HPS

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Parallel Python

MPI for Python

Learning Objectives

- Understand Python MPI libraries and communication
- Run Python code in parallel on multiple machines
- Improve Numpy code via MPI parallelization

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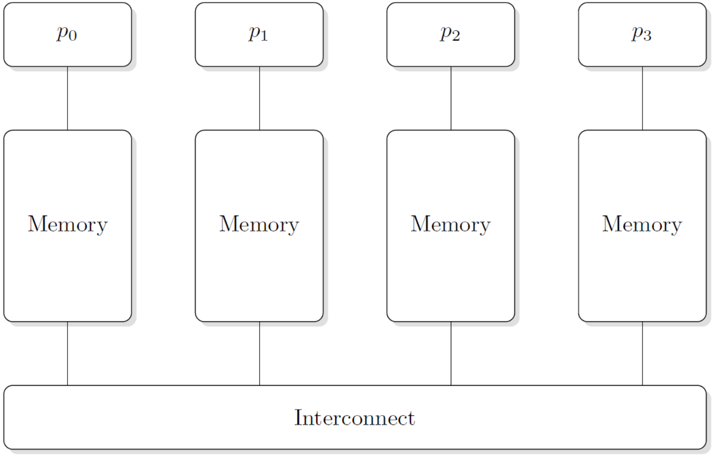
Repetition - MPI

MPI is used for distributed memory systems



Execution of an MPI Program

- Launching an MPI-parallelized Pythonscript (e.g., with mpirun, mpiexec . . .) will start *n* Python interpreters
- All processes contain the same code, thus they are independent and identical processes

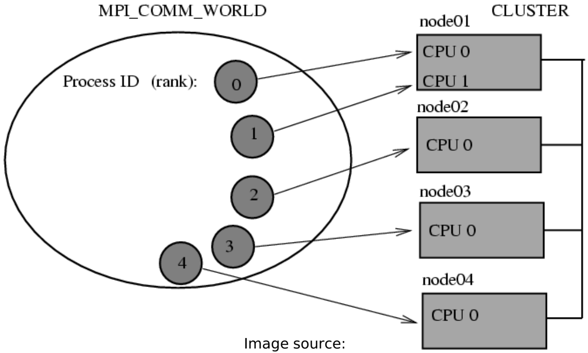


Image source:
https://lsi.vc.ehu.eus/pablogn/docencia/manuales/linuxcourse.rutgers.edu/lessons/HPC_1/sec_4.php.html

Ranks and Communicators

- Rank: Unique id given to one process to distinguish between them
- Communicator: Group of processes
  - Communication takes always place in a certain communicator
  - Rank of a process can be different in different communicators

minimal-mpi.py

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
size = comm.get_size()
rank = comm.get_rank()

If rank == 0:
        # do stuff that only process 0 should do
```

Sending and Receiving Data - Example

send-recv.py

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank == 0:
        data = {'a': 1, 'b': 2, 'c':'test string'}
        comm.send(data,dest=1,tag=11)
elif rank == 1:
        data = comm.recv(source=0,tag=11)
        print(data)
```

run send-recv

```
$ mpirun -n 2 python3 send-recv.py
{'a': 1, 'b': 2, 'c': 'test string'}
```

Sending and Receiving Data - Summary

- Arbitrary Python objects can be sent and received without the manual need for serialization from the user
  - MPI functions pickle under the hood
- `send(data,dest,tag)`
  - `data`: Data, i.e. a Python object to send
  - `dest`: Rank of the destination process
  - `tag`: Arbitrary id for this message
- `recv(source,tag)`
  - `source`: Rank of the sending process
  - `tag`: ID of the message, must match the tag in the send function
  - The **return value** is the send data
- There are also the non-blocking functions `isend` and `irecv`

Sending and Receiving Data - Summary

- Objects need to be serialized to a byte stream when sending
- Byte stream needs to be deserialized on the receiving process
    - Additional overhead for communication
- Specifically in scientific computing it is necessary to be able to efficiently exchange large amounts of data
- For this contiguous NumPy arrays can be communicated with a largely reduced overhead
- Use `Send(data,dest,tag)` and `Recv(data,source,tag)`
    - Notice the **capitalized Send** and **Recv**
- Data array has to exist beforehand on the receiving process

Sending and Receiving NumPy Arrays

numpy-send-recv.py

```python
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
if rank == 0:
        data = numpy.arange(100, dtype=numpy.float)
        comm.Send(data,dest=1,tag=11)
elif rank == 1:
        data = numpy.empty(100,dtype=numpy.float)
        comm.Recv(data, source=0,tag=11)
```

Summary

- send/recv for all general Python objects, slow
- Send/Recv for continuous arrays, fast

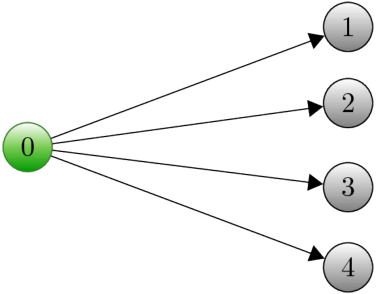
Collective Communication - Broadcast

broadcast.py

```python
from mpi4py import MPI

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

if rank == 0:
        data = {'key1' : [7, 2.72, 2+3j],
                'key2' : ( 'abc', 'xyz')}
else:
        data = None
data = comm.bcast(data, root=0)
```



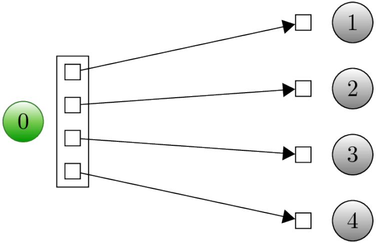
Collective Communication - Scatter

scatter.py

```
from mpi4py import MPI

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

if rank == 0:
        data = [(i+1)**2 for i in range(size)]
else:
        data = None
data = comm.scatter(data, root=0)
assert data == (rank+1)**2
```



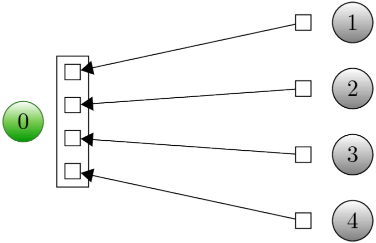
Collective Communication - Gather

gather.py

```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:
        for i in range(size):
                assert data[i] == (i+1)**2
else:
        assert data is None
```



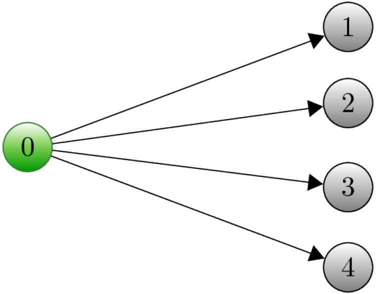
Collective Communication - Broadcasting a Numpy Array

broadcast-numpy.py

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

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

if rank == 0:
        data = np.arange(100, dtype='i')
else:
        data = np.empty(100, dtype='i')
comm.Bcast(data, root=0)
for i in range(100):
        assert data[i] == i
```



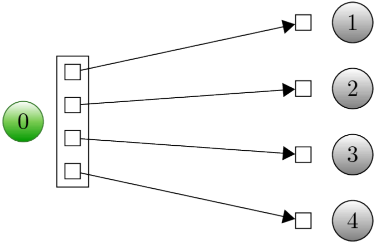
Collective Communication - Scatter a Numpy Array

scatter-numpy.py

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

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

sendbuf = None
if rank == 0:
        sendbuf = np.empty([size, 100], dtype='i')
        sendbuf.T[:,:] = range(size)
recvbuf = np.empty(100, dtype='i')
comm.Scatter(sendbuf, recvbuf, root=0)
assert np.allclose(recvbuf, rank)
```

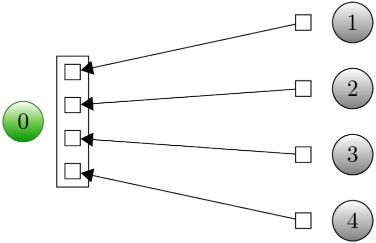


Collective Communication - Gather a Numpy Array

gather.py

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

comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()
sendbuf = np.zeros(100, dtype='i') + rank
recvbuf = None
if rank == 0:
        recvbuf = np.empty([size, 100], dtype='i')
comm.Gather(sendbuf, recvbuf, root=0)
if rank == 0:
        for i in range(size):
                assert np.allclose(recvbuf[i,:], i)
```



Exceptions and Deadlocks

- Upon import, mpi4py is being automatically initialized
- Avoid a deadlock by using `-m mpi4py`

deadlock.py

```python
from mpi4py import MPI
assert MPI.COMM_WORLD.Get_size() > 1
rank = MPI.COMM_WORLD.Get_rank()
if rank == 0:
        1/0
        MPI.COMM_WORLD.send(None, dest=1, tag=42)
elif rank == 1:
        MPI.COMM_WORLD.recv(source=0, tag=42)
```

```
$ mpirun -n 10 python3 deadlock.py
Traceback (most recent call last):
        ZeroDivisionError: division by zero
```

```
$ mpirun -n 10 python3 -m mpi4py deadlock.py
Traceback (most recent call last):
```

Dynamic Process Management Ia

- MPI-2 provides a process model, which allows for creating new processes and establishing communication between them and the existing MPI application
- Useful for sequential applications built on top of parallel modules or in a client/server model

communicator.py

```
from mpi4py import MPI
import numpy
import sys

comm = MPI.COMM_SELF.Spawn(sys.executable,
args=['cpi.py'],
maxprocs=5)

N = numpy.array(100, 'i')
comm.Bcast([N, MPI.INT], root=MPI.ROOT)
PI = numpy.array(0.0, 'd')
comm.Reduce(None, [PI, MPI.DOUBLE],
op=MPI.SUM, root=MPI.ROOT)
print(PI)
comm.Disconnect()
```

Dynamic Process Management Ib

- communicatior.py will run as the boss-rank, and cpi.py (see next slide) as the worker ranks
- Note as usual the matching broadcast and reduce calls
- This calcualtes Pi by approximating an integral thru the trapezoid method. Each rank does a portion of the integral.

communicator.py

```
from mpi4py import MPI
import numpy
import sys

comm = MPI.COMM_SELF.Spawn(sys.executable,
args=['cpi.py'],
maxprocs=5)

N = numpy.array(100, 'i')
comm.Bcast([N, MPI.INT], root=MPI.ROOT)
PI = numpy.array(0.0, 'd')
comm.Reduce(None, [PI, MPI.DOUBLE],
op=MPI.SUM, root=MPI.ROOT)
print(PI)
comm.Disconnect()
```

Dynamic Process Management II

cpi.py

```
from mpi4py import MPI
import numpy
comm = MPI.Comm.Get_parent()
size = comm.Get_size(); rank = comm.Get_rank()

N = numpy.array(0, dtype='i')
comm.Bcast([N, MPI.INT], root=0)
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 = numpy.array(s * h, dtype='d')
comm.Reduce([PI, MPI.DOUBLE], None,
                op=MPI.SUM, root=0)
comm.Disconnect()
```

Further Reading

Single Most important Source:

`https://mpi4py.readthedocs.io/en/stable/index.html`