`	status	Status object

Point-to-Point Communication Routines

- Blocking vs. Non-blocking
- Synchronous vs. Asynchronous
- Determinism
- Deadlocks, or Race Conditions

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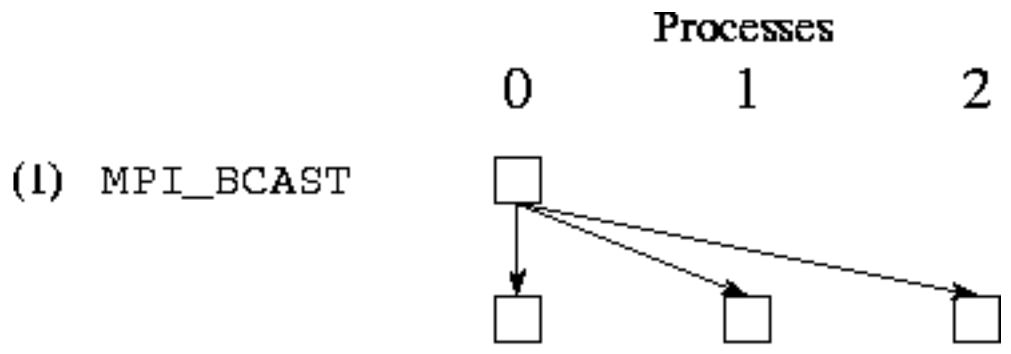
Collective Communication Routines

- Broadcast:



C	`MPI_Bcast (&buffer,count,datatype,root,comm)`
Fortran	`MPI_BCAST (buffer,count,datatype,root,comm,ierr)`

Arguments:

Intent	Argument	Type	Description
INOUT	`buffer`	choice	Address of input data array, or output data array at root
IN	`count`	integer(≥ 0)	Number of array elements to receive
IN	`datatype`	handle	Type of data to recv
IN	`root`	integer	Rank (task ID) of root task
IN	`comm`	handle	Communicator

Collective Communication Routines

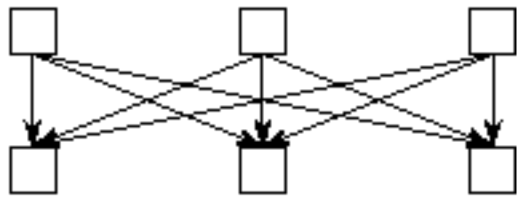
- Reduction:
  - This operation takes the data in the same variable on each processor, or array of variables, and performs an operation on all of the variables, for example computing the sum or finding the maximum value.
  - The result is either collected at the root process (MPI_Reduce) or distributed to all processes (MPI_Allreduce).
-

C	`MPI_Reduce (&sendbuf,&recvbuf,count,datatype,op,root,comm)`
Fortran	`MPI_REDUCE (sendbuf,recvbuf,count,datatype,op,root,comm,ierr)`

Arguments:

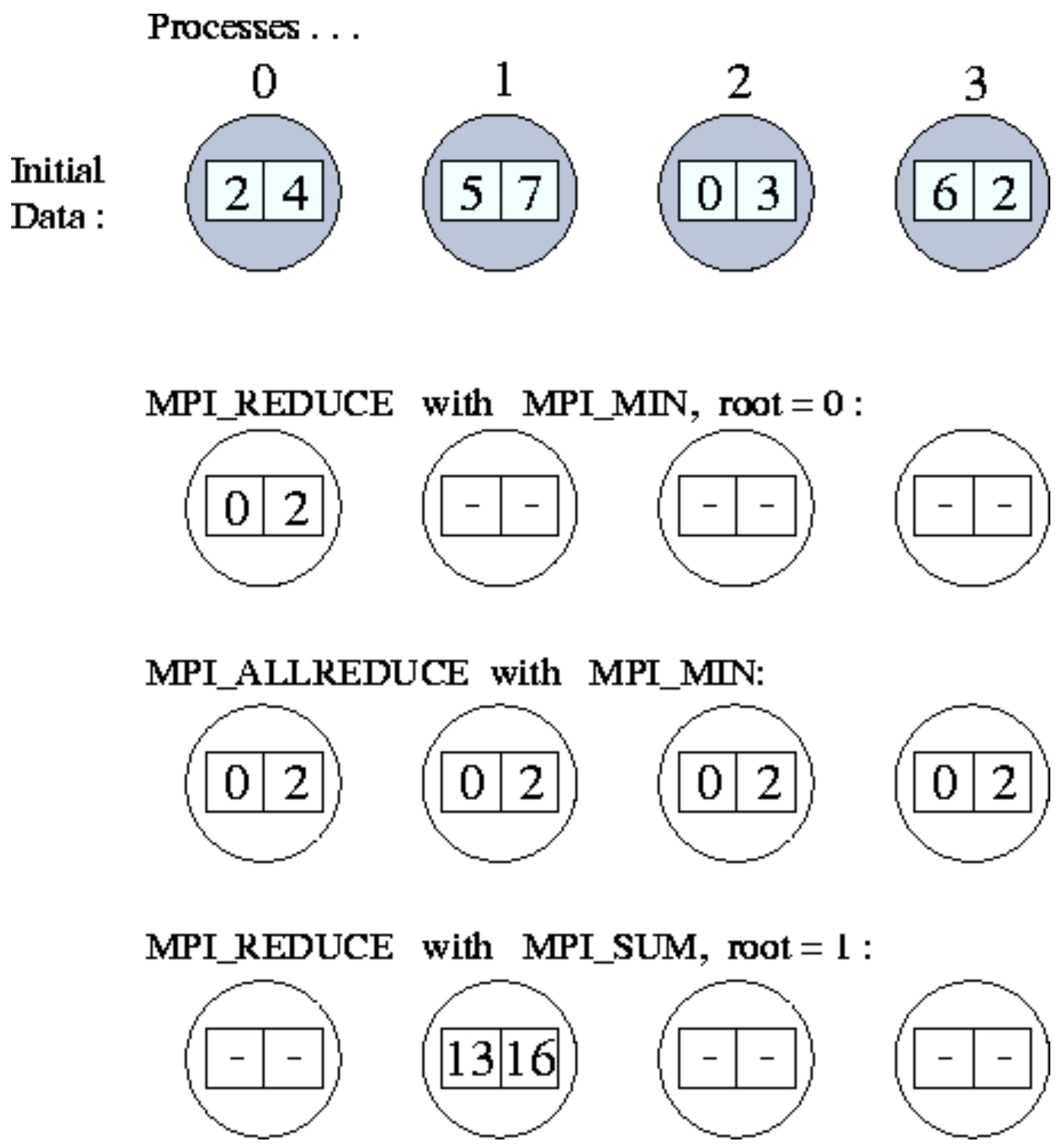
Intent	Argument	Type	Description
IN	`sendbuf`	choice	Address of input data array to send
OUT	`recvbuf`	choice	Address of output data array for result at root
IN	`count`	integer(≥ 0)	Number of array elements to receive
IN	`datatype`	handle	Type of data to recv
IN	`op`	handle	Operation to perform
IN	`root`	integer	Rank (task ID) of root task
IN	`comm`	handle	Communicator

(4) MPI_REDUCEALL



Collective Communication Routines

- Example of Reduction Operation:



Processes . . .
0
1
2
3
Initial Data :
2 4
5 7
0 3
6 2
MPI_REDUCE with MPI_MIN, root = 0 :
0 2
- -
- -
- -
MPI_ALLREDUCE with MPI_MIN:
0 2
0 2
0 2
0 2
MPI_REDUCE with MPI_SUM, root = 1 :
- -
13 16
- -
- -

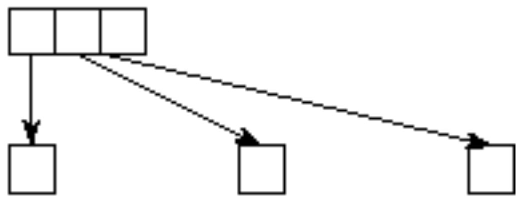
Collective Communication Routines

- Barrier: Wait for all tasks to synchronize

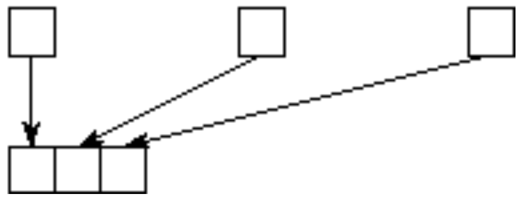
C	`MPI_Barrier (comm)`
Fortran	`MPI_BARRIER (comm,ierr)`

- Others: Scatter and Gather

(2) MPI_SCATTER



(5) MPI_GATHER



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Asynchronous Communication Routines

- Asynchronous communication allows an MPI task continue with local computational operations while waiting for a message to be sent or delivered

- This can be very computationally efficient, but requires care in ensuring data is only used after a message has been received.

- Some of the MPI calls are MPI_ISEND, MPI_IPROBE, and MPI_IRECV.

References

Information on Message Passing Interface (MPI)

- Designing and Building Parallel Programs, Ian Foster
http://www.mcs.anl.gov/~itf/dbpp/
-Somewhat dated (1995), but an excellent online textbook with detailed discussion about many aspects of HPC. This presentation borrowed heavily from this reference

- Message Passing Interface (MPI), Blaise Barney
  https://computing.llnl.gov/tutorials/mpi/
  -Excellent tutorial on the use of MPI, with both Fortran and C example code