Collective Communication

Pedro Ojeda, Xin Li, Joachim Hein

HPC2N, Umeå University

LUNARC & Centre of Mathematical Sciences

Lund University

PDC, KTH

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

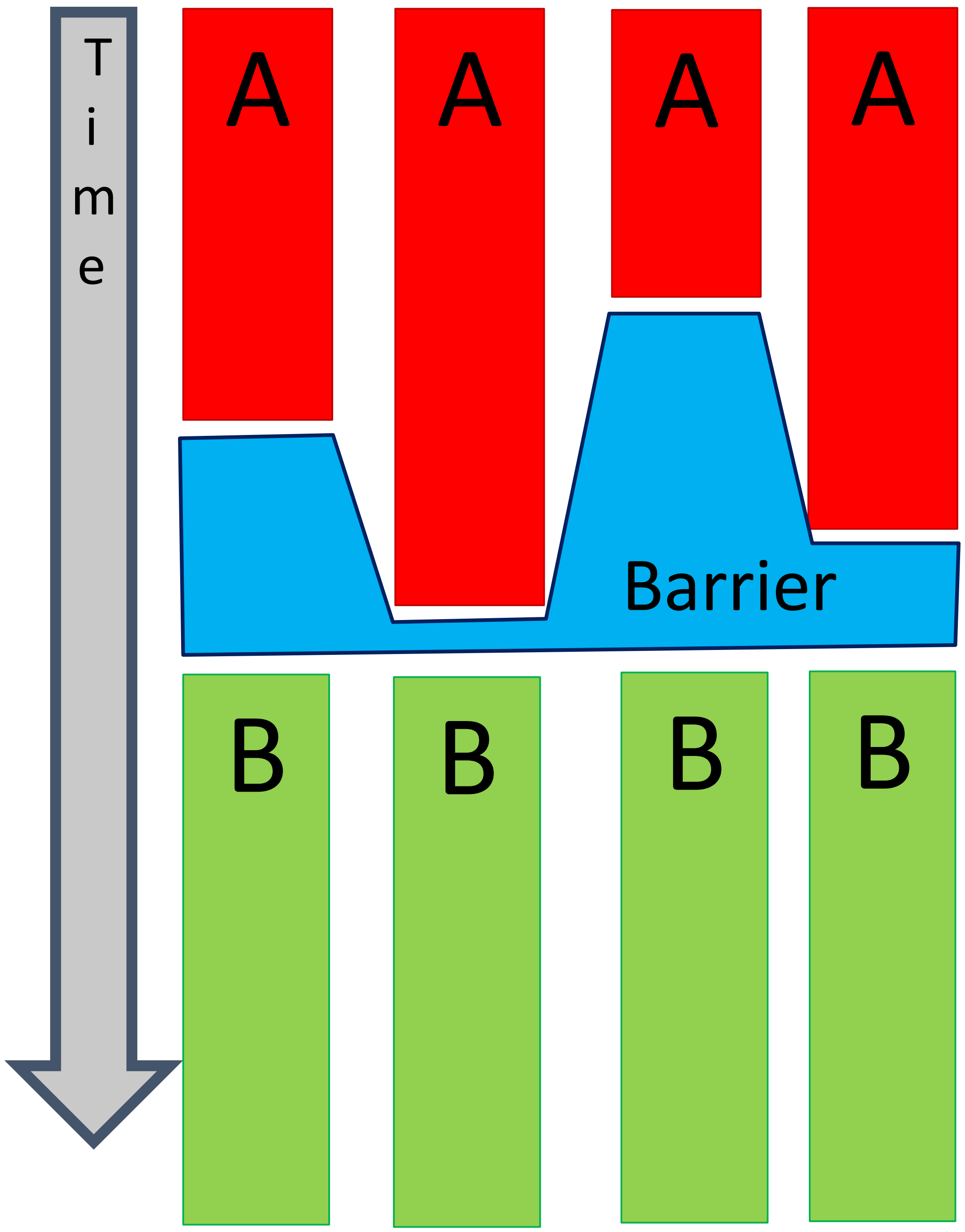
Ref. An introduction to parallel programming, Peter S. Pacheco

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()
```

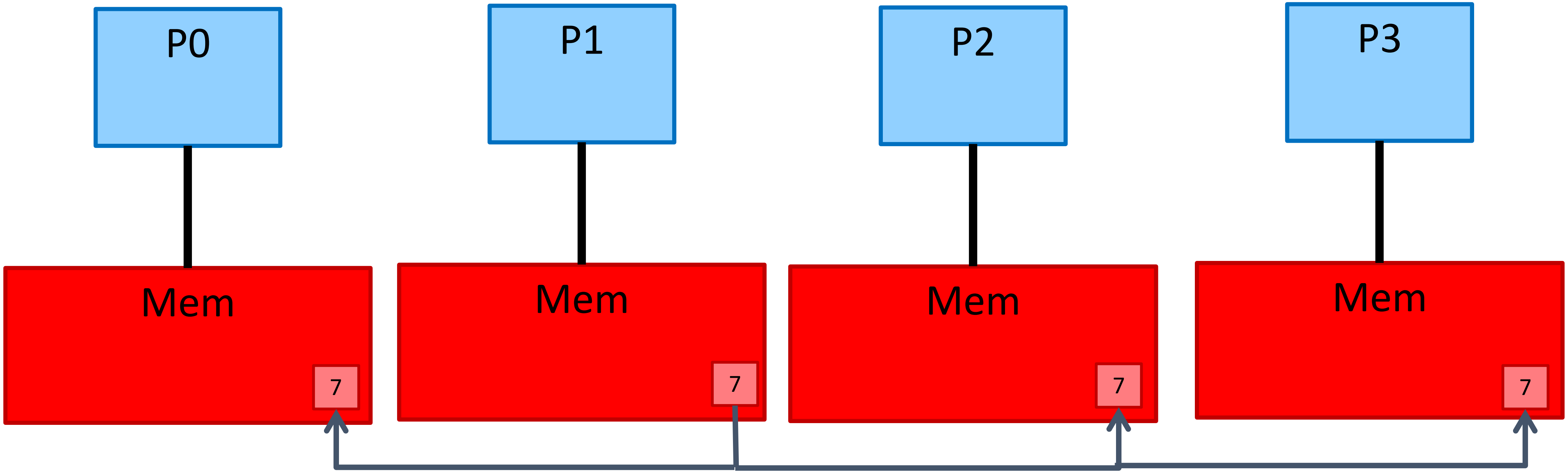
- Typically no good reason to use, except
  - Performance measurement/Benchmarking
  - Single sided communication – not in this course

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)
```

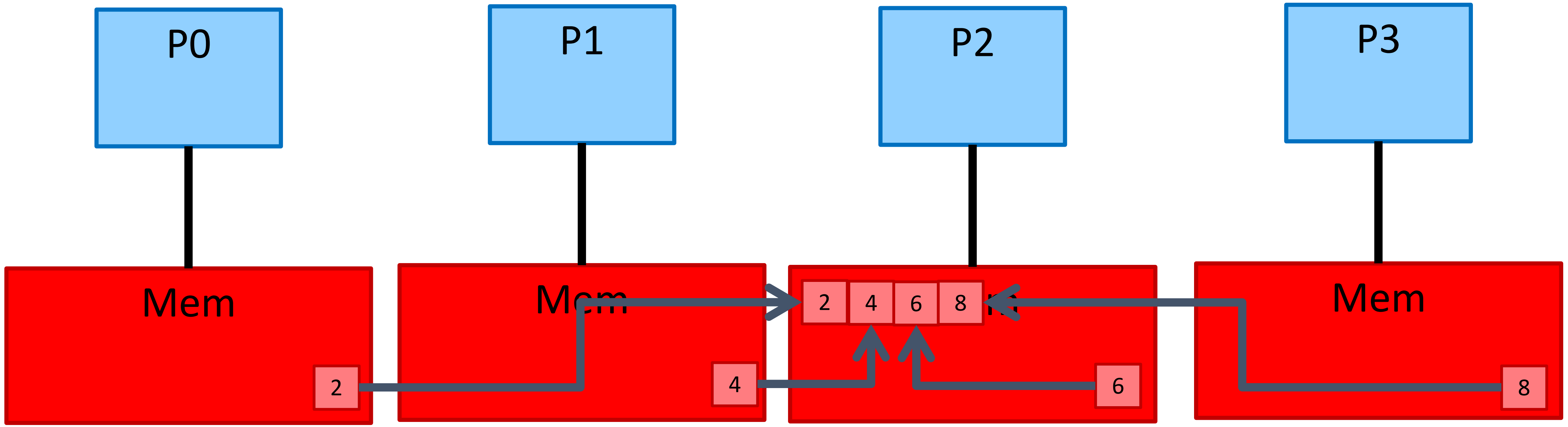
In C	In Fortran

<pre>#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;
}</pre>
	<pre>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</pre>

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	In Fortran

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);
}
	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,root,MPI_COMM_WORLD, ierr)
	
	if(myrank == 0) then
	  do i=1,size_recvbuf
	    print *, "Array", recvbuf(i)
	  enddo
	  deallocate (recvbuf)
	endif

In Python

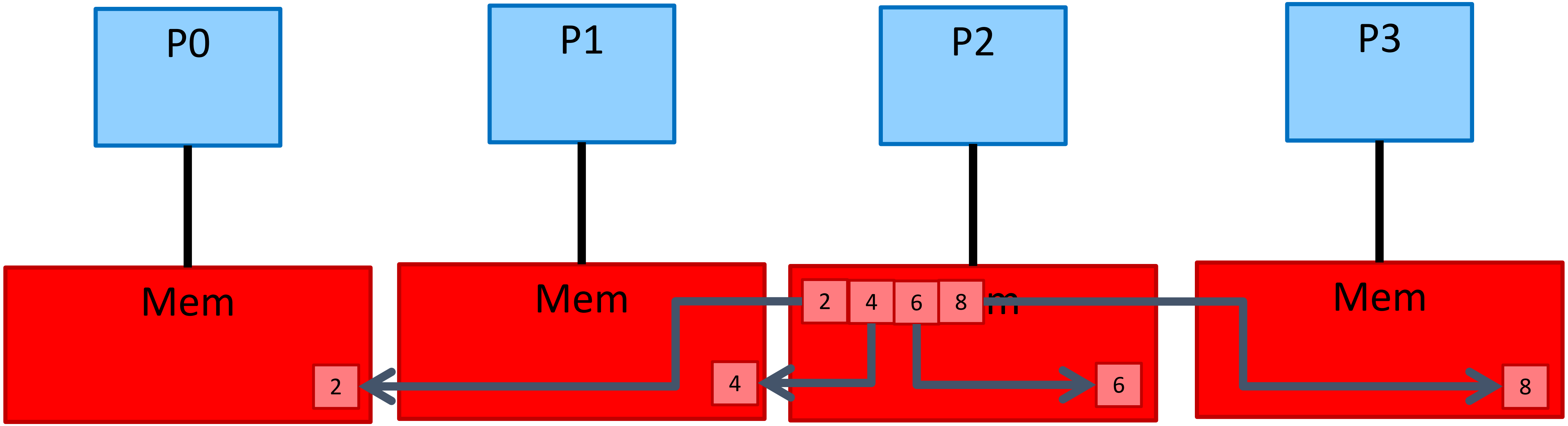
```
from mpi4py import MPI

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.

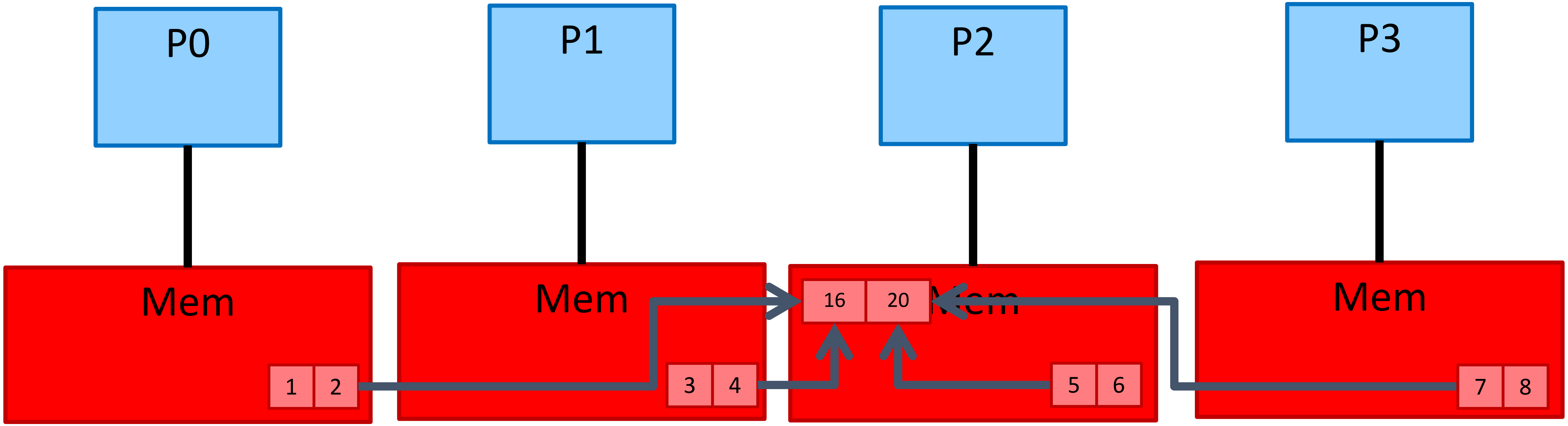
In C	In Fortran

float *sendbuf=NULL;
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();
	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

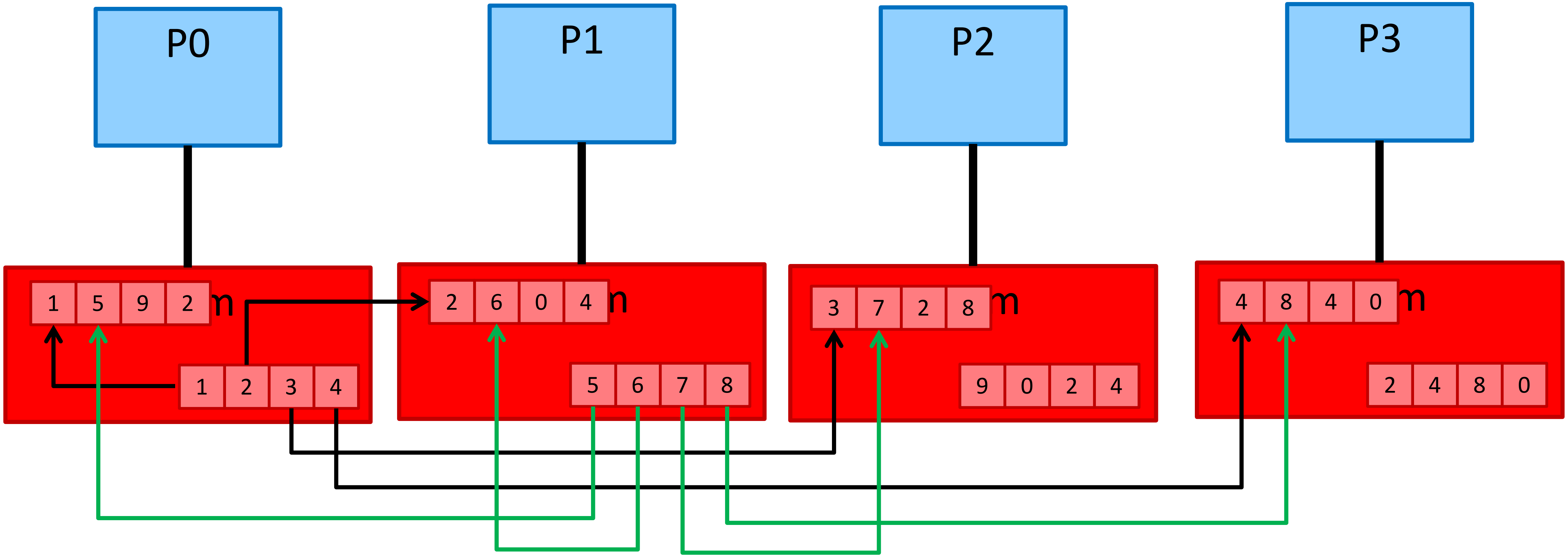
Example:

```
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 **not** 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 **<u>not</u>** 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

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

Exercise 3 (challenge)

Write a parallel code to compute the volume under the surface of the function f=sin(x+y) in the region $x^2 + y^2 = \pi^2$