MPI Basics with Python

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Outline

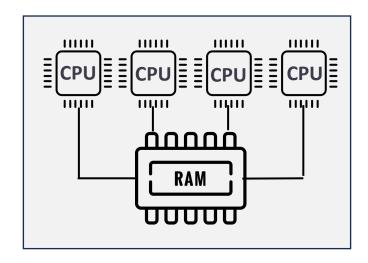
- Parallel Computing
- What is MPI
- Running programs in parallel
- Dividing work among workers
- Point to point communication
- Collective communication

Parallel Computing:

Parallel computing is when <u>multiple</u> <u>processors</u> or <u>computers</u> work together to solve a problem at the same time.

Main difference between these two cases is the underlying memory

Multiple processors:
Shared Memory

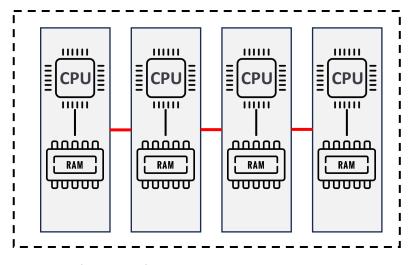


All access the same memory

Multi-Processing

OpenMP programming

Multiple computers: **Distributed Memory**



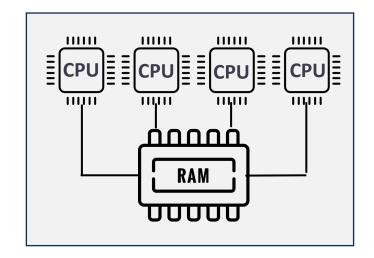
Each CPU has a separate memory
All CPUs communicate via network
MPI programming

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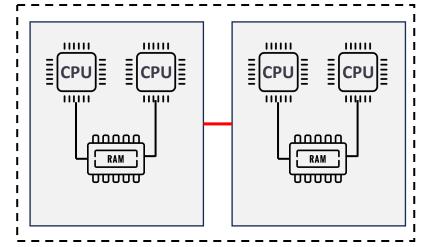


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Multi-Processing

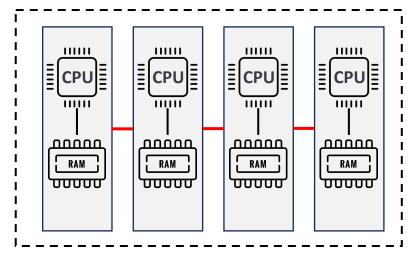
OpenMP programming

Hybrid



A combination of both MPI+OpenMP hybrid programming

Multiple computers: **Distributed Memory**



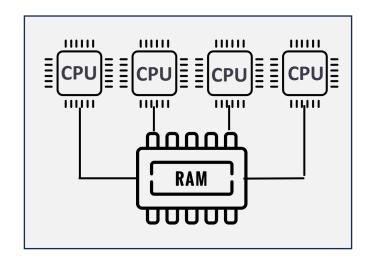
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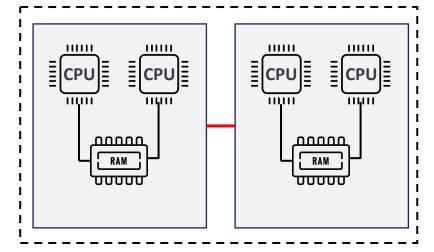


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Multi-Processing

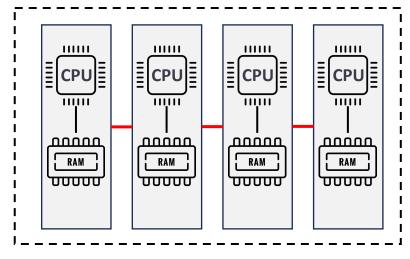
OpenMP programming

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Multiple computers: **Distributed Memory**



Each CPU has a separate memory All CPUs communicate via network MPI programming

This is our focus here!

What is MPI?

- Message Passing Interface
- Defines a standard for programs to communicate with each other
- Describes a set of functions and their expected behavior
- MPI_Send() is described but not implemented
- Implementation is left to others

3.2 Blocking Send and Receive Operations

3.2.1 Blocking Send

The syntax of the **blocking send** procedure is given below.

MPI_SEND(buf, count, datatype, dest, tag, comm)

| IN | buf | initial address of send buffer (choice) |
|----|----------|---|
| IN | count | number of elements in send buffer (non-negative integer) $$ |
| IN | datatype | datatype of each send buffer element (handle) |
| IN | dest | rank of destination (integer) |
| IN | tag | message tag (integer) |
| IN | comm | communicator (handle) |
| | | |

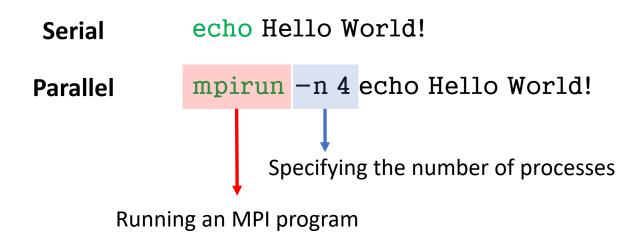
C binding

Official description for MPI_Send

What is MPI?

- There are many MPI implementations
- Each implementation must be compliant with MPI description
- On Discovery/Endeavour you will find
 - openmpi
 - mpich
 - intel-mpi
 - mvapich
- Each solves the same problems but in different ways

```
int MPI_Send(const void *buf, int count, MPI_Datatype type, int dest,
             int tag, MPI Comm comm)
   int rc = MPI_SUCCESS;
   SPC_RECORD(OMPI_SPC_SEND, 1);
   MEMCHECKER (
       memchecker_datatype(type);
       memchecker_call(&opal_memchecker_base_isdefined, buf, count, type);
       memchecker comm(comm);
   );
   if ( MPI_PARAM_CHECK ) {
       OMPI_ERR_INIT_FINALIZE(FUNC_NAME);
       if (ompi comm invalid(comm)) {
            return OMPI_ERRHANDLER_NOHANDLE_INVOKE(MPI_ERR_COMM, FUNC_NAME)
       } else if (count < 0) {</pre>
            rc = MPI ERR COUNT;
       } else if (tag < 0 || tag > mca pml.pml max tag) {
            rc = MPI ERR TAG;
       } else if (ompi comm peer_invalid(comm, dest) &&
                   (MPI_PROC_NULL != dest)) {
            rc = MPI_ERR_RANK;
       } else {
            OMPI_CHECK_DATATYPE_FOR_SEND(rc, type, count);
            OMPI CHECK USER BUFFER(rc, buf, type, count);
       OMPI ERRHANDLER CHECK(rc, comm, rc, FUNC NAME);
```



The name "mpirun" is not part of the standard, other names include:

SLURM: srun

Mpich2: mpiexec

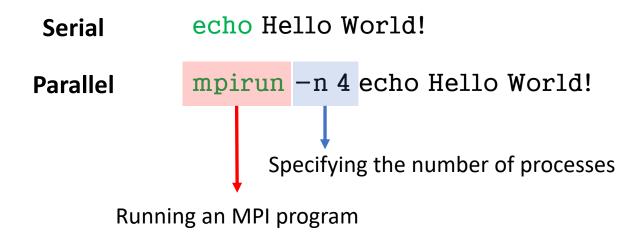
IBM SP: poe

Stampede2: ibrun

If you don't have enough CPUs to run this command on your machine, you may get:

There are not enough slots available in the system

Solution: mpirun -- oversubscribe -n 4 echo Hello World!

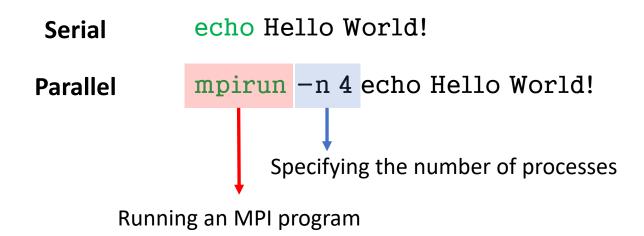


- MPI copies a program several times and run them individually
- How to tell a program, it is being executed by an MPI command and all pieces should work together?
 - In C and Fortran:

Start the program with function: MPI_INIT and clean up with: MPI_FINALIZE

• In Python:

Handled by the library: from mpi4py import MPI



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• In Python:

Handled by the library: from mpi4py import MPI

• np = MPI.COMM_WORLD.Get_size() Total number of processes

Rank of each process (between 0,np-1)

myrank = MPI.COMM_WORLD.Get_rank()

Hello World MPI

```
from mpi4py import MPI

comm = MPI.COMM_WORLD

rank = comm.Get_rank()

print(f"Hello from rank {rank}")
```

- Each process will:
 - Start up
 - Find out their "rank" number
 - Print rank to screen
- See examples/hello_world for code

Hello World MPI

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Getting Compute resources

- MPI programs must be run in Slurm jobs
- Each "rank" must be given a Slurm "task"
- Use reservation for this workshop:
- #SBATCH --reservation=bootcamp
- #SBATCH --account=hpcsuppt_613
- #SBATCH --partition=gpu
- We will be using mpi4py and numpy
- If not installed, use pip install mpi4py numpy

Run from interactive job

```
$ salloc --ntasks=4 --reservation=bootcamp
--account=hpcsuppt_613 --time=1:00:00 --partition=gpu
$ module load usc
$ module load python
$ srun python3 hello_world_mpi.py
Hello from rank 0!
Hello from rank 2!
Hello from rank 3!
Hello from rank 1!
```

Run from batch job

```
#!/bin/bash
#SBATCH --ntasks=4
#SBATCH --partiton=debug
#SBATCH --mem-per-cpu=2GB

module load usc
module load python
srun python3 hello_world_mpi.py
```

- Use interactive job to help build job script
- Everything we did in interactive job
- Output saved to slurm-xxxxx.out file

Serial Print from 0 to 9

Parallel Print from 0 to 9 with 3 processes, each process prints "its rank", and "its portion of the numbers"

Last process carries whatever is left

Initializing the MPI

Finding:

- Total *number* of processes
- *Rank* of each process

Split the work:

- *How many* numbers each process needs to write
- The range of numbers each process needs to write

0 1 2 3 4 5 6 7 8 9

Maximum number / total number of CPUs

$$np = 10 / 3 = 3.33$$

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Maximum number / total number of CPUs

$$np = 10 / 3 = 3.33$$

Each process takes np=3 numbers
Last process takes the rest 4

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Split the work:

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- The range of numbers each process needs to write

0 1 2 3 4 5 6 7 8 9

0 1 2 3 4 5 6 7 8 9

rank 0 rank 1 rank 2

Each process takes **np=3** numbers
Last process takes the rest 4

Serial Print from 0 to 9

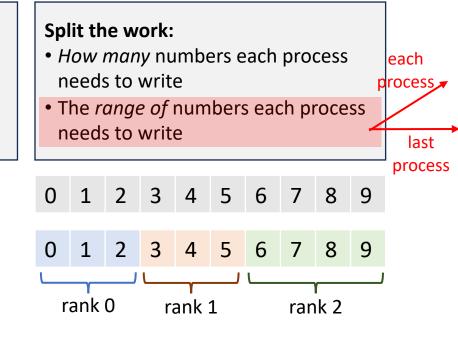
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Initializing the MPI

Finding:

- Total *number* of processes
- *Rank* of each process



Each process takes **np=3** numbers
Last process takes the rest 4

rank * np \leq range < r(ank+1) * np rank * np \leq range < max

Serial Print from 0 to 9

Parallel Print from 0 to 9 with 3 processes, each process prints "its rank", and "its portion of the numbers"

Last process carries whatever is left

from mpi4py import MPI

Initializing the MPI

Serial Print from 0 to 9

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Parallel Print from 0 to 9 with 3 processes, each process prints "its rank", and "its portion of the numbers"

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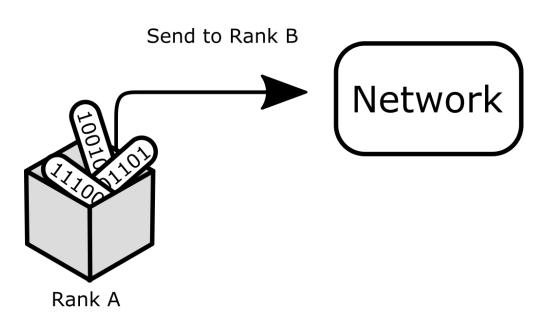
Initializing the MPI from mpi4py import MPI max=10Finding: • Total *number* of processes ntotal = MPI.COMM WORLD.Get size() • *Rank* of each process myrank = MPI.COMM WORLD.Get rank() Split the work: np = max//ntotal #gives the quotient • How many numbers each remainder=max % ntotal process needs to write if (myrank is ntotal-1): print ('myrank=', myrank, ' start=', myrank*np, ' end=', (myrank+1)*np+remail • The *range of* numbers each else:

print ('myrank=', myrank, ' start=', myrank*np, ' end=', (myrank+1)*np)

process needs to write

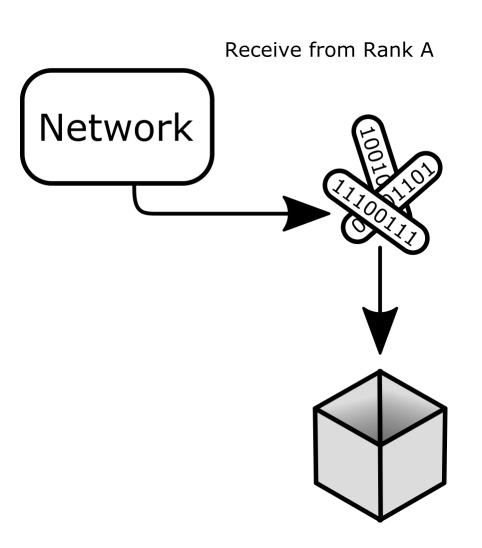
Point to Point Communication - Send

- Simplest way to send data
- comm.send(buf, dest, tag)
- Different parts
 - buf the thing you want to send
 - dest rank to send to
 - tag label for data
- Send will wait for successful receive before continuing



Point to Point Communication - Recv

- Simplest way to receive data
- comm.recv(buf, source=ANY_SOURCE, tag=ANY_TAG)
- Different parts
 - buf container for data
 - source rank data is expected from
 - tag label for data
- Recv will wait for data before continuing
- Recv will only accept data from dest with matching tag



Send/Recv example

```
from mpi4py import MPI
comm = MPI.COMM WORLD
rank=comm.Get rank()
print(f'Rank {rank} starting up ...')
good tag=7
data = None
if rank == 0:
    print(f'Rank {rank}: Sending data to rank 1 with tag {good tag}')
    comm.send(data, dest=1, tag=good tag)
if rank == 1:
    #data=None
    print(f'Rank {rank}: Waiting for data from rank 1 with tag {good tag}')
    data=comm.recv(source=0, tag=good tag)
    print(f'Rank {rank}: Got data: {data} from rank 0 with tag {good tag}')
print(f'Rank {rank} shutting down with data={data}.')
```

Send/Recv example - Initialize

```
from mpi4py import MPI
comm = MPI.COMM WORLD
rank=comm.Get rank()
print(f'Rank {rank} starting up ...')
good tag=7
data = None
if rank == 0:
   data=412
    print(f'Rank {rank}: Sending data to rank 1 with tag {good_tag}')
    comm.send(data, dest=1, tag=good tag)
if rank == 1:
    #data=None
    print(f'Rank {rank}: Waiting for data from rank 1 with tag {good tag}')
    data=comm.recv(source=0, tag=good tag)
    print(f'Rank {rank}: Got data: {data} from rank 0 with tag {good tag}')
print(f'Rank {rank} shutting down with data={data}.')
```

Send/Recv example - Rank 0

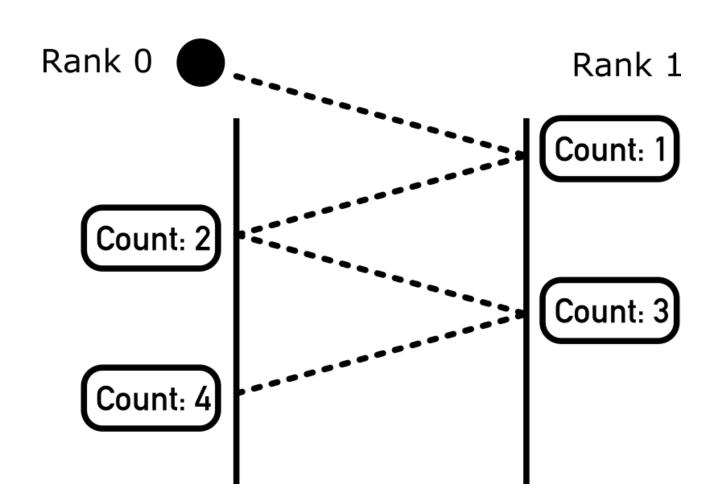
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rank=comm.Get rank()
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good tag=7
data = None
if rank == 0:
    data=412
    print(f'Rank {rank}: Sending data to rank 1 with tag {good tag}')
    comm.send(data, dest=1, tag=good tag)
if rank == 1:
    #data=None
    print(f'Rank {rank}: Waiting for data from rank 1 with tag {good tag}')
    data=comm.recv(source=0, tag=good tag)
    print(f'Rank {rank}: Got data: {data} from rank 0 with tag {good tag}')
print(f'Rank {rank} shutting down with data={data}.')
```

Send/Recv example - Rank 1

```
from mpi4py import MPI
comm = MPI.COMM WORLD
rank=comm.Get rank()
print(f'Rank {rank} starting up ...')
good tag=7
data = None
if rank == 0:
    data=412
    print(f'Rank {rank}: Sending data to rank 1 with tag {good_tag}')
    comm.send(data, dest=1, tag=good tag)
if rank == 1:
    #data=None
    print(f'Rank {rank}: Waiting for data from rank 1 with tag {good tag}')
    data=comm.recv(source=0, tag=good tag)
    print(f'Rank {rank}: Got data: {data} from rank 0 with tag {good tag}')
print(f'Rank {rank} shutting down with data={data}.')
```

MPI Ping Pong

- Classic MPI example
- Two ranks alternate sending a message
- Counter is incremented on receipt
- Stop after a N rounds



MPI Ping Pong - Code

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
world_size = MPI.COMM_WORLD.Get_size()
if world_size !=2:
    print("Only two can play")
    sys.exit(1)
print(f'Rank {rank} starting up...')
counter = 0
max\_counter = 10
if rank == 0:
    partner = 1
if rank == 1:
    partner = 0
while counter < max_counter:</pre>
    counter=comm.recv(source=partner)
    print(f'Rank {rank}: Got message {counter} from rank {partner}')
    counter = counter + 1
    print(f'Rank {rank}: sending message {counter} to rank {partner}')
    comm.send(counter,dest=partner)
```

MPI Ping Pong - Initialize

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
world_size = MPI.COMM_WORLD.Get_size()
if world_size !=2:
    print("Only two can play")
    sys.exit(1)
print(f'Rank {rank} starting up...')
if rank == 0:
    partner = 1
if rank == 1:
    partner = 0
```

MPI Ping Pong - Send/Receive loop

```
counter = 0
max_counter = 10

while counter < max_counter:
    counter=comm.recv(source=partner)
    print(f'Rank {rank}: Got message {counter} from rank {partner}')
    counter = counter + 1

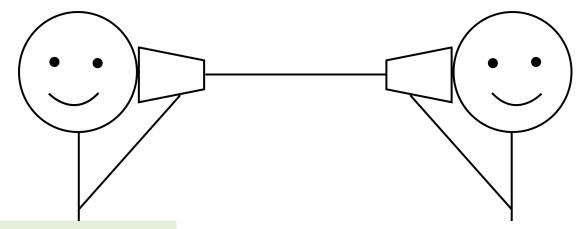
print(f'Rank {rank}: sending message {counter} to rank {partner}')
    comm.send(counter, dest=partner)</pre>
```

MPI Ping Pong

- Something is wrong with this example!
- Run the program on your own
- What could you change to make it work?

Deadlock

- Both ranks are "receiving"
- Can't proceed until done



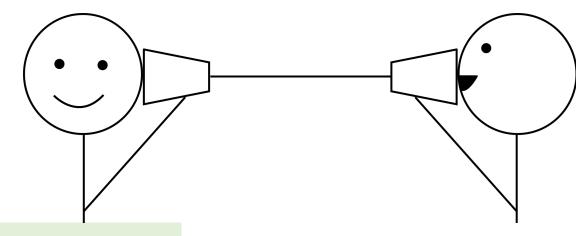
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    comm.send(counter, dest=partner)</pre>
```

Deadlock

Be careful with message coordination



```
counter = 0
max_counter = 10

if rank == 0:
    comm.send(counter,dest=partner)

while counter < max_counter:
    counter=comm.recv(source=partner)
    print(f'Rank {rank}: Got message {counter} from rank {partner}')

    print(f'Rank {rank}: sending message {counter} to rank {partner}')
    comm.send(counter,dest=partner)
    counter = counter + 1</pre>
```

| 0 | | | 0 | 0 | | |
|---|---|---|---|---|---|---|
| | | | | | | |
| | | | | | 0 | 0 |
| | 0 | | | | | |
| | 0 | | | | | |
| | | 0 | | | 0 | |
| | | | | | | |
| | | | 0 | | | |

Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

Initializing the MPI

Finding:

- Total *number* of processes
- Rank of each process

| 0 | | | 0 | 0 | | |
|---|---|---|---|---|---|---|
| | | | | | | |
| | | | | | 0 | 0 |
| | 0 | | | | | |
| | 0 | | | | | |
| | | 0 | | | 0 | |
| | | | | | | |
| | | | 0 | | | |

Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

Initializing the MPI

Finding:

- Total *number* of processes
- Rank of each process

Creating the matrix

Split the work:

- The *range of* elements each process needs to read
- Calculate

| 0 | | | 0 | 0 | | |
|---|---|---|---|---|---|---|
| | | | | | | |
| | | | | | 0 | 0 |
| | 0 | | | | | |
| | 0 | | | | | |
| | | 0 | | | 0 | |
| | | | | | | |
| | | | 0 | | | |

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| 0 | | | 0 | 0 | | |
|---|---|---|---|---|---|---|
| | | | | | | |
| | | | | | 0 | 0 |
| | 0 | | | | | |
| | 0 | | | | | |
| | | 0 | | | 0 | |
| | | | | | | |
| | | | 0 | | | |

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| 0 | | | 0 | | 0 | | |
|---|------|-----|---|----|-----|---|---|
| | rank | 0: | | ra | nk1 | | |
| | | | | | | 0 | 0 |
| | 0 | | | | | | |
| | 0 | | | | | | |
| ı | rank | 2:0 | | ra | nk3 | 0 | |
| | | | | | | | |
| | | | 0 | | | | |

Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

Initializing the MPI

Finding:

- Total *number* of processes
- *Rank* of each process

Creating the matrix

Split the work:

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- Calculate

Calculation

| 0 | | | 0 | | 0 | | |
|---|------|----|---|----|------|---|---|
| | rank | 0: | | ra | nk1 | | |
| | nz=3 | 3 | | r | 1z=3 | 0 | 0 |
| | 0 | | | | | | |
| | 0 | | | | | | |
| ı | rank | | | ra | nk3 | 0 | |
| | nz=3 | 3 | | r | 1z=1 | | |
| | | | 0 | | | | |

Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

Initializing the MPI

Finding:

- Total *number* of processes
- *Rank* of each process

Creating the matrix

Split the work:

- The *range of* elements each process needs to read
- Calculate

 o
 o

 rank0:
 rank1:

 nz=3
 nz=3

 o
 o

 rank2:0
 rank3:

 nz=3
 nz=1

Calculation

Sending the results to rank0

Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

Initializing the MPI

Finding:

- Total *number* of processes
- *Rank* of each process

Creating the matrix

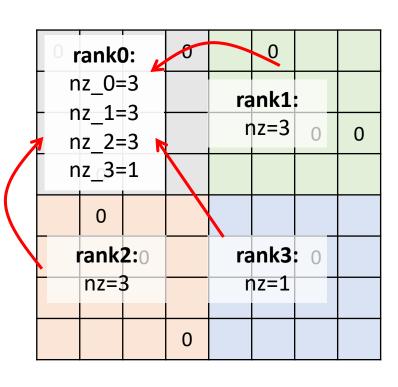
Split the work:

- The *range of* elements each process needs to read
- Calculate

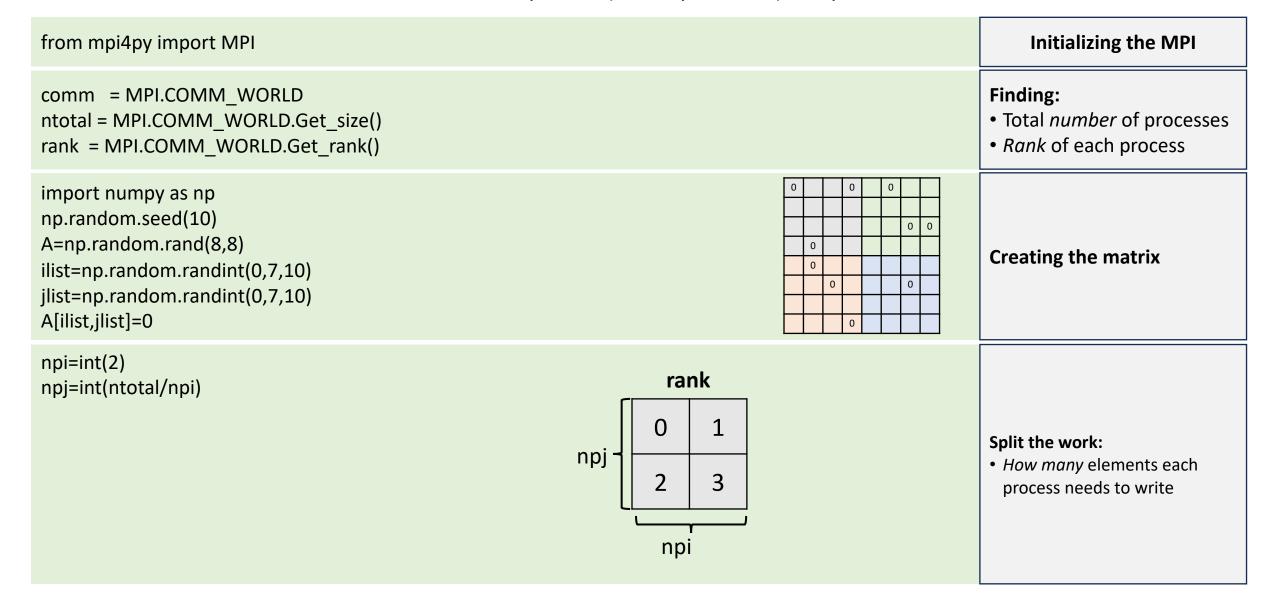
Calculation

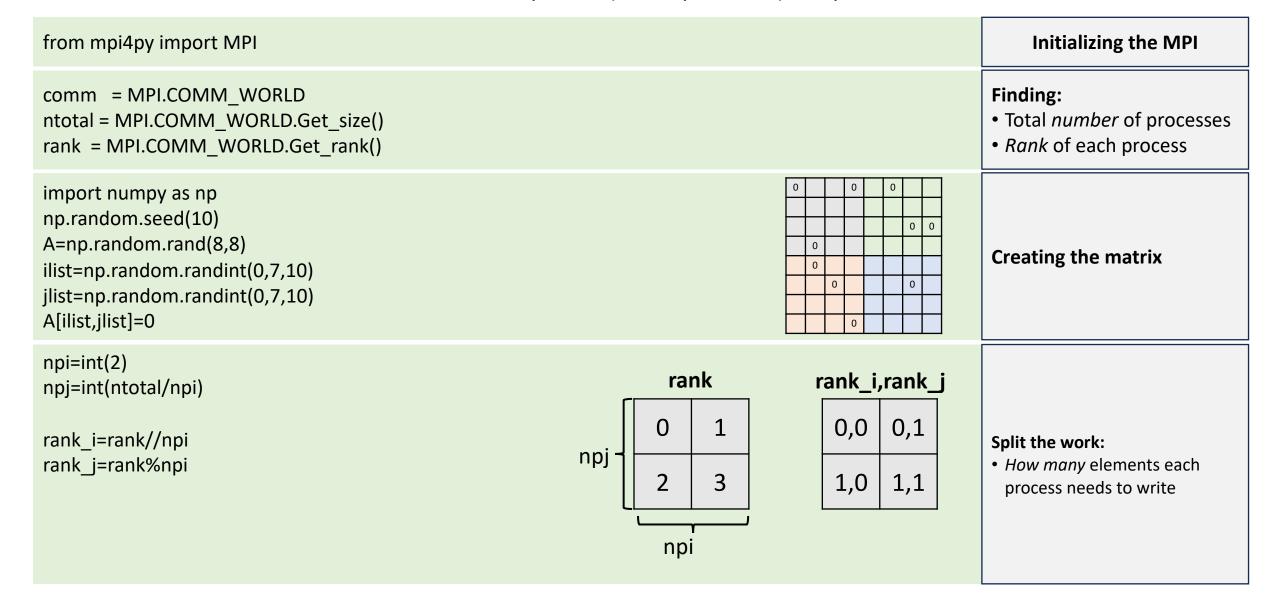
Sending the results to rank0

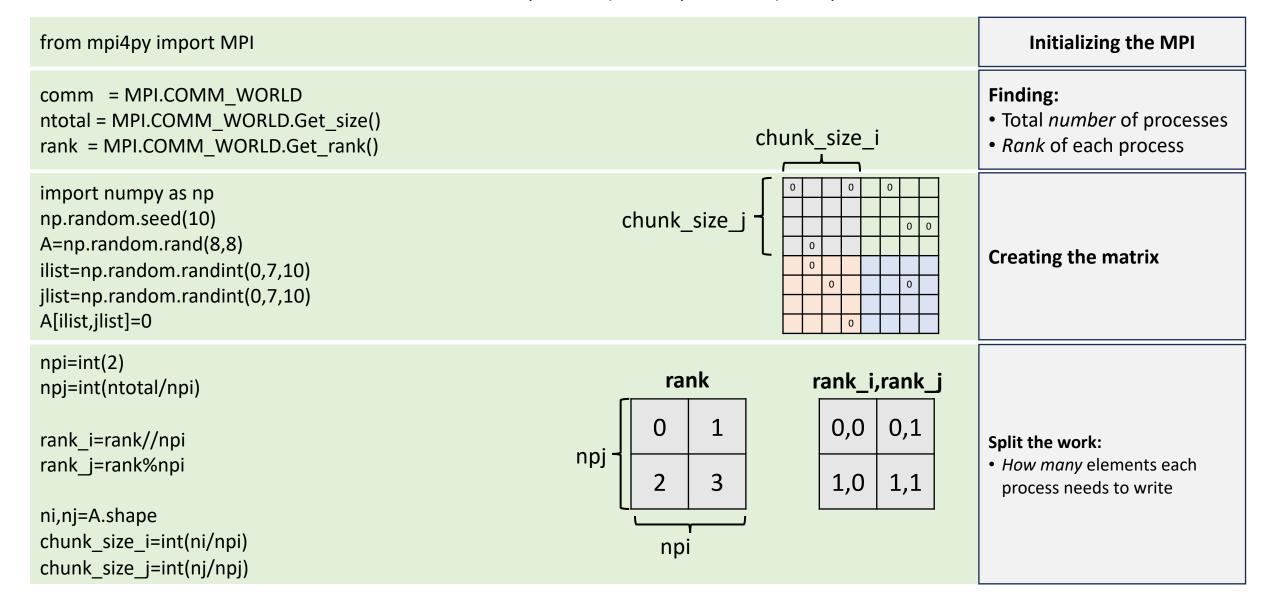
Receiving the results by rank0

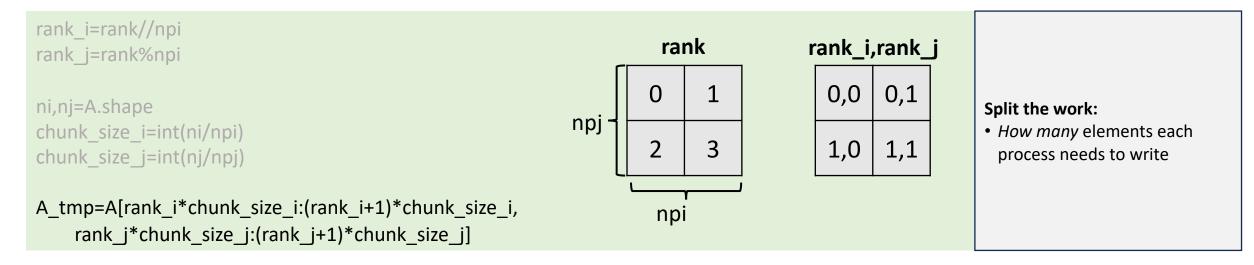


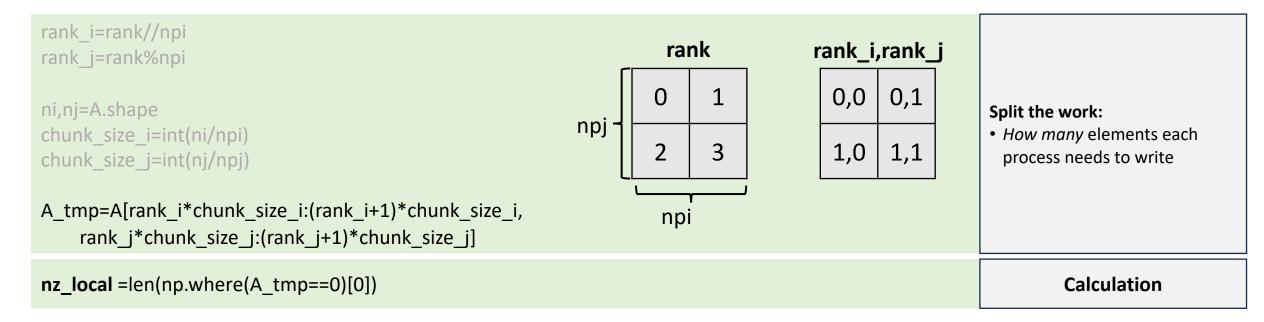
| Initializing the MPI | Finding: • Total number processes • Rank of each | | Creating the matrix | Split the work: The range of elements each process needs to read Calculate | nz | ank0 2_tota 3+3+ 10 | al= | 8 | 0 nk1: z=3 | 0 | 0 |
|-------------------------|--|--------------------------------------|------------------------|--|----|------------------------------|-----|---|------------------|---|---|
| Calculation | Sending the results to rank0 | Receiving the results by rank0 | Calculation in rank0 | Printing the results by rank0 | | 0 ranka nz=3 | | 0 | nk3: z=1 | 0 | |







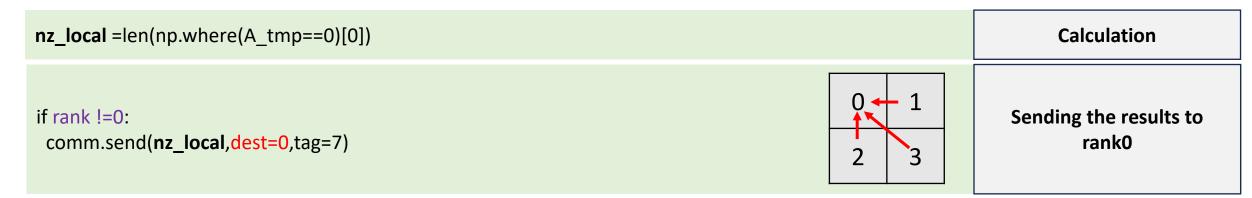


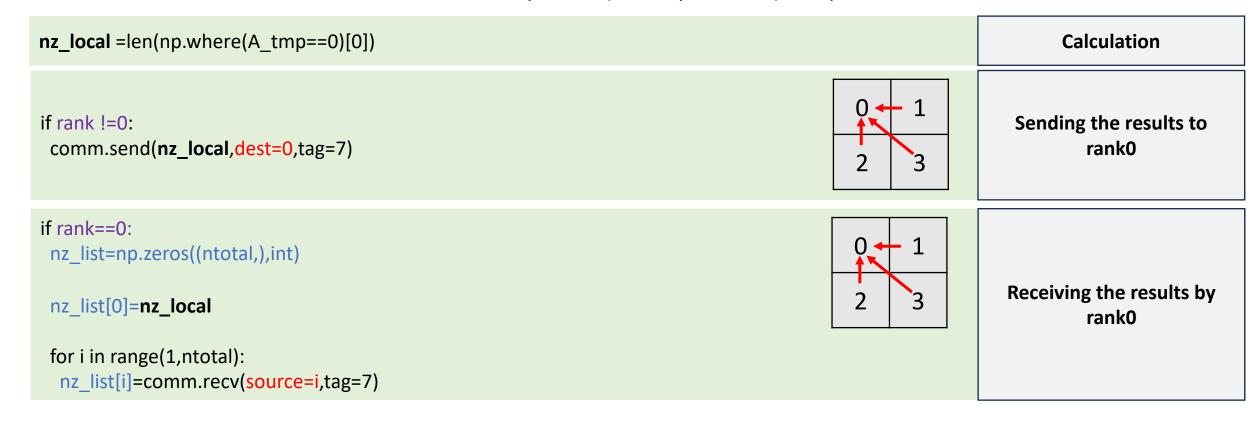


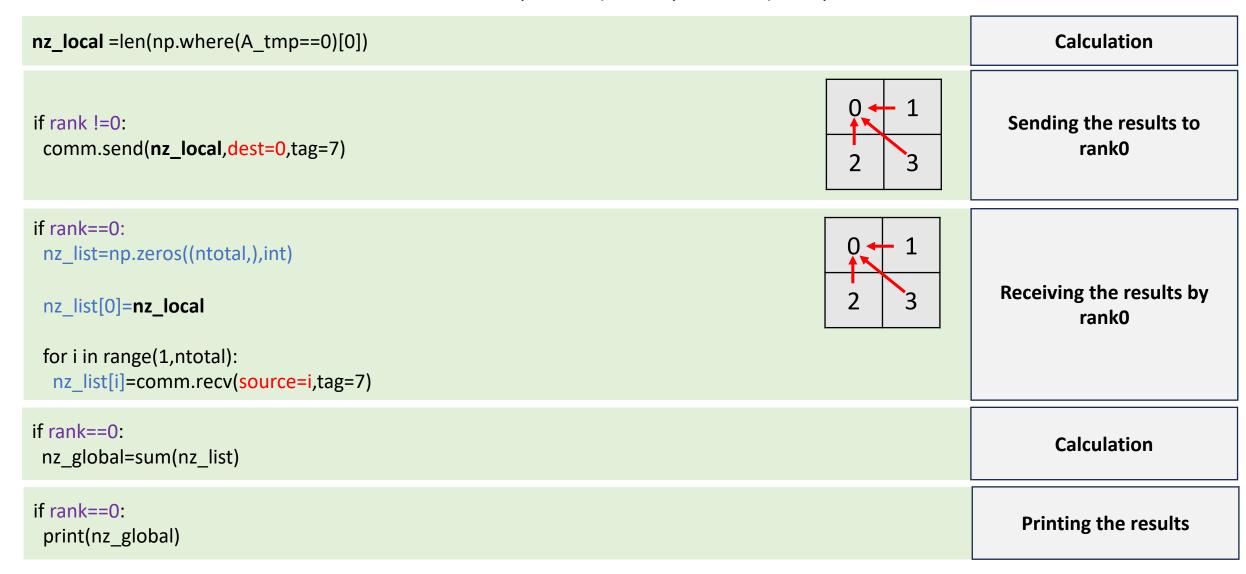
Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results

nz_local =len(np.where(A_tmp==0)[0])

Calculation

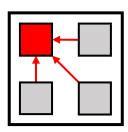


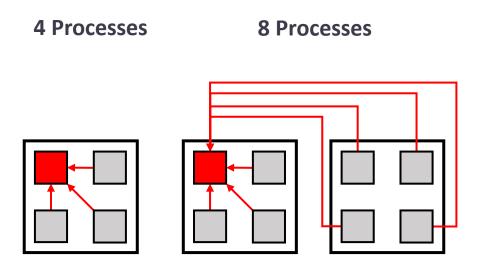


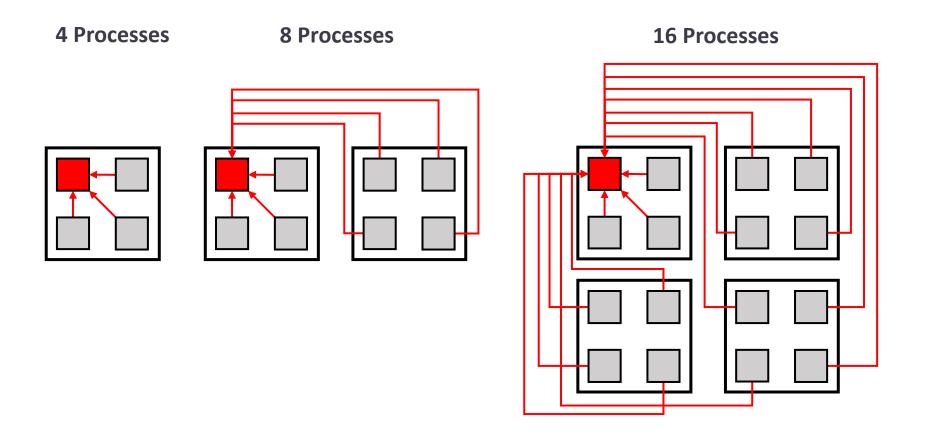


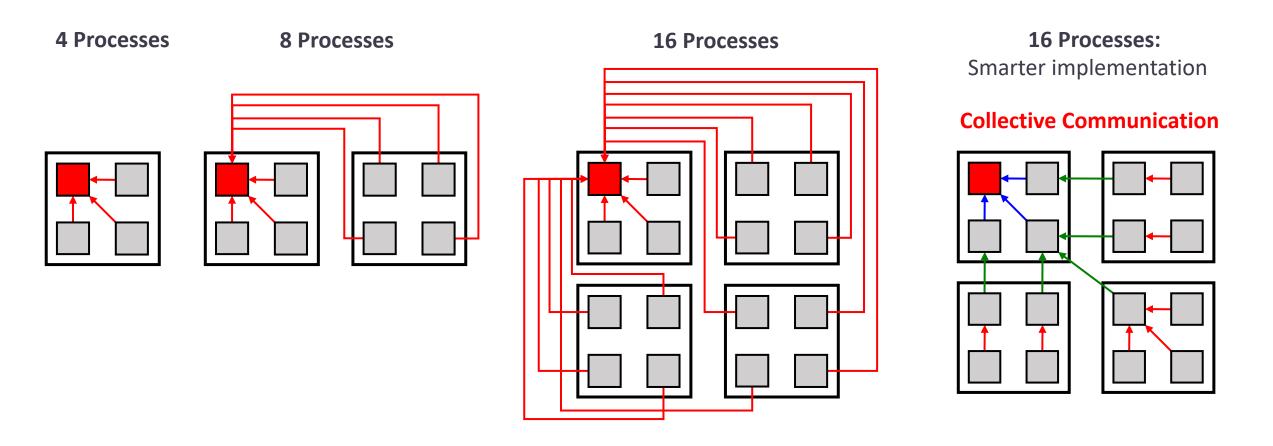
Count the number of zero elements of a matrix in parallel (with 4 processes) and print the results What if we had more processes?

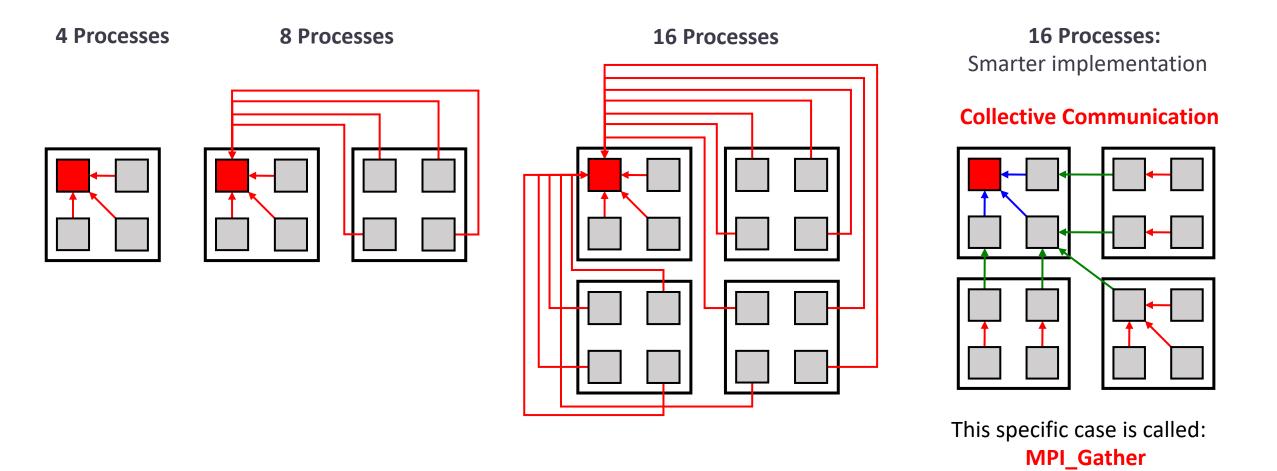
4 Processes

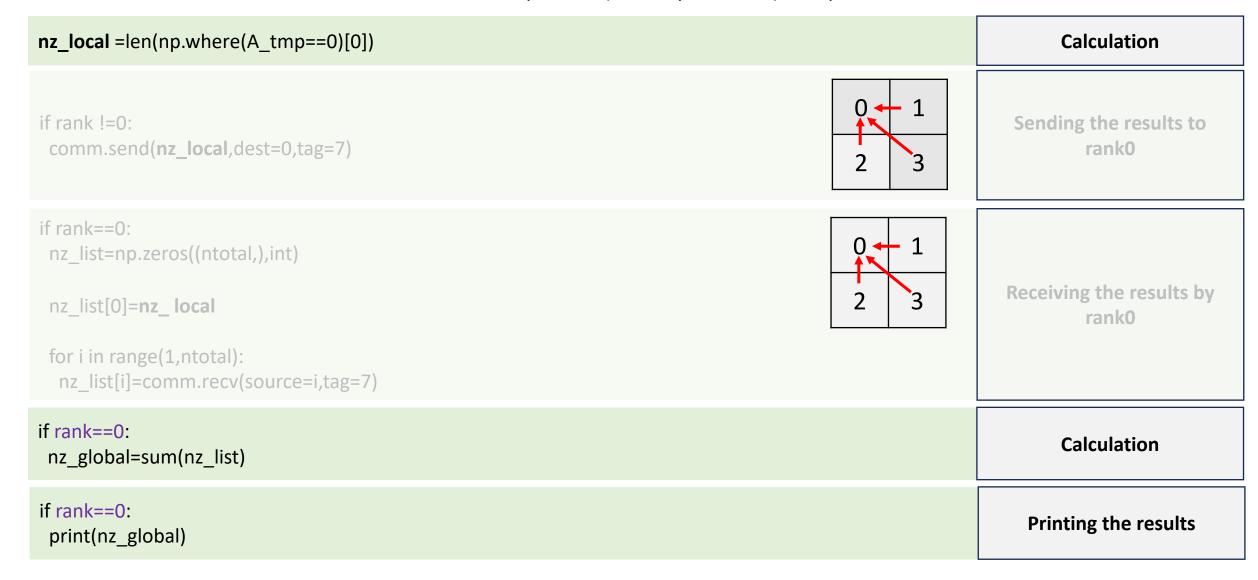






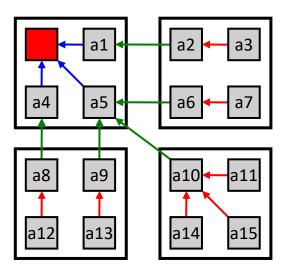




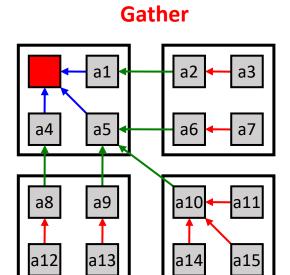


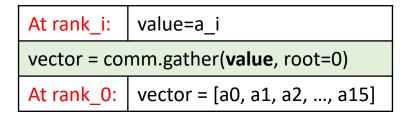
| nz_local =len(np.where(A_tmp==0)[0]) | Calculation |
|---|----------------------|
| nz_list = comm.gather(nz_local, root=0) | Gather nz_local |
| if rank==0: nz_global=sum(nz_list) | Calculation |
| if rank==0: print(nz_global) | Printing the results |

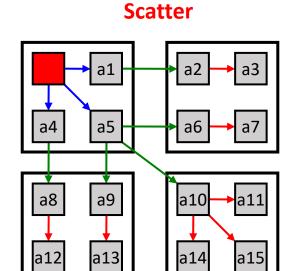
Gather



| At rank_i: | value=a_i | | | |
|-------------------------------------|-----------------------------|--|--|--|
| vector = comm.gather(value, root=0) | | | | |
| At rank_0: | vector = [a0, a1, a2,, a15] | | | |

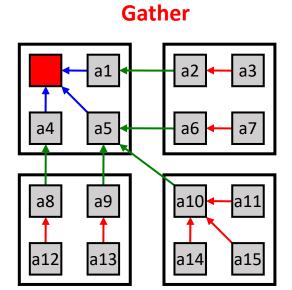


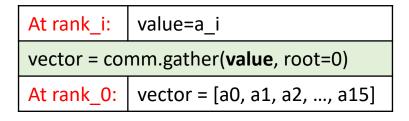


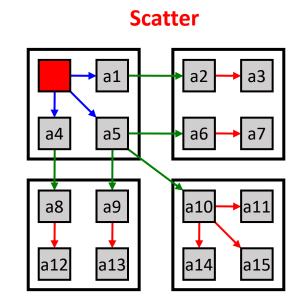


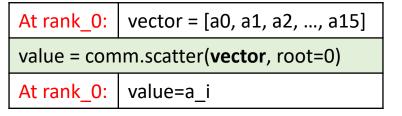
```
At rank_0:
            vector = [a0, a1, a2, ..., a15]
value = comm.scatter(vector, root=0)
At rank_0:
            value=a_i
```

a15

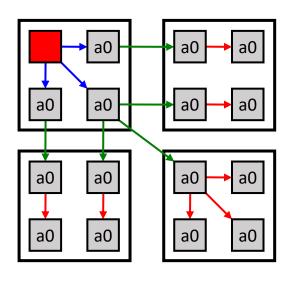




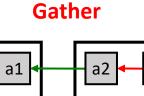


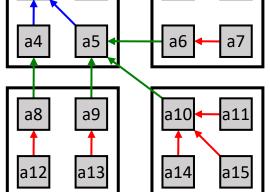


Broadcast



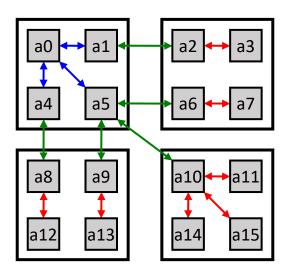
| At rank_0: value=a_0 | | | |
|----------------------|--------------------------------------|--|--|
| value = com | nm.broadcast(value , root=0) | | |
| At rank_i: | value=a_0 | | |





| At rank_i: | value=a_i |
|--------------|-----------------------------------|
| vector = cor | mm.gather(value , root=0) |
| At rank_0: | vector = [a0, a1, a2,, a15] |

Allgather



| At rank_i: | value=a_i | | | |
|--------------------------------|---------------------------|--|--|--|
| vector = comm.allgather(value) | | | | |
| At rank_i: | vector=[a0, a1, a2,, a15] | | | |

Type of collective operations

Data Movement

- Broadcast
- Scatter/Gather
- Allgather/AlltoAll

Computation

- Reduce
- Allreduce
 - SUM
 - MIN/MAX
 - ...
- Scan

Synchronization

- Barrier

Thank you!

- Questions?
- carc-support@usc.edu
- Office hours: LVL 3L and Zoom 2:30-5pm Every Tuesday
- Thanks to Marco for help on these slides!