An Introduction to MPI Programming

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Topics

- Introduction
- Initialising MPI & basic concepts
- Compiling and running a parallel program on the Cray
- Practical: "Hello World" MPI program
- Synchronisation
- Practical
- Data types and tags
- Basic sends and receives
- Practical
- Collective communications
- Reduction Operations
- MPI References



Introduction (1 of 4)

- Message Passing evolved in the late 1980's
- Cray was dominate in supercomputing
 - with very expensive shared-memory vector processors
- Many companies tried new approaches to HPC
- Workstation and PC Technology was spreading rapidly
- "The Attack of the Killer Micros"
- Message Passing was a way to link them together
 - many different flavours PVM, PARMACS, CHIMP, OCCAM
- Cray recognised the need to change
 - switched to MPP using cheap DEC Alpha microprocessors (T3D/T3E)
- But application developers needed portable software



Introduction (2 of 4)

- Message Passing Interface (MPI)
 - The MPI Forum was a combination of end users and vendors (1992)
 - defined a standard set of library calls in 1994
 - Portable across different computer platforms
 - Fortran and C Interfaces
- Used by multiple tasks to send and receive data
 - Working together to solve a problem
 - Data is decomposed (split) into multiple parts
 - Each task handles a separate part on its own processor
 - Message passing to resolve data dependencies
- Works within a node and across Distributed Memory Nodes
- Can scale to thousands of processors
 - Subject to constraints of Amdahl's Law



Introduction (3 of 4)

The MPI standard is large

- Well over 100 routines in MPI version 1
- Result of trying to cater for many different flavours of message passing and a diverse range of computer architectures
- And an additional 100+ in MPI version 2 (1997)
- And many more additions in MPI version 3 (2012)
- MPI version 1 works whatever version of MPI you have

Many sophisticated features

- Designed for both homogenous and heterogeneous environments
- But most people only use a small subset
 - IFS was initially parallelised using Parmacs
 - This was replaced by about 10 MPI (version 1) routines
 - Hidden within "MPL" library



Introduction (4 of 4)

- This course will look at just a few basic routines
 - Fortran Interface Only
 - MPI version 1.2
 - SPMD (Single Program Multiple Data)
 - As used at ECMWF in IFS
- A mass of useful material on the Web
 - MPI standard
 - Lots of useful information about MPI's behaviour & implementation
 - http://www.mpi-forum.org/docs/mpi-1.1/mpi-11-html/mpi-report.html
 - Open MPI documentation
 - A nice easy guide to the API (contains MPI v2 too), including Fortran interface
 - http://www.open-mpi.org/doc/v1.10/



SPMD

The SPMD model is by far the most common

- <u>Single Program Multiple Data</u>
- One program executes multiple times simultaneously
- The problem is divided across the multiple copies
- Each work on a subset of the data

MPMD

- <u>Multi Program Multiple Data</u>
- Different executable on different processors
- Useful for coupled models for example
- Part of the MPI 2 standard
- Not currently used by IFS
- Can be mimicked in SPMD mode
 - Top level branch deciding which "program" (subroutine) this task will run



Some definitions

Task

- one running instance (copy) of a program
- Equivalent to a UNIX process
- Basic unit of an MPI parallel execution
- May run on one processor
 - Or across many if OpenMP is used as well (threads)
 - Or many tasks on one processor (not a good idea!)

Master

- the master task is the first task in a parallel program : TaskID=0

Slave

- all other tasks in a parallel program
- Nothing intrinsically different between master/slave but the parallel program may treat them differently



The simplest MPI program......

- Lets start with "hello world"
- Introduces
 - 4 essential housekeeping routines
 - the "use mpi" statement
 - the concept of Communicators

```
program hello
implicit none
print *,"Hello world"
end
```



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror, ntasks, mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK(MPI_COMM_WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



use mpi: The MPI header file

use mpi

- The MPI header file
- Always include in any routine calling an MPI function
- Contains declarations for constants used by MPI
- May contain interface blocks, so compiler will tell you if you make an obvious error in arguments to MPI library
 - This is not mandated by the standard so you shouldn't rely on it.
 You may want to test Cray's mpi to see if it does!
- In Fortran77 use "include 'mpif.h" instead



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror, ntasks, mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK (MPI COMM WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



MPI_INIT

```
integer:: ierror
call MPI INIT(ierror)
```

- Initializes the MPI environment
- Expect a return code of zero for ierror
 - If an error occurs the MPI layer will normally abort the job
 - best practise would check for non zero codes
 - we will ignore for clarity but see later slides for MPI_ABORT
- On the Cray all tasks execute the code before MPI_INIT
 - this is an implementation dependent feature
 - try not to do anything that alters the state of the system before this, eg. I/O



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror, ntasks, mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK (MPI COMM WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



MPI_COMM_WORLD

- An MPI communicator
- Constant integer value from "use mpi"
- MPI_COMM_WORLD means all tasks
 - many MPI programs only use MPI_COMM_WORLD
 - All our examples only use MPI_COMM_WORLD
- Communicators define sets or groups of tasks
 - dividing programs into subsets of tasks often not necessary
 - IFS also creates and uses some additional communicators
 - useful when doing collective communications
 - Useful if you want to dedicate a subset of tasks to a special job (eg. I/O server)
 - advanced topic



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror,ntasks,mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK (MPI COMM WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



MPI_COMM_SIZE

```
integer:: ierror,ntasks
call MPI COMM SIZE(MPI COMM WORLD, ntasks, ierror)
```

- Returns the number of parallel tasks in the variable "ntasks"
 - the number of tasks is defined from the aprun command which starts the parallel executable
- Value can be used to help decompose the problem
 - in conjunction with Fortran allocatable/automatic arrays
 - avoid the need to recompile for different processor numbers



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror,ntasks,mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK (MPI COMM WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



MPI_COMM_RANK

```
integer:: ierror, mytask
call MPI_COMM_RANK(MPI_COMM_WORLD, mytask, ierror)
```

- Returns the rank of the task in mytask
 - In the range 0 to ntasks-1
 - Easy to make mistakes with this as Fortran arrays normally run 1:n
 - Used as a task identifier when sending/receiving messages



Hello World with MPI

```
program hello
implicit none
use mpi
integer:: ierror,ntasks,mytask
call MPI INIT (ierror)
call MPI COMM SIZE (MPI COMM WORLD, ntasks, ierror)
call MPI COMM RANK (MPI COMM WORLD, mytask, ierror)
print *,"Hello world from task ",mytask," of ",ntasks
call MPI FINALIZE(ierror)
end
```



MPI_FINALIZE

```
integer:: ierror
call MPI_FINALIZE(ierror)
```

- Tell the MPI layer that we have finished
- Any MPI call after this is an error
 - Like MPI_INIT, the MPI standard does not mandate what happens after an MPI_FINALIZE – cannot guarantee that all tasks still execute after this point
- Does not stop the program at least one (probably all!) tasks will continue to run



MPI_ABORT

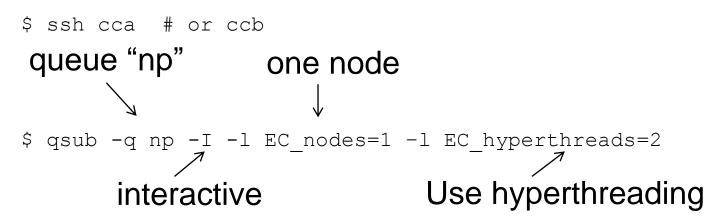
```
integer:: ierror
call MPI_ABORT(MPI_COMM_WORLD,ierror)
```

- Causes all tasks to abort
- Even if only one task makes call



PBSPro and MPI

- Many varied ways of defining your requirements
- For the exercises we'll keep it as simple as possible
 - Create an interactive shell in which you can run parallel jobs in up to one node (48 hyperthreaded CPUs)
 - You won't need to wait every time you run an executable!
 - Don't forget to log out when you're finished!
 - Not recommended for regular use!





Compiling an MPI Program

- Very easy using modules
 - Automatically adds all the flags/libraries required for MPI

```
$ module load PrgEnv-cray # Use Cray compilers
$ module load PrgEnv-intel # Use Intel compilers
$ module load PrgEnv-gnu # Use Gnu compilers
----
$ ftn hello.f90 # produces a.out
$ ftn Or c hello.f90 # produces hello.o
$ ftn hello.o -o hello.exe # produces hello.exe
```



Running an MPI Program

aprun

- Details and many options covered in other lectures
- Here we will use a very simple form
- Run from the MOM node (where your interactive shell is running), launches the parallel executable on the parallel (ESM) node(s)

```
$ aprun -n 4 <executable>
```



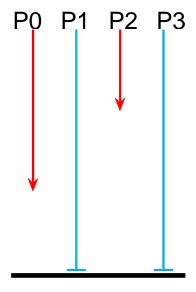
First Practical

- Copy all the practical exercises to your account on cca or ccb:
 - cd \$HOME
 - mkdir mpi_course ; cd mpi_course
 - cp -r ~trx/mpi.2016/*.
- Exercise1a
 - Run your own Hello World program with MPI
- See the README for details

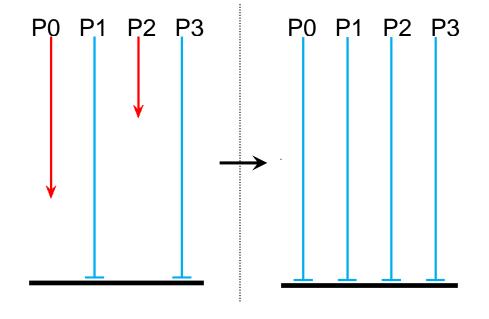
```
integer:: ierror
call MPI BARRIER(MPI COMM WORLD, ierror)
```

 Forces all tasks (in a communicator group) to synchronise (wait for each other)



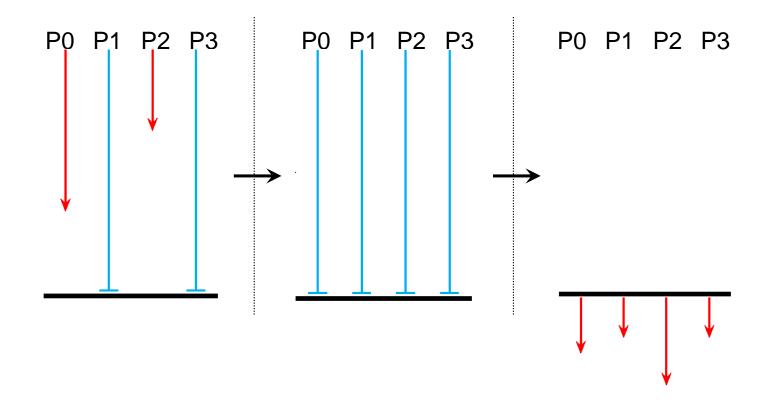








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- Possible uses:
 - for timing points
 - to improve output of prints
 - can be used to force ordering of events
 - to separate different communications phases
- A task waits in the barrier until every task has reached it
- Then all tasks exit the call together at the same time
- Deadlock if one task does not reach the barrier
 - MPI_BARRIER will wait until the task reaches its cpu limit
- What happens if different tasks call MPI_BARRIER in different parts of the code?
 - Could be desired behaviour, or it could be highly confusing bug!



Second Practical

- Forcing the ordering of output
- Exercise 1b see the README file for more details…



Basic Sends and Receives

- MPI_SEND
 - sends a message from one task to another
- MPI_RECV
 - receives a message from another task
- A message is just data with some form of identification
 - think of it as an email the body and some headers
 - To: Where the message should be sent to
 - Subject: Some description of the contents (in MPI, a "tag")
 - Body: The data itself (can be any size), various Fortran types
- You program the logic to send and receive messages
 - the sender and receiver are working together
 - every send must have a corresponding receive



MPI Datatypes

- MPI can send variables of any Fortran type
 - integer, real, real*8, logical,
 - it needs to know the type
- There are predefined constants used to identify types
 - MPI_INTEGER, MPI_REAL, MPI_REAL8, MPI_LOGICAL......
 - Defined by "use mpi"
- Also user defined data types
 - MPI allows you create types created out of basic Fortran types (rather like a Fortran 90 structure)
 - Allows strided (non contiguous) data to be communicated
 - advanced topic not covered here



MPI Tags

- All messages are given an integer TAG value
 - standard says maximum value is at least 32768 (2^31)
- This helps to identify a message (like an email's "subject")
- Particularly useful when sending multiple messages
- You decide what tag values to use
 - Good idea (helps spot problems) to use separate ranges of tags in different communication areas, eg:
 - 1000, 1001, 1002..... in routine a
 - 2000, 2001, 2002.... in routine b



MPI_SEND

• SBUF	the array being sent	input
• COUNT	the number of elements to send	input
• MPI_TYPE	type of SBUF eg MPI_REAL	input
• DEST	the task id of the receiver	input
• TAG	the message identifier	input



MPI_RECV

• RBUF	the array being received	output
• COUNT	the length of RBUF	input
• MPI_TYPE	type of RBUF eg MPI_REAL	input
• SOURCE	the task id of the sender	input
• TAG	the message identifier	input



STATUS

information about the message

output

More on MPI_RECV

- MPI_RECV will block (wait) until the message arrives
 - if message never sent then deadlock
 - task will wait until it reaches cpu time limit, and then dies
- Order in which messages are received
 - For a given pair of processors using the same communicator, the MPI standard guarantees the messages will be received in the same order they were sent
- This means you need to be careful
 - If you are receiving multiple messages from the same task, you MUST do the MPI_RECVs in the same order as the MPI_SENDs
 - Otherwise the first MPI_RECV will wait forever, and eventually die
 - What happens if you don't know the ordering of the MPI_SENDs?



How to be less specific on MPI_RECV

- The source and tag can be more open
 - MPI_ANY_SOURCE means receive from any sender
 - MPI_ANY_TAG means receive any tag
 - Useful in more complex communication patterns
 - Used to receive messages in a more random order
 - helps smooth out load imbalance
 - May require over-allocation of receive buffer
- But how do we know what message we've received?
 - status (MPI_SOURCE) will contain the actual sender
 - status (MPI_TAG) will contain the actual tag



An example: task 0 sends a message to task 1

```
subroutine transfer(values,len,mytask)
implicit none
use mpi
integer:: mytask,len,source,dest,tag,ierror,status(MPI STATUS SIZE)
real:: values(len)
tag = 12345
if (mytask.eq.0) then
   dest = 1
   call MPI_SEND(values,len,MPI_REAL,dest,tag,MPI COMM WORLD,ierror)
elseif(mytask.eq.1) then
   source = 0
   call MPI RECV(values,len,MPI REAL,source,tag,MPI COMM WORLD,status,ierror)
endif
end
```



Third Practical

- Sending and receiving a message
- Exercise 1c see the README file for more details...



Collective Communications (1)

- SEND/RECV is pairwise communication
- Often we want to do more complex communication patterns
- For example
 - Send the same message from one task to many other tasks
 - Receive messages from many tasks onto many other tasks
- We could write this with MPI SEND & MPI RECV
 - How?
 - Why not?



Collective Communications

- MPI contains many Collective Communications routines
 - called by all tasks (in a communicator group) together
 - replace multiple send/receive calls
 - easier to code and understand
 - can be more efficient
 - the MPI library may optimise the data transfers
- We will look at MPI BCAST and MPI GATHER
- Other routines will be summarised
- The diagrams are schematic
 - Help to conceptualise the data movement
 - The MPI library and machine hardware may actually be doing a more complex (and hopefully efficient!) communication pattern
- IFS uses a few collective routines, sometimes we hand code our own



FORTRAN TYPE:: buff

integer:: count, root, ierror

call MPI BCAST(buff,count, MPI TYPE, root, MPI COMM WORLD, ierror)

ROOT task doing broadcast input

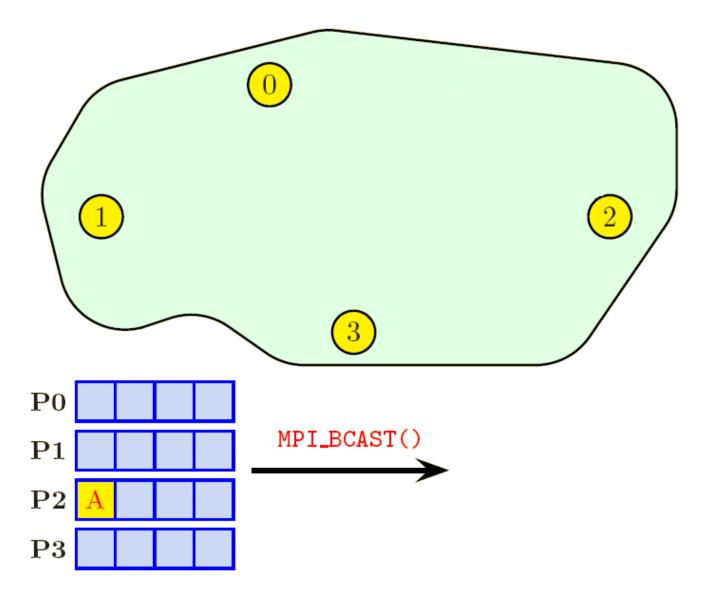
BUFF array being broadcast input/output

COUNT the number of elements input

MPI TYPE the kind of variable input

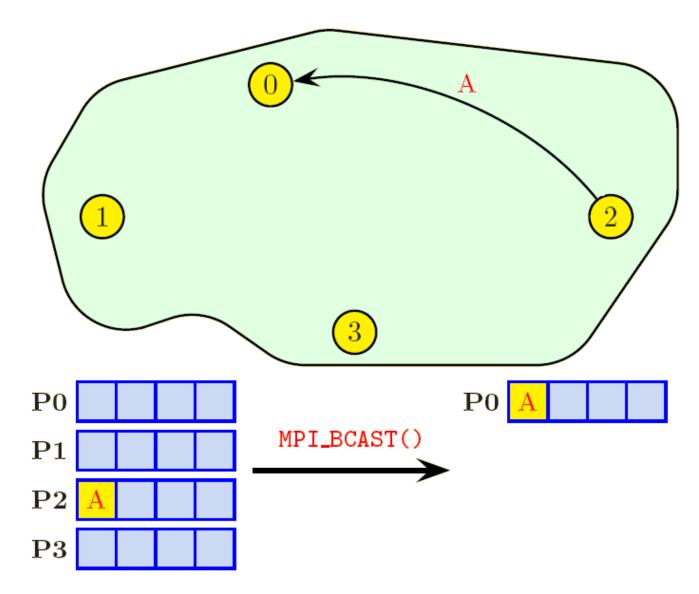
The contents of buff are sent from task id root to all other tasks. Each task receives the full array. Equivalent to putting MPI_SEND in a loop and matching MPI_RECVs





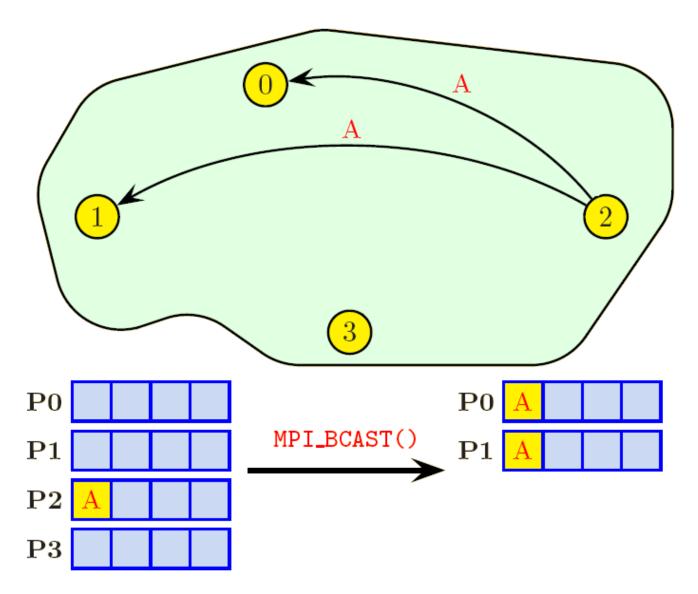






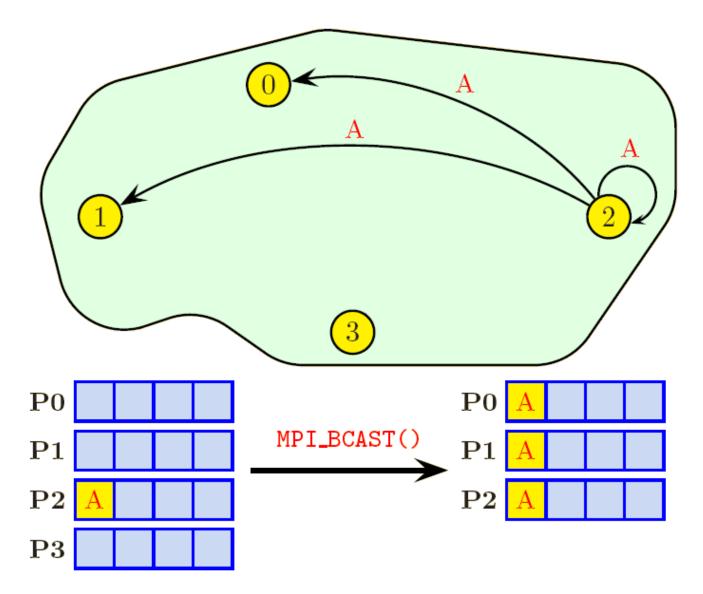






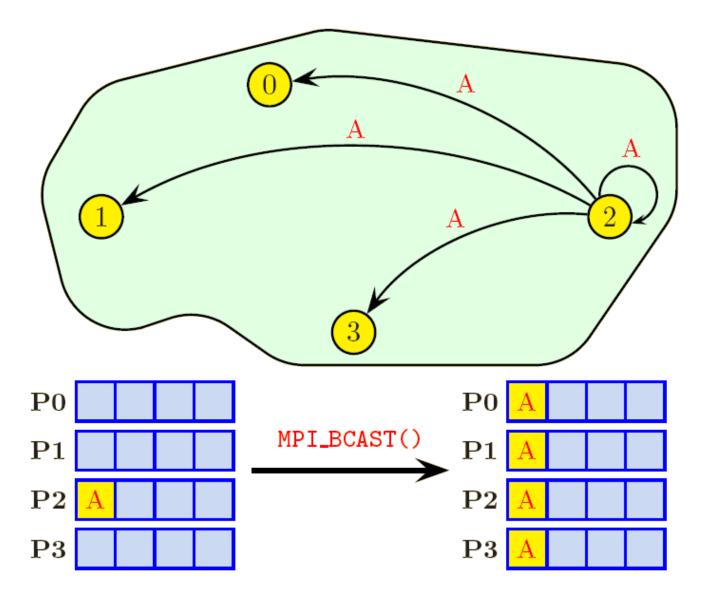












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ROOT task doing gather input

SBUFF array being sent input

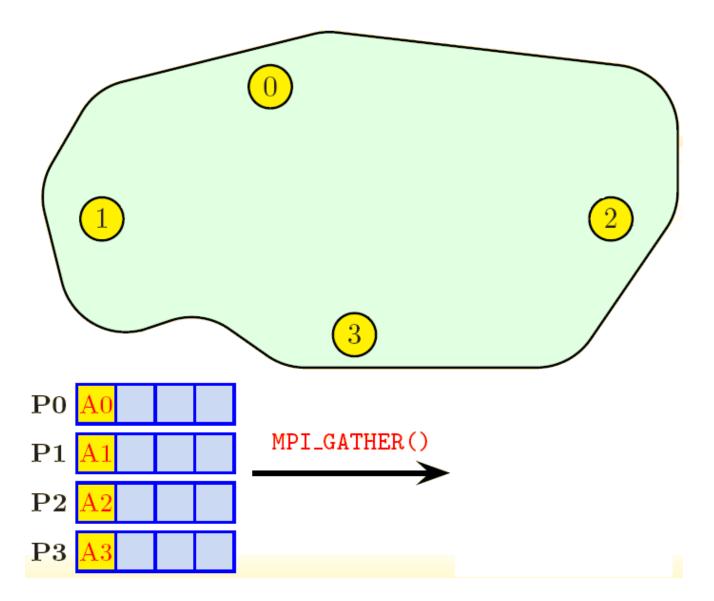
RBUFF array being received output

• [S/R] COUNT number of items to/from input

each task

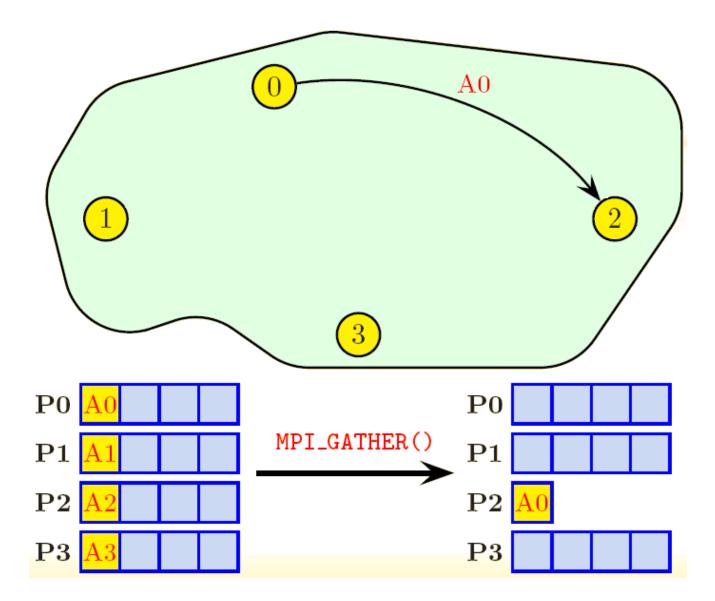
The contents of sbuff are sent from every task to task id root and received (concatenated in rank order) in array rbuff. Could also be done by putting MPI_RECV in a loop.





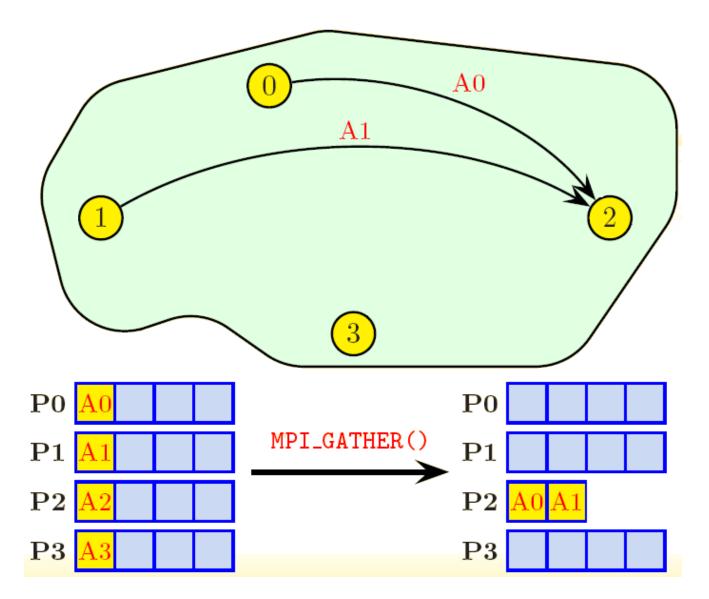






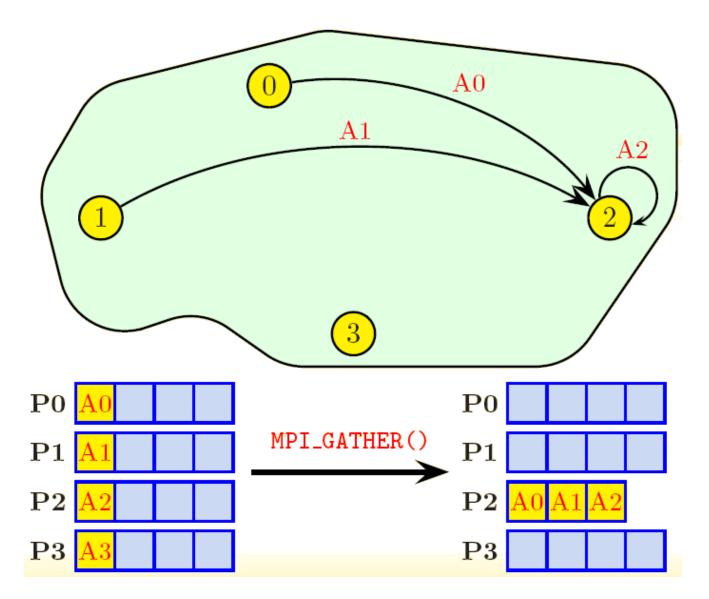
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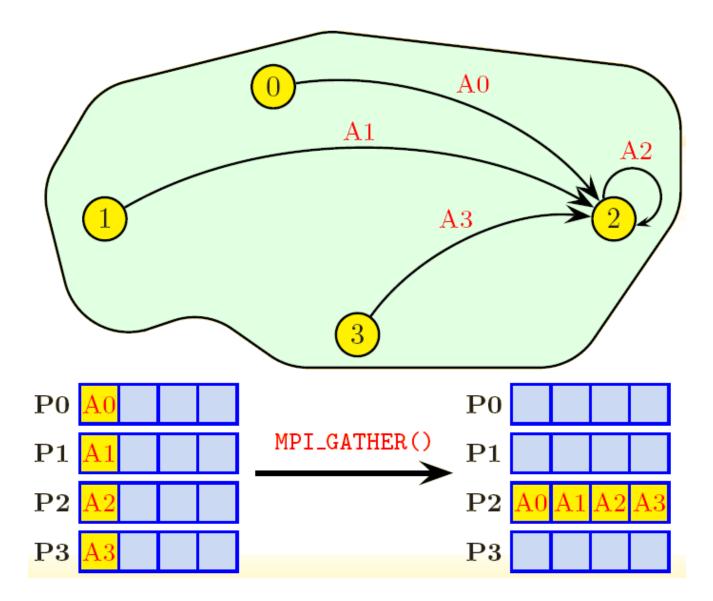












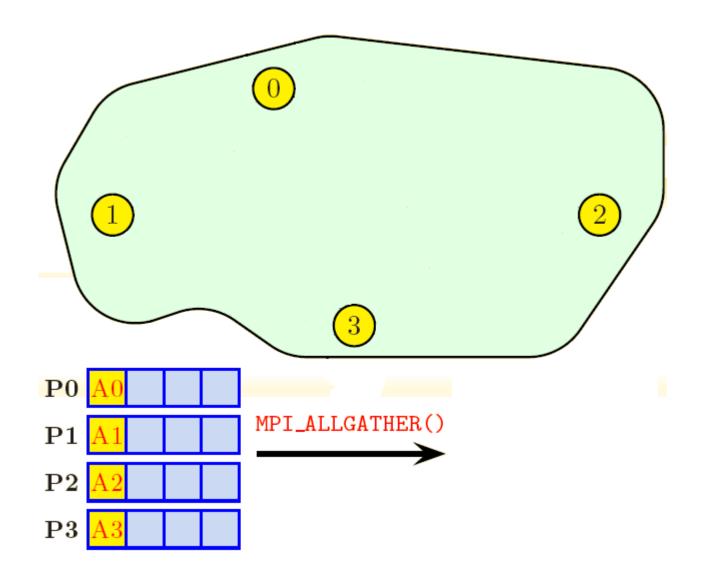
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Gather Routines

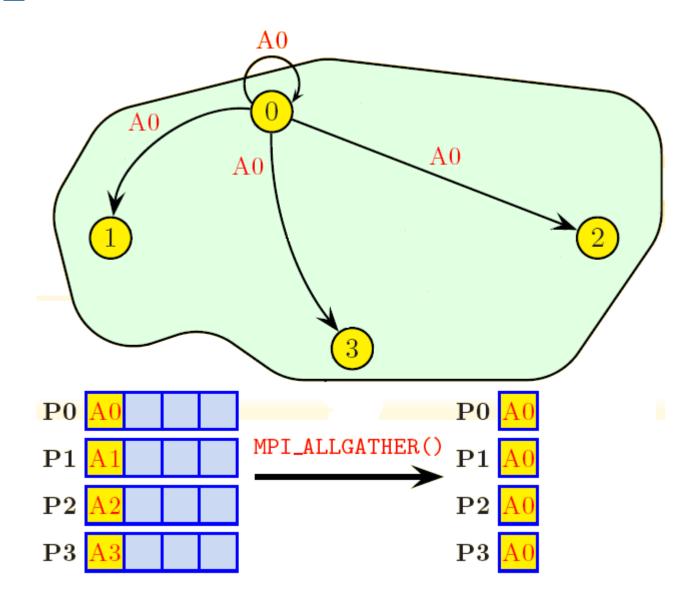
- MPI ALLGATHER
 - gather arrays of equal length into one array on <u>all</u> tasks
 - Equivalent to doing MPI_GATHER followed by MPI_BCAST
- MPI GATHERV
 - gather arrays of different lengths into one array on one task
- MPI ALLGATHERV
 - gather arrays of different lengths into one array on <u>all</u> tasks
- Where do you think these may be useful?





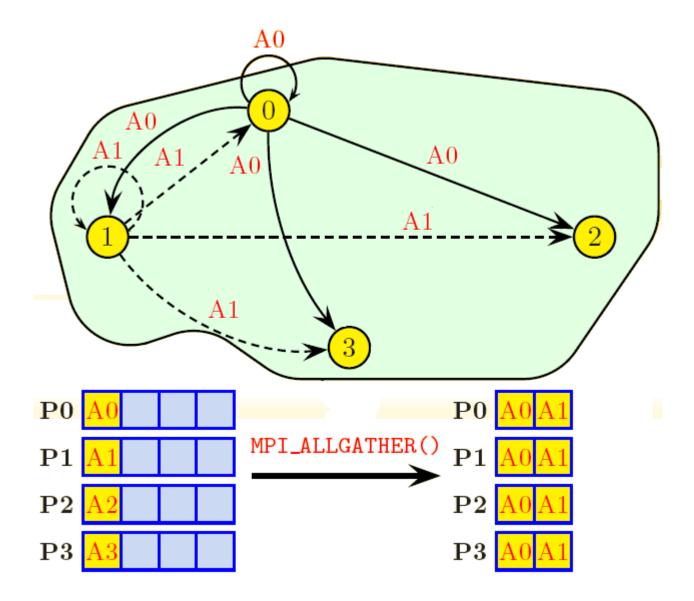






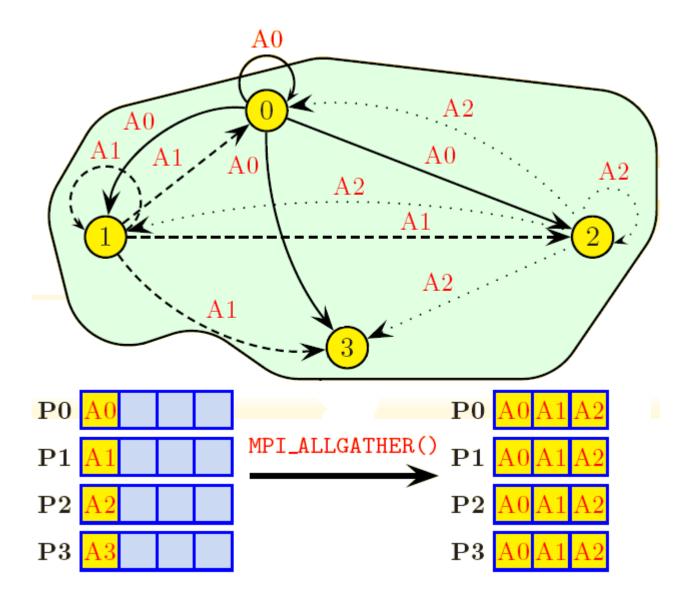






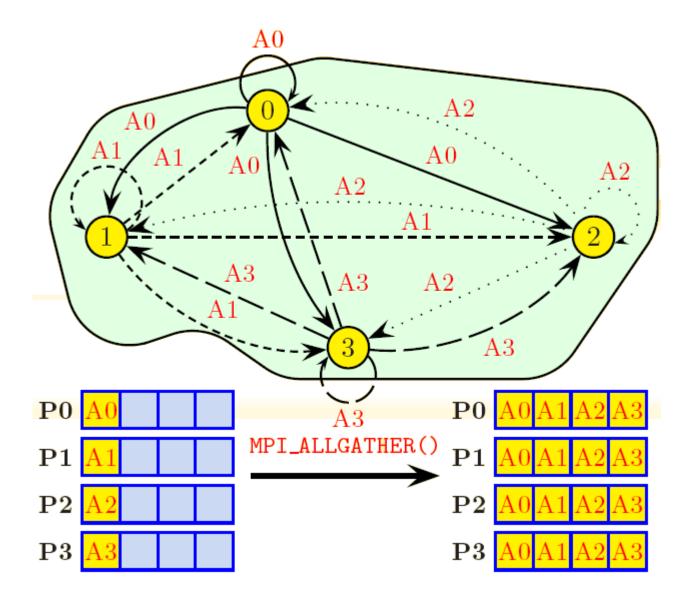
















Scatter Routines

- MPI SCATTER
 - divide one array on one task equally amongst all tasks
 - each task receives the same amount of data
- MPI_SCATTERV
 - divide one array on one task <u>unequally</u> amongst all tasks
 - each task can receive a different amount of data
- Where do you think they might be useful?



ROOT task doing scatter input

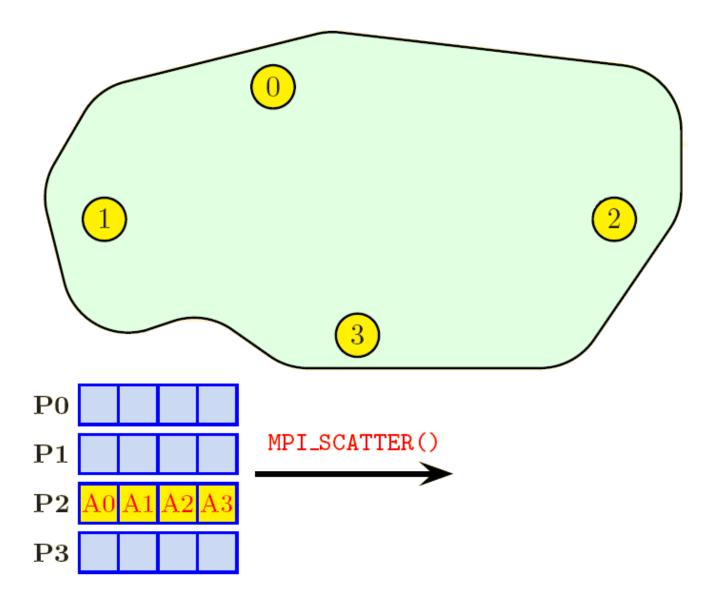
SBUFF array being sent input

RBUFF array being received output

• [S/R] COUNT number of items to/from input each task

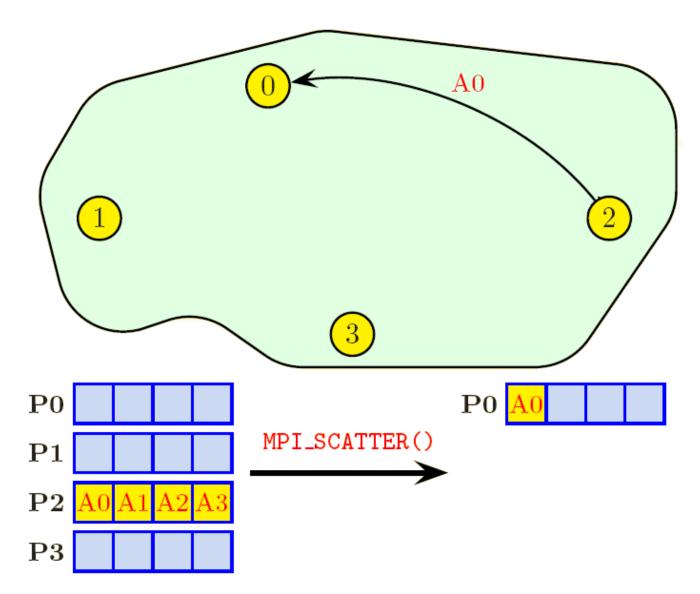
The contents of sbuff on task id root are equally split and each task receives its part in array rbuff. Could also be done by putting MPI_SEND in a loop.





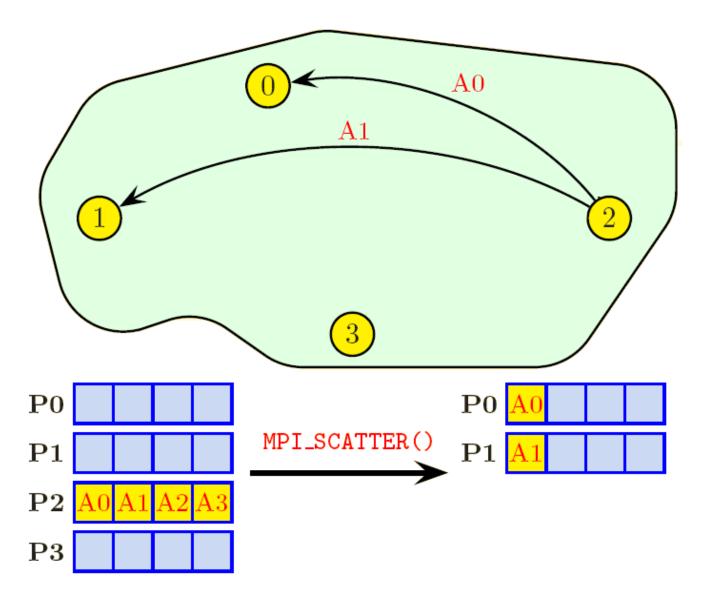






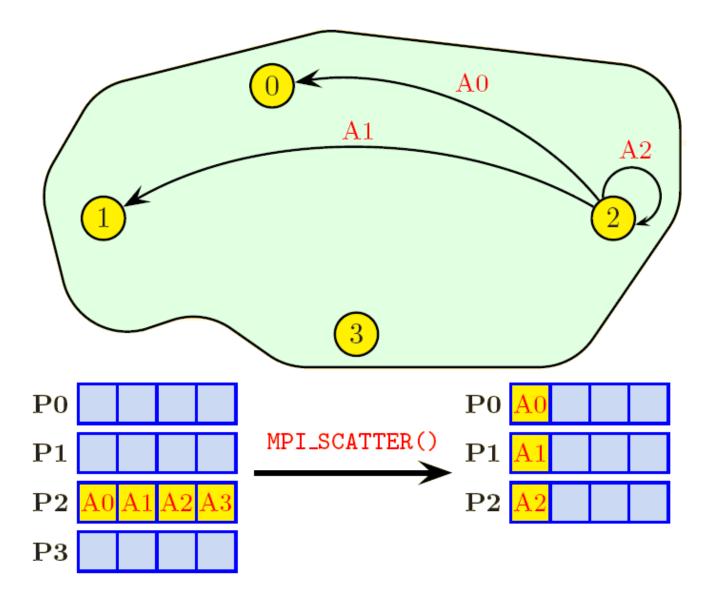






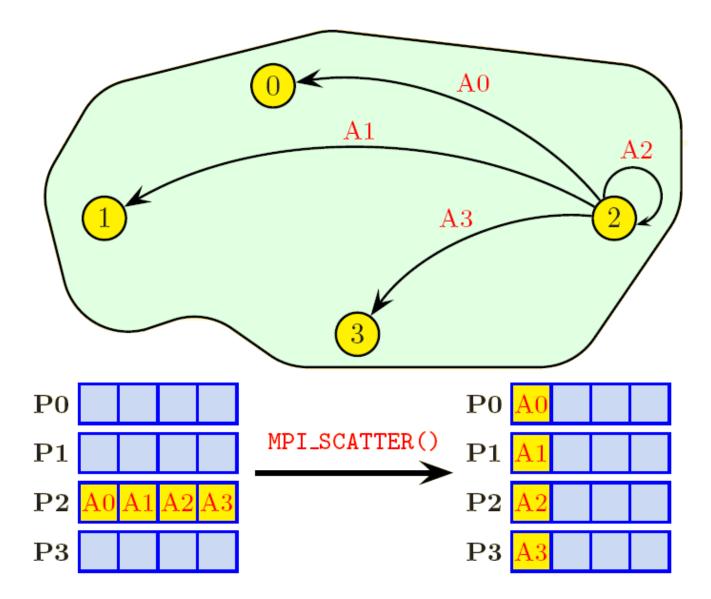












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All to All Routines

- MPI_ALLTOALL
 - every task sends equal length parts of an array to all other tasks
 - every task receives equal parts from all other tasks
 - transpose of data over the tasks
- MPI_ALLTOALLV
 - as above but parts are different lengths



MPI_ALLTOALL

SBUFF array being sent input

RBUFF array being received output

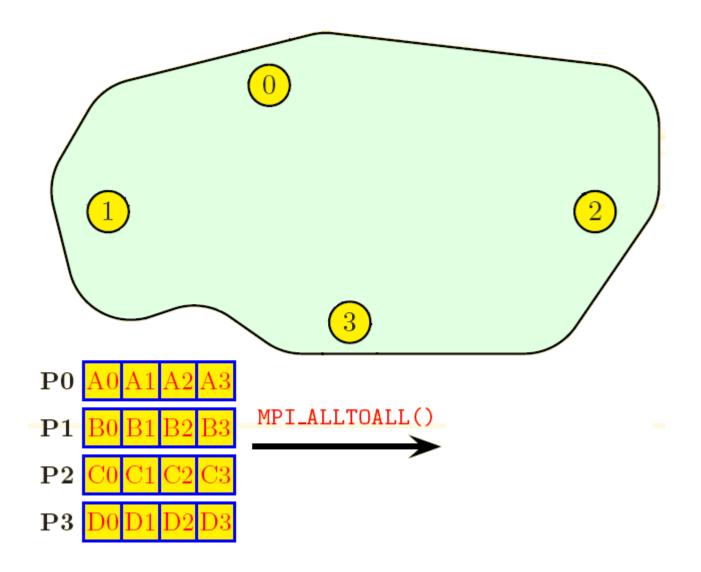
• [S/R] COUNT number of items to/from input

each task

The contents of sbuff on each task are equally split and each task receives an equal part into array rbuff. Could also be done by putting MPI_SEND/MPI_RECV in a loop.



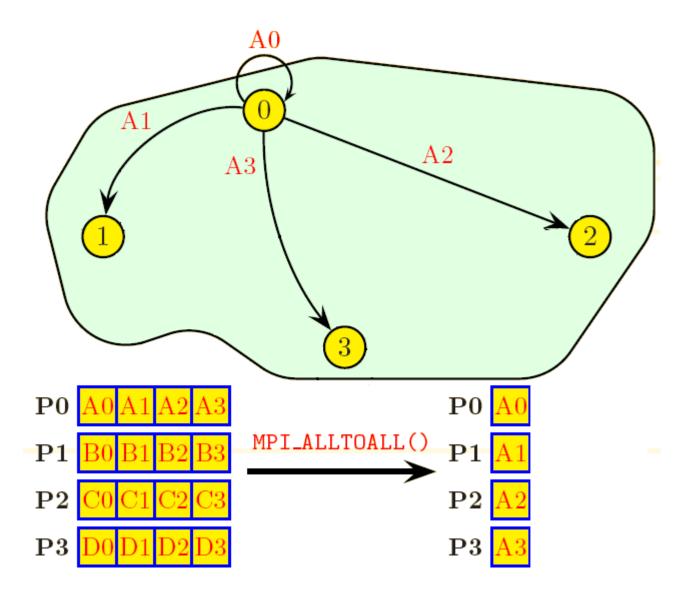
MPI_ALLTOALL







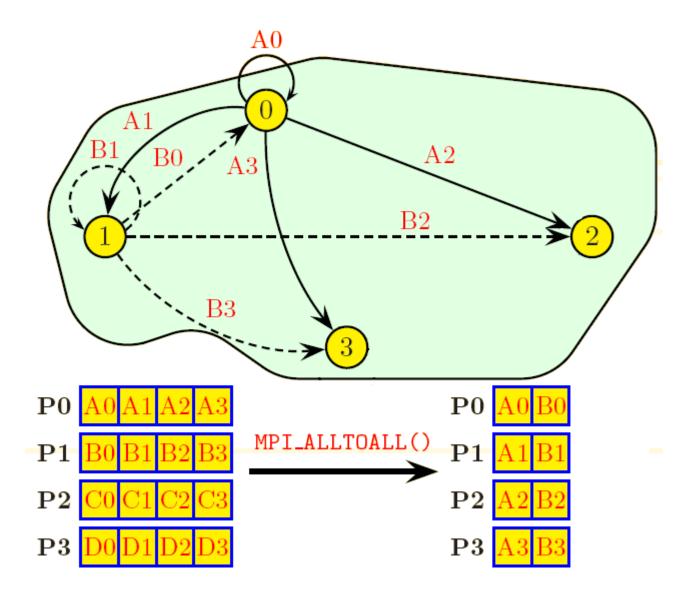
MPI_ALLTOALL







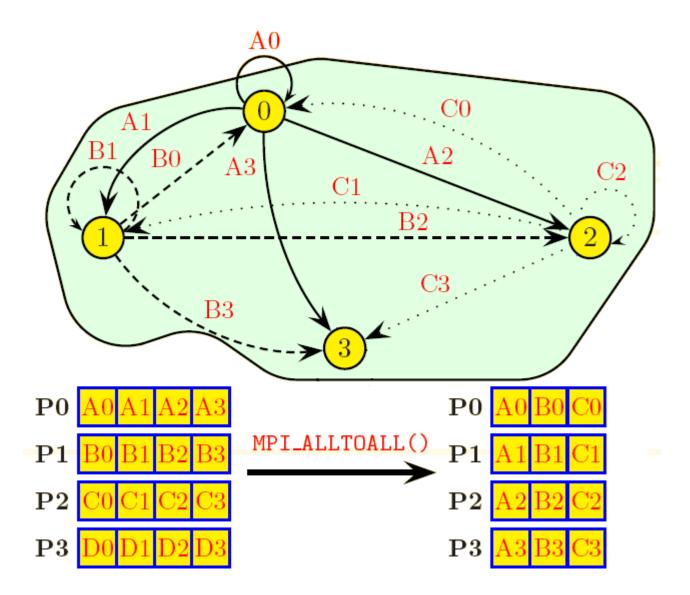
MPI_ALLTOALL







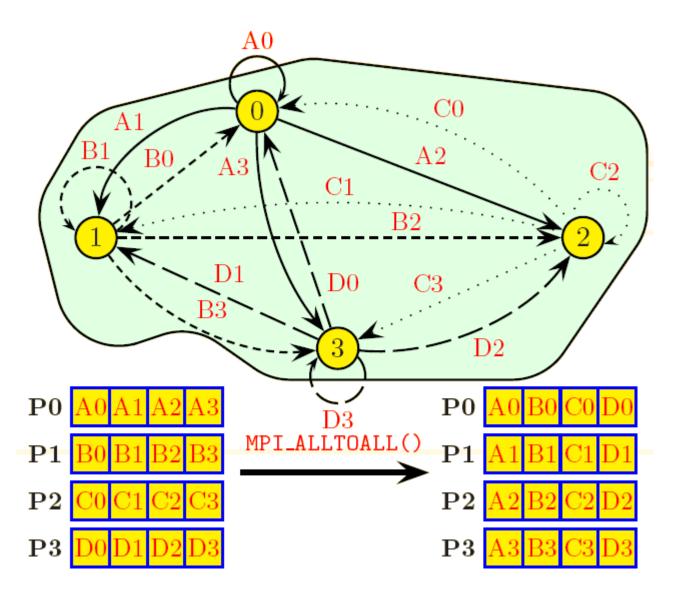
MPI_ALLTOALL







MPI_ALLTOALL







Reduction routines

- Perform both communications and simple maths
 - Global sum, min, max,
- Beware reproducibility
 - MPI makes no guarantee of reproducibility
 - Eg. Summing an array of real numbers from each task
 - May be summed in a different order each time
 - You may need to write your own order preserving summation if reproducibility is important to you.
- MPI REDUCE
 - every task sends data and result is computed on the "root" task
- MPI_ALLREDUCE
 - every task sends, result is computed and broadcast back to all tasks. Equivalent to MPI_REDUCE followed by MPI_BCAST



MPI_REDUCE

SBUFF array to be reduced input

RBUFF result of reduction output

• COUNT number of items to be input

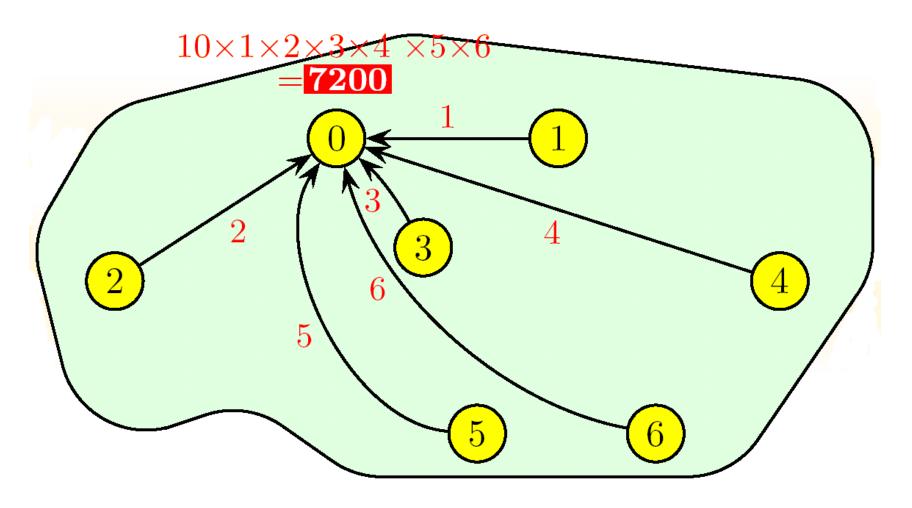
reduced

The contents of sbuff from all tasks are reduced according to OP_TYPE and the result is sent to RBUFF task root.

OP_TYPE can be MPI_MAX, MPI_MIN, MPI_SUM, MPI_IPROD, MPI_IAND, MPI_BAND, MPI_IOR, MPI_BOR, MPI_LXOR, MPI_BXOR, MPI_MAXLOC, MPI_MINLOC



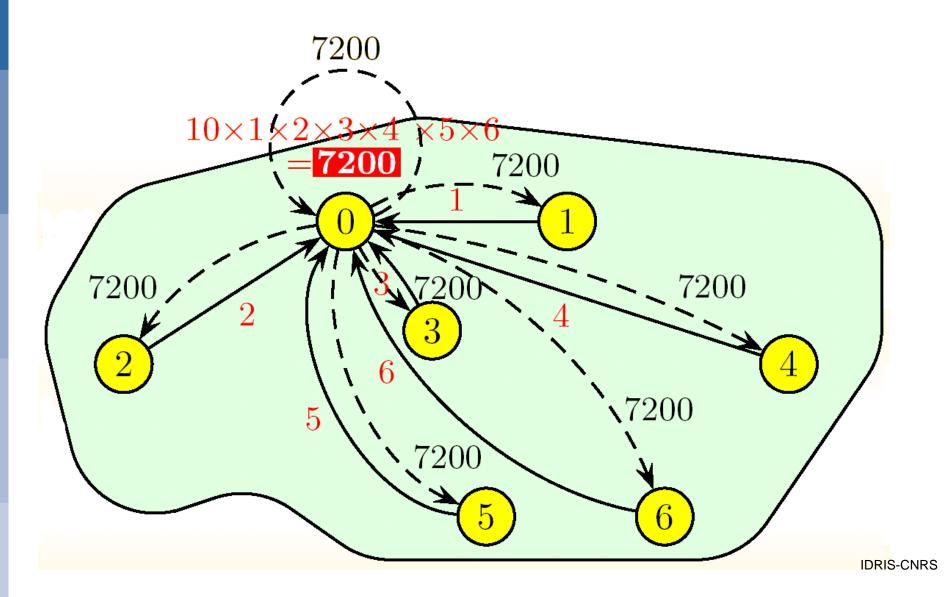
MPI_REDUCE



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MPI_ALLREDUCE





Back to "simple" send & receives

- What happens after you do MPI_SEND?
 - When does the next instruction get executed?
- What happens after you do MPI_RECV?
 - When does the next instruction get executed?



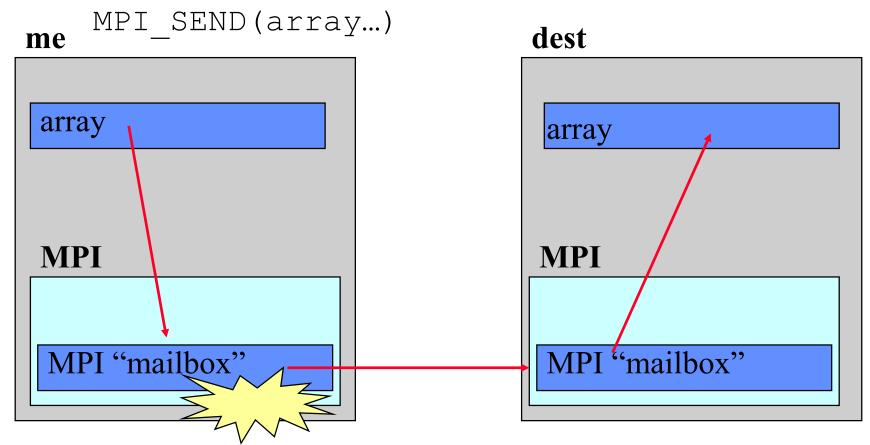
Blocking v Non-blocking communication

Blocking communication

- Call to MPI "sending" routine does not return until the "send" buffer (array) is safe to use again
 - This does not necessarily mean the data has been sent and received by the remote task (although it might!)
- Call to MPI "receiving" routine does not return until the "receive" buffer has received all the data in the incoming message
- Non-blocking communication
 - Call to MPI routine returns immediately
 - Further MPI calls are required to check the progress of the communication
 - Allows other work to be done during communication
- Cray's MPI_SEND can sometimes be blocking and sometimes non-blocking!



MPI_SEND : Eager protocol



MPI_SEND completes when "array" is copied into "mailbox" on the sending task

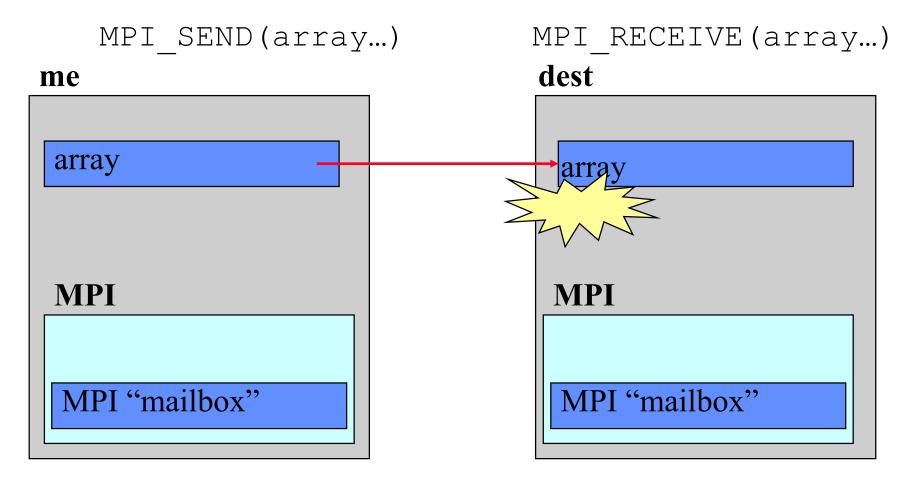


MPI_SEND : Eager protocol

- The MPI layer has copied the data elsewhere
 - using internal buffer/mailbox space on the sending task
- MPI_SEND returns as soon as the message has been copied
 - The message is then "in transit" but not necessarily in the receivers array
- Used for short messages
 - By default "short" is 8192 bytes (8Kb) on the Cray
 - Can be modified by envioronment vairable
 - \$ export MPICH_GNI_MAX_EAGER_MSG_SIZE=X (bytes)
 - Maximum permitted value 131072 bytes (128Kb)
- No need to worry if the remote task has done an "MPI_RECEIVE"



MPI_SEND: Rendezvous protocol



MPI_SEND completes when "array" is copied into "array" on the receiving task



MPI_SEND: Rendezvous protocol

- MPI_SEND does not return until the message has been successfully received by the remote task
- Used for long messages
 - By default "long" is >8192 bytes on the Cray
- Need to ensure that remote task is doing an "MPI_RECEIVE" otherwise we may deadlock...
 - Easily done!
 - eg. ping-pong example 2 tasks exchanging messages...

```
if (me .eq.0) then
  other=1
else
  other=0
endif

call MPI_SEND(sbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,ierror)
call MPI_RECV(rbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,stat,ierror)
```



Solutions to Send/Send deadlocks

- My advice avoid MPI_SEND/MPI_RECV!
 - Behaviour is implementation dependent code may work, but then stop working when message size changes or move to another platform
- Pair up sends and receives (next slide shows how…)
 - But this is not very efficient
- use MPI SENDRECV
 - Hopefully more efficient
- use a buffered send (like the eager protocol, but user space buffering)
 - MPI_BSEND
- use asynchronous sends/receives (recommended)
 - MPI ISEND **or** MPI IRECV



Paired Sends and Receives

- More complex code, and close synchronisation
- Less efficient
 - task 1 has to wait until it has received message from task 0 before it can send its message

```
if (me .eq. 0) then
   other=1
   call MPI_SEND(sbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,ierror)
   call MPI_RECV(rbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,stat,ierror)
   else
   other=0
   call MPI_RECV(rbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,stat,ierror)
   4 call MPI_SEND(sbuff,n,MPI_REAL8,other,tag,MPI_COMM_WORLD,ierror)
   endif
    time
```

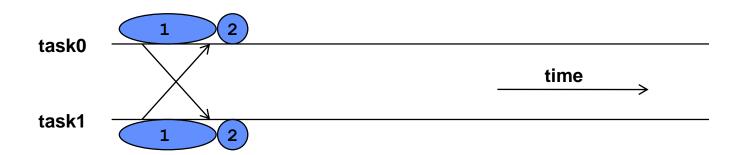


task1

MPI_SENDRECV

- Simpler to code & hopefully more efficient
- Still implies close synchronisation
- 1 call MPI_SENDRECV(sbuff,n,MPI_REAL8,other,1, & rbuff,n,MPI_REAL8,other,1, & MPI_COMM_WORLD,stat,ierror)







MPI_BSEND

- This performs a send using an additional buffer
 - the buffer is allocated by the program via MPI_BUFFER_ATTACH
 - done once as part of the program initialisation
 - MPI_BSEND completes as soon as message is copied into buffer
- Typically quick to implement
 - add the MPI BUFFER ATTACH call
 - how big to make the buffer?
 - change MPI_SEND to MPI_BSEND everywhere
- But introduces additional memory copy
 - extra overhead
 - not recommended for production codes
 - One day your buffer won't be big enough!



MPI_IRECV / MPI_ISEND

- Uses Non Blocking Communications
- "I" stands for immediate
 - the call returns immediately
- Routines return without completing the operation
 - the operations run asynchronously (in the background)
 - Must NOT reuse the buffer (send/receive array) until safe to do so
- Later test that the operation completed
 - via an integer identification handle passed to MPI_WAIT

```
call MPI_IRECV(rbuff,n,MPI_REAL8,other,1,MPI_COMM_WORLD, request, ierror)
call MPI_SEND (sbuff,n,MPI_REAL8,other,1,MPI_COMM_WORLD,ierror)
call MPI_WAIT(request, stat,ierr)
```

Alternatively could have used MPI ISEND and MPI RECV



Non Blocking Communications

Routines include

- MPI_ISEND
- MPI IRECV
- MPI WAIT
- MPI_WAITALL
 - Waits for a number of outstanding communications to complete



Final Practical

- exercise2
- A "simple" numerical model
- See the README for details
- See copies of MPI standard for details of arguments required for various MPI routines you might want to use.
- Ask if you need help or don't understand anything!

