Collective Communication

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Overview

- Introduces the most important collective communication operations within MPI
- Discusses their MPI application interfaces

Collective calls I

- So far discussed: point-to-point communication
  - One sending process
  - One receiving process
- Often required: Communication in a group of processes
- Examples:
  - Distribution of simulation parameters
  - Averages of distributed data structures

Collective calls II

- All collective calls can be built up of point-to-point calls

- On a well tuned system you should not be able to beat the performance of a collective using MPI point-to-point
  - Some systems offer dedicated hardware for collectives (e.g. IBM BlueGene L and P)[1]
- Whenever there is a collective: Use it

- There are no non-blocking collective calls in MPI 2.x
  - Introduced in MPI 3.0

[1]The Int. Jour. of High Perf. Comp., S. Kumar (2014)

Collective and point-to-point calls differences

- The collective function must be called by all the processes
- Arguments passed to the collective functions by the processes need to match their counterparts (for instance, the root rank)
- Point-to-point calls use tags and communicators to establish message transfer. Collective calls are matched by the order in which they appear
- Don’t use the same buffer for input and output

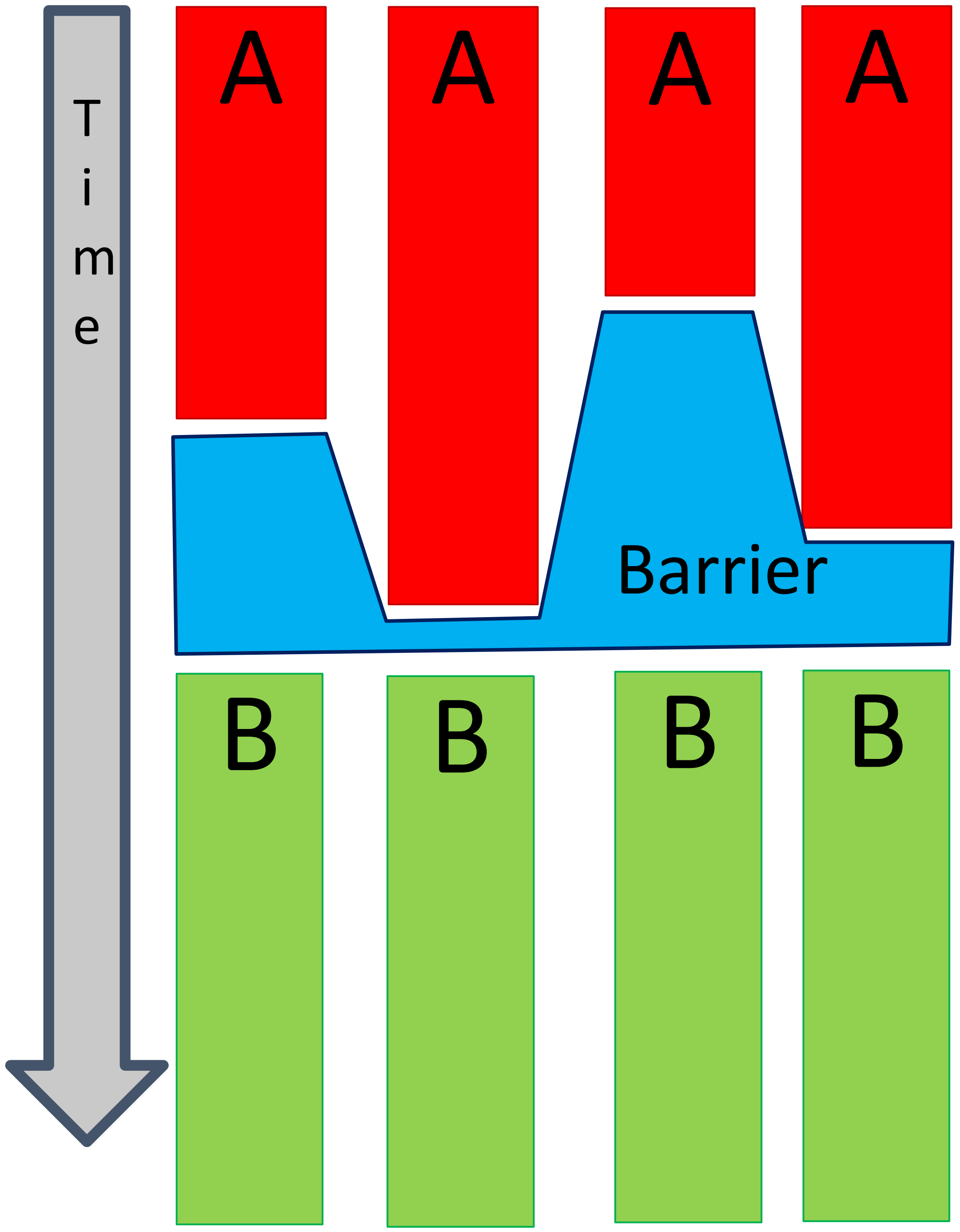
Ref. An introduction to parallel programming, Peter S. Pacheco

Barrier

- Program (each Proc:)

```
Call calc_A()
Call barrier(comm)
Call calc_B()
```

- Tasks wait in barrier until last finished `calc_A`



MPI_Barrier

In C:

```
int MPI_Barrier(MPI_Comm comm)
```

In Fortran 90:

```
MPI_BARRIER(COMM, IERROR)
 INTEGER:: COMM, IERROR
```

In Python:

```
comm.barrier()
```

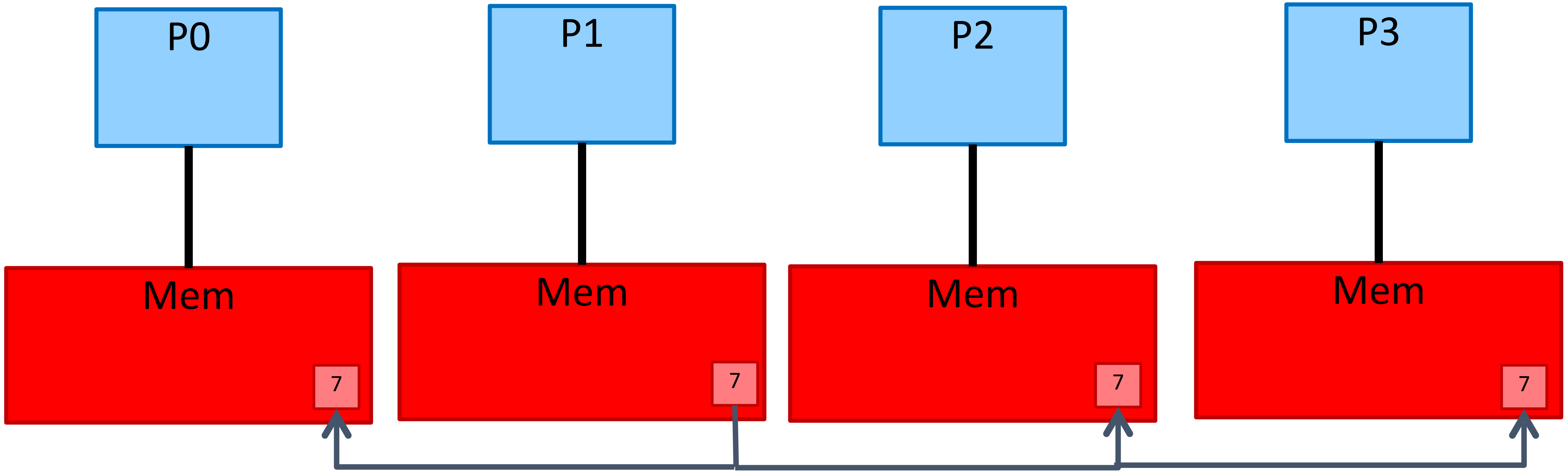
- Typically no good reason to use, except
  - Performance measurement/Benchmarking
  - Single sided communication – not in this course

In C	In Fortran
`#include "mpi.h"`	`program main`
`#include <stdio.h>`	`use mpi`
`int main(int argc, char *argv[])`	`implicit none`
`{`	
`int myrank, numprocs, ierr;`	`integer myrank, numprocs, ierr`
`MPI_Init(&argc,&argv);`	`call MPI_INIT(ierr)`
`MPI_Comm_size(MPI_COMM_WORLD,&numprocs);`	`call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)`
`MPI_Comm_rank(MPI_COMM_WORLD,&myrank);`	`call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)`
`ierr = MPI_Barrier(MPI_COMM_WORLD);`	`call MPI_Barrier(  MPI_COMM_WORLD, ierr)`
`MPI_Finalize();`	`call MPI_FINALIZE(ierr)`
`return 0;`	
`}`	`end`

In Python

```
from mpi4py import MPI

comm = MPI.COMM_WORLD

numprocs = comm.Get_size()
myrank = comm.Get_rank()

comm.Barrier()
```

Broadcast



MPI_Bcast in C

```
int MPI_Bcast(void* buf, int count, MPI_Datatype
 datatype, int root,      MPI_Comm comm )
```

• `buf:`	address of buffer (send on root, receive else)
• `count:`	number of data
• `datatype:`	type of data
• `root:`	root rank – rank of task sending data
• `comm:`	communicator – every task in comm gets data

Remark: Depending on your rank, this is a send **or** receive

MPI_Bcast in Fortran 90

```
MPI_BCAST(BUF, COUNT, DATATYPE, ROOT, COMM, & IERROR)
 <type>::  BUF
 INTEGER:: COUNT, DATATYPE, ROOT, COMM, IERROR
```

• `buf:`	buffer (send on root, receive else)
• `count:`	number of data
• `datatype:`	type of data
• `root:`	root rank – rank of task sending data
• `comm:`	communicator – every task in comm gets data

Remark: Depending on your rank, this is a send **or** receive

bcast in Python

```
comm.bcast(obj, root=root)
```

- `obj`: the Python object to broadcast
- `root`: root rank – rank of task sending data

Remark: Depending on your rank, this is a send **or** receive

The Python object will be returned by `bcast`. Example:

```
data = comm.bcast(data, root=0)
```

In C

```c
#include "mpi.h"
#include <stdio.h>

int main(int argc, char *argv[])
{
int myrank, numprocs, ierr, alpha;

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);

if (myrank == 0) {
  printf("Type some integer\n");
  scanf("%d", &alpha);
}

MPI_Bcast(&alpha, 1, MPI_INT, 0, MPI_COMM_WORLD);
printf("Value of alpha on each rank %d\n", alpha);

MPI_Finalize();
return 0;
}
```

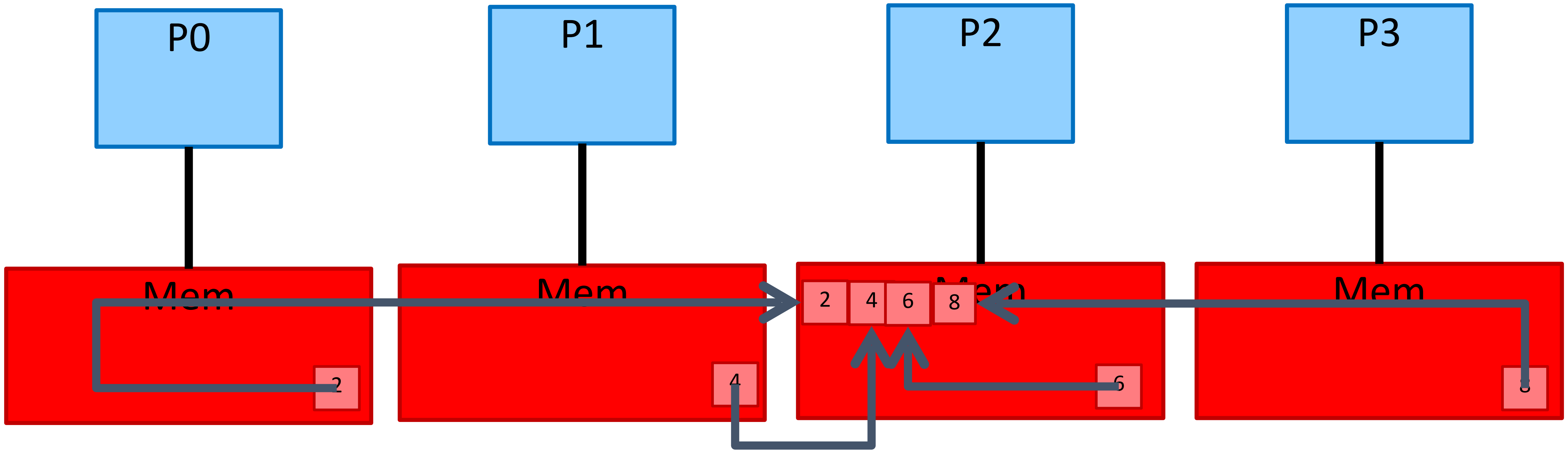
In Fortran

```fortran
program main
use mpi
implicit none


integer myrank, numprocs, ierr, alpha

call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

if (myrank .eq. 0) then
  print *, 'Type some integer'
  read(*,*) alpha
endif

call MPI_BCAST(alpha, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, ierr)
print *, 'Value of alpha on each rank', alpha

call MPI_FINALIZE(ierr)
end
```

In Python

```
from mpi4py import MPI

comm = MPI.COMM_WORLD

numprocs = comm.Get_size()
myrank = comm.Get_rank()

if myrank == 0:
    alpha = int(input("Type some integer:\n"))
else:
    alpha = None

alpha = comm.bcast(alpha, root=0)

print("Value of alpha on rank {:d} is: {:d} ".format(myrank,
alpha))
```

Gather



- Collects data from all processors into a large array on root
- Order: 1st all data from rank 0, followed by all data from rank 1, followed by all data from rank 2, ...

- This is not a scalable call - think again if you want to use
  - On 10000 cores you easily run out of memory

MPI_Gather in C

```
int MPI_Gather(void* sendbuf, int sendcount, MPI_Datatype
  sendtype, void* recvbuf, int recvcount, MPI_Datatype
  recvtype, int root, MPI_Comm comm)
```

• `sendbuf:`	address of send buffer
• `sendcount:`	number of elements in send buffer
• `sendtype:`	type of data
• `recvbuf:`	address of receive buffer (only root)
• `recvcount:`	number of data received from **each** task
• `recvtype:`	type of data
• `root:`	root rank – rank collecting the data
• `comm:`	communicator – every task has to send

MPI_Gather in Fortran 90

```
MPI_GATHER(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT,
  RECVTYPE, ROOT, COMM, IERROR)
<type>:: SENDBUF, RECVBUF
INTEGER:: SENDCOUNT, SENDTYPE, RECVCOUNT, RECVTYPE, ROOT,
  COMM, IERROR
```

• `SENDBUF:`	send buffer
• `SENDCOUNT:`	number of elements in send buffer
• `SENDTYPE:`	type of data
• `RECVBUF:`	receive buffer (significant only on root)
• `RECVCOUNT:`	number of data received from **each** task
• `RECVTYPE:`	type of data
• `ROOT:`	root rank – rank collecting the data
• `COMM:`	communicator – every task has to send

gather in Python

```
comm.gather(obj, root=root)
```

• `obj:`	the Python object to gather
• `root:`	root rank – rank collecting the data

A `list` will be returned by `gather`.

Example:

```
   a = comm.Get_rank()
   b = comm.gather(a, root=0)
```

`b` on the root rank is a `list` containing `a` from all MPI processes.

In C

```
root = 0;
counts = 3; //nr. of elements to be sent/received
size_recvbuf = counts * numprocs; //size receiving buffer
//allocating receiving buffer: counts elements per rank
if( myrank == 0) recvbuf = malloc(size_recvbuf * sizeof(float));

//initializing sending buffer
float
sendbuf[4]={1.0*myrank,2.0*myrank,3.0*myrank,4.0*myrank};
MPI_Gather(sendbuf,counts,MPI_FLOAT,recvbuf,counts,MPI_FLOAT,
root,MPI_COMM_WORLD);

if (myrank == 0) {
  for( i = 0; i < size_recvbuf; i++)
     printf("Array %.3f \n", recvbuf[i]);

  free(recvbuf);
}
```

In Fortran

```
root = 0
counts =3 !nr. of elements to be sent/received
size_recvbuf = counts * numprocs !size receiving buffer
!allocating receiving buffer: 2 elements per rank
if (myrank == 0 ) allocate( recvbuf(size_recvbuf) )

!initializing sending buffer
sendbuf = (/1.0*myrank,2.0*myrank,3.0*myrank,4.0*myrank /)
call
MPI_Gather(sendbuf,counts,MPI_REAL,recvbuf,counts,MPI_REAL,ro
ot,MPI_COMM_WORLD, ierr)

if(myrank == 0) then
  do i=1,size_recvbuf
     print *, "Array", recvbuf(i)
  enddo
  deallocate ( recvbuf )
endif
```

In Python

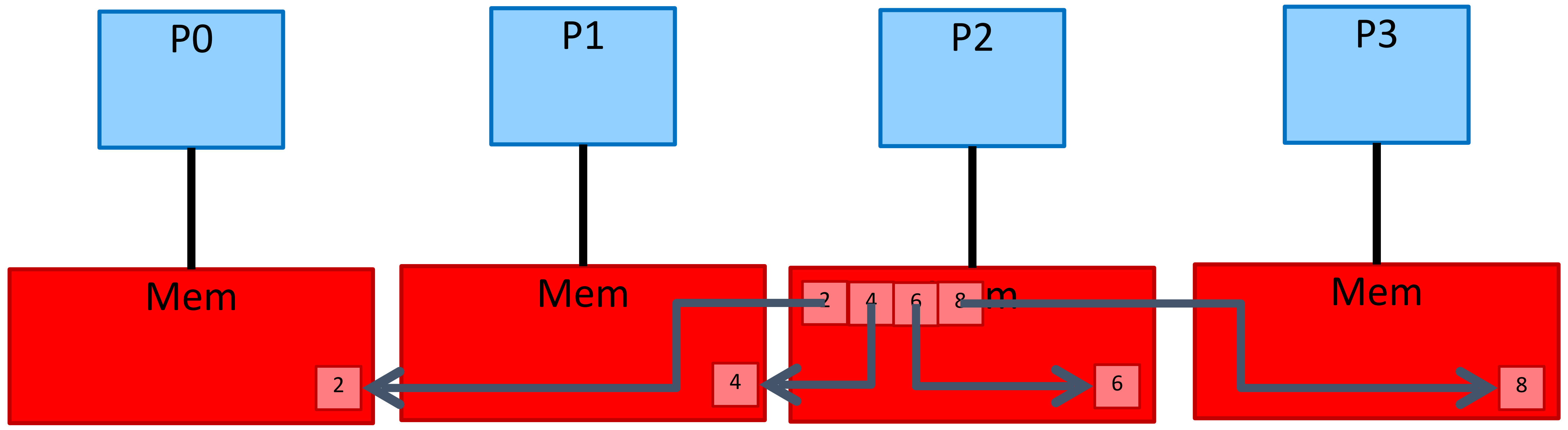
```
from mpi4py import MPI

comm = MPI.COMM_WORLD

numprocs = comm.Get_size()
myrank = comm.Get_rank()

send_data = [1.0*myrank, 2.0*myrank, 3.0*myrank, 4.0*myrank]
send_count = 3

recv_data = comm.gather(send_data[:send_count], root=0)

if myrank == 0:
    for entry in recv_data:
        for number in entry:
            print("Array: {:.3f} ".format(number))
```

Deadlock in collectives

- Consider the following code snipped:
- At least on rank 6, the gather can not finish, it needs input from rank 5
- Rank 6 will wait forever

```
if (rank /= 5) then
 call CalcA(a)
 call MPI_GATHER(a,7,&
  MPI_REAL,b,7,MPI_REAL,&
  6,mcomm,merror)
else
 call CalcB(a)
endif

if (rank == 6) then
 call Vcalc(b)
endif
```

Scatter



- Distributes data from a large array on root
- Order: 1st lot of data go to rank 0, followed by all data for rank 1, followed by all data for rank 2, ...
- “Inverse” of gather
- This is not a scalable call - think again if you want to use
  - On 10000 cores you easily run out of memory

MPI_Scatter in C

```
int MPI_Scatter(void* sendbuf, int sendcount,
 MPI_Datatype sendtype, void* recvbuf, int recvcount,
 MPI_Datatype recvtype, int root, MPI_Comm comm)
```

• `sendbuf:`	address of send buffer (only root significant)
• `sendcount:`	number of elements send to **each** task
• `sendtype:`	type of data
• `recvbuf:`	address of receive buffer
• `recvcount:`	number of data received from root
• `recvtype:`	type of data
• `root:`	root rank – rank sending the data
• `comm:`	communicator – every task receives

MPI_Scatter in Fortran 90

```
MPI_Scatter(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF, RECVCOUNT,
  RECVTYPE, ROOT, COMM, IERROR)
<type>:: SENDBUF, RECVBUF
INTEGER:: SENDCOUNT, SENDTYPE, RECVCOUNT, RECVTYPE, ROOT,
  COMM, IERROR
```

• `SENDBUF:`	send buffer (significant only on root)
• `SENDCOUNT:`	number of elements send to **each** task
• `SENDTYPE:`	type of data
• `RECVBUF:`	receive buffer
• `RECVCOUNT:`	number of data received from root
• `RECVTYPE:`	type of data
• `ROOT:`	root rank – rank sending the data
• `COMM:`	communicator – every task receives

scatter in Python

```
comm.scatter(obj, root=root)
```

- `obj`: The Python object (should be a list) to scatter
- `root`: root rank – rank sending the data

`obj` should be a list that contains the objects to be sent to each process.

`len(obj)` should be equal to the number of processes.

Example:

```
   b = comm.scatter(a, root=0)
```

`a` on the root rank should be a `list` containing Python objects.

After scatter, `b` is the object on each process.

In C	In Fortran
float *sendbuf=NULL;	real, pointer :: sendbuf(:)
float recvbuf[4];	real recvbuf(4)
MPI_Init(&argc,&argv);	call MPI_INIT(ierr)
MPI_Comm_size(MPI_COMM_WORLD,&numprocs);	call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);	call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

In C

```c
float *sendbuf=NULL;
float recvbuf[4];
MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);

root = 0;
counts = 3; //nr. of elements to be sent/received
size_sendbuf = counts * numprocs; //size receiving buffer
if( myrank == 0) {
  sendbuf = malloc(size_sendbuf * sizeof(float));
  for( i = 0; i < size_sendbuf; i++)
     sendbuf[i] = 1.0*i;
}

MPI_Scatter(sendbuf,counts,MPI_FLOAT,recvbuf,counts,MPI_FLOAT,
root,MPI_COMM_WORLD);

if( myrank == 0) {
  free(sendbuf);
}
MPI_Finalize();
```

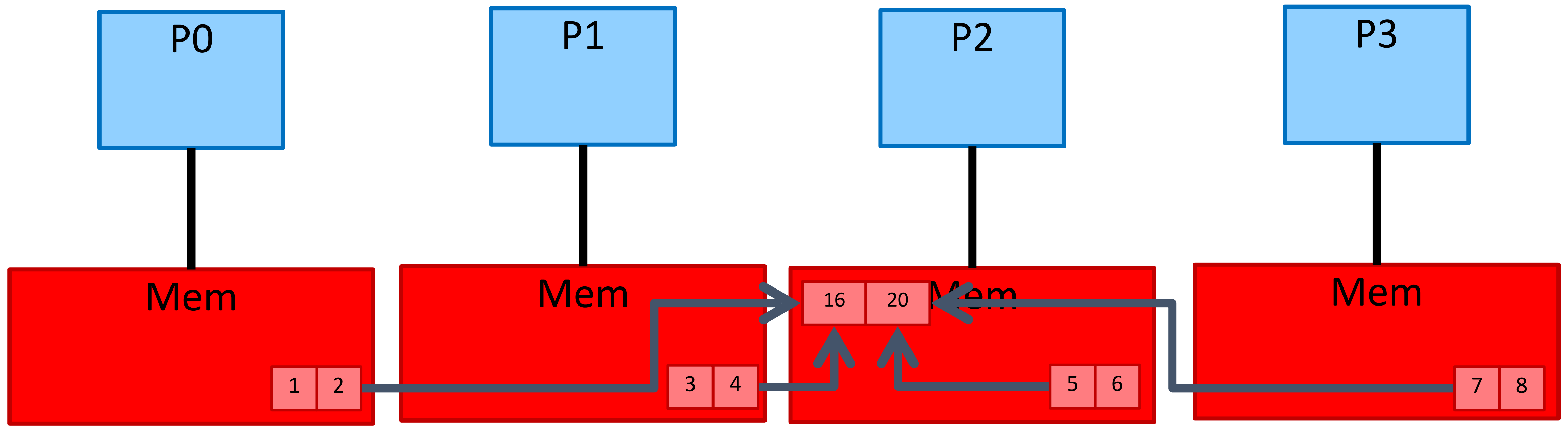
In Fortran

```fortran
real, pointer :: sendbuf(:)
real recvbuf(4)
call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

root = 0
counts =3 !nr. of elements to be sent/received
size_sendbuf = counts * numprocs !size receiving buffer
if (myrank == 0 ) then
   allocate( sendbuf(size_sendbuf) )
   do i=1,size_sendbuf
      sendbuf(i) = 1.0*i-1.0
   enddo
endif
call MPI_Scatter (sendbuf, counts,MPI_REAL,recvbuf,counts,
MPI_REAL,root,MPI_COMM_WORLD, ierr)

if(myrank == 0) then
  deallocate ( sendbuf )
endif
Call MPI_FINALIZE(ierr)
```

In Python

```
from mpi4py import MPI

comm = MPI.COMM_WORLD

numprocs = comm.Get_size()
myrank = comm.Get_rank()

send_count = 3
send_size = send_count * numprocs

if myrank == 0:
   send_data = []
   for i in range(numprocs):
      send_data.append([i * send_count + j for j in range(send_count)])
else:
   send_data = None

comm.scatter(send_data, root=0)
```

Reduce



- Example: Vector addition for count of 2
- Combines data from all processors into data structure on root

- This is a widely used scalable call
  - Structures on each processor task count independent

MPI_Reduce in C

```
int MPI_Reduce(void* sendbuf, void* recvbuf,
 int count, MPI_Datatype datatype, MPI_Op op,
 int root, MPI_Comm comm)
```

`sendbuf:`	send buffer
`recvbuf:`	receive buffer (significant only on root)
`count:`	length of send and receive buffer
`datatype:`	data type of data – required for correct op
`op:`	handle of operation (more later)
`root:`	rank of root process
`comm:`	communicator, every rank contributes

Option: Constant **`MPI_IN_PLACE`** as sendbuf on root

MPI_Reduce in Fortran 90

```
MPI_REDUCE(SENDBUF, RECVBUF, COUNT, DATATYPE, OP, ROOT, &
 COMM, IERROR)
 <type>::  SENDBUF, RECVBUF
 INTEGER:: COUNT, DATATYPE, OP, ROOT, COMM, IERROR
```

• `sendbuf:`	send buffer
• `recvbuf:`	receive buffer (significant only on root)
• `count:`	length of send and receive buffer
• `datatype:`	data type of data – required for correct op
• `op:`	handle of operation (more later)
• `root:`	rank of root process
• `comm:`	communicator, every rank contributes

Option: Constant **`MPI_IN_PLACE`** as sendbuf on root

Predefined reduction operations

Name	Function	MPI data types
`MPI_MAX`	Maximum	C integer, Fortran integer, Floating point
`MPI_MIN`	Minimum	C integer, Fortran integer, Floating point
`MPI_SUM`	Sum	C integer, Fortran integer, Floating point, Complex
`MPI_PROD`	Product	C integer, Fortran integer, Floating point, Complex
`MPI_LAND`	Logical and	C integer, Fortran logical
`MPI_BAND`	Bit-wise and	C integer, Fortran logical, Byte
`MPI_LOR`	Logical or	C integer, Fortran logical
`MPI_BOR`	Bit-wise or	C integer, Fortran logical, Byte
`MPI_LXOR`	Logical xor	C integer, Fortran logical
`MPI_BXOR`	Bit-wise xor	C integer, Fortran logical, Byte

reduce in Python

```
comm.reduce(obj, op=op, root=root)
```

• `obj:`	The Python object to reduce
• `op:`	handle of operation (more later)
• `root:`	rank of root process

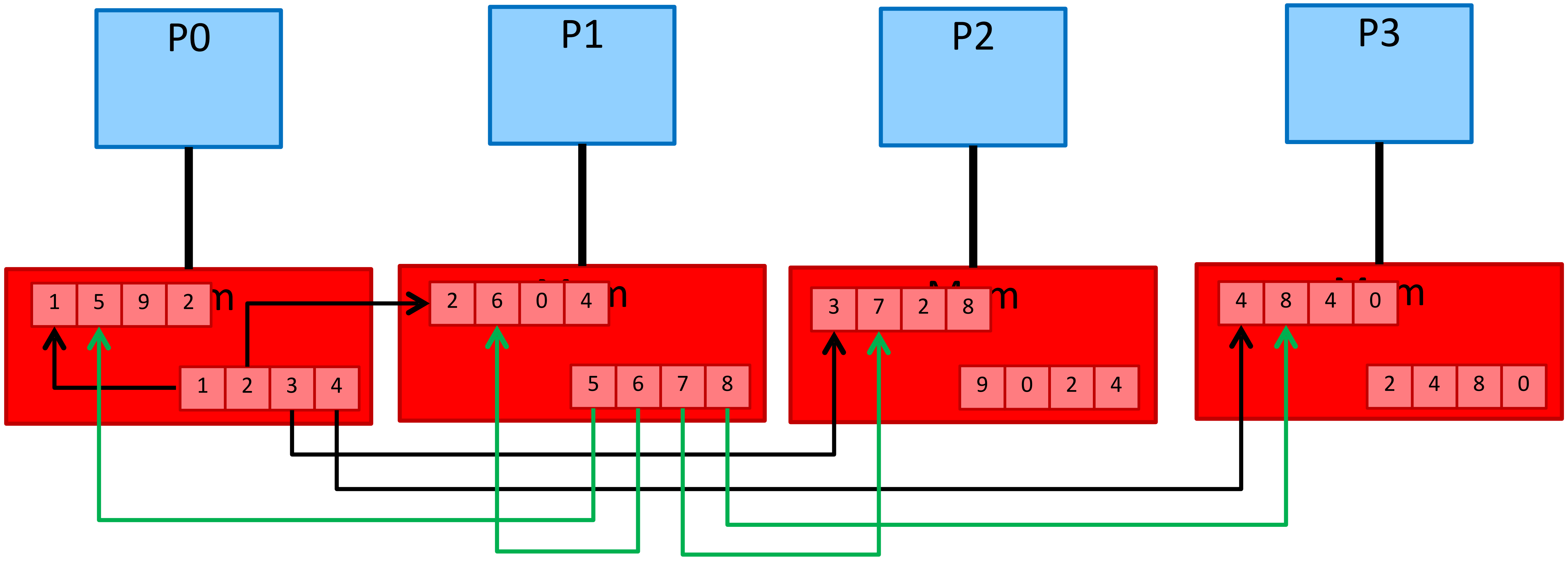
Example:

```
  pi = comm.reduce(partial_pi, op=MPI.SUM, root=0)
```

Predefined reduction operations in Python

Name	Function	MPI data types
`MPI.MAX`	Maximum	C integer, Fortran integer, Floating point
`MPI.MIN`	Minimum	C integer, Fortran integer, Floating point
`MPI.SUM`	Sum	C integer, Fortran integer, Floating point, Complex
`MPI.PROD`	Product	C integer, Fortran integer, Floating point, Complex
`MPI.LAND`	Logical and	C integer, Fortran logical
`MPI.BAND`	Bit-wise and	C integer, Fortran logical, Byte
`MPI.LOR`	Logical or	C integer, Fortran logical
`MPI.BOR`	Bit-wise or	C integer, Fortran logical, Byte
`MPI.LXOR`	Logical xor	C integer, Fortran logical
`MPI.BXOR`	Bit-wise xor	C integer, Fortran logical, Byte

All-to-all (the worse of the worst)



- Every processor sends to every other processor
- 1st portion of send buffer → rank 0, 2nd portion → rank 1, etc.
- 1st portion in recv buffer ← rank 0, 2nd portion ← rank 1, etc.
- *Extremely important in spectral codes, e.g. parallel FFT*

MPI_Alltoall in C

```
int MPI_Alltoall(void* sendbuf, int sendcount,
 MPI_Datatype sendtype, void* recvbuf, int recvcount,
 MPI_Datatype recvtype, MPI_Comm comm)
```

• `sendbuf:`	Address of send buffer
• `sendcount:`	Number of elements send from each task
• `sendtype:`	Data type of send buffer
• `recvbuf:`	Address of receive buffer
• `recvcount:`	Number of elements received f. each task
• `recvtype:`	Data type of receive buffer
• `comm:`	Communicator, every task sends and recvs

Rem: The counts are **<u>not</u>** the buffer size!

MPI_Alltoall in Fortran 90

```
MPI_ALLTOALL(SENDBUF, SENDCOUNT, SENDTYPE, RECVBUF,
 RECVCOUNT, RECVTYPE, COMM, IERROR)
 <type>:: SENDBUF, RECVBUF
 INTEGER:: SENDCOUNT, SENDTYPE, RECVCOUNT, RECVTYPE, COMM,
 IERROR
```

• `sendbuf:`	Address of send buffer
• `sendcount:`	Number of elements send form each task
• `sendtype:`	Data type of send buffer
• `recvbuf:`	Address of receive buffer
• `recvcount:`	Number of elements received f. each task
• `recvtype:`	Data type of receive buffer
• `comm:`	Communicator, every task sends and recvs

Rem: The counts are **not** the buffer size!

alltoall in Python

```
comm.alltoall(obj)
```

- `obj`: The Python object (should be a list)

`obj` should be a list that contains the objects to be sent to each process.

`len(obj)` should be equal to the number of processes.

Example:

```
    b = comm.alltoall(a)
```

`a` should be a `list` containing Python objects.

After scatter, `b` is a `list` containing the result of `alltoall` operation.

Variations: Allgather and Allreduce

- The are "**`All`**" versions for calls which receive only on root:
  - **`MPI_Allgather (or comm.allgather in Python)`**
  - **`MPI_Allreduce (or comm.allreduce in Python)`**
- Every task has a receive buffer – the result is know on every task
- These calls can be thought of as
  - **`MPI_Gather`** followed by **`MPI_Bcast`**
  - **`MPI_Reduce`** followed by **`MPI_Bcast`**
- The **`root`** argument is omitted from the interface
- "**`All`**"-communications can take longer to complete
  - Only use them if you need them

Advanced topic: Vector collectives

- The calls of this lecture: Same count on all tasks

- Vector collectives relax this condition:
  - **`MPI_Gatherv`**
  - **`MPI_Scatterv`**
  - **`MPI_Allgatherv`**
  - **`MPI_Alltoallv`**

- These calls go beyond the scope of this course

Non blocking collectives in MPI 3.x

- Similar to non-blocking point-to-point communication:
  - Non-blocking call (e.g. **`MPI_Ibcast`**) initiates communication
  - A completion call (e.g. **`MPI_Wait`**) ensures that local part of communication is finalised
    - Send buffers can be overwritten
    - Receive buffers contain data
- Allows for
  - Overlapping communication and calculation
  - Avoiding synchronisation if MPI library avoids sync.
    - The call **`MPI_Ibarrier`** has to avoid synchronisation
  - Avoiding dead locks (e.g. overlapping communicators)

Summary

- Discussed collective communications:
  - Barrier
  - Broadcast
  - Gather/Scatter
  - Reduction
  - Alltoall
- Variations of the above (all-version, vector-version)
- Non-blocking collective communication in MPI 3.0

2D Integration

In this example you will calculate the double integral:

$$\int_0^{\pi}\int_0^{\pi} \sin(x+y)dxdy = 0$$

One way to parallelize this calculation is by dividing the integration range in one of the variables, let's say "x", evenly between N processes and do the regular integration over the other variable "y" in this case.

This problem is useful for two reasons, first we know the exact value of the integral (0) and second because it includes a double integral, the computation is heavier enough to detect the effects of a parallel implementation.

Exercise 1

Create a version of your π^2-code using collective calls

- Time the communication times
- Compare performance of the versions using
  - Point-to-point
  - Collectives

Remarks:

- You might need a barrier in the beginning of your code to absorb differences in ” task wake up”
- You might need to run repeatedly

Exercise 2

Modify your *messages around a ring* code to use a collective to add the send-buffers onto rank 0

Compare the performance with original code