Primena super-računara u astronomiji

Basic scalar optimization techniques

- Do less work
- Avoid expensive operations
- Shrink the working set
- Elimination of common subexpressions
- Avoiding branches

Basic scalar optimization techniques

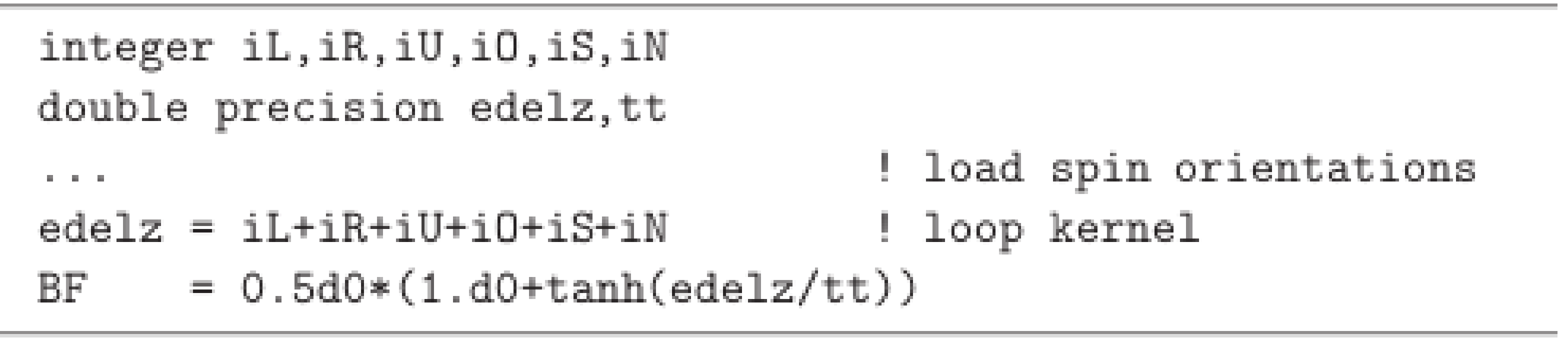
- **Do less work!**

```
~~logical FLAG~~
~~FLAG = .false.~~
~~do i=1,N~~
~~        If (complex_func(A(i)) < THRESHOLD) then~~
~~                FLAG = .true.~~
~~        endif~~
~~enddo~~
```

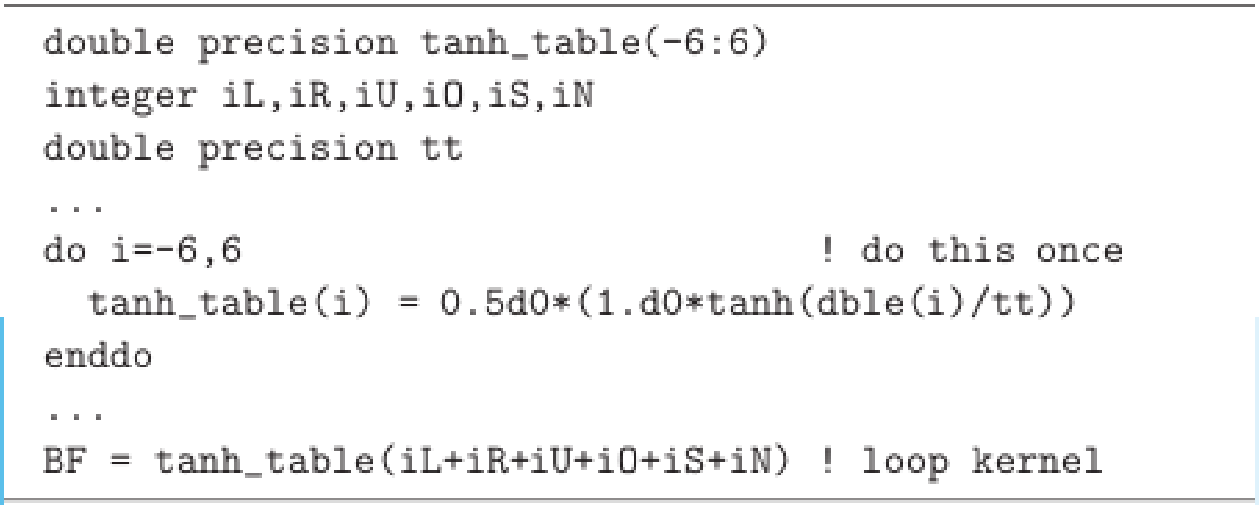
```
logical FLAG
FLAG = .false.
do i=1,N
        If (complex_func(A(i)) < THRESHOLD) then
                FLAG = .true.
                exit
        endif
enddo
```

Basic scalar optimization techniques

- **Avoid expensive operations!**
  - Examples for “strong” operations are **trigonometric** and **exponential** functions
  - Use x*x instead of x^2



```
integer iL,iR,iU,iO,iS,iN
double precision edelz,tt
...                                 ! load spin orientations
edelz = iL+iR+iU+iO+iS+iN           ! loop kernel
BF    = 0.5d0*(1.d0+tanh(edelz/tt))
```



```
double precision tanh_table(-6:6)
integer iL,iR,iU,iO,iS,iN
double precision tt
...
do i=-6,6                             ! do this once
  tanh_table(i) = 0.5d0*(1.d0*tanh(dble(i)/tt))
enddo
...
BF = tanh_table(iL+iR+iU+iO+iS+iN) ! loop kernel
```

Basic scalar optimization techniques

- **Shrink the working set!**
  - The **working set** of a code is the amount of memory it uses in the course of a calculation
  - Shrinking the working set by whatever means is a good thing because it raises the probability for cache hits
  - If and how this can be achieved and whether it pays off performancewise depends heavily on the algorithm and its implementation
  - **Example**: the previous code used standard four-byte integers to store the spin orientations. The working set was thus much larger than the **L2** cache of most processor. By changing the array definitions to use **integer*1** for the spin variables, the working set could be reduced by nearly a factor of four, and became comparable to cache size

Basic scalar optimization techniques

- **Elimination of common subexpressions!**
  - Common subexpression elimination is an optimization that is often considered a task for compilers
  - Basically one tries to save time by pre-calculating parts of complex expressions and assigning them to temporary variables before a loop starts

```
! inefficient
do i=1,N
  A(i)=A(i)+s+r*sin(x)
enddo
```

$\longrightarrow$

```
tmp=s+r*sin(x)
do i=1,N
  A(i)=A(i)+tmp
enddo
```

Basic scalar optimization techniques

- **Avoiding branches!**
  - If for some reason compiler optimization fails or is inefficient, performance will suffer.
  - This can easily happen if the loop body contains conditional branches

```
do j=1,N
        do i=1,N
                if(i.ge.j) then
                        sign=1.d0
                else if(i.lt.j) then
                        sign=-1.d0
                else
                        sign=0.d0
                endif
                C(j) = C(j) + sign * A(i,j) * B(i)
        enddo
enddo
```

Basic scalar optimization techniques

- **Avoiding branches!**
  - By using two different variants of the inner loop, the conditional has effectively been moved outside

```
do j=1,N
        do i=j+1,N
                C(j) = C(j) + A(i,j) * B(i)
        enddo
enddo
do j=1,N
        do i=1,j-1
                C(j) = C(j) - A(i,j) * B(i)
        enddo
enddo
```

PYTHON

MPI paralelization in Python

- In MPI, the processes involved in the execution of a parallel program are identified by a sequence of non-negative integers called **ranks**
- If we have a number **p** of processes that runs a program, the processes will then have a rank that goes from 0 to p-1
- The function MPI that comes to us to solve this problem has the following function calls:

```
rank = comm.Get_rank()
```

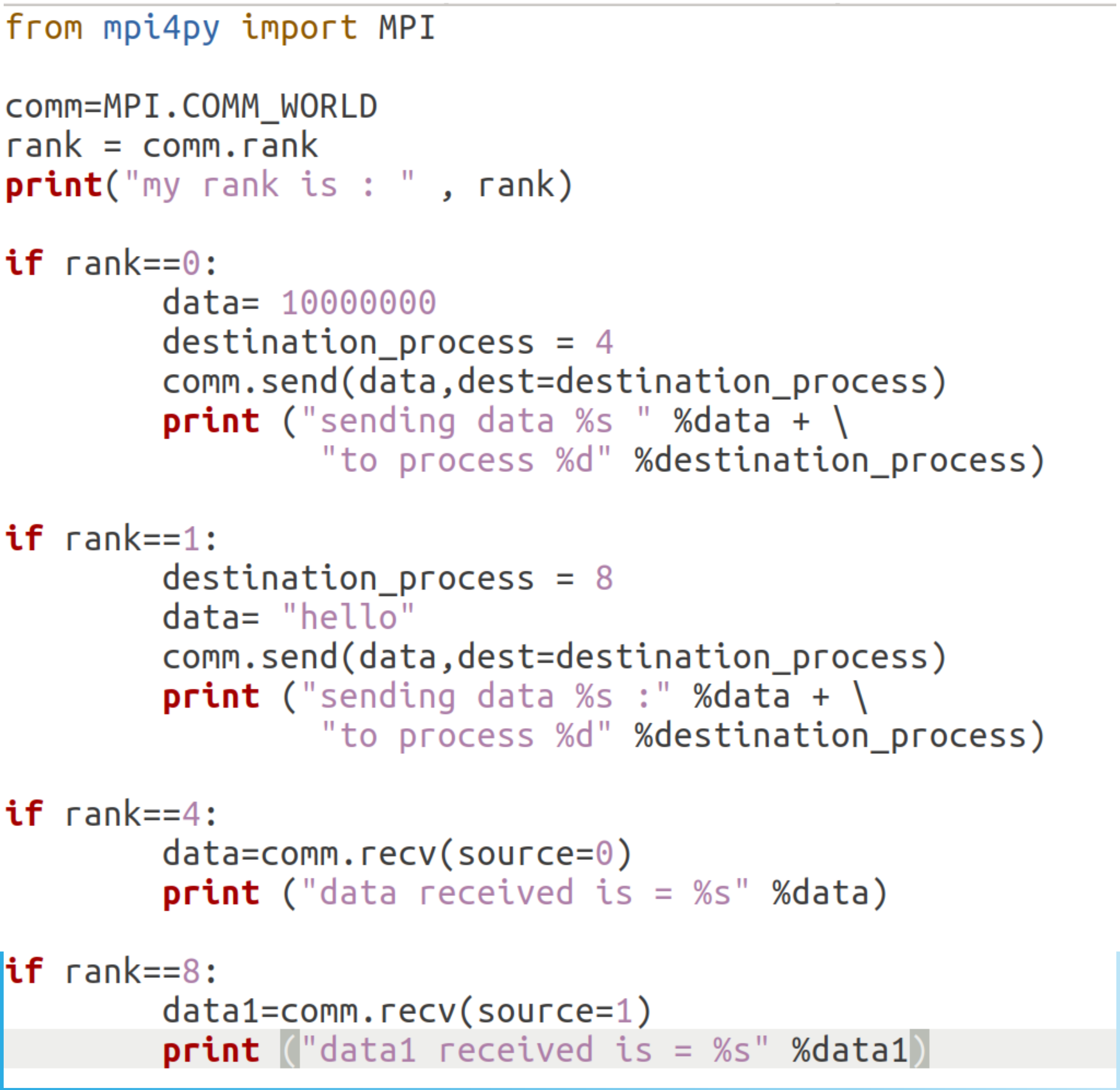
- The comm argument is called a communicator, as it defines its own set of all processes that can communicate together, namely:

```
comm = MPI.COMM_WORLD
```

Point-to-point communication

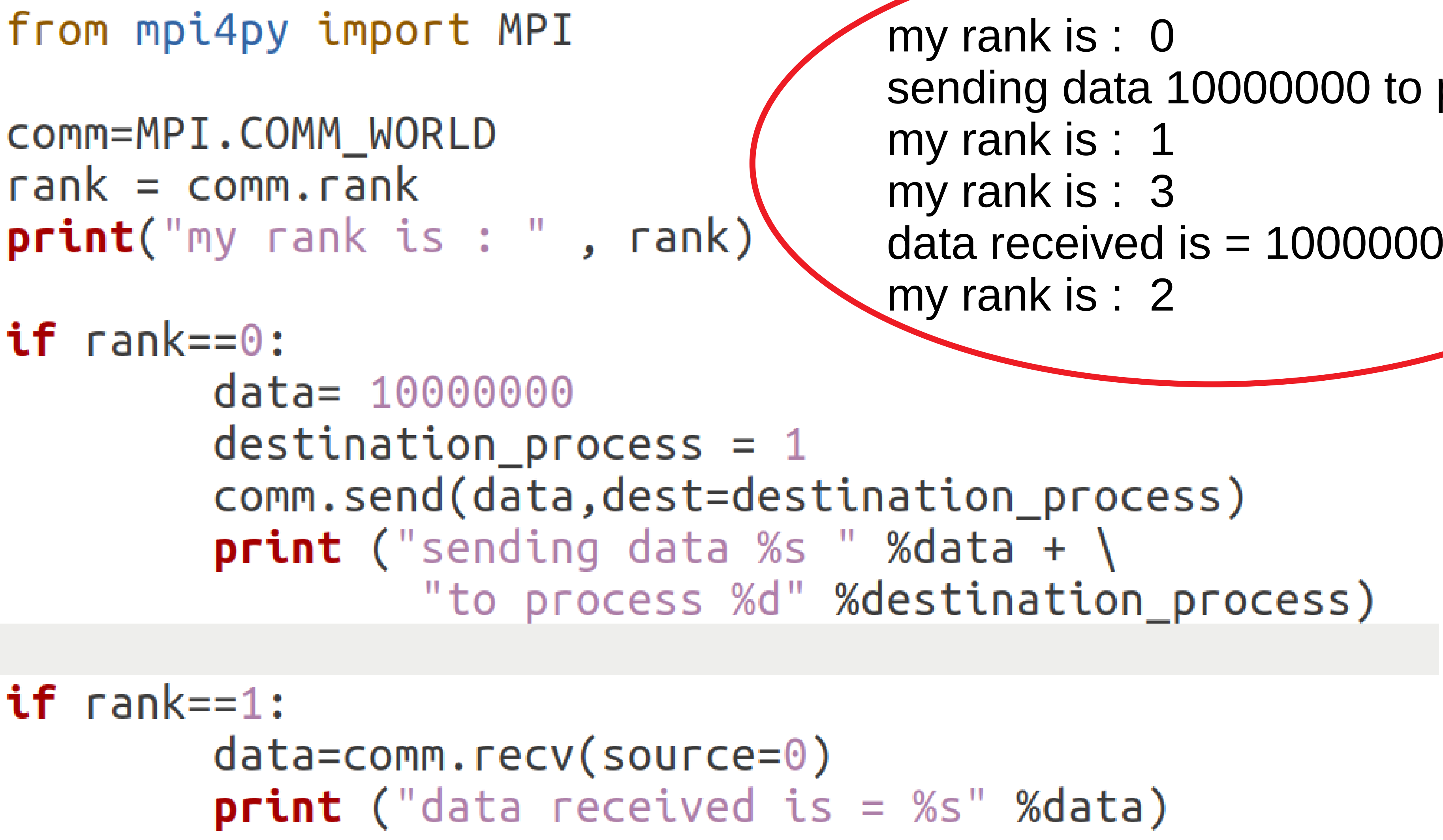
- The point-to-point communication is a mechanism that enables data transmission between two processes: a process receiver, and process sender
- The Python module **mpi4py** enables point-to-point communication via two functions:
    - Comm.Send(data, process_destination)
    - Comm.Recv(process_source)

Point-to-point communication



```
from mpi4py import MPI

comm=MPI.COMM_WORLD
rank = comm.rank
print("my rank is : " , rank)

if rank==0:
        data= 10000000
        destination_process = 4
        comm.send(data,dest=destination_process)
        print ("sending data %s " %data + \
                "to process %d" %destination_process)

if rank==1:
        destination_process = 8
        data= "hello"
        comm.send(data,dest=destination_process)
        print ("sending data %s :" %data + \
                "to process %d" %destination_process)

if rank==4:
        data=comm.recv(source=0)
        print ("data received is = %s" %data)

if rank==8:
        data1=comm.recv(source=1)
        print ("data1 received is = %s" %data1)
```

Point-to-point communication



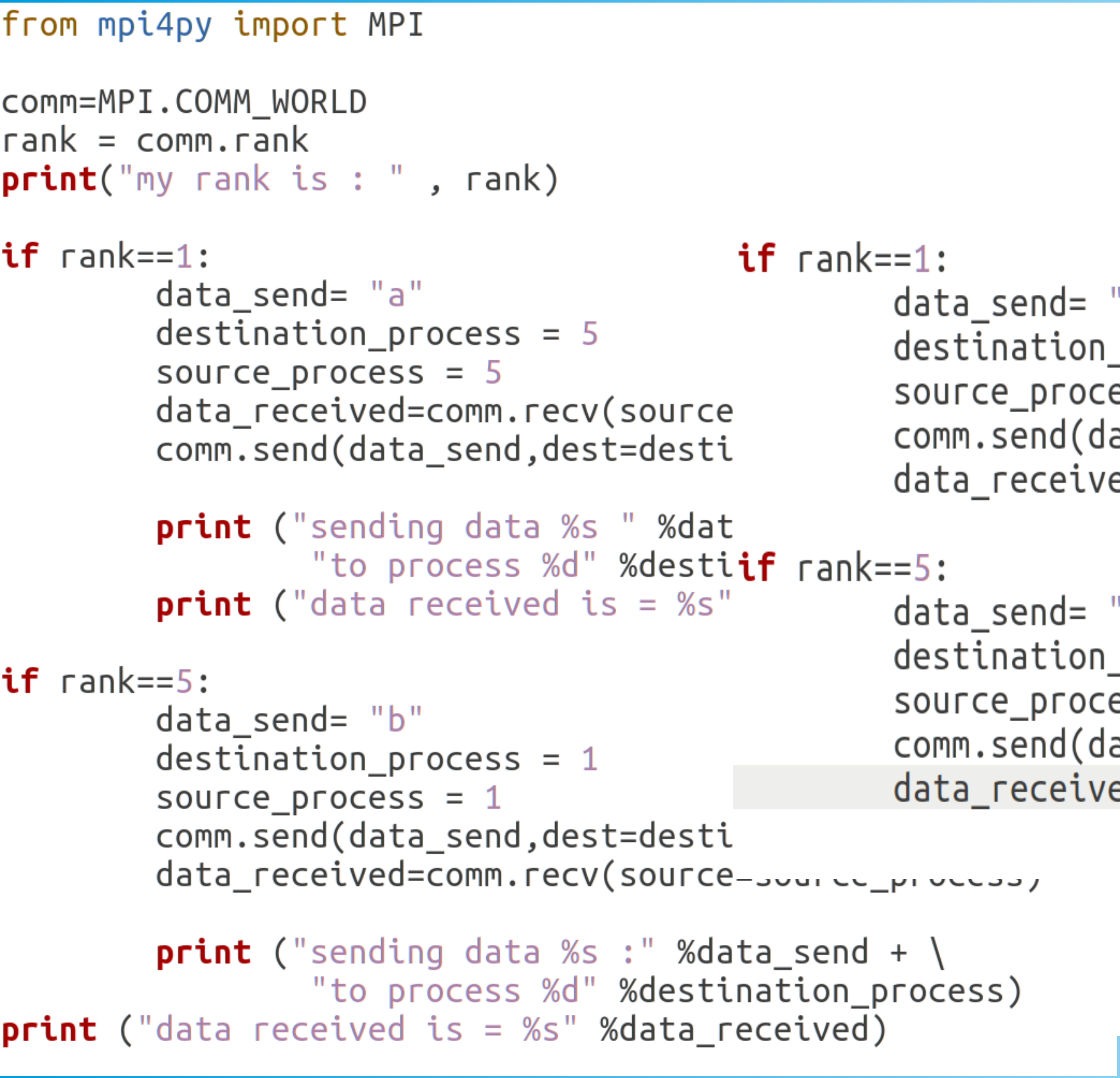
```python
from mpi4py import MPI

comm=MPI.COMM_WORLD
rank = comm.rank
print("my rank is : " , rank)

if rank==0:
        data= 10000000
        destination_process = 1
        comm.send(data,dest=destination_process)
        print ("sending data %s " %data + \
                "to process %d" %destination_process)

if rank==1:
        data=comm.recv(source=0)
        print ("data received is = %s" %data)
```

```
my rank is :  0
sending data 10000000 to process 1
my rank is :  1
my rank is :  3
data received is = 10000000
my rank is :  2
```

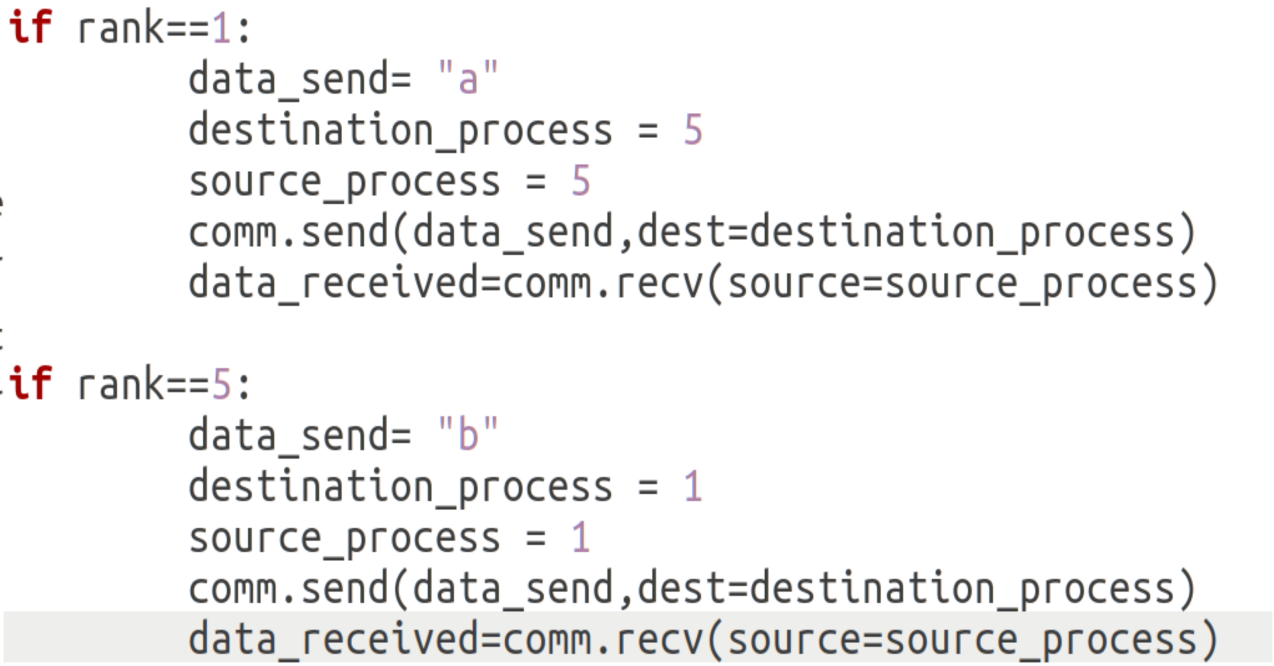
Avoiding deadlock problems

- The deadlock is a situation where two (or more) processes block each other and wait for the other to perform a certain action that serves to another, and vice versa
- The **mpi4py** module doesn't provide any specific functionality to resolve this but only some measures, which the developer must follow to avoid problems of deadlock

Avoiding deadlock problems



```
from mpi4py import MPI

comm=MPI.COMM_WORLD
rank = comm.rank
print("my rank is : " , rank)

if rank==1:
        data_send= "a"
        destination_process = 5
        source_process = 5
        data_received=comm.recv(source
        comm.send(data_send,dest=desti

        print ("sending data %s " %dat
                "to process %d" %desti
        print ("data received is = %s"

if rank==5:
        data_send= "b"
        destination_process = 1
        source_process = 1
        comm.send(data_send,dest=desti
        data_received=comm.recv(source=source_process)

        print ("sending data %s :" %data_send + \
                "to process %d" %destination_process)
print ("data received is = %s" %data_received)
```



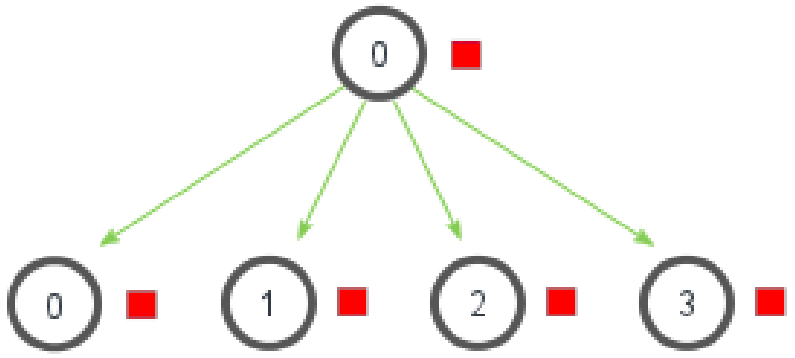
```
if rank==1:
        data_send= "a"
        destination_process = 5
        source_process = 5
        comm.send(data_send,dest=destination_process)
        data_received=comm.recv(source=source_process)

if rank==5:
        data_send= "b"
        destination_process = 1
        source_process = 1
        comm.send(data_send,dest=destination_process)
        data_received=comm.recv(source=source_process)
```

Collective communication using broadcast

- A communication method that involves all the processes belonging to a communicator is called a **collective communication**
- A collective communication generally involves more than two processes.
- Here we will call the collective communication broadcast, wherein a single process sends the same data to any other process.
- The **mpi4py** functionalities in the broadcast are offered by the following method:

```
buf = comm.bcast(data_to_share, rank_of_root_process)
```

- This function simply sends the information contained in the message process root to every other process that belongs to the comm communicator; each process must, however, call it by the same values of root and comm



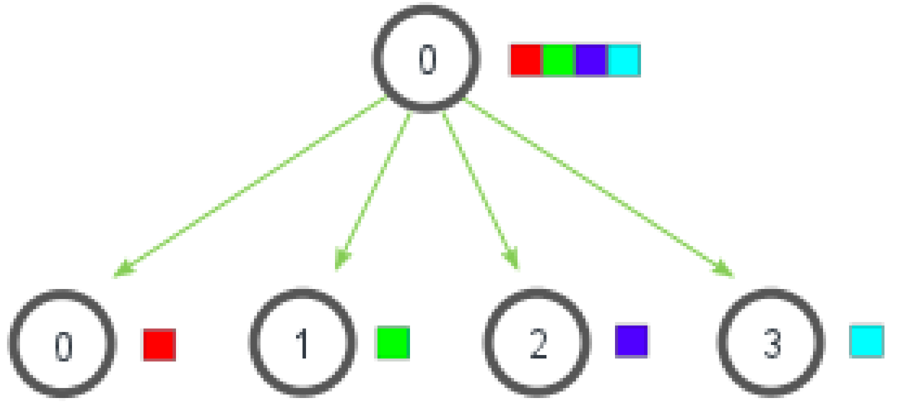
Collective communication using broadcast

```
process = 0 variable shared = 100
process = 1 variable shared = 100
process = 3 variable shared = 100
process = 2 variable shared = 100
```

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
        variable_to_share = 100

else:
        variable_to_share = None

variable_to_share = comm.bcast(variable_to_share, root=0)
print("process = %d" %rank + " variable shared = %d " \
                        %variable_to_share)
```

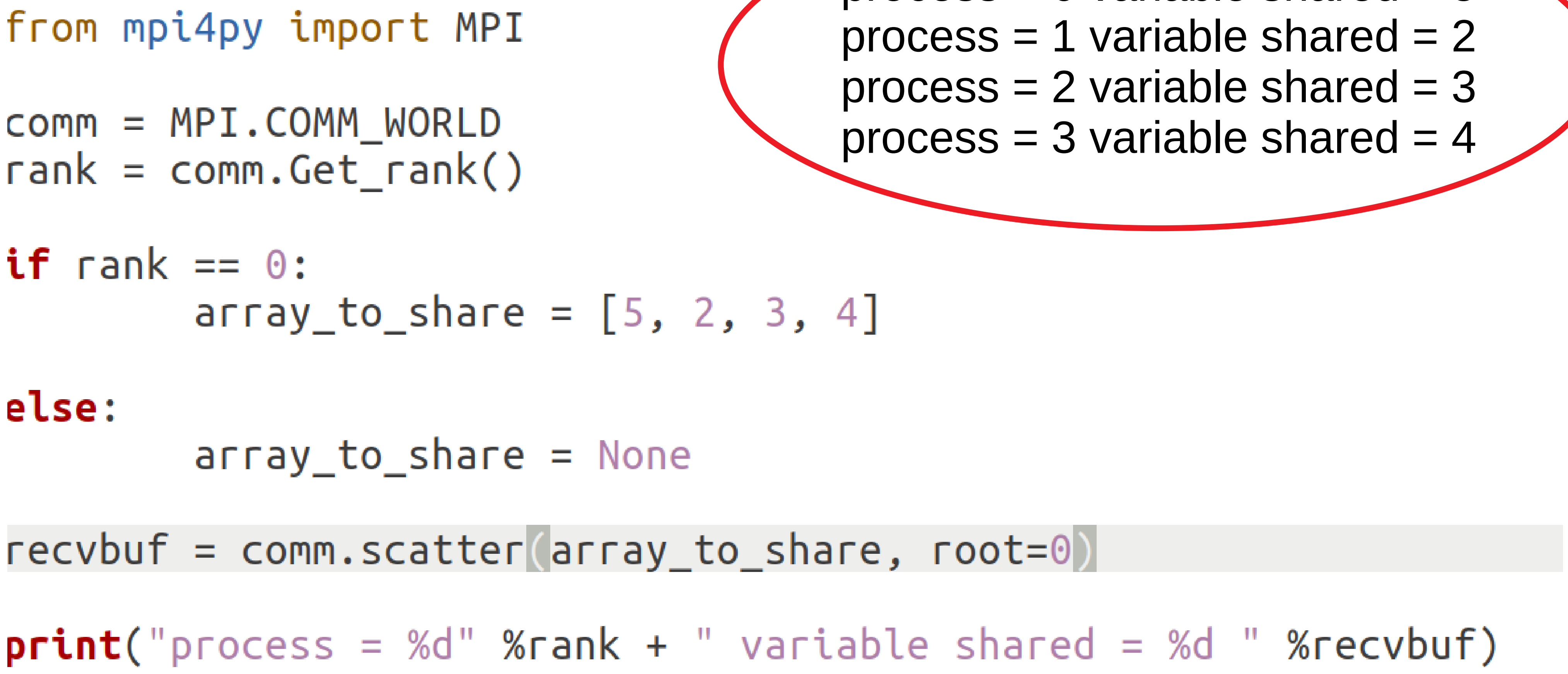
Collective communication using scatter

- The scatter functionality is very similar to a broadcast
- There is one major difference: while comm.bcast sends the same data to all listening processes, comm.scatter can send the chunks of data in an array to different processes
- The comm.scatter function takes the elements of the array and distributes them to the processes according to their rank, for which the first element will be sent to the process zero, the second element to the process 1, and so on
- The function implemented in **mpi4py** is as follows:
  - recvbuf = comm.scatter(sendbuf, rank_of_root_process)



Collective communication using scatter

```
process = 0 variable shared = 5
process = 1 variable shared = 2
process = 2 variable shared = 3
process = 3 variable shared = 4
```

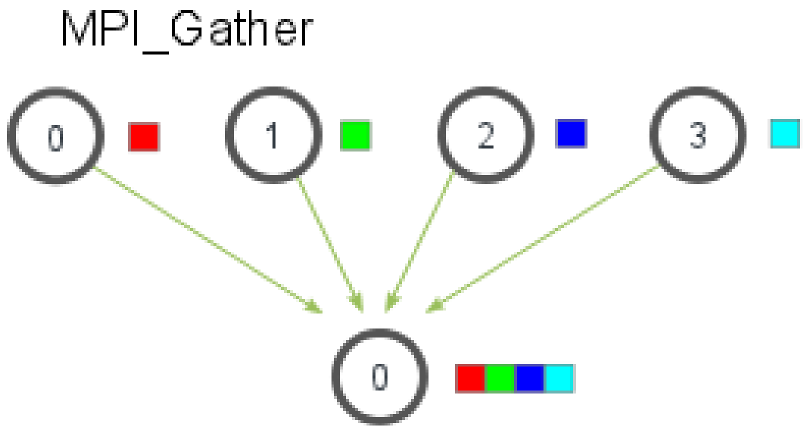


```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
        array_to_share = [5, 2, 3, 4]

else:
        array_to_share = None

recvbuf = comm.scatter(array_to_share, root=0)

print("process = %d" %rank + " variable shared = %d " %recvbuf)
```

- **One of the restrictions to comm.scatter is that you can scatter as many elements as the processors you have available or specify in the execution statement !**

Collective communication using gather

- The gather function performs the inverse of the scatter functionality. In this case, all processes send data to a root process that collects the data received.
- The gather function implemented in **mpi4py** is, as follows:
  - recvbuf = comm.gather(sendbuf, rank_of_root_process)



Collective communication using gather

```
rank = 0 ...receiving data to other process
 process 0 receiving 4 from process 1
 process 0 receiving 9 from process 2
 process 0 receiving 16 from process 3
```

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
data = (rank+1)**2

data = comm.gather(data, root=0)
if rank == 0:
        print ("rank = %s " %rank +\
                "...receiving data to other process")

        for i in range(1,size):
                data[i] = (i+1)**2
                value = data[i]
                print(" process %s receiving %s from process %s"\
                        %(rank , value , i))
```

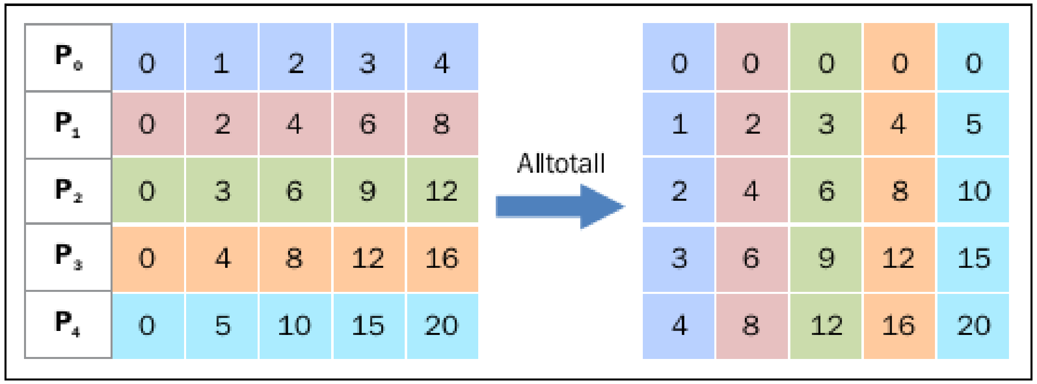
Collective communication using Alltoall

- The **Alltoall** collective communication combines the scatter and gather functionality.
- In **mpi4py**, there are three types of **Alltoall** collective communication:
  - comm.Alltoall (sendbuf, recvbuf): The all-to-all scatter/gather sends data from all-to-all processes in a group
  - comm.Alltoallv (sendbuf, recvbuf): The all-to-all scatter/gather vector sends data from all-to-all processes in a group, providing different amount of data and displacements
  - comm.Alltoallw (sendbuf, recvbuf): Generalized all-to-all communication allows different counts, displacements, and datatypes for each partner

Collective communication using Alltoall

```python
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()

a_size = 1
senddata = (rank+1)*numpy.arange(size,dtype=int)
recvdata = numpy.empty(size*a_size,dtype=int)
comm.Alltoall(senddata,recvdata)

print(" process %s sending %s receiving %s"\
        %(rank , senddata , recvdata))
```

```
process 0 sending [0 1 2 3] receiving [0 0 0 0]
process 2 sending [0 3 6 9] receiving [2 4 6 8]
process 3 sending [ 0  4  8 12] receiving [ 3  6  9 12]
process 1 sending [0 2 4 6] receiving [1 2 3 4]
```



P_0	0	1	2	3	4
P_1	0	2	4	6	8
P_2	0	3	6	9	12
P_3	0	4	8	12	16
P_4	0	5	10	15	20

0	0	0	0	0
1	2	3	4	5
2	4	6	8	10
3	6	9	12	15
4	8	12	16	20

The reduction operation

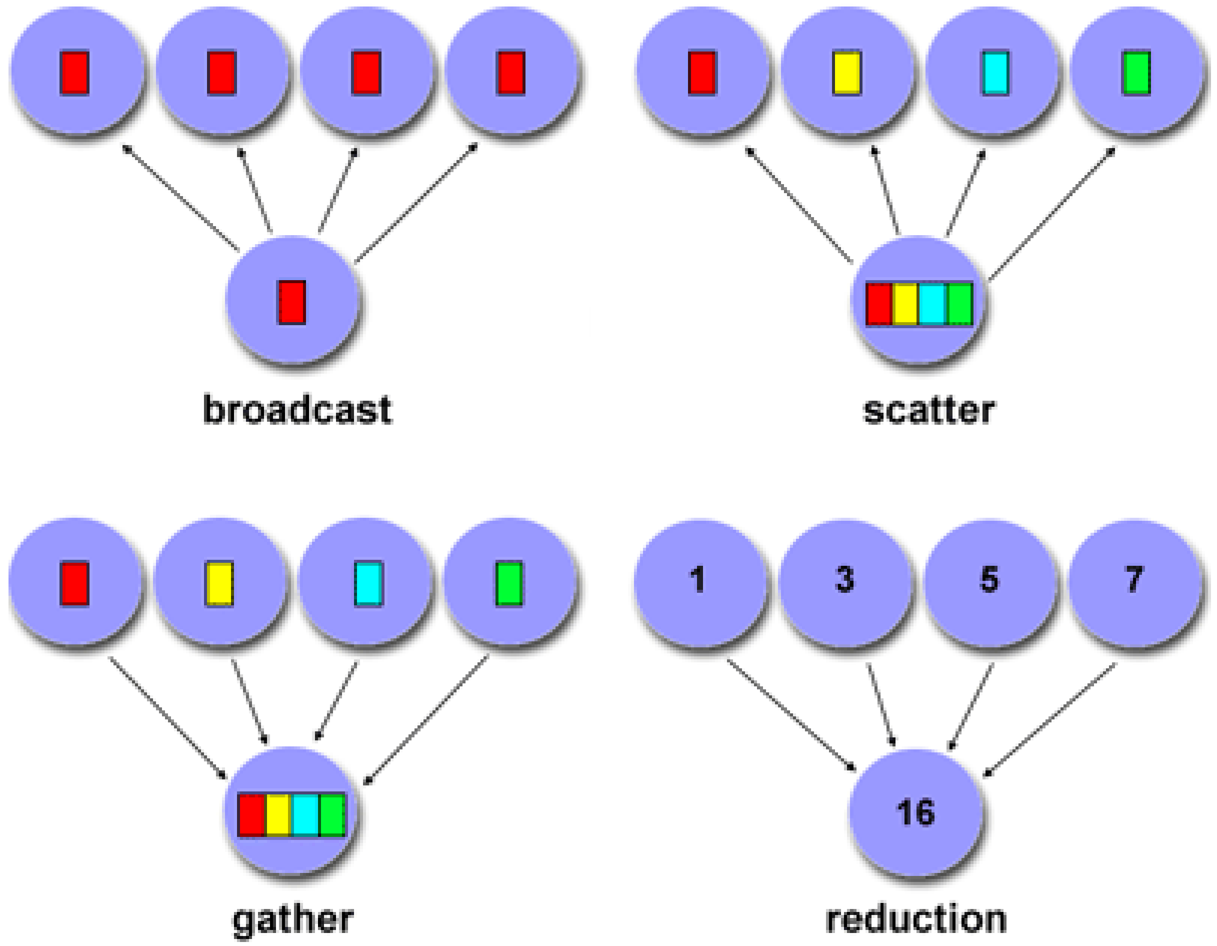
- Similar to comm.gather, comm.reduce takes an array of input elements in each process and returns an array of output elements to the root process
- However, the output elements contain the reduced result
- In **mpi4py**, the reduction operation is defined through the following statement:
  - comm.Reduce(sendbuf, recvbuf, rank_of_root_process, op = type_of_reduction_operation)
- Note that the difference with the comm.gather statement resides in the **op** parameter, which is the operation that you wish to apply to your data
- The **mpi4py** module contains a set of reduction operations that can be used
- Some of the reduction operations defined by MPI are:
  - MPI.MAX - This returns the maximum element
  - MPI.MIN - This returns the minimum element
  - MPI.SUM - This sums up the elements
  - MPI.PROD - This multiplies all elements

The reduction operation

```
process 0 sending [0 1 2]
 process 1 sending [0 2 4]
 process 3 sending [0 4 8]
 process 2 sending [0 3 6]
on task 2 after Reduce: data =  [0 0 0]
on task 0 after Reduce: data =  [ 0 10 20]
on task 1 after Reduce: data =  [0 0 0]
on task 3 after Reduce: data =  [0 0 0]
```

```python
import numpy
import numpy as np
from mpi4py import MPI

comm = MPI.COMM_WORLD

size = comm.size
rank = comm.rank

array_size = 3
recvdata = numpy.zeros(array_size,dtype=numpy.int)
senddata = (rank+1)*numpy.arange(array_size,dtype=numpy.int)
print(" process %s sending %s " %(rank , senddata))
comm.Reduce(senddata,recvdata,root=0,op=MPI.SUM)
print ('on task',rank,'after Reduce: data = ',recvdata)
```

Overview



broadcast
scatter
gather
1
3
5
7
16
reduction