JÜLICH
FORSCHUNGSZENTRUM

Session 12: Introduction to MPI (4PY)

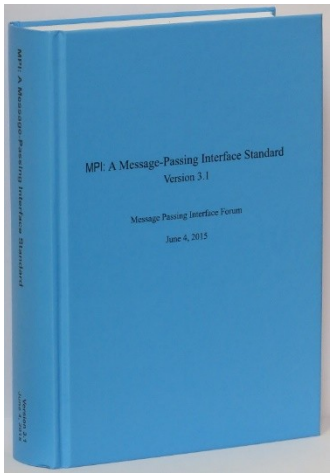
October 9th 2018, Alexander Peyser (Lena Oden)

Overview

- Introduction
  - Basic concepts
  - mpirun
- Hello world
- Wrapping numpy arrays
- Common Pitfalls

Introduction

- MPI: de facto standard for parallel programming in HPC systems since 1994 (MPI 1.0)
- Currently at MPI 3.1
- MPI is a standard with different implementation
    - OpenMPI
    - MPICH
    - Mvapich
    - ….
- Distributed memory systems (process parallel)
- Message-passing
- Goals: performance, scalability, portability
    - Shared memory, sockets, Infiniband…
- Standard is C (C++ bindings deprecated)
- MPI4PY: Layer above in Python



Getting started

- Requires an MPI Installation + mpi4py
- **Communicator**: The “context” processes use to talk with each other
  - groups processes
  - Separation of concerns
- Process can be in more than one communicator

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

- **MPI_COMM_WORLD (MPI.COMM_WORLD)**
  - Basic communicator, created at start time

Introduction: mpirun

- MPI programs are started with a specialized runner application
  - Sets up the environment and starts the instances
  - Distributes processes across nodes

mpirun –np 2 python hello_world.py <args>

mpirun : MPI runner applications
-np 2 : number of parallel mpi processes to start
python hello_world.py : Your application
<args> : Arguments (argv and argc stay the same.)

Note: On clusters with SLURM use srun instead on mpirun

Hello world

```
from mpi4py import MPI

# Communicator that contains all mpi processes
comm = MPI.COMM_WORLD

rank = comm.Get_rank()
size = comm.Get_size()
name = MPI.Get_processor_name()

print("Rank {0} out of {1} on {2}".format(
      rank, size, name))
```

```
$ srun -np 2 python3 hello_world.py
Rank 0 out of 2 on ANDREASPC
Rank 1 out of 2 on ANDREASPC
```

Blocking Point-to-Point

- Simple principle:
  - One process sends a message (comm.send)
  - Another process receives the message (comm.recv)
- Blocking, until **locally** completed
- Tag for matching (Should always be set, if possible)

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=1)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
    print(data)
```

MPI4Py: *pickle based vs. arrays*

- MPI4Py supports both:
  - generic Python objects
  - buffer-like objects (e.g. numpy)

- Generic objects
  - Data are pickled before transfer
  - Needs time and memory
- Buffer-like objects
  - Send(), Recv()
  - Tuple/triple for the data
    [data, MPI.DOUBLE]
    [data, count, MPI.DOUBLE]

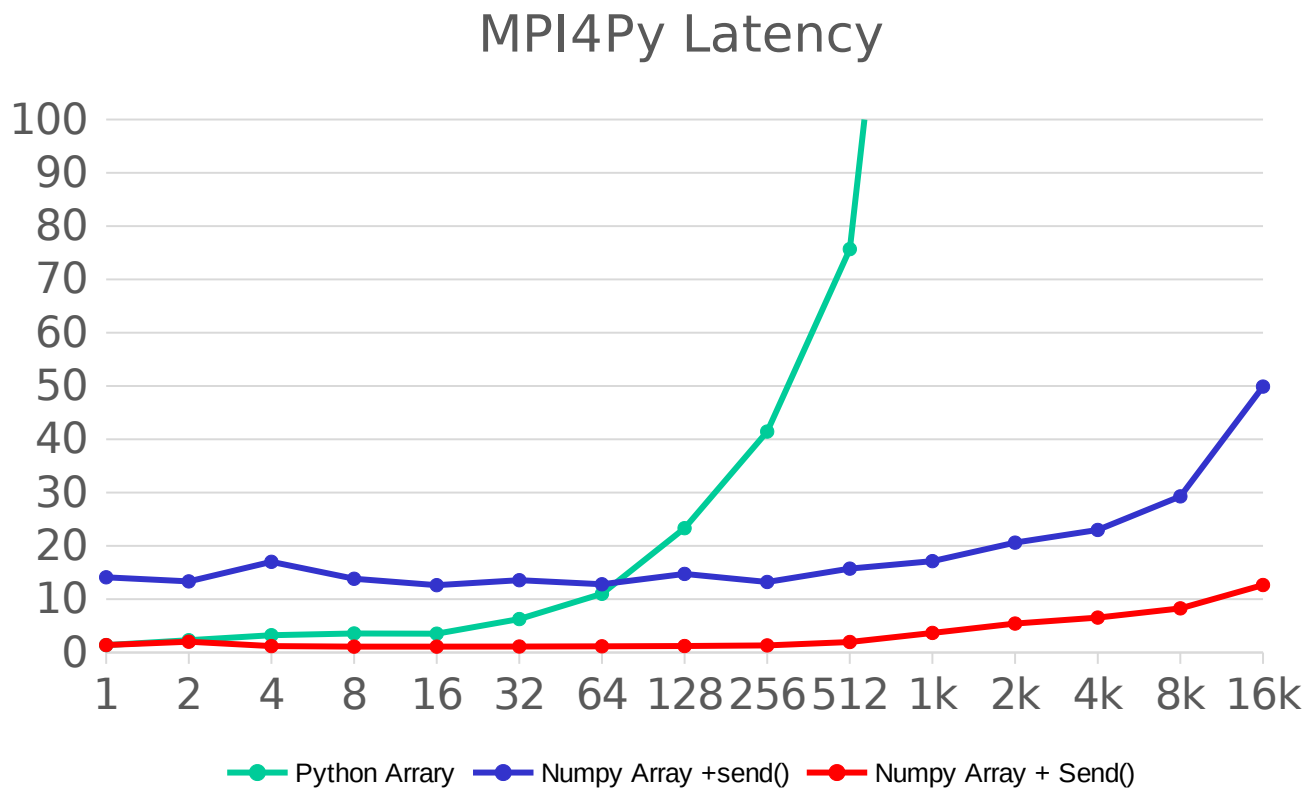
Example: Send/Recv with numpy

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
     data = np.array([1,2,4,5], dtype='int')
  comm.send(data, dest=1, tag=1)
elif rank is 1:
    data = comm.recv(source=0, tag=1)
    print(data)
```

Example: Send/Recv with numpy

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
     data = np.array([1,2,4,5], dtype='int’)
     comm.Send([data, MPI.INT], dest=1, tag=11)
elif rank is 1:
    data=np.zeros(4, dtype='int')
    comm.Recv(([data, MPI.INT],source=0, tag=11)
    print(data)
```

Performance Comparison



Non-Blocking Point to Point

- Non-blocking version of Send/Recv
- Start a send/recv operations
- Completed later (wait)
- Used to overlap computation and communication
- Avoiding Deadlocks

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
req = {}

if rank == 0:
    data = np.array([1,2,4,5], dtype='int’)
    req[0]= comm.Isend([data, MPI.INT], dest=1, tag=11)
elif rank == 1:
    data=np.zeros(4, dtype='int’)
    req[0] = comm.Irecv([data, MPI.INT],source=0, tag=11)
req[0].wait()
#MPI.Request.waitall(req)
```

Exercise 1: Deadlocks

```
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()
#modify this function so we don't have a deadlock
send_data1 = np.array([1,2,4,5], dtype='int')
send_data2 = np.array([5,7,8,9], dtype='int')
recv_data1 =np.zeros(4, dtype='int')
recv_data2 =np.zeros(4, dtype='int')
next = (rank + 1)%size
prev = (size + rank -1) % size
comm.Send([send_data1, MPI.INT], dest=next, tag=11)
comm.Recv([recv_data2, MPI.INT], source=next, tag=12)
comm.Send([send_data2, MPI.INT], dest=prev, tag=12)
comm.Recv([recv_data1, MPI.INT], source=prev, tag=11)
```

Caution

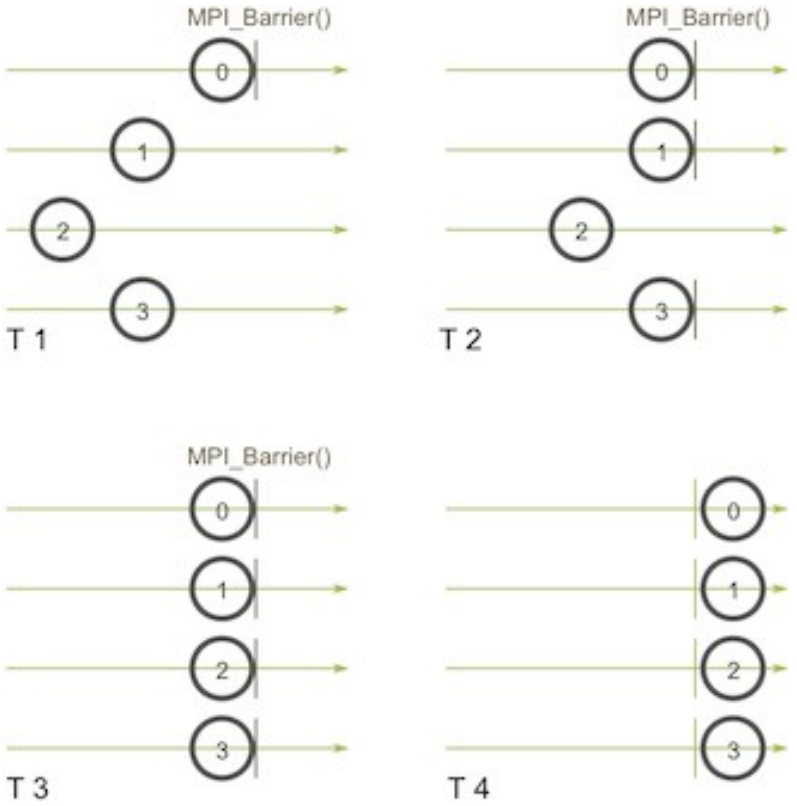
- Send/Recv are only locally blocking
- Send may return, before the other process has received the data
  - Depends on the Message size and the MPI-implementation
  - (buffered send vs. rendezvous protocol)
- Using non-blocking communication does NOT necessarily mean that communication is handled in the background
  - May require “poking” of the MPI Progress Engine
  - Depends on MPI implementation and message size
  - Req.test()
- Wait is usually busy wait (in HPC, we prefer our threads to sleep)

Collective Operations

- A communication call to collective send/recv messages in a communicator
  - Barrier
  - Bcast
  - Scatter
  - Gather
  - Allgather
  - Reduce/Allreduce
- Forces a synchronization between Processes
  - Can also be a reason for slow-down
  - Usually, a busy waiting model (HPC)

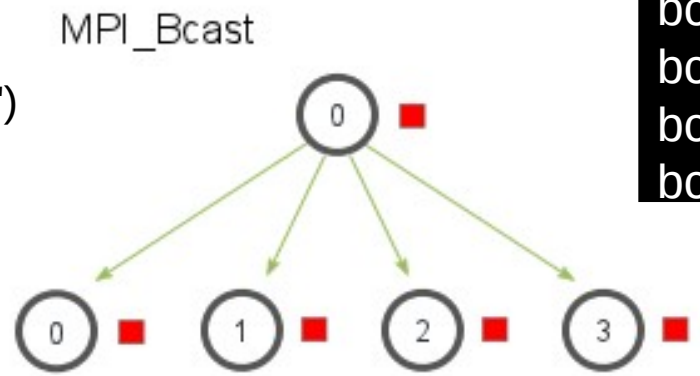
Barrier

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
comm.Barrier()
#comm.barrier()
```

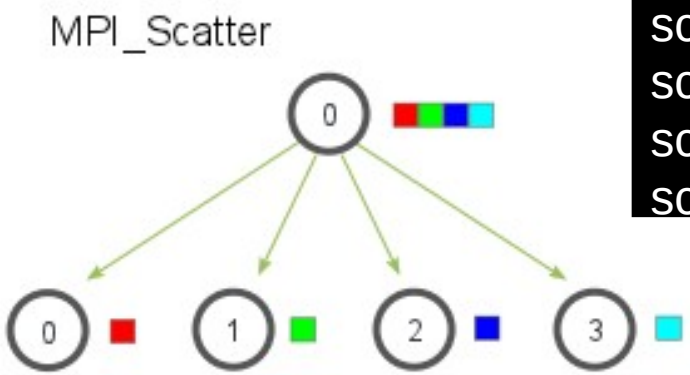


Bcast and Scatter

```
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank is 0:
    data = np.array([2,2,3,4], dtype='int')
else:
    data = np.zeros(1, dtype='int')

comm.Bcast([data,MPI.INT], root=0)
print("bcast", rank, data)
if rank is 0:
    comm.Scatter([data, MPI.INT],
                 [data,MPI.INT],
                 root=0)
else:
    comm.Scatter(None,
                 [data,MPI.INT],
                 root=0)
print("scatter", rank, data)
```



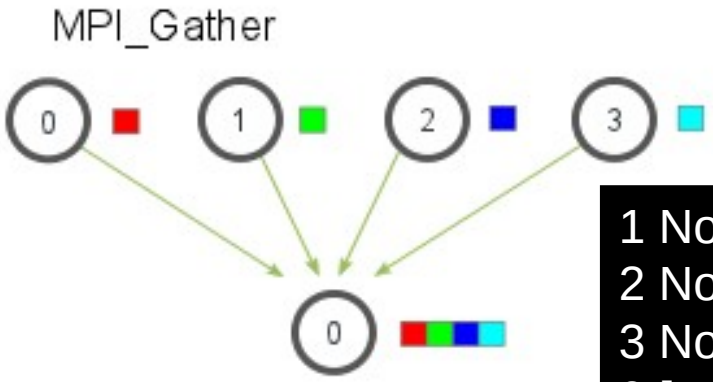

```
bcast 0 [2 2 3 4]
bcast 1 [2 2 3 4]
bcast 3 [2 2 3 4]
bcast 2 [2 2 3 4]
```




```
scatter 0 [2 2 3 4]
scatter 1 [2 0 0 0]
scatter 2 [3 0 0 0]
scatter 3 [4 0 0 0]
```

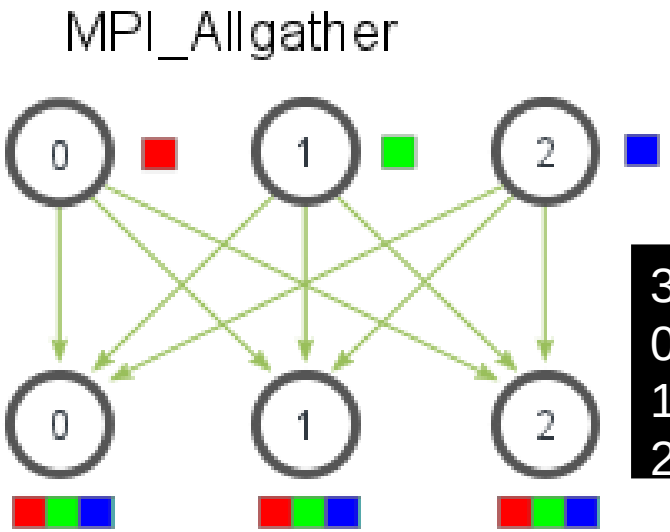
Gather and Allgather

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

data = (rank+1)**2
data = comm.gather(data, root=0)

print(rank, data)
```




```
1 None
2 None
3 None
0 [1, 4, 9,
```

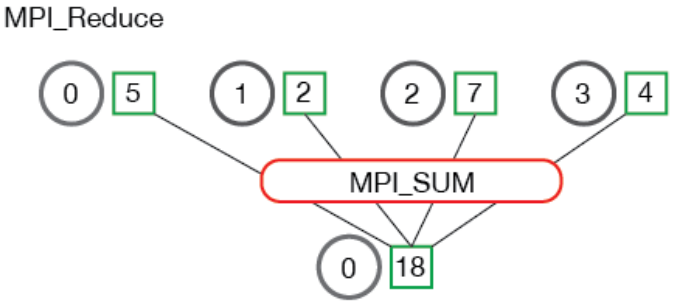
```
ata = np.array(rank, dtype='int')
gather = np.zeros(4, dtype='int')
comm.Allgather([data,MPI.INT],
               [gather, MPI.INT])
print(rank, gather)
```

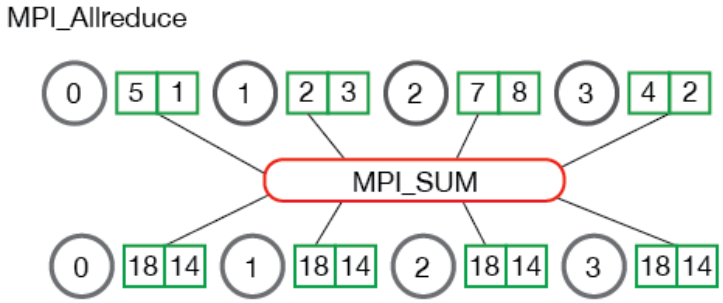



```
3 [0 1 2 3]
0 [0 1 2 3]
1 [0 1 2 3]
2 [0 1 2 3]
```

Reduce/Allreduce

```
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
data = np.array(rank, dtype='int')
result = np.zeros(1, dtype='int')
comm.Reduce([data, MPI.DOUBLE],
            [result, MPI.DOUBLE],
            op=MPI.SUM, root=0)
print("reduce", rank, result)

comm.Allreduce([data, MPI.DOUBLE],
               [result,
                 MPI.DOUBLE],
               op=MPI.SUM)
print("allreduce", rank, result)
```





Reduce/Allreduce

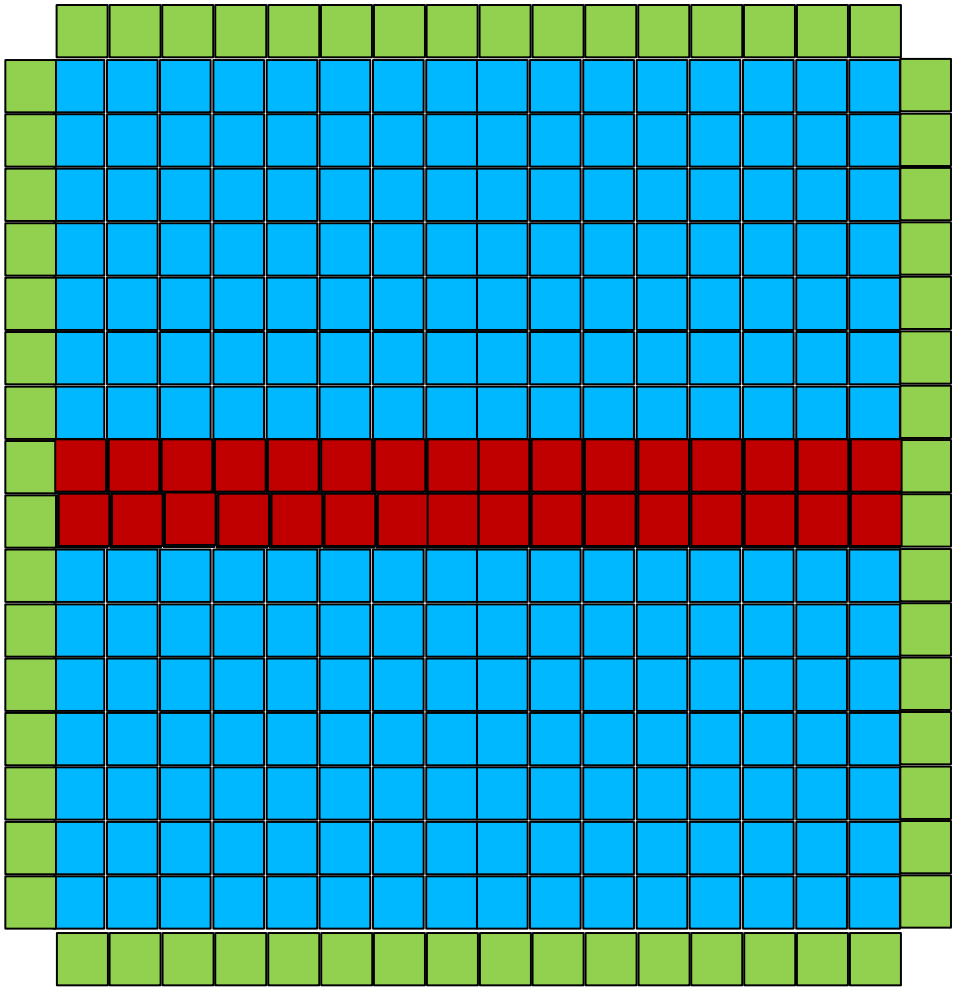
```
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
data = np.array(rank, dtype='int')
result = np.zeros(1, dtype='int')
comm.Reduce([data, MPI.DOUBLE],
            [result, MPI.DOUBLE],
            op=MPI.SUM, root=0)
print("reduce", rank, result)

comm.Allreduce([data, MPI.DOUBLE],
               [result,
                 MPI.DOUBLE],
               op=MPI.SUM)
print("allreduce", rank, result)
```

```
reduce 1 [0]
reduce 3 [0]
reduce 2 [0]
reduce 0 [6]
allreduce 2 [6]
allreduce 3 [6]
allreduce 1 [6]
allreduce 0 [6]
```

Exercise 2: Computing Pi in Parallel

```
If rank is 0
    N = np.array(10000, 'i')

#Distribute N Across all nodes

start = time.time()
h = 1.0 / N; s = 0.0
for i in range(rank, N, size):
    x = h * (i + 0.5)
    s += 4.0 / (1.0 + x**2)
PI = np.array(s * h, dtype=‘d’)

#collect result with the reduce function
end = time.time()
if rank is 0:
    print ("I get for PI {0}").format(PI_ALL)
    print("I needed {0} seconds").format(end-start)
```

Exercise 3: 2-D Stencil



Tips: Send/recv partial arrays

```
req[0] =comm.Isend([grid1[1][:],MPI.DOUBLE], dest=top, tag=2)

req[1]= comm.Irecv([grid1[my_m+1][:],MPI.DOUBLE], source=btm, tag=2)
```

Further reading and resources used

https://en.wikipedia.org/wiki/Message_Passing_Interface

https://www.nesi.org.nz/sites/default/files/mpi-in-python.pdf

Thank you for your attention





References and further reading: