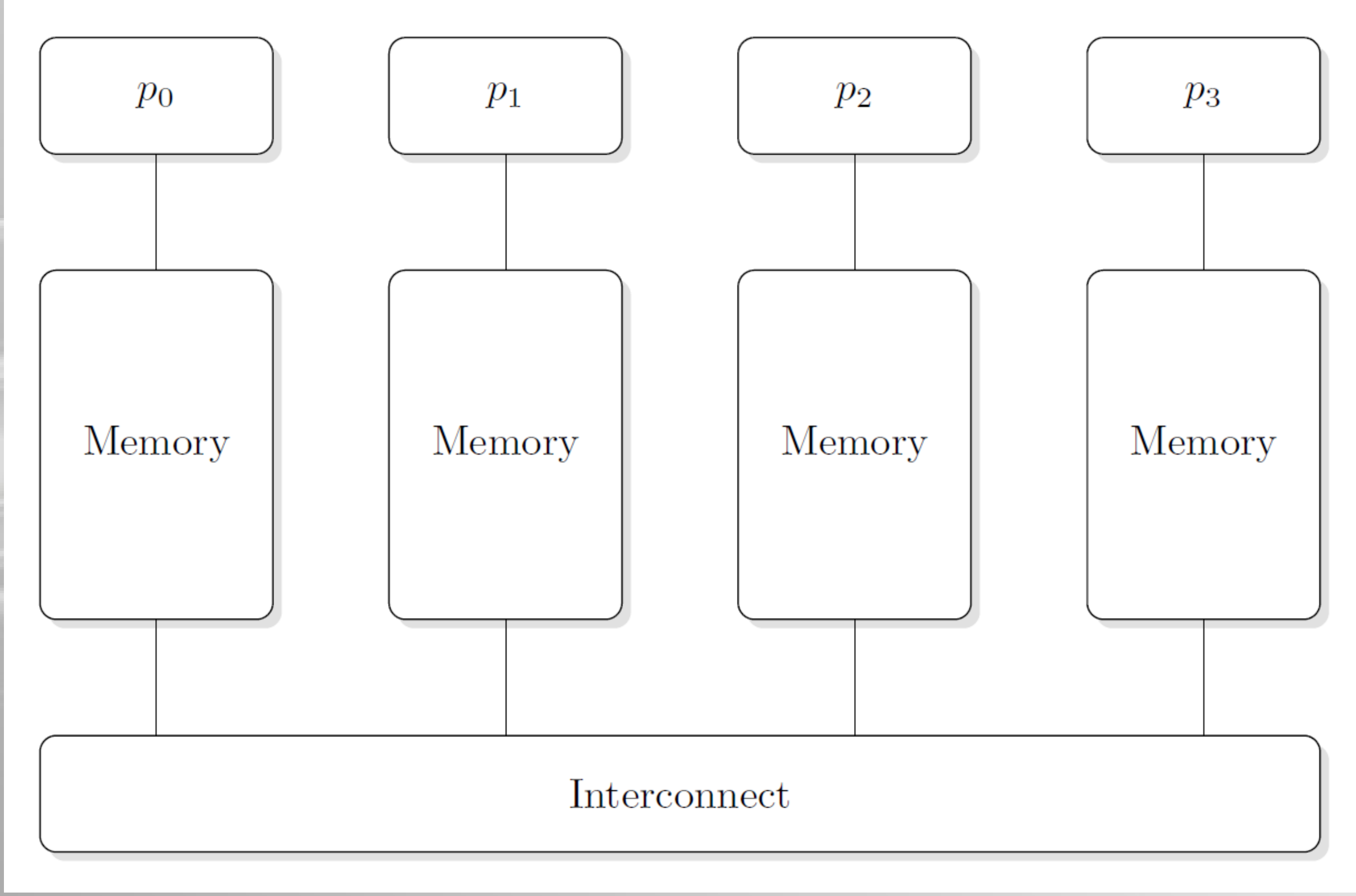
Python + MPI

Hendrik Nolte

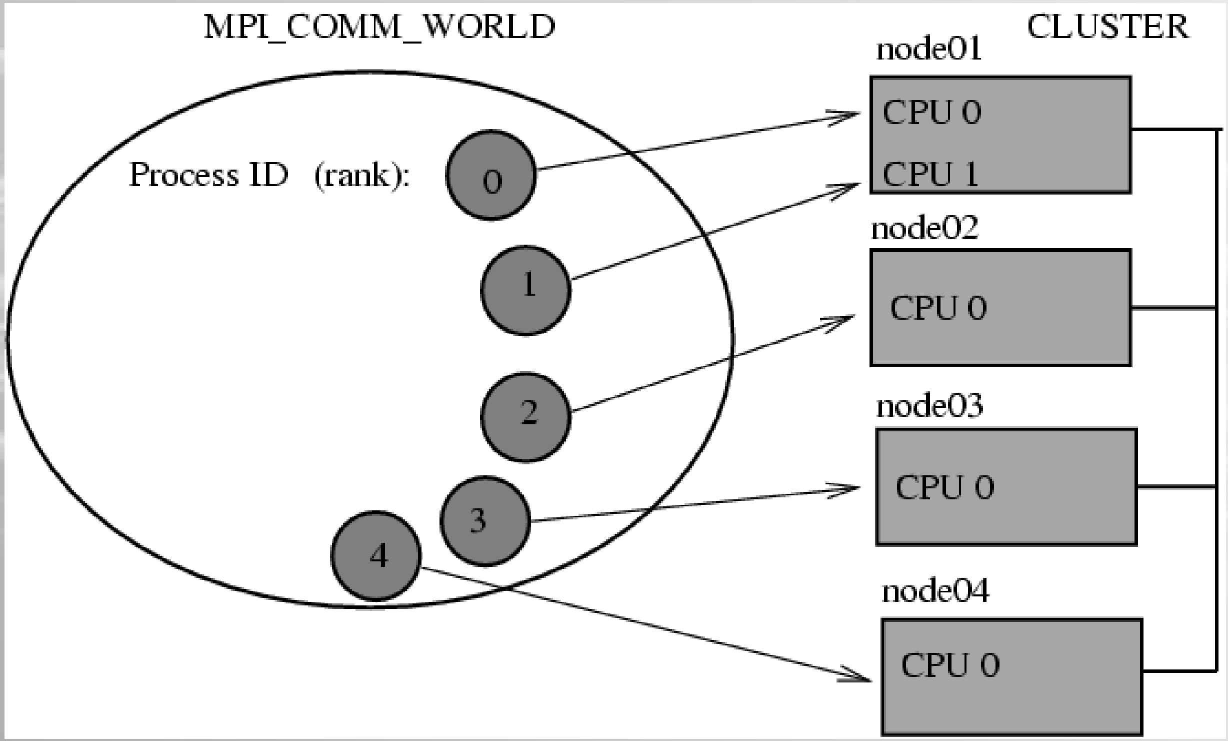
Repetition - MPI

MPI is used for a distributed memory system



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



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

```
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

```
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)
```

```
$ mpirun -n 2 python3 mpi_example_1.py
{'a': 1, 'b': 2, 'c': 'test string'}
```

Sending and Receiving Data - Summary

- Arbitrary Python objects can be send 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

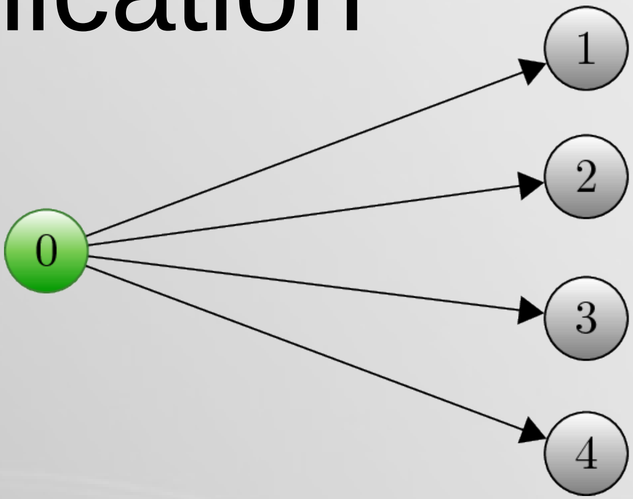
```
from mpi4py import MPI
import numpy

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

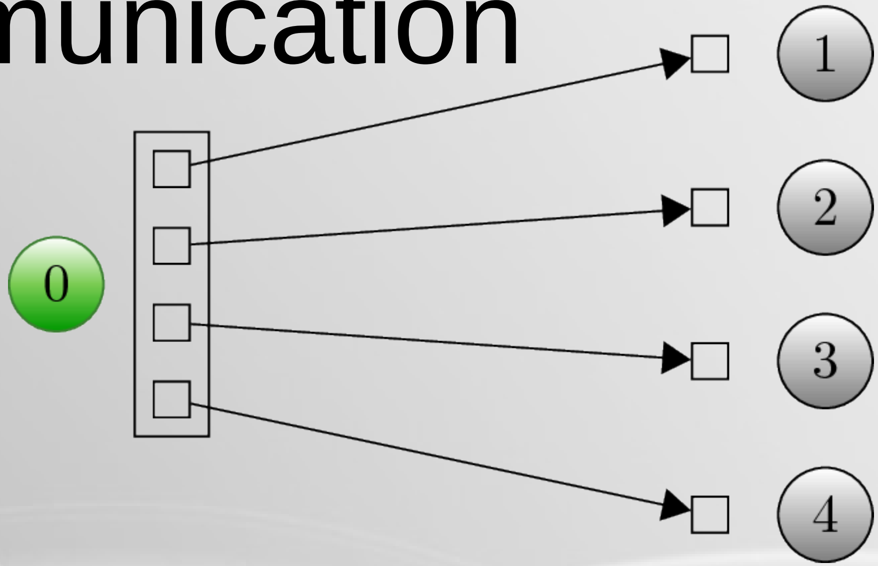
Broadcast



```
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

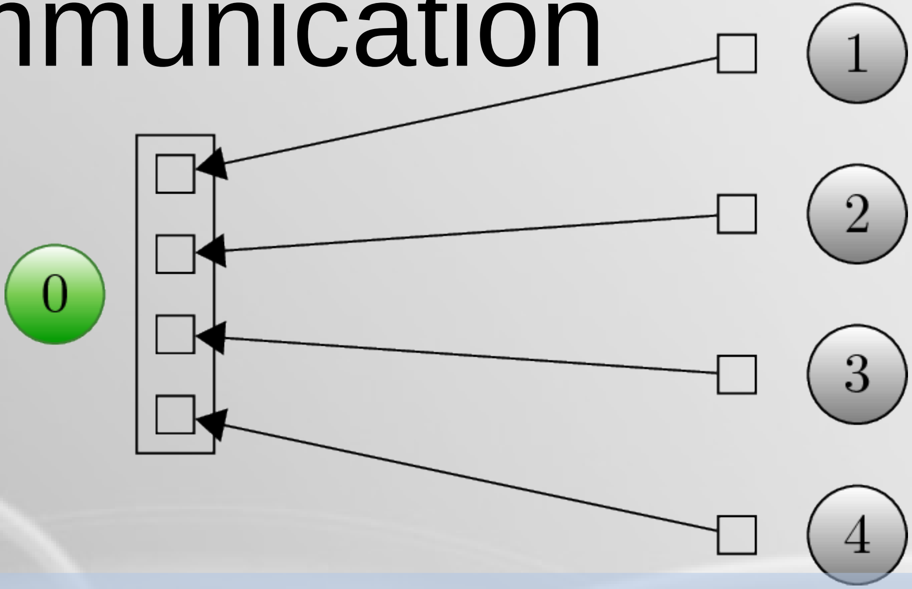
Scattering



```
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

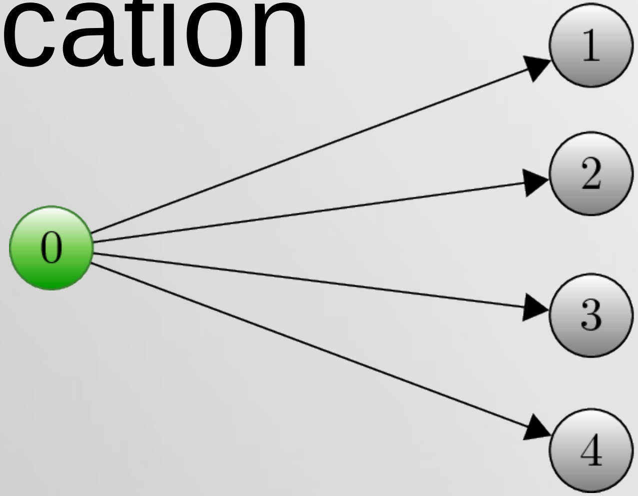
Gather



```
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

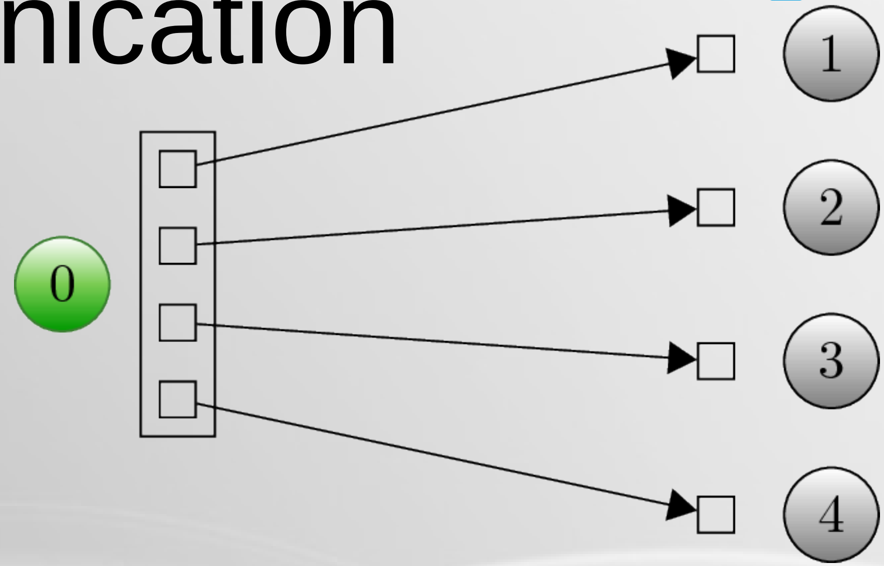
Broadcasting a NumPy array



```
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

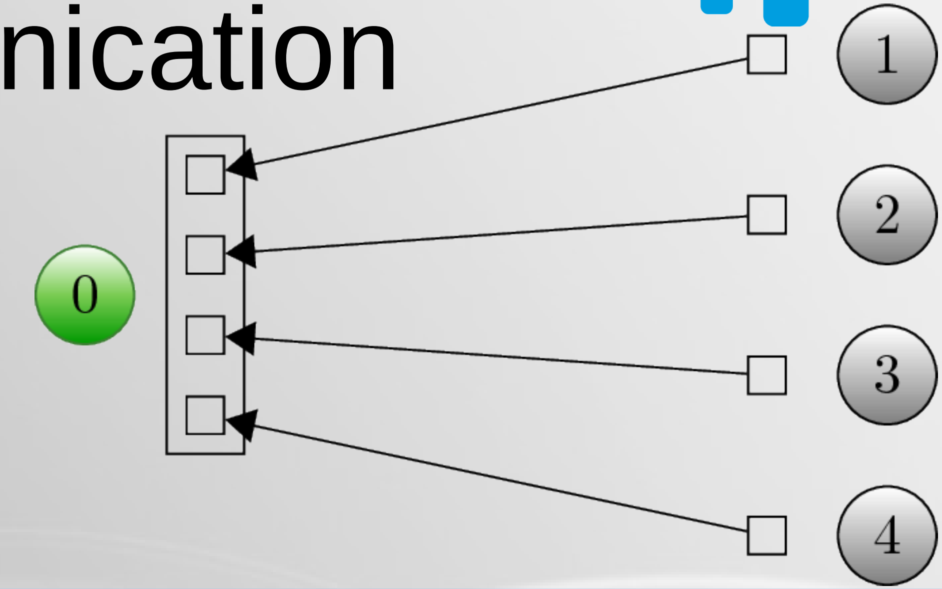
Scattering a NumPy array



```
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

Gathering a NumPy array



```
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

```
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)
```

- Using

```
$ mpirun -n 10 python3 deadlock_example.py
Traceback (most recent call last):
  File "deadlock_example.py", line 5, in <module>
    1/0
ZeroDivisionError: division by zero
```

Gives a Deadlock, rather use

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

Dynamic Process Management I

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

```
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

```
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()
```

Q&A

Single Most important Source:

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