An Introduction to MPI Programming

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Topics

- Introduction
- Initialising MPI
- Data Types and Tags
- Basic Send/Receive

- Practical 1

- Receive Part 2
- Collective CommunicationsReferences

- Practical 2

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 (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
- **Works within SMP and across Distributed Memory Nodes**
- **Can scale to hundreds 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)
- 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 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 on the ECMWF IBM
- A mass of useful material on the Web

SPMD

- The SPMD model is by far the most common
  - Single Program Multiple Data
  - One program executes multiple times simultaneously
  - The problem is divided across the multiple copies
  - Each work on a subset of the data
- MPMD
  - Multi Program Multiple Data
  - Different executable on different processors
  - Useful for coupled models for example
  - Part of the MPI 2 standard
  - Not currently used by IFS

Some definitions

- Task
  - one running instance (copy) of a program
  - same as a UNIX process
  - IBM Loadleveler talks about tasks not processes
  - Basic unit of an MPI parallel execution
- Master
  - the master task is the first task in a parallel program
  - task id is 0
- Slave
  - all other tasks in a parallel program
  - Nothing intrinsically different between master/slave – but the parallel programming 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

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
```

MPIF.H

```
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 IBM'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 IBM all tasks execute the code before `MPI_INIT`
  - this is an implementation dependent feature

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`"
- Communicators define subsets of tasks
  - dividing programs into subsets of tasks often not necessary
  - IFS also creates and uses some additional communicators
    - useful when doing collective communications
  - advanced topic
- `MPI_COMM_WORLD` means all tasks
  - many MPI programs only use `MPI_COMM_WORLD`

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 ntasks**
  - **the number of tasks is defined in a loadleveler directive**
- **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
- Does not stop the task

MPI_ABORT

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

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

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 envelope (the identification, address etc.) and the contents (data)
  - data can be of various Fortran types
  - data length can be zero bytes to MB's
  - messages have tag identifiers
- 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)
  - permits send/receive to non contiguous buffers
  - advanced topic

MPI Tags

- All messages are given an integer TAG value
  - standard says maximum value is at least 32768 (2^31)
  - `CALL MPI_Comm_get_attr (MPI_COMM_WORLD,MPI_TAG_UB, maxtag, flag, error)`
- This helps to identify a message
- Used to ensure messages are read in the right order
  - standard says nothing about the order of message arrival
- You decide what tag values to use
  - Enables you to keep track of multiple messages
  - Good ideas to use separate ranges of tags eg:
    - 1000, 1001, 1002..... in routine a
    - 2000, 2001, 2002.... in routine b

MPI_SEND

```
FORTRAN_TYPE:: sbuf
integer:: count, dest, tag, ierror
call MPI_SEND( sbuf, count, MPI_TYPE, dest, tag, &
               MPI_COMM_WORLD, ierror)
```

SBUF	**the array being sent**	**input**
COUNT	**the number of elements to send**	**input**
MPI_TYPE	**the kind of variable eg `MPI_REAL`**	**input**
DEST	**the task id of the receiver**	**input**
TAG	**the message identifier**	**input**

MPI_RECV

```
FORTRAN_TYPE:: rbuf
integer:: count, source, tag, status(MPI_STATUS_SIZE),ierror
call MPI_RECV( rbuf, count, MPI_TYPE, source, tag, &
               MPI_COMM_WORLD, status, ierror)
```

RBUF	**the array being received**	**output**
COUNT	**the length of RBUF**	**input**
MPI_TYPE	**the kind of variable eg MPI_REAL**	**input**
SOURCE	**the task id of the sender**	**input**
TAG	**the message identifier**	**input**
STATUS	**information about the message**	**output**

A simple example

```
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
```

Compiling an MPI Program

- **Use mpxlf90_r compiler**
  - **automatically finds the "`use mpi`" file and loads appropriate libraries**

```
$ mpxlf90_r -c hello.f
$ mpxlf90_r hello.o -o hello
```

Loadleveler and MPI

- **Define your task requirements as loadleveler directives**

```
#@ job_type = parallel
#@ class = np

#@ node = 2
#@ total_tasks = 64

or

#@ node = 2
#@ tasks_per_node = 32
```

First Practical

- Copy all the practical exercises to your account:
  - `cd $HOME`
  - `mkdir mpi_course ; cd mpi_course`
  - `cp –r ~trx/mpi.2012/* .`
- Exercise1a
  - A simple message passing exchange based on “hello world”
- See the README for details

More on MPI_RECV

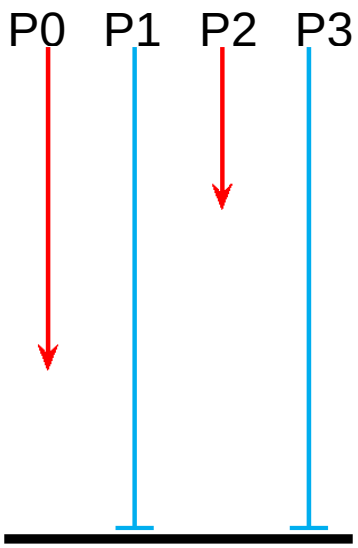
- `MPI_RECV` will block waiting for the message
  - if message never sent then deadlock
    - task will wait until it reaches cpu time limit, and is killed
- The source and tag can be less specific
  - `MPI_ANY_SOURCE` means receive from any sender
  - `MPI_ANY_TAG` means receive any tag
  - Used to receive messages in a more random order
  - helps smooth out load imbalance
  - May require over-allocation of receive buffer
- `status(MPI_SOURCE)` will contain the actual sender
- `status(MPI_TAG)` will contain the actual tag

MPI_BARRIER

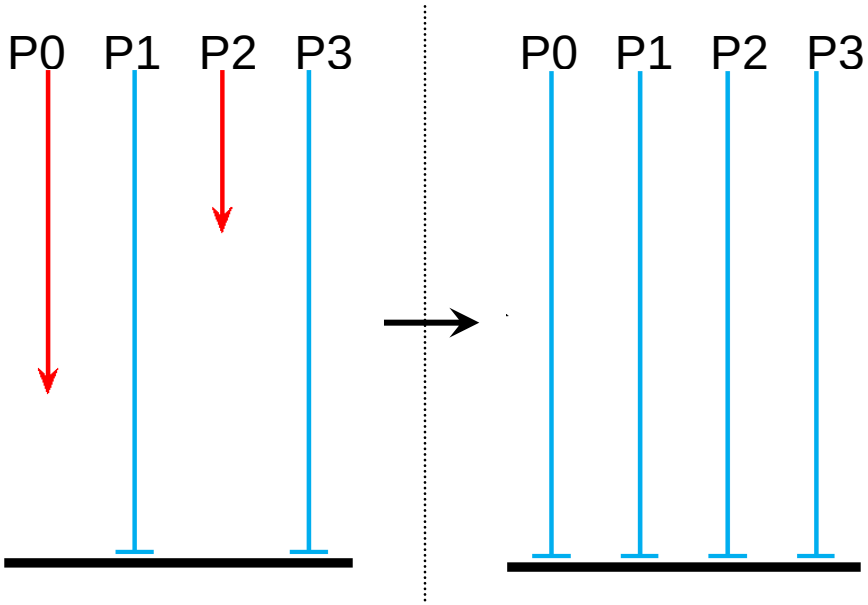
```
integer:: ierror
call MPI_BARRIER(MPI_COMM_WORLD,ierror)
```

- Forces all tasks (in a communicator group) to synchronise
  - for timing points
  - to improve output of prints
  - to separate different communications phases
- A task waits in the barrier until all tasks reach it
- Then every task completes the call together
- Deadlock if one task does not reach the barrier
  - `MPI_BARRIER` will wait until the task reaches its cpu limit

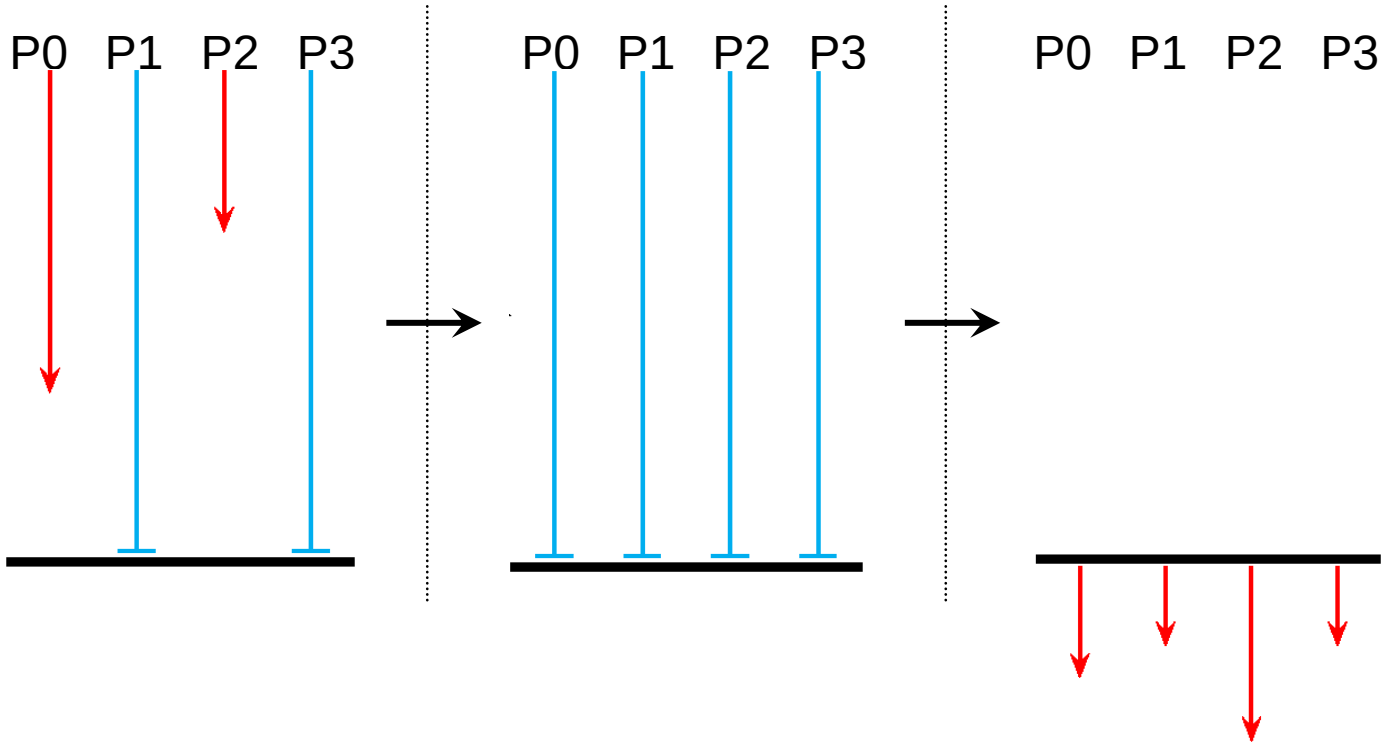
MPI_BARRIER



MPI_BARRIER



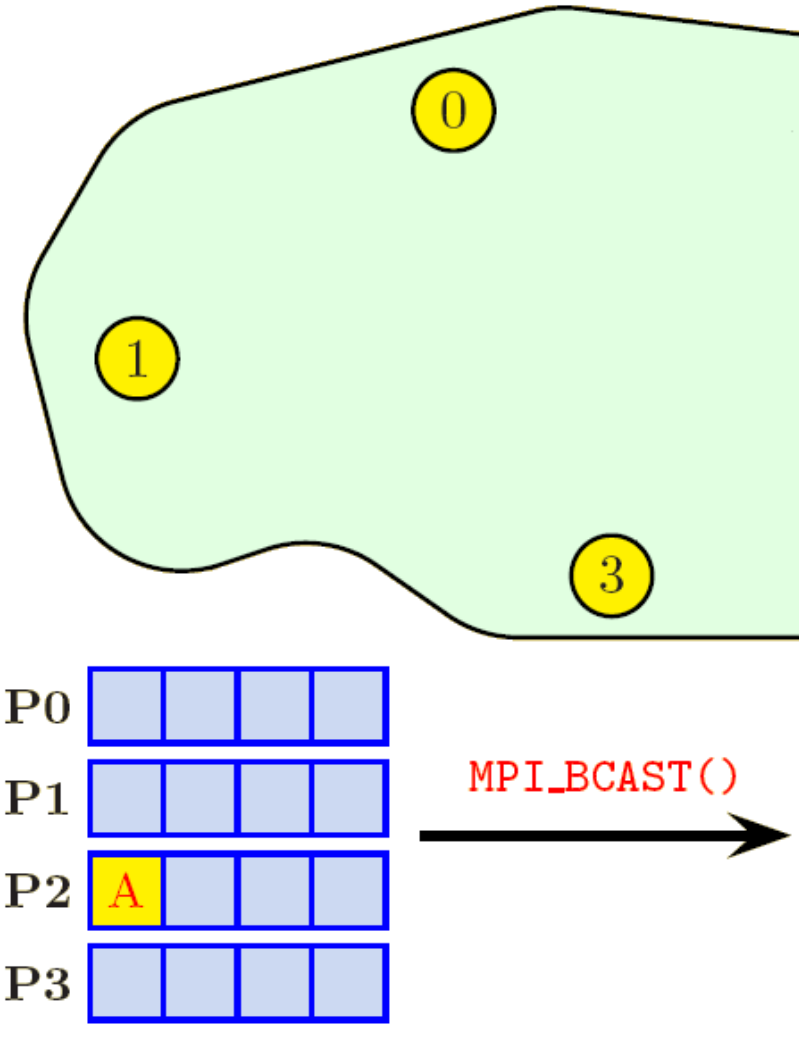
MPI_BARRIER



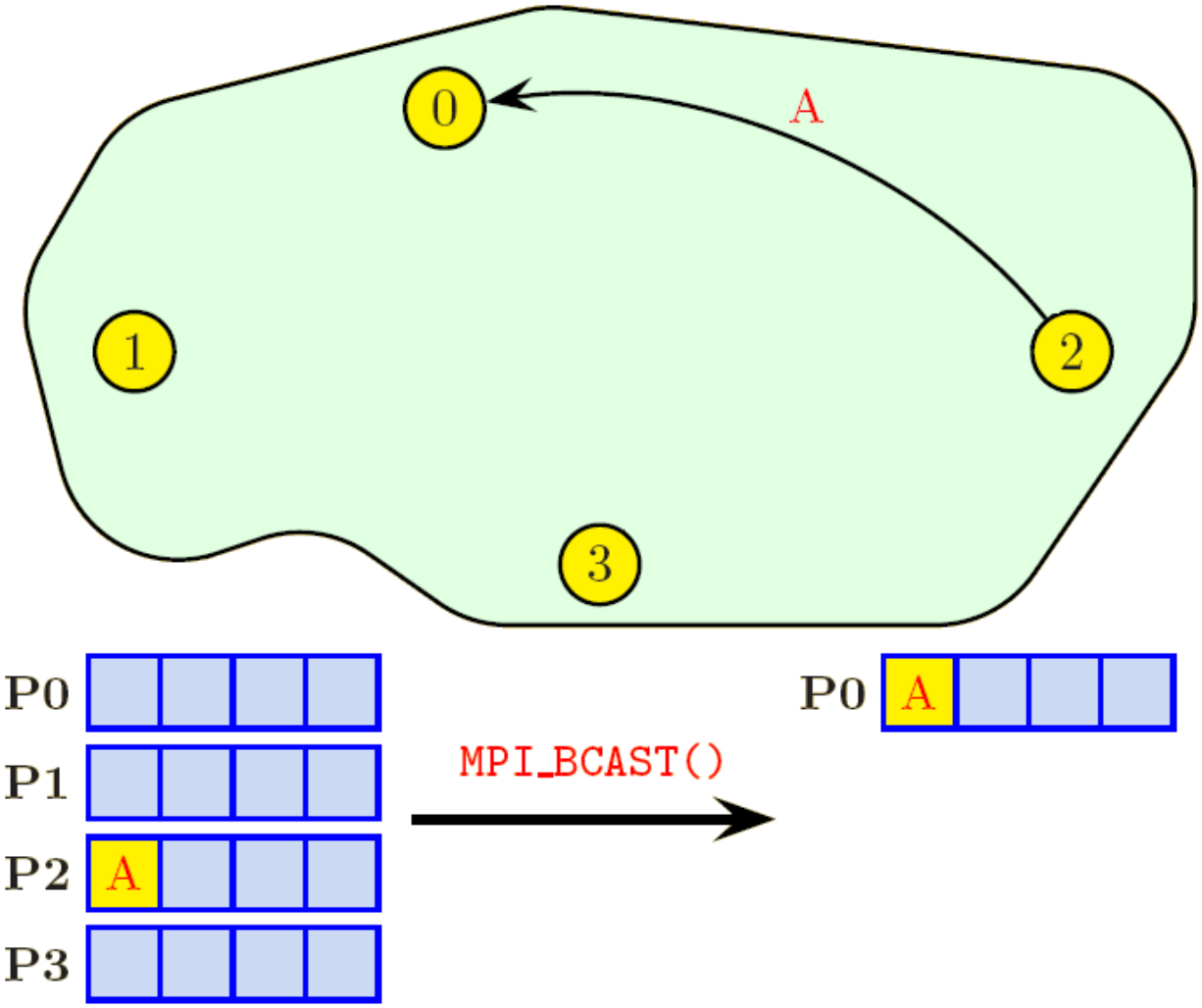
Collective Communications

- MPI contains Collective Communications routines
  - called by all tasks together
  - replace multiple send/recv 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
- IFS uses some collective routines

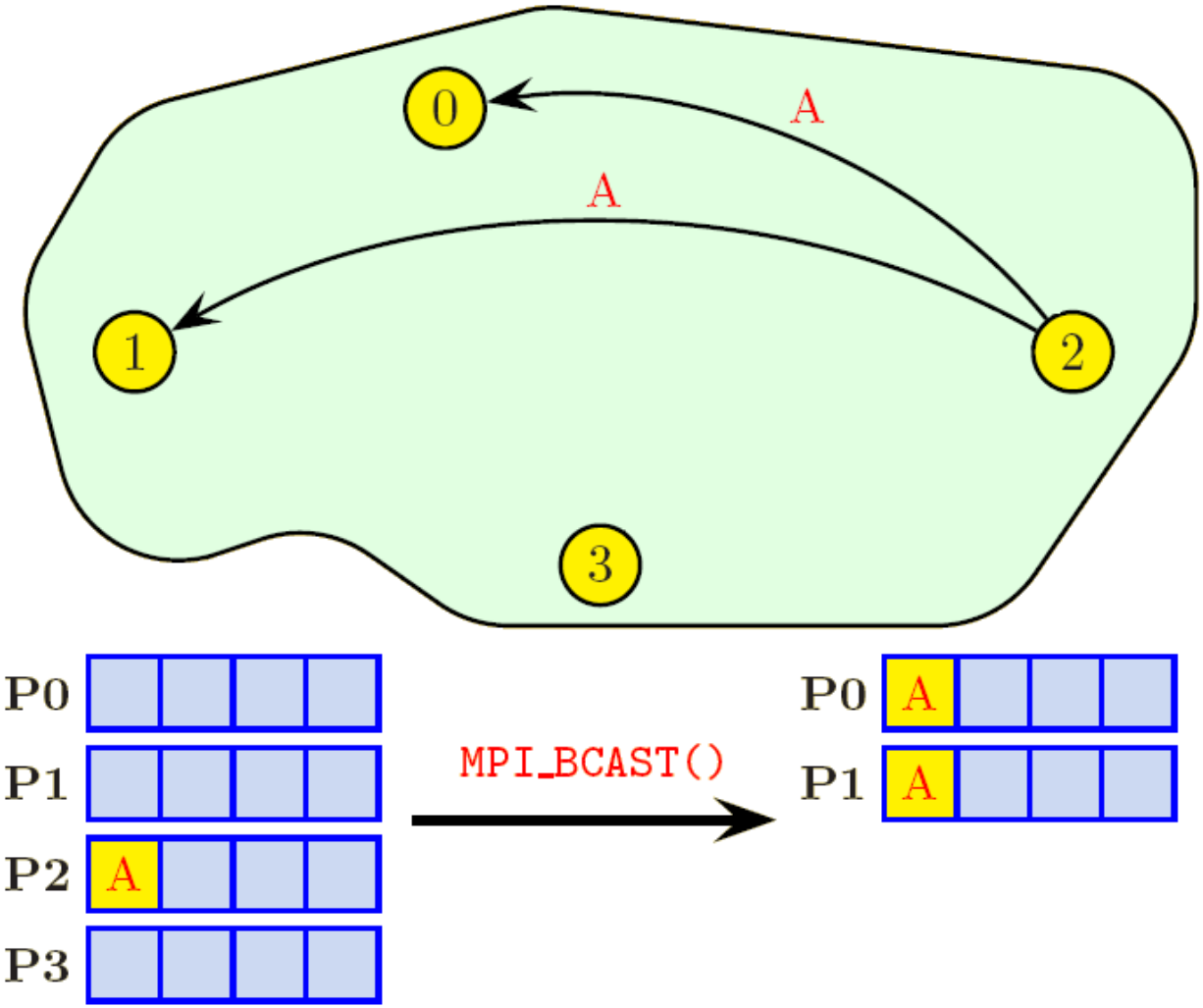
MPI_BCAST



MPI_BCAST



MPI_BCAST



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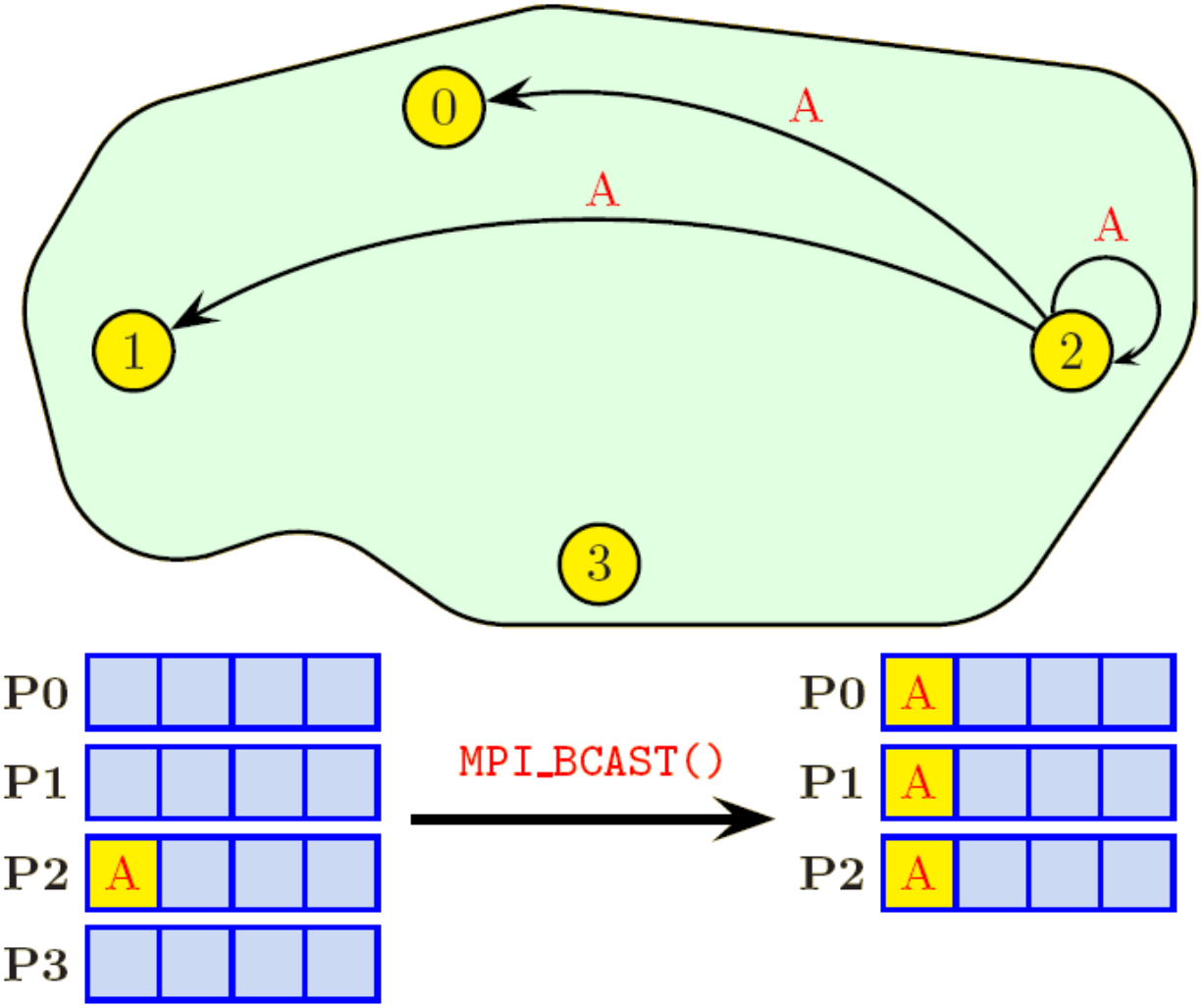

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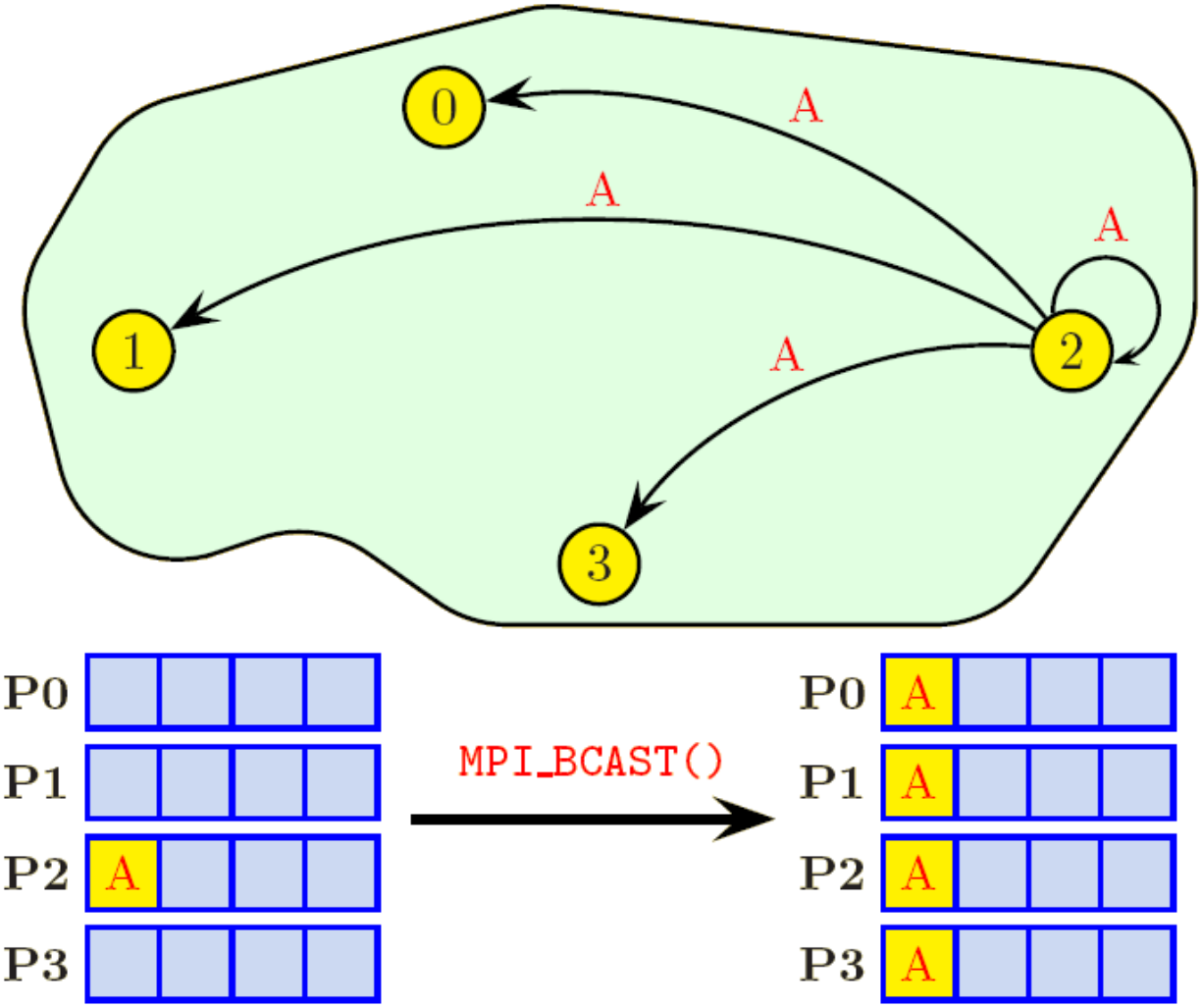


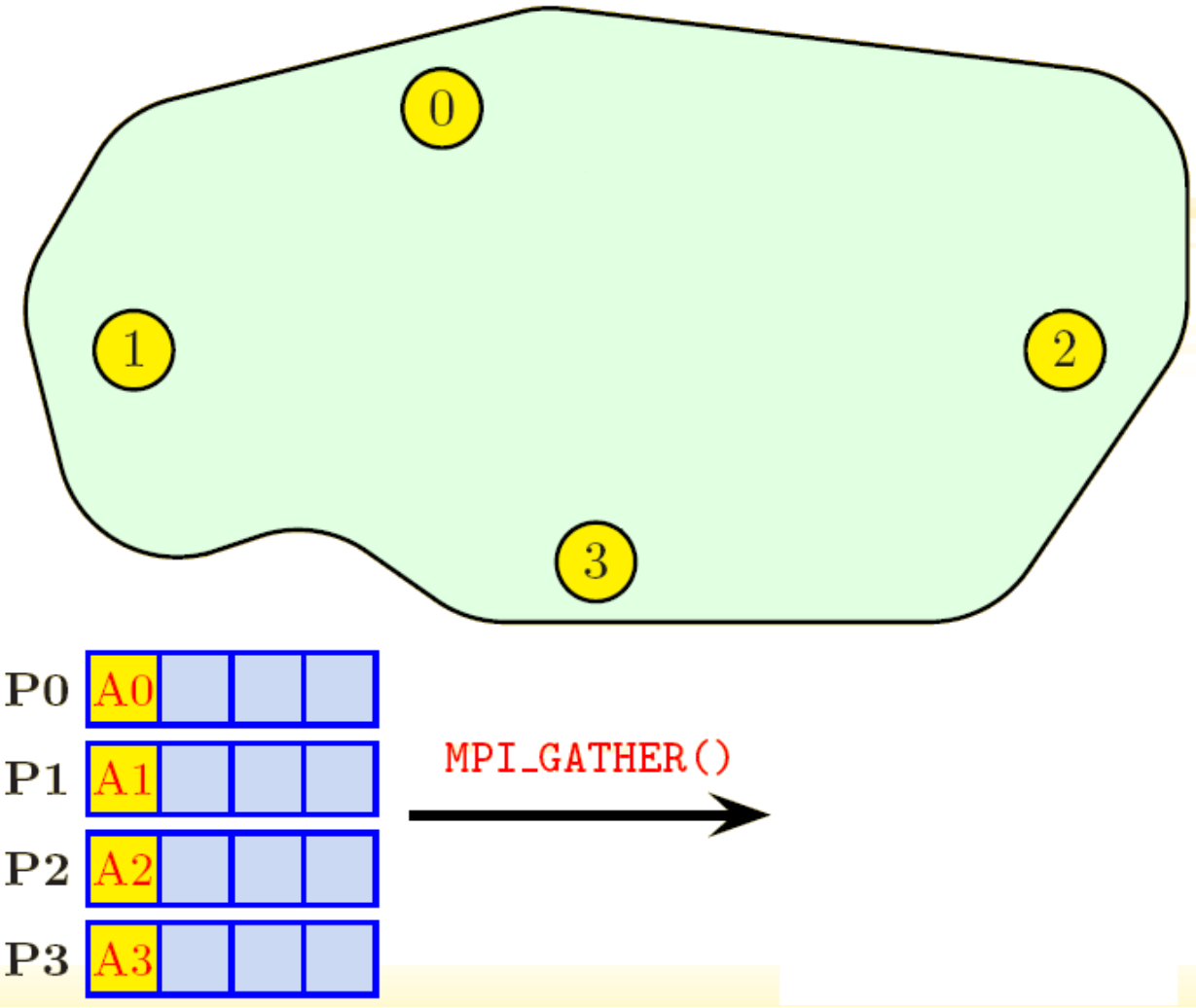
MPI_BCAST

```
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. Could also be done by putting `MPI_SEND` in a loop.

MPI_GATHER



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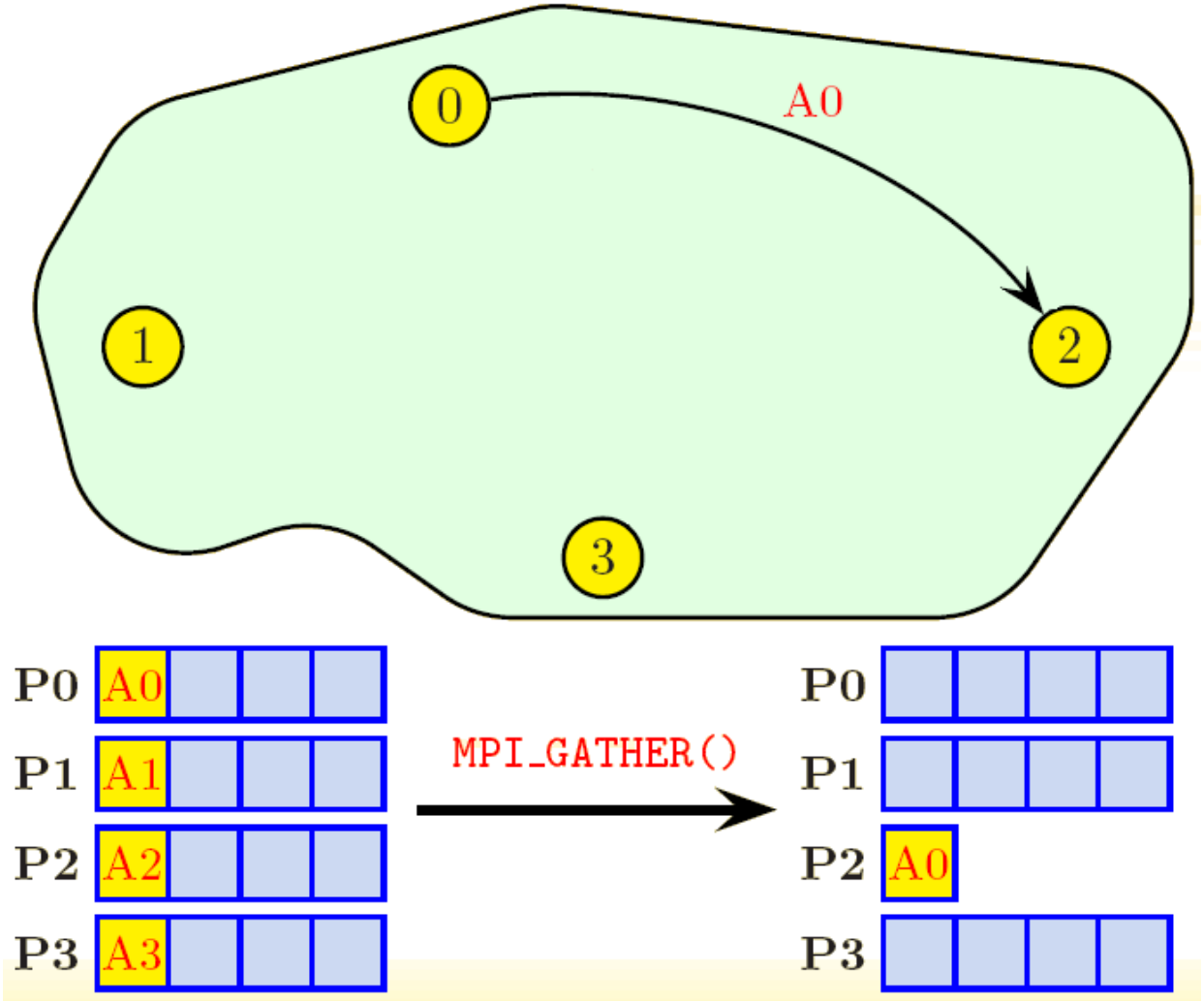

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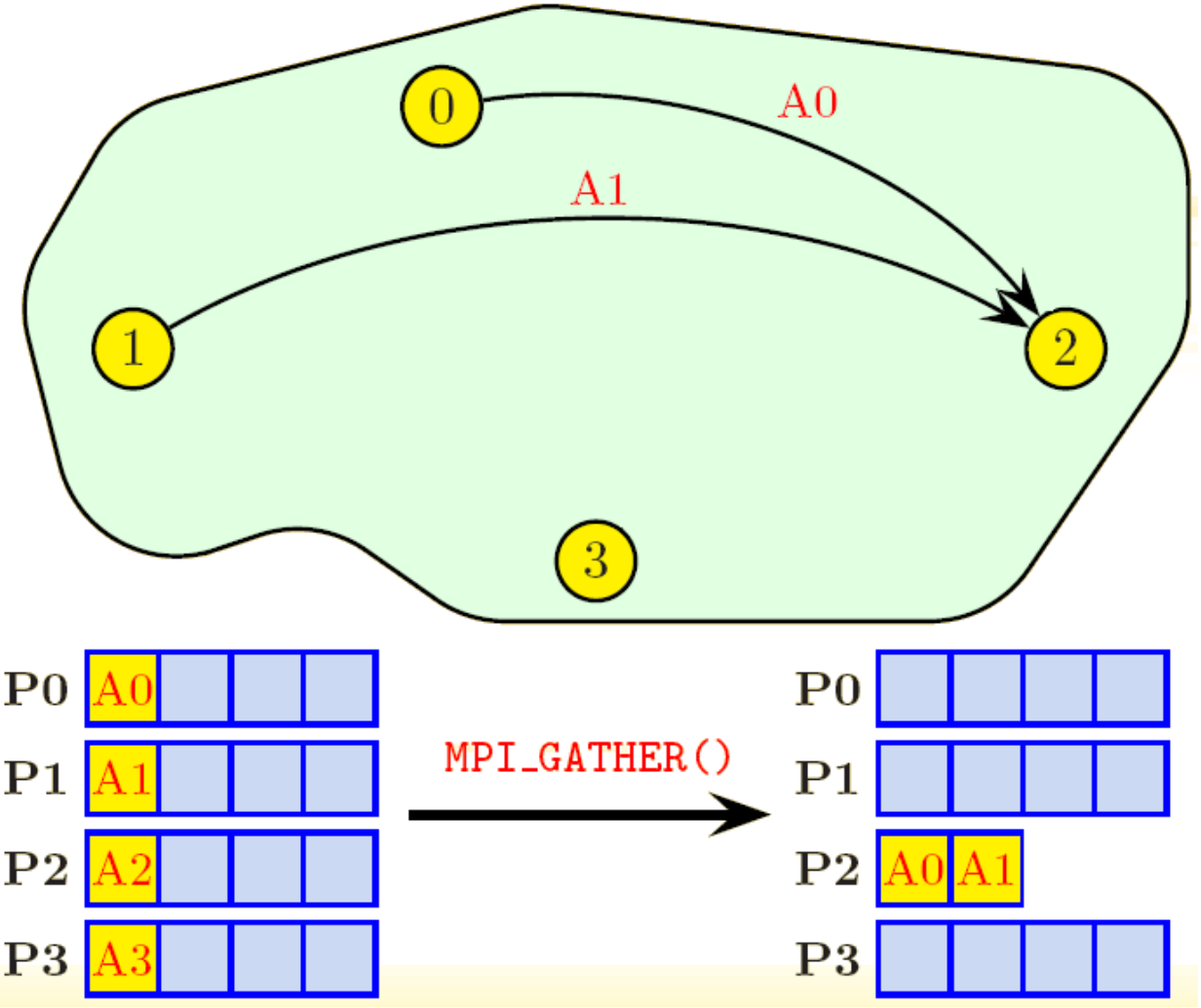

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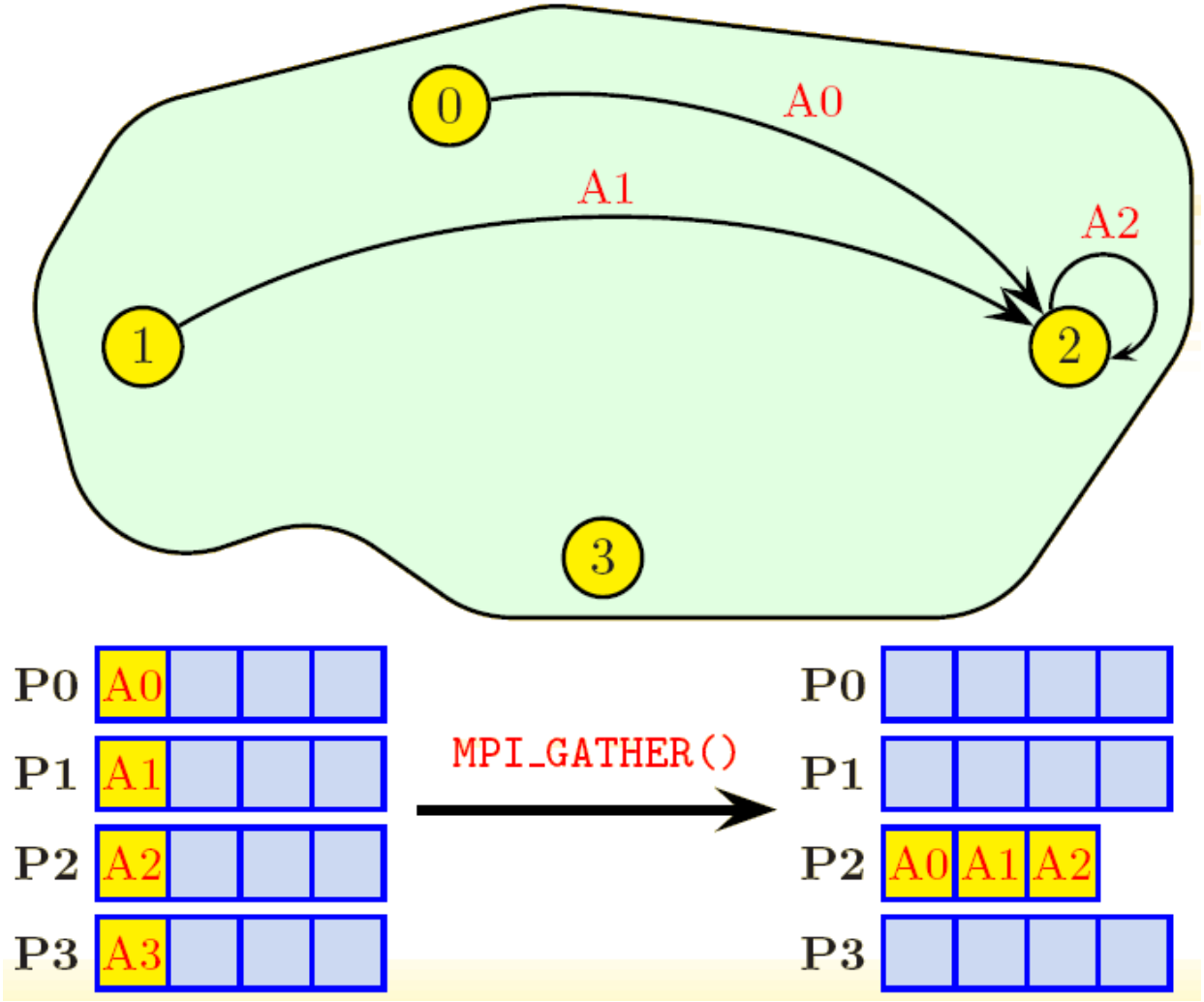
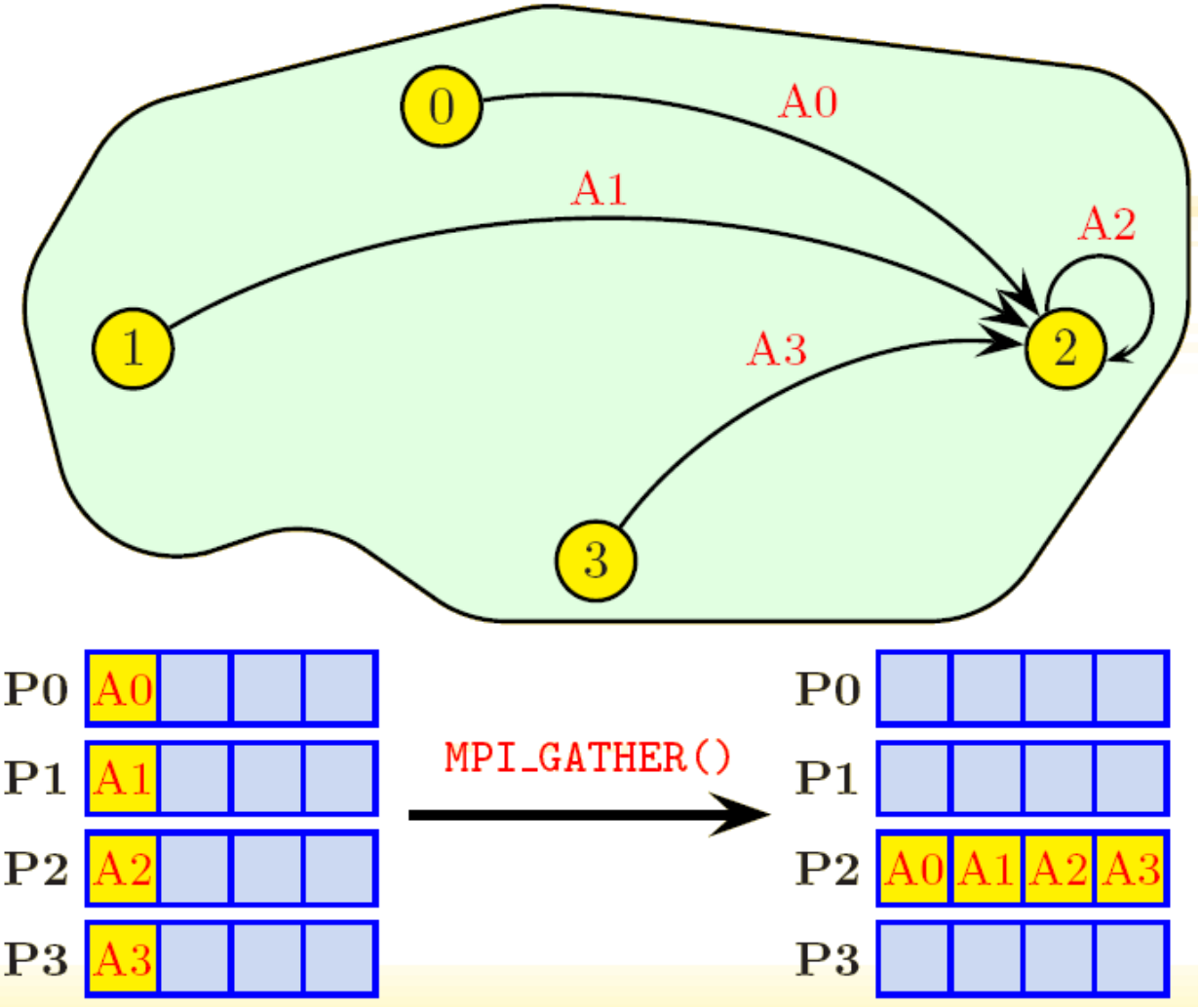


MPI_GATHER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1
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MPI_GATHER()
P0
P1
P2
P3
A0
A1
A2
A3

MPI_GATHER

```
FORTRAN_TYPE:: sbuff, rbuff
integer:: count, root, ierror
call MPI_GATHER( sbuff,scount,MPI_TYPE, &
                 rbuff,rcount,MPI_TYPE,root,MPI_COMM_WORLD,ierror)
```

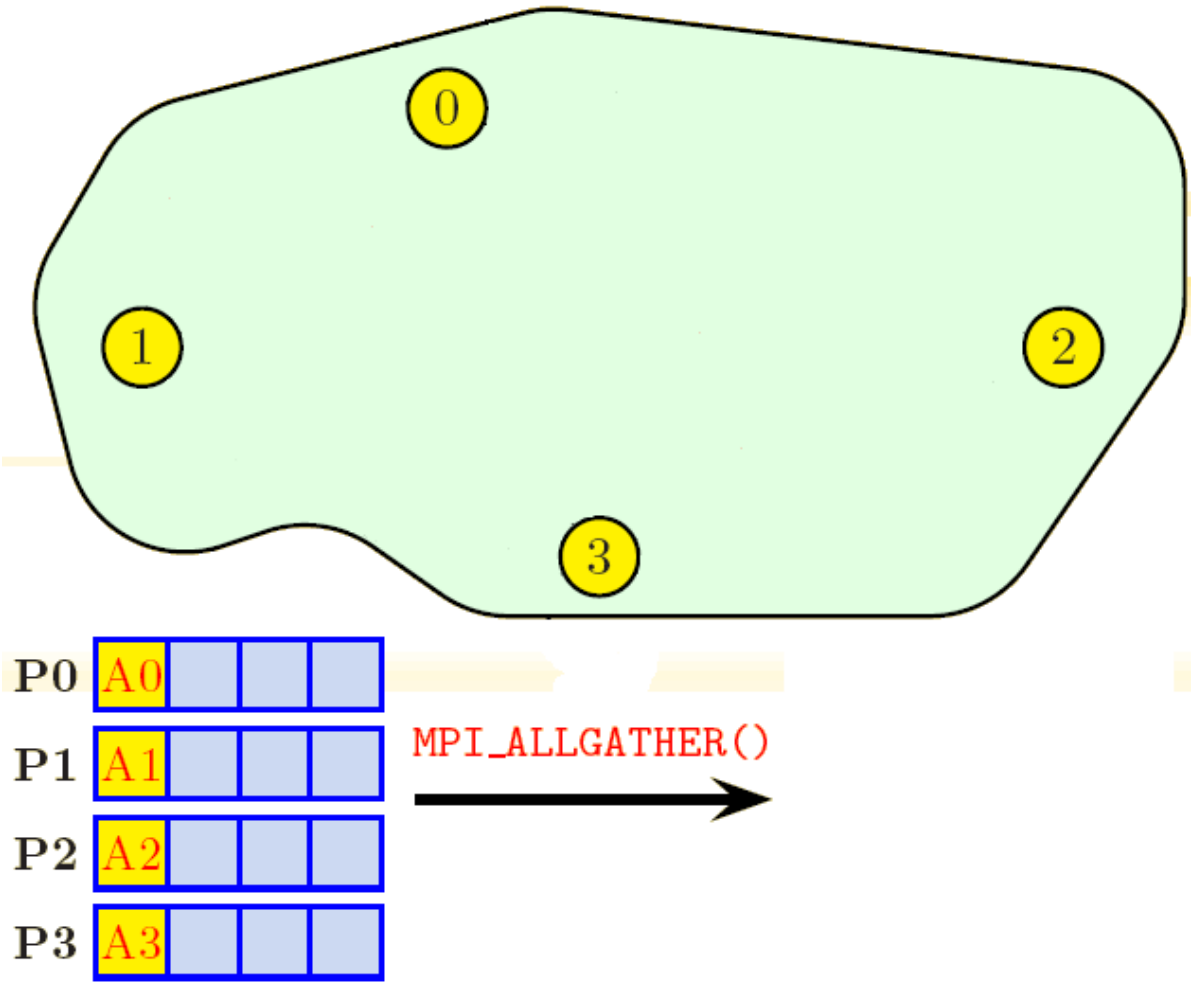
ROOT	**task doing gather**	**input**
SBUFF	**array being sent**	**input**
RBUFF	**array being received**	**output**
[S/R]COUNT	**number of items to/from each task**	**input**

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.

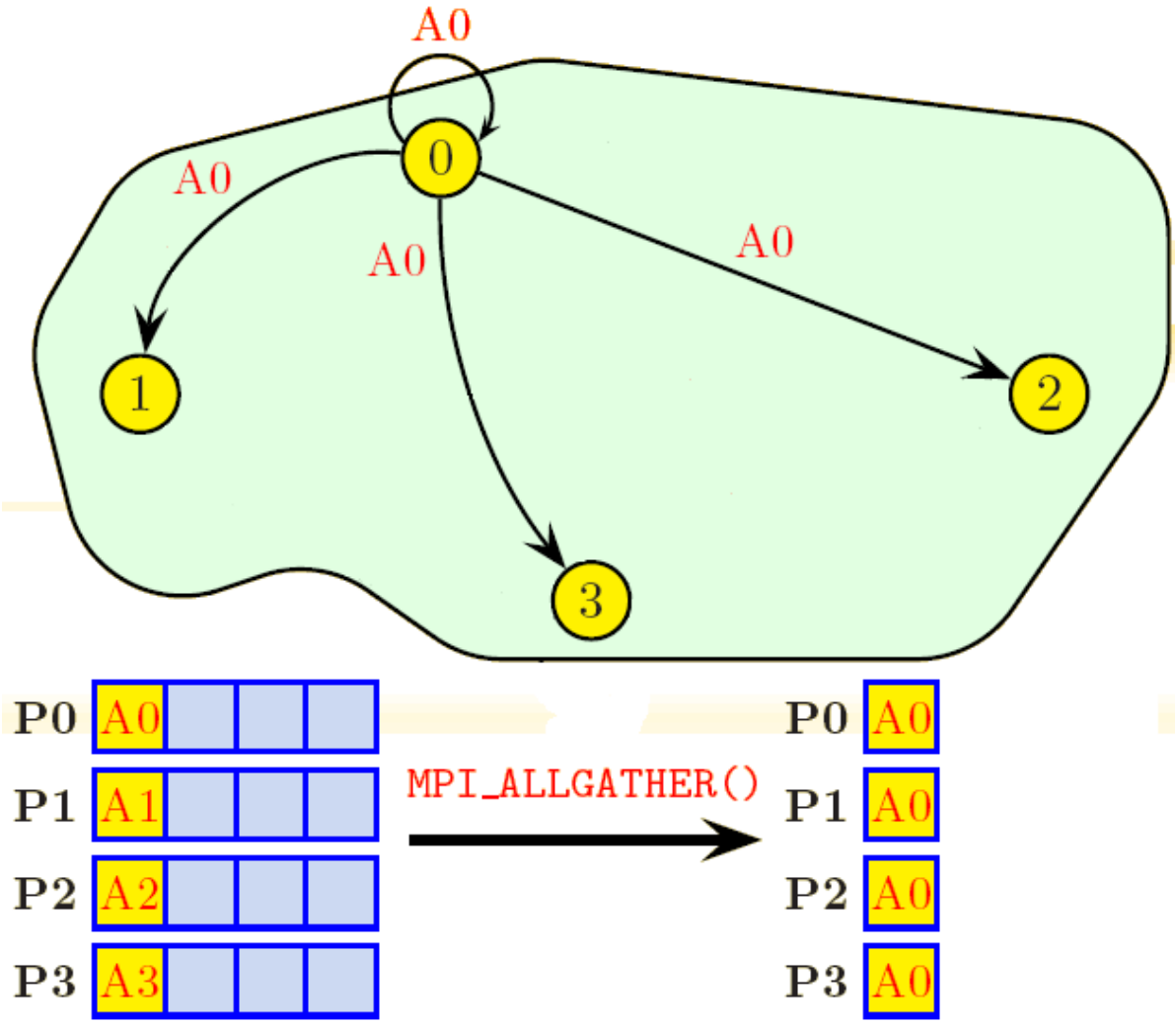
Gather Routines

- **MPI_ALLGATHER**
  - gather arrays of equal length into one array on all tasks
  - Simpler and more efficient than 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 all tasks

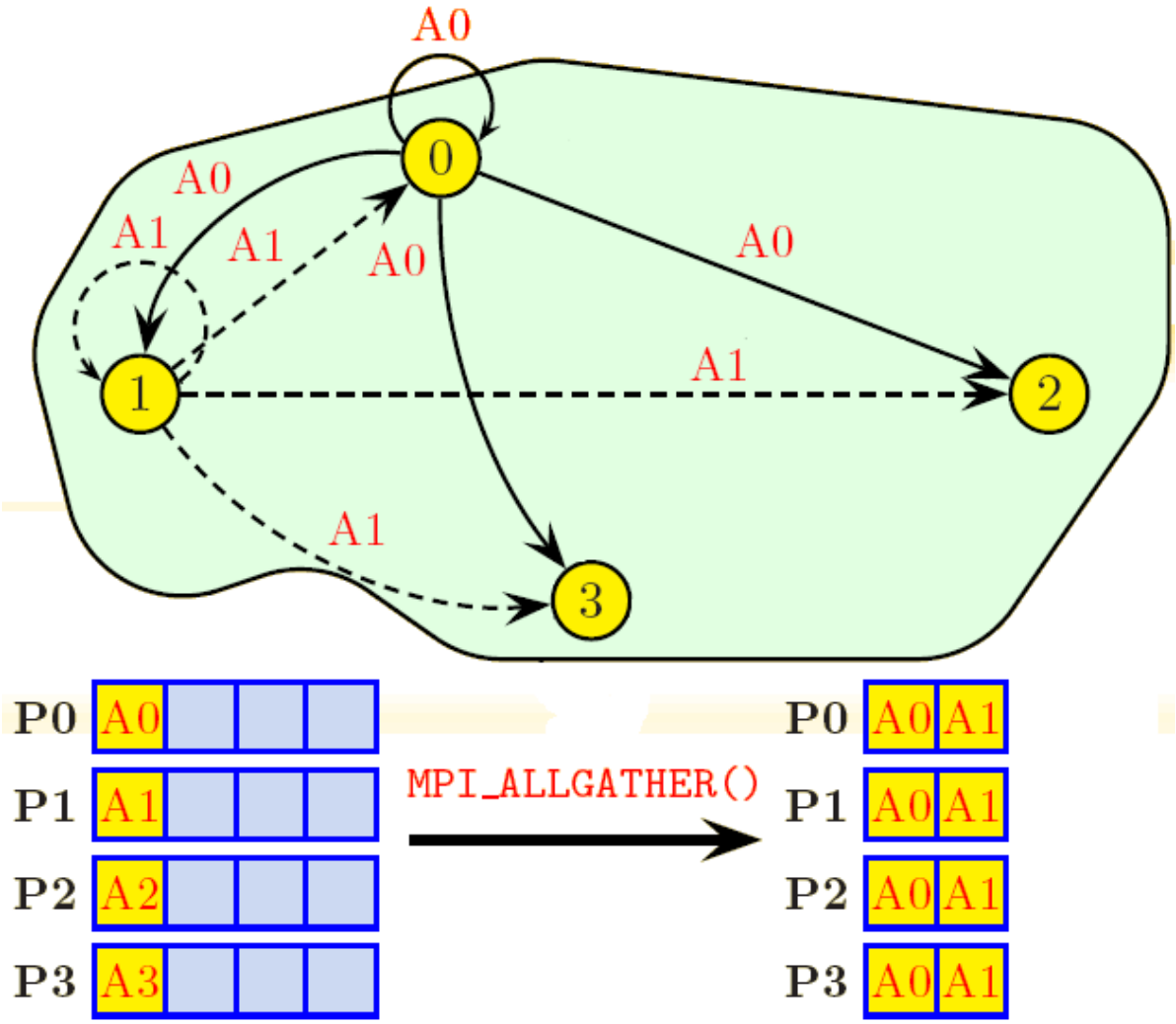
MPI_ALLGATHER



MPI_ALLGATHER



MPI_ALLGATHER



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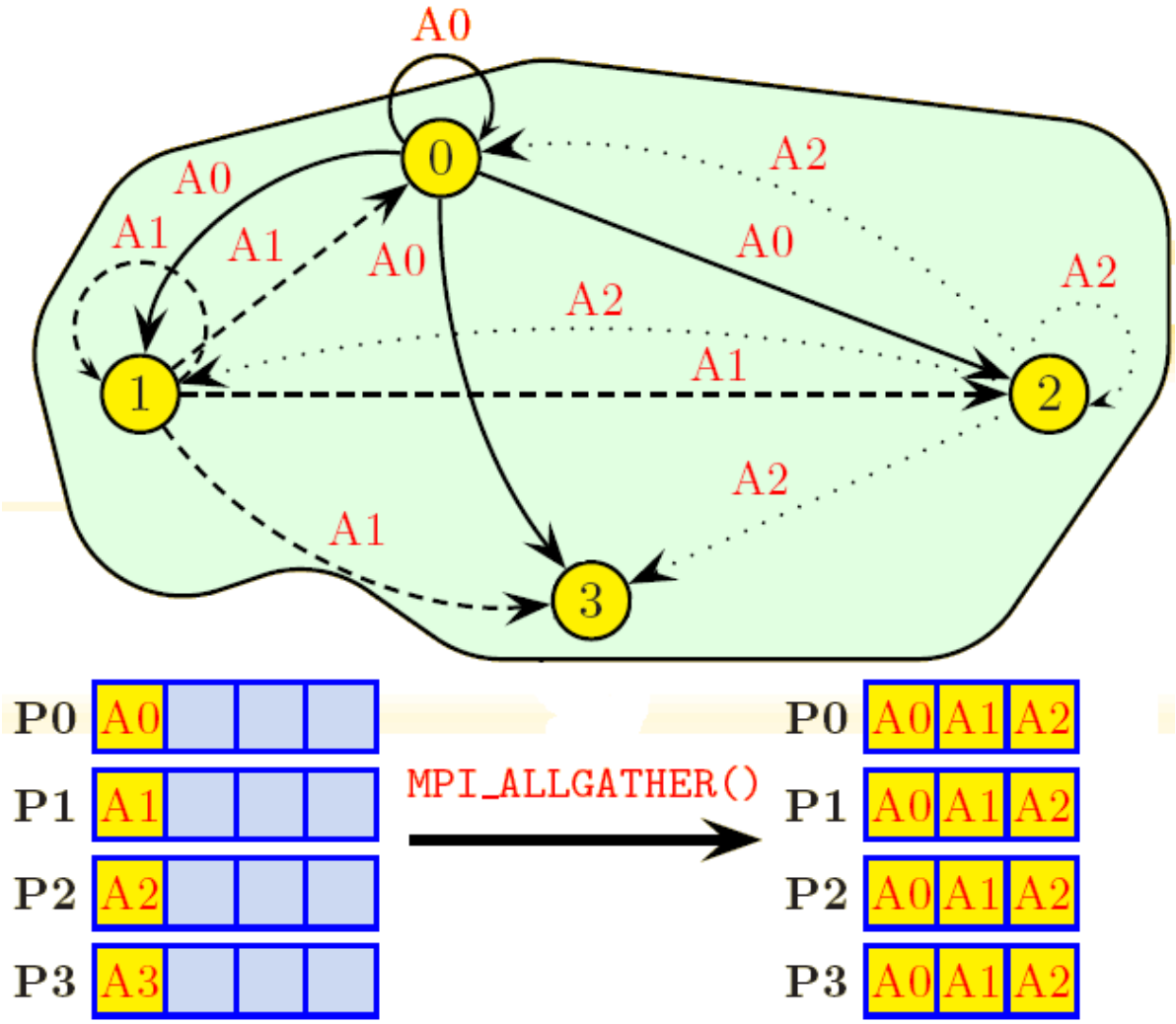
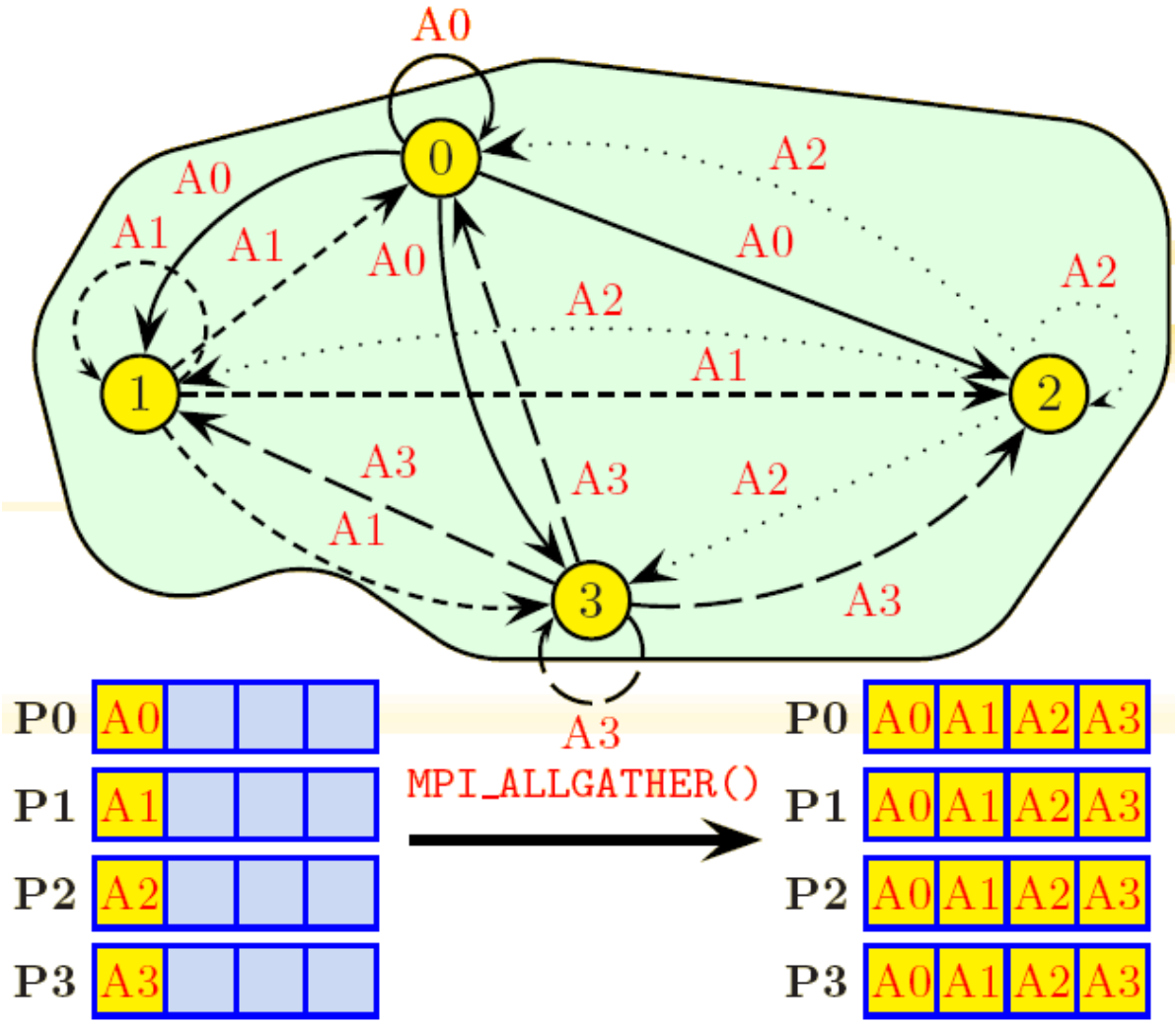
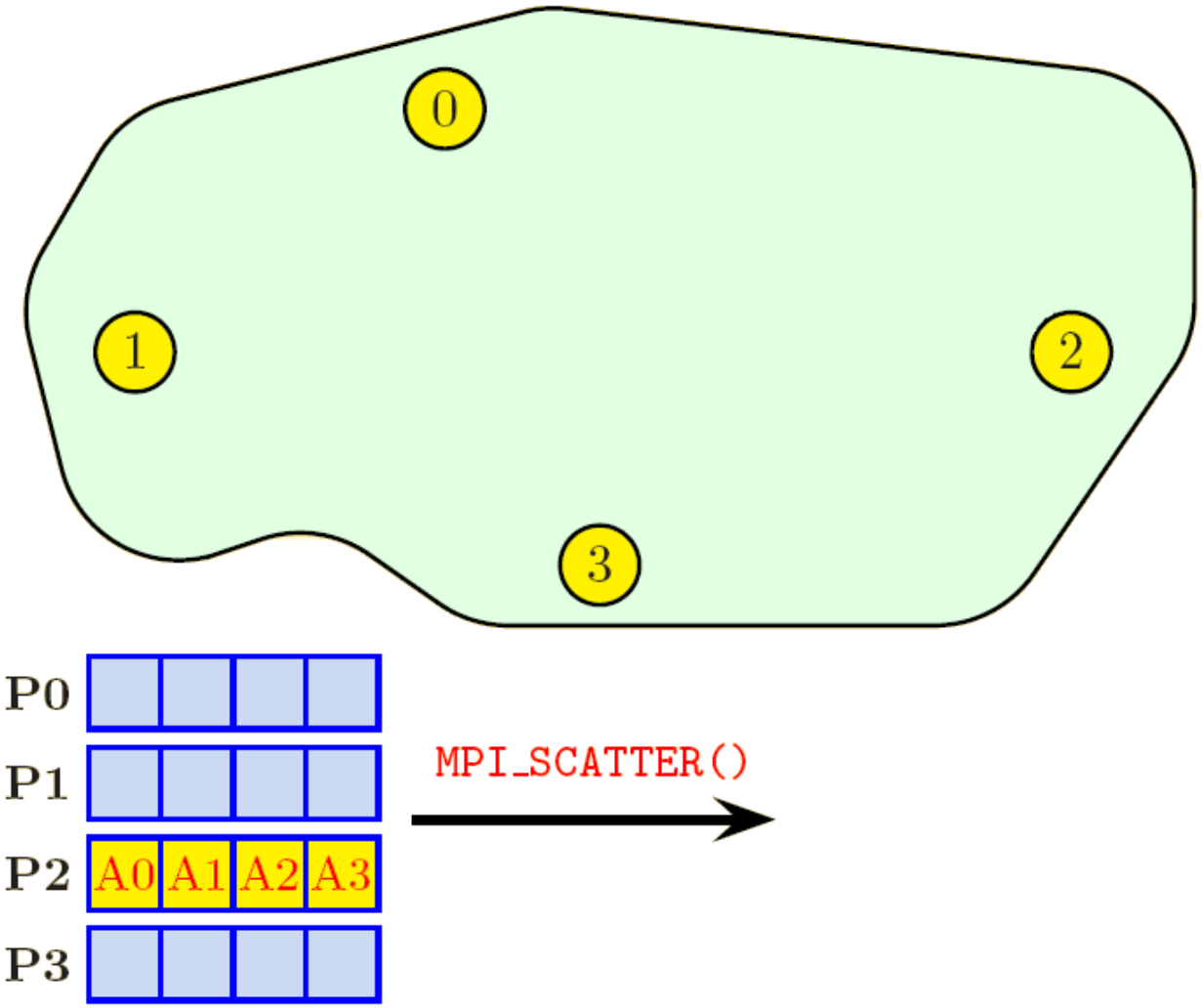


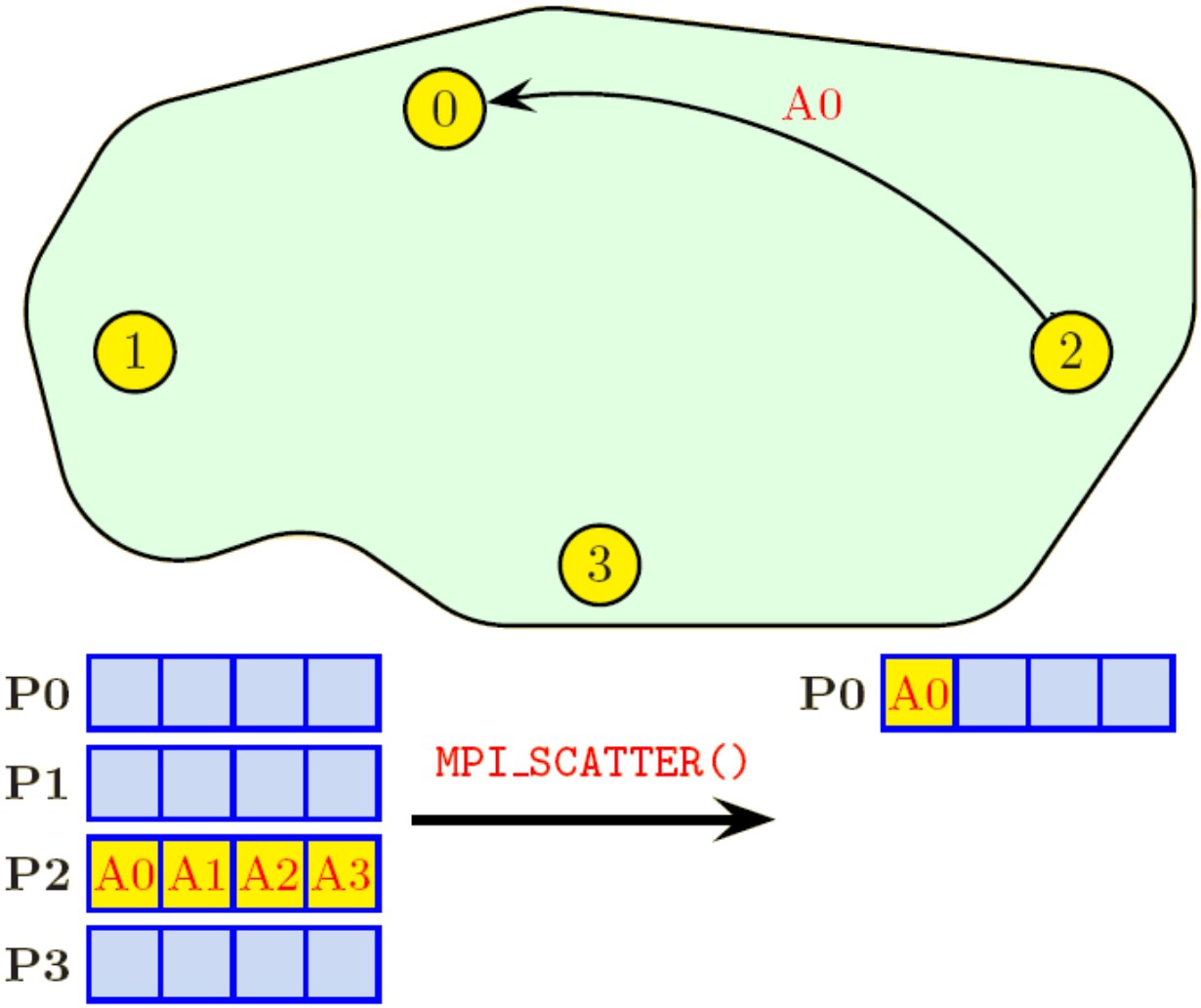
MPI_ALLGATHER



MPI_SCATTER



MPI_SCATTER



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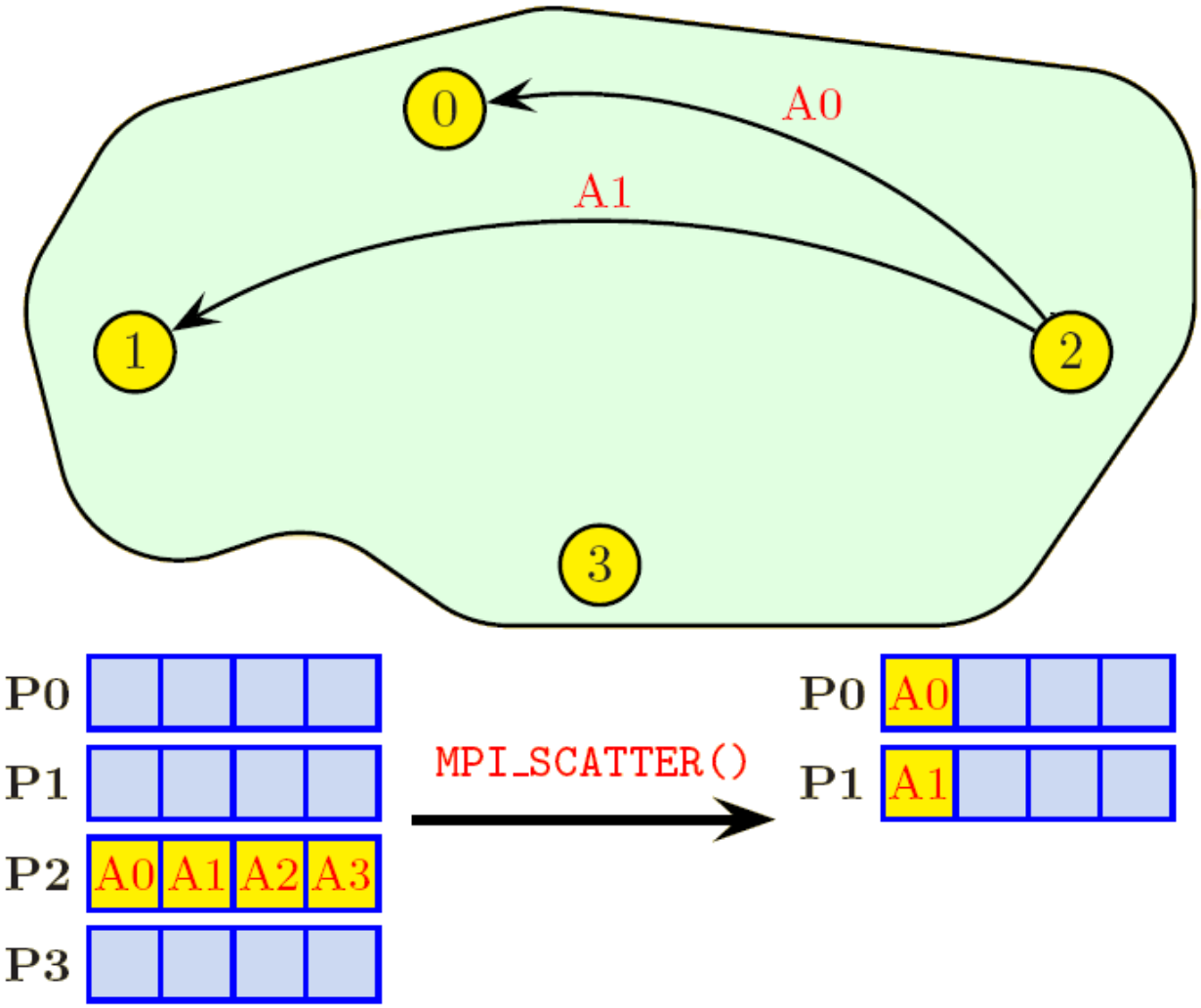

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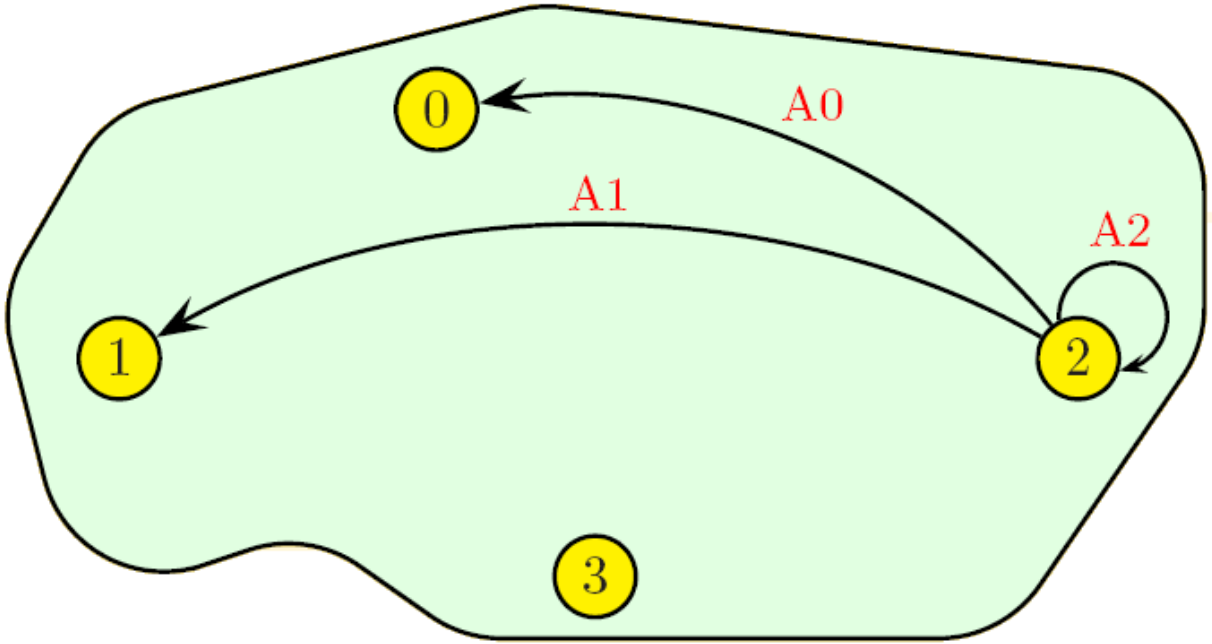
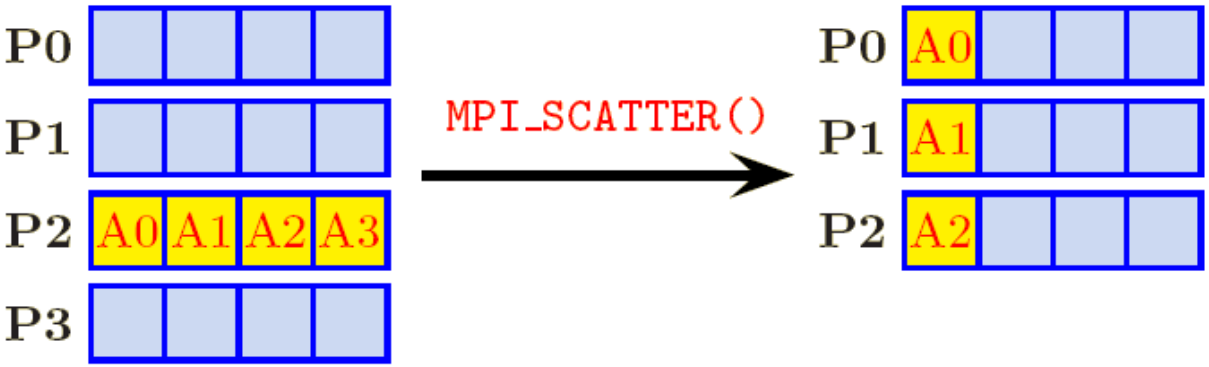
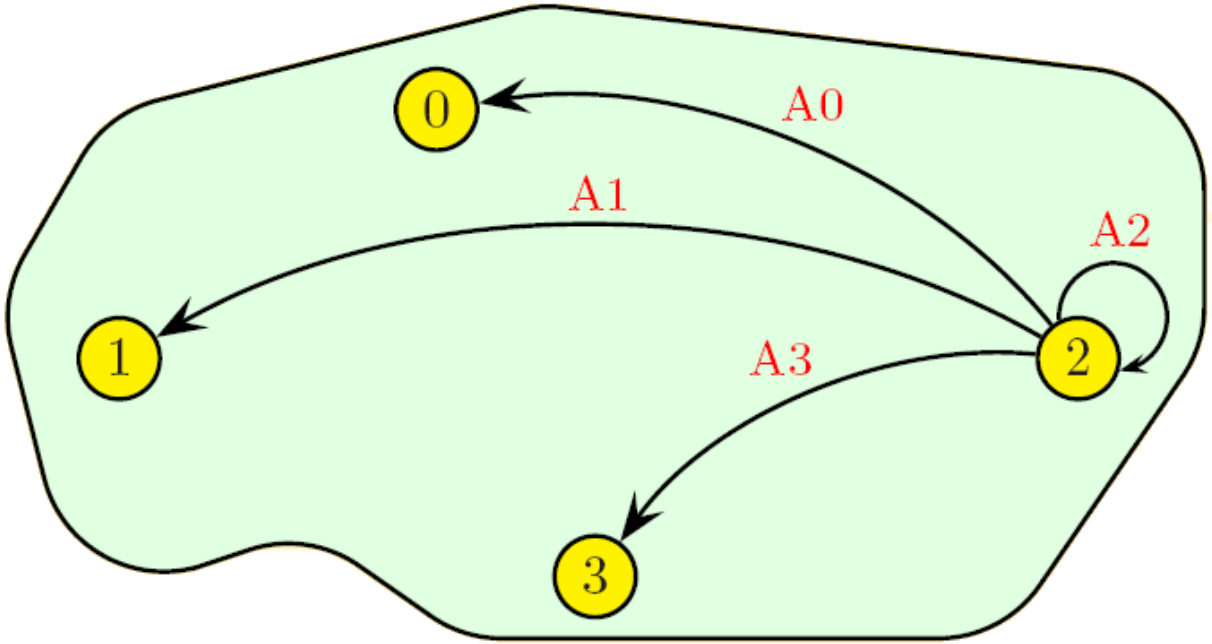
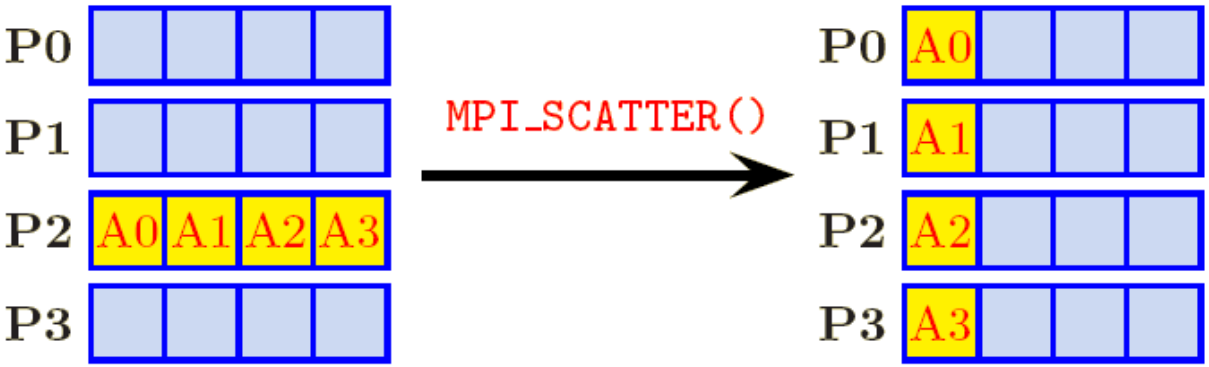




MPI_SCATTER


0
A0
A1
A2
1
2
A3
3


P0
P1
P2
A0 A1 A2 A3
P3
MPI_SCATTER()
P0 A0
P1 A1
P2 A2
P3 A3

MPI_SCATTER

```
FORTRAN_TYPE:: sbuff, rbuff
integer:: count, root, ierror
call MPI_SCATTER( sbuff,scount,MPI_TYPE, &
                  rbuff,rcount,MPI_TYPE,root,MPI_COMM_WORLD,ierror)
```

ROOT	**task doing scatter**	**input**
SBUFF	**array being sent**	**input**
RBUFF	**array being received**	**output**
[S/R]COUNT	**number of items to/from each task**	**input**

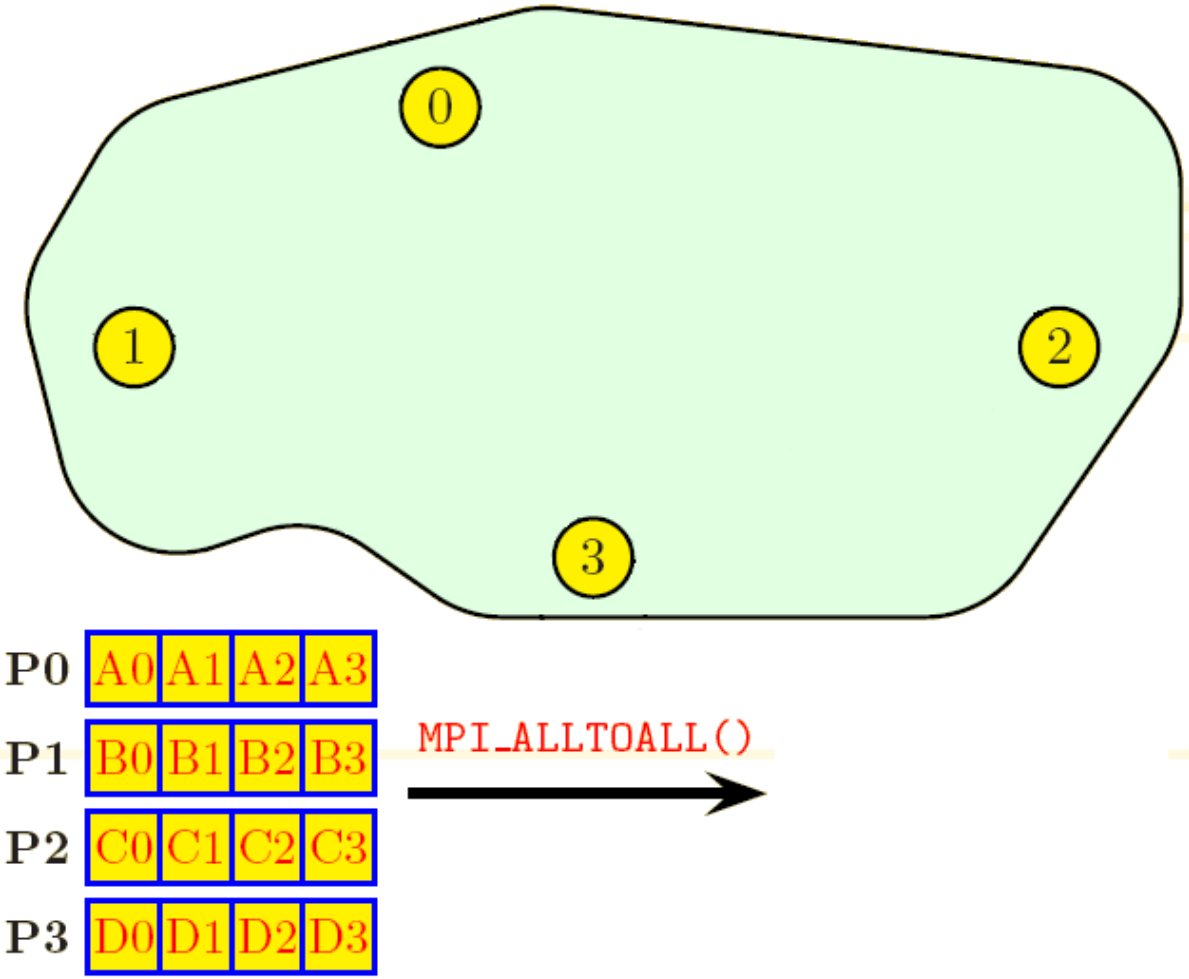
The contents of `sbuff` on task id `root` are equally split and each task receives its part in array `rbuff`. Could also be done by putting `MPI_SEND` in a loop.

Scatter Routines

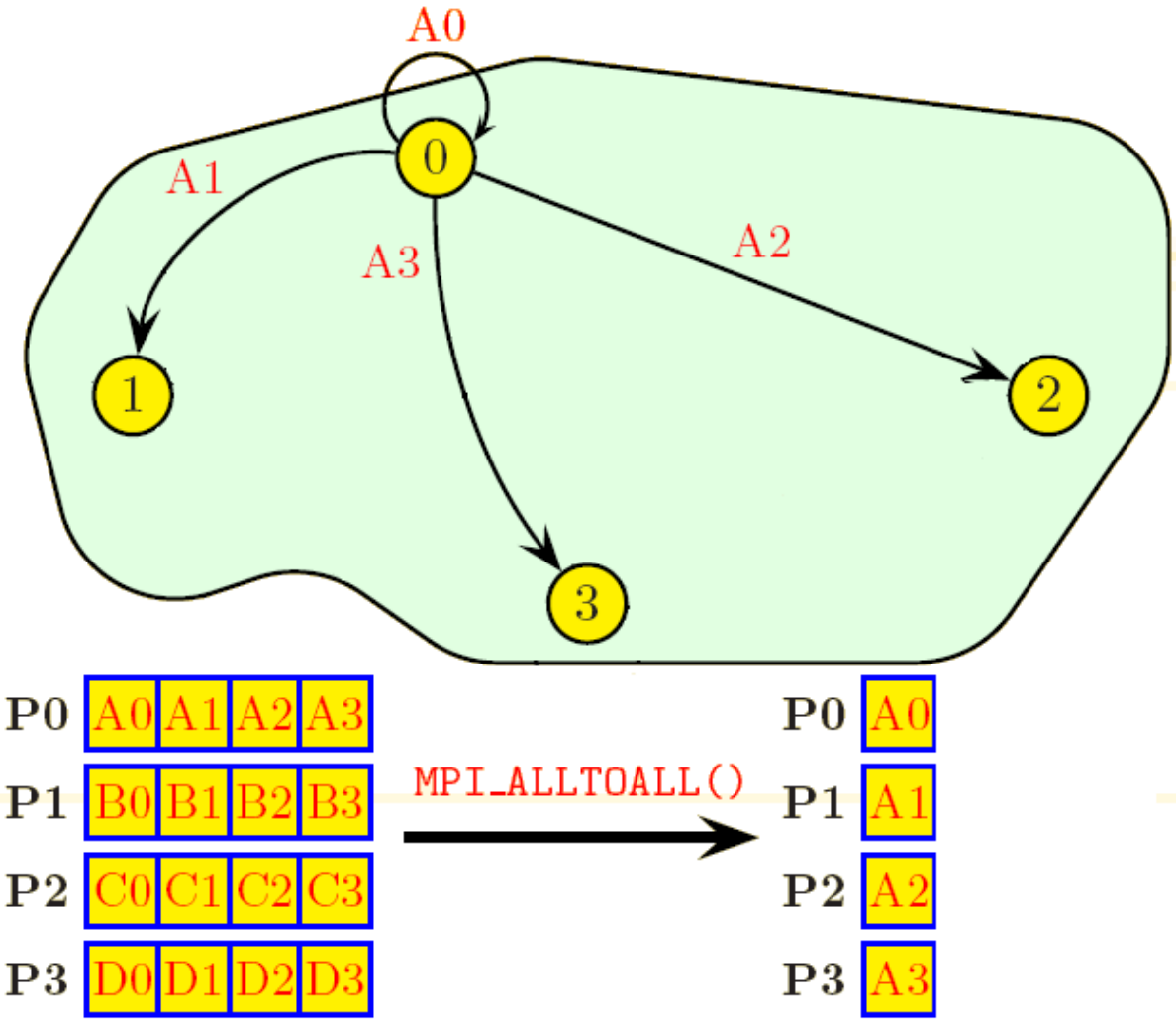
- **`MPI_SCATTER`**
  - divide one array on one task equally amongst all tasks
  - each task receives the same amount of data

- **`MPI_SCATTERV`**
  - divide one array on one task unequally amongst all tasks
  - each task can receive a different amount of data

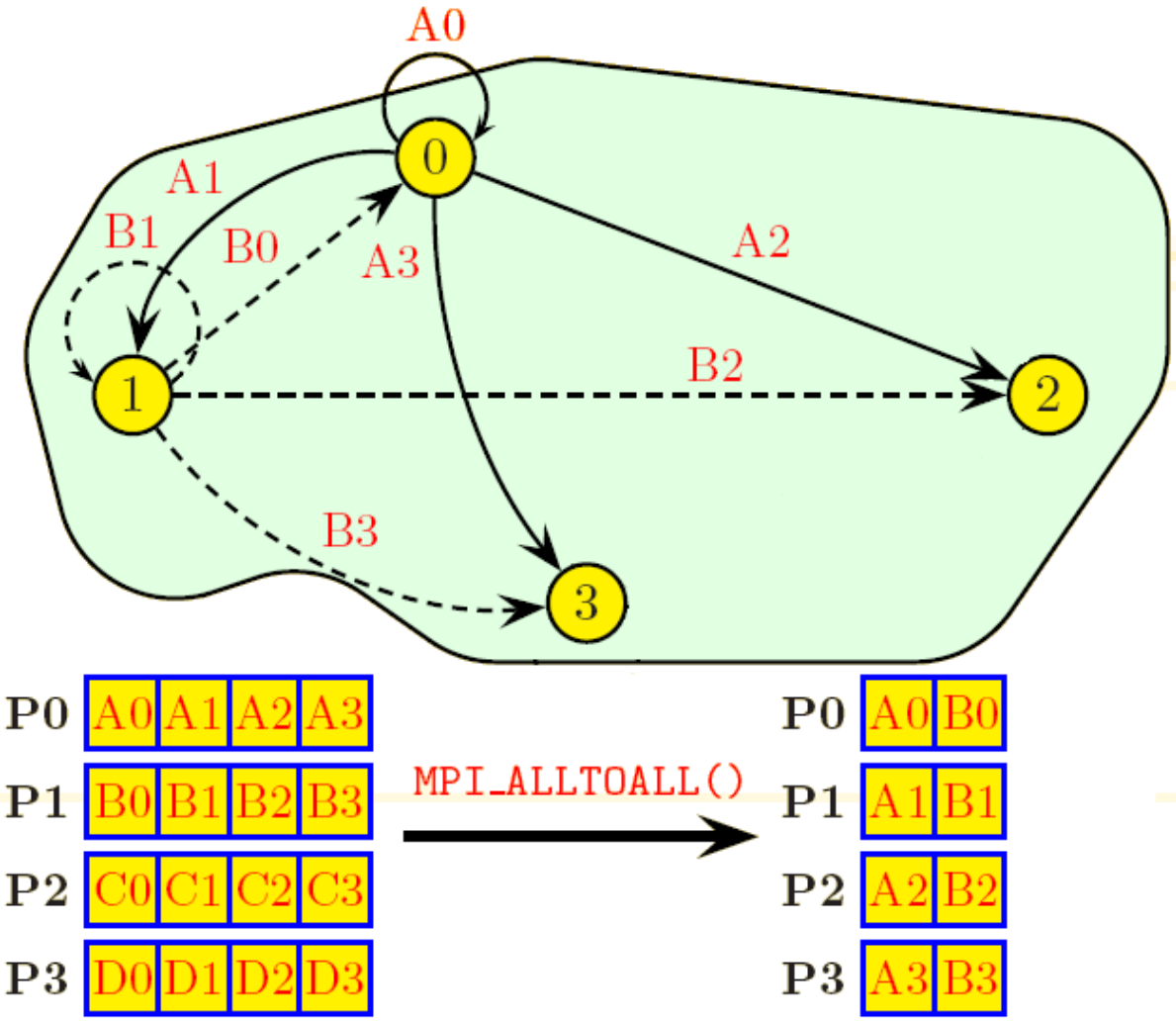
MPI_ALLTOALL



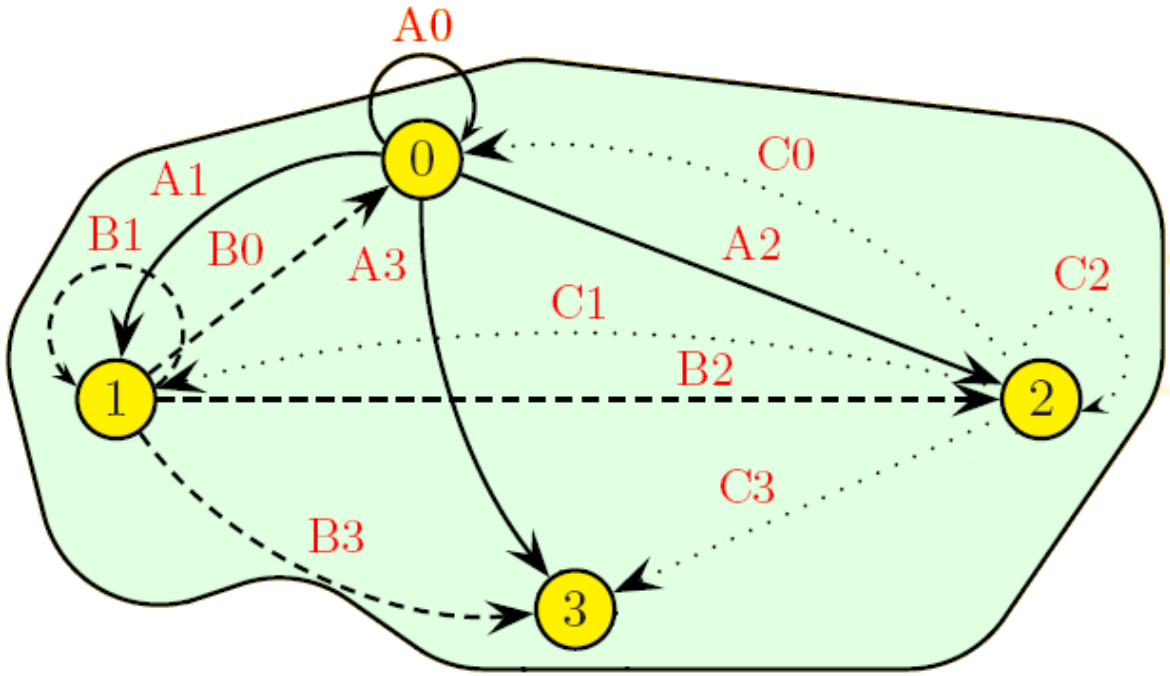
MPI_ALLTOALL

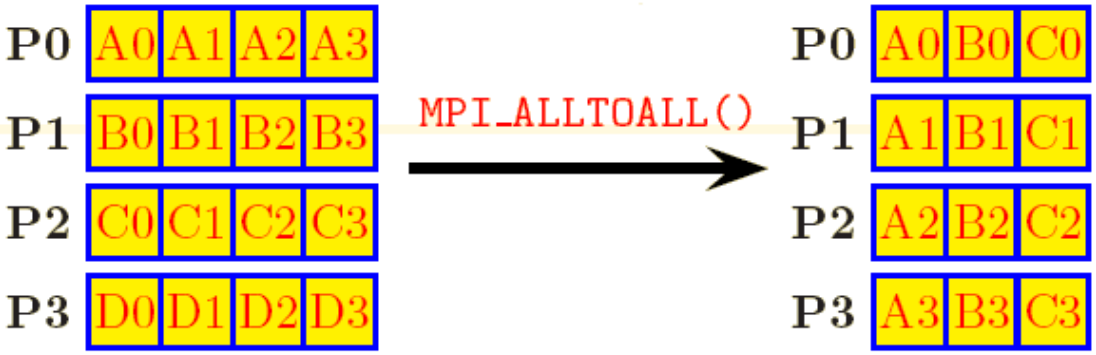


MPI_ALLTOALL

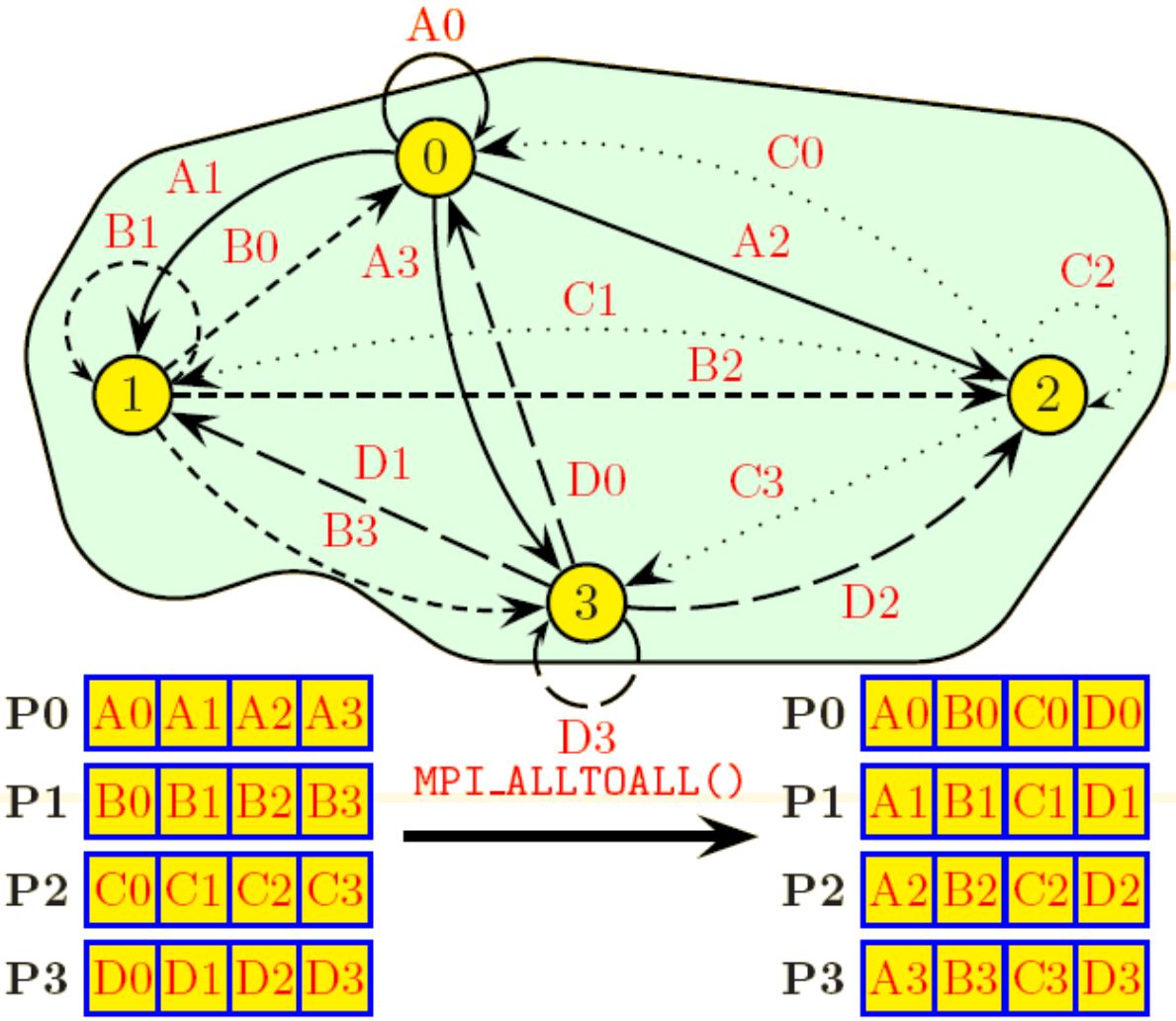


MPI_ALLTOALL





MPI_ALLTOALL



MPI_ALLTOALL

```
FORTRAN_TYPE:: sbuff, rbuff
integer:: count, root, ierror
call MPI_SCATTER( sbuff,scount,MPI_TYPE, &
                  rbuff,rcount,MPI_TYPE,MPI_COMM_WORLD,ierror)
```

- **SBUFF** — array being sent — input
- **RBUFF** — array being received — output
- **[S/R]COUNT** — number of items to/from each task — input

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.

All to All Routines

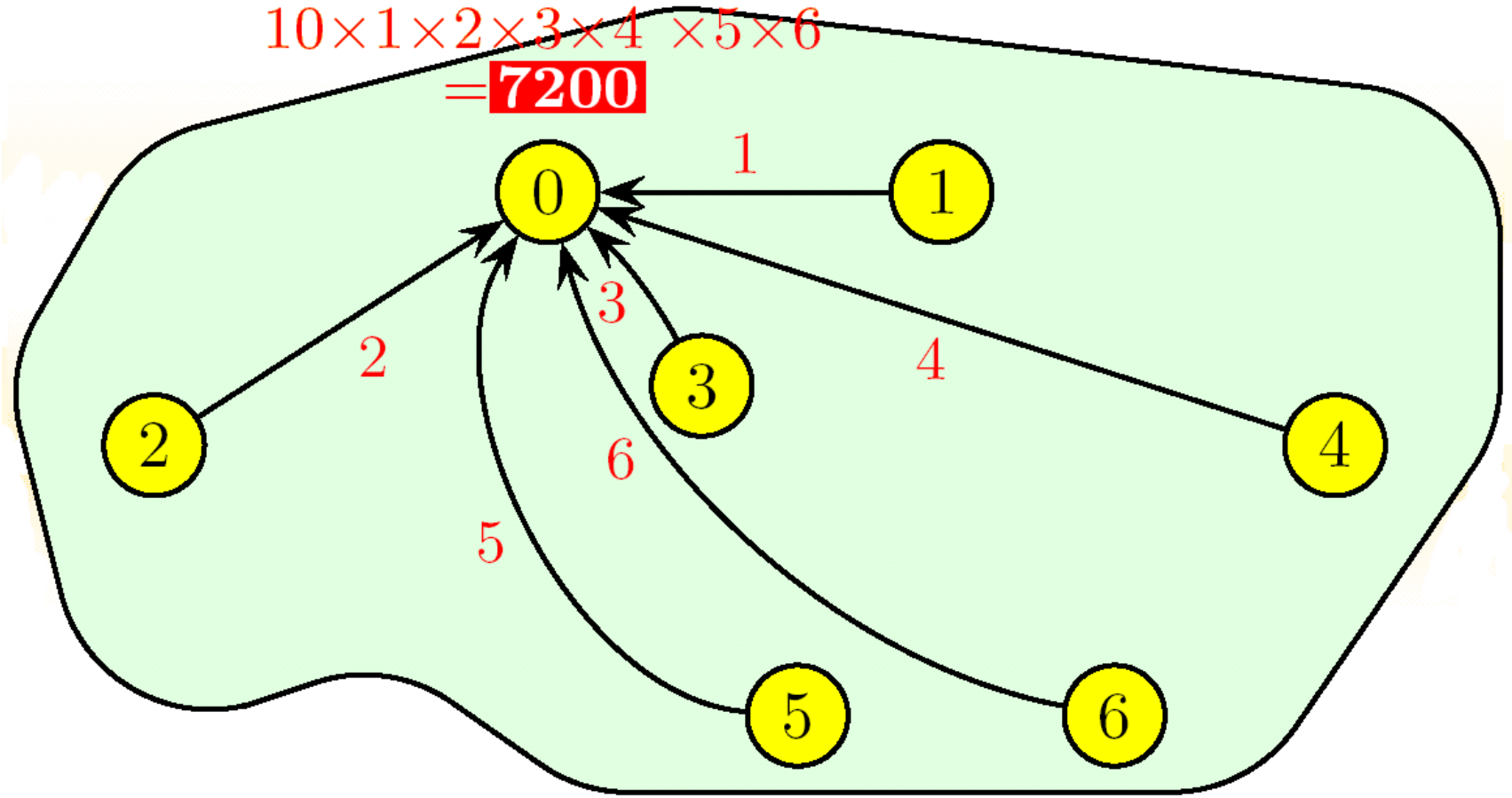
- **MPI_ALLTOALL**
  - every task sends equal length parts of an array to all other tasks
  - every task receives equal parts from all other tasks
  - transpose of data over the tasks

- **MPI_ALLTOALLV**
  - as above but parts are different lengths

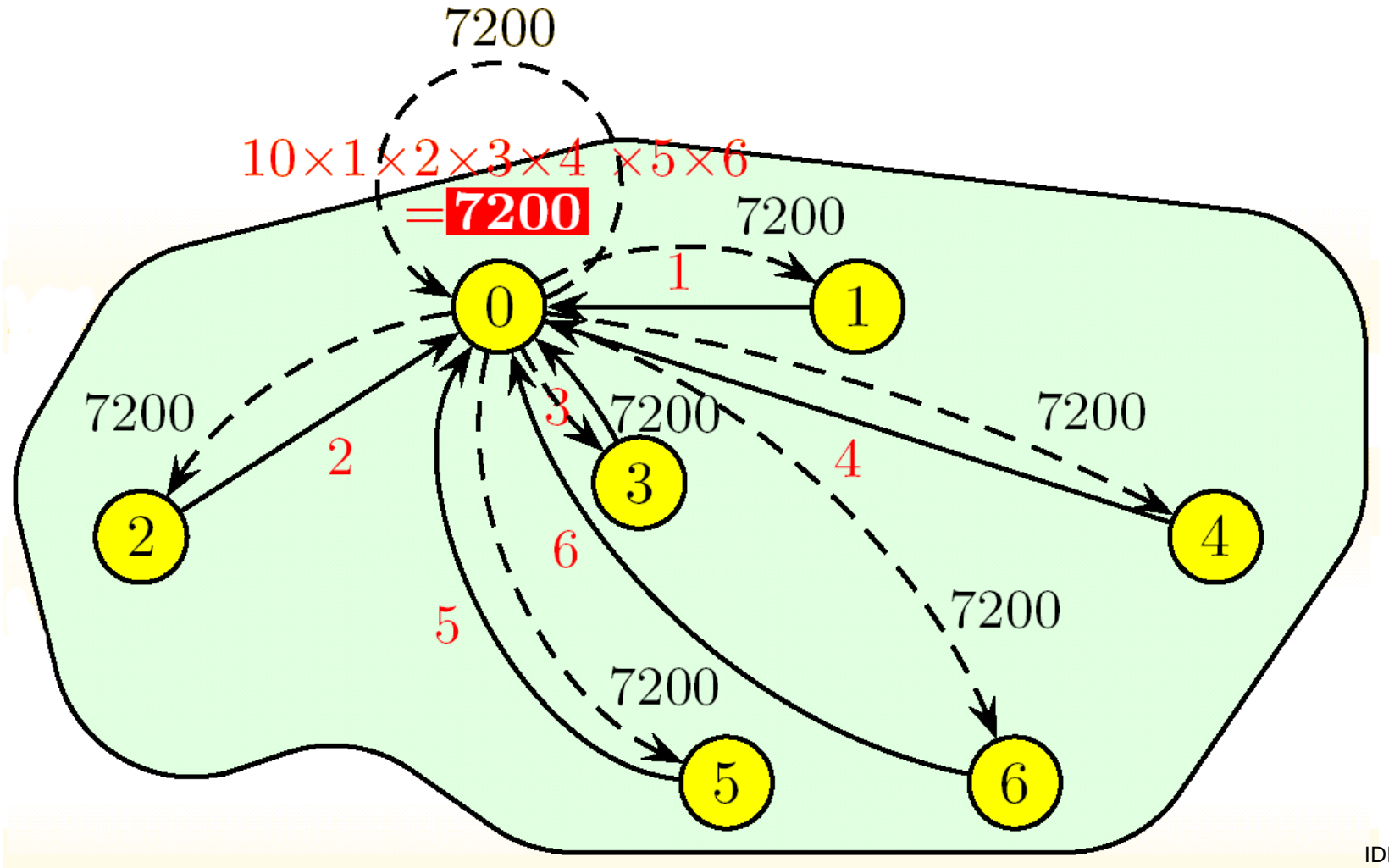
Reduction routines

- Perform both communications and simple math
  - 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



MPI_ALLREDUCE



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MPI_REDUCE

```
FORTRAN_TYPE:: sbuff, rbuff
integer:: count, root, ierror
call MPI_REDUCE( sbuff,rbuff,count,MPI_TYPE,OP_TYPE, &
                 root,MPI_COMM_WORLD,ierror)
```

- **SBUFF** — array to be reduced — input
- **RBUFF** — result of reduction — output
- **COUNT** — number of items to be reduced — input

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 References

- **Using MPI (2nd edition) by William Gropp, Ewing Lusk and Anthony Skjellum; Copyright 1999 MIT; MIT Press ISBN 0-262-57132-3**
- **The Message Passing Interface Standard on the web at**

  `www-unix.mcs.anl.gov/mpi/index.html`

- **IBM Parallel Environment for AIX Manuals**

  `www.ibm.com/servers/eserver/pseries/library/sp_books/pe.html`

  - IBM PE Hitchhikers Guide (sample programs also available)
  - MPI Programming Guide
  - MPI Subroutine Reference

- **Further Training Material**

  `www.epcc.ed.ac.uk/library/training`

  - Decomposing the Potentially Parallel
  - MPI Course

Second Practical

- exercise1b
- See the README for details