PARALLEL PROGRAMMING WITH PYTHON USING MPI4PY

Outline

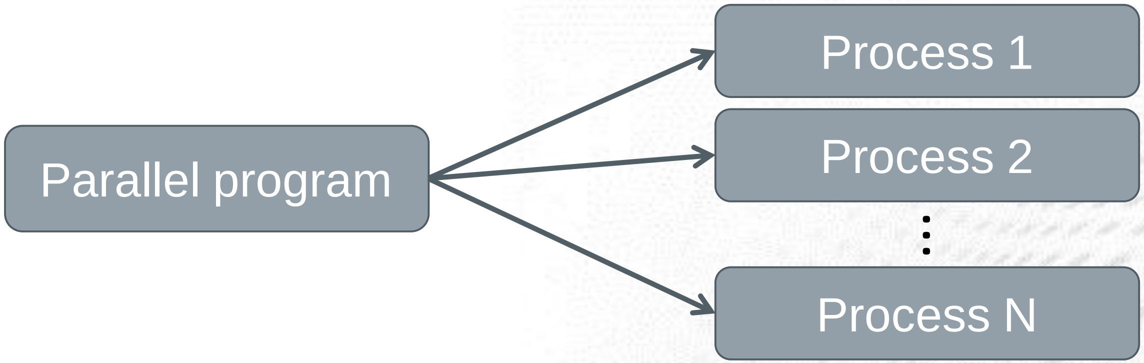
- Brief introduction to message passing interface (MPI)
- Python interface to MPI – mpi4py
- Performance considerations

Message passing interface

- MPI is an application programming interface (API) for communication between separate processes
- The most widely used approach for distributed parallel computing
- MPI programs are portable and scalable
  - the same program can run on different types of computers, from PC's to supercomputers
- MPI is flexible and comprehensive
  - large (over 120 procedures)
  - concise (often only 6 procedures are needed)
- MPI standard defines C and Fortran interfaces
- **mpi4py** provides (an unofficial) Python interface

Execution model in MPI

- Parallel program is launched as set of **independent, identical processes**



- All the processes contain the same program code and instructions
- Processes can reside in different nodes or even in different computers
- The way to launch parallel program is implementation dependent
  – mpirun, mpiexec, aprun, poe, ...
- When using Python, one launches N Python interpreters
  – mpirun -np 32 python parallel_script.py

MPI Concepts

- rank: id number given to process
  - it is possible to query for rank
  - processes can perform different tasks based on their rank

mpi.py

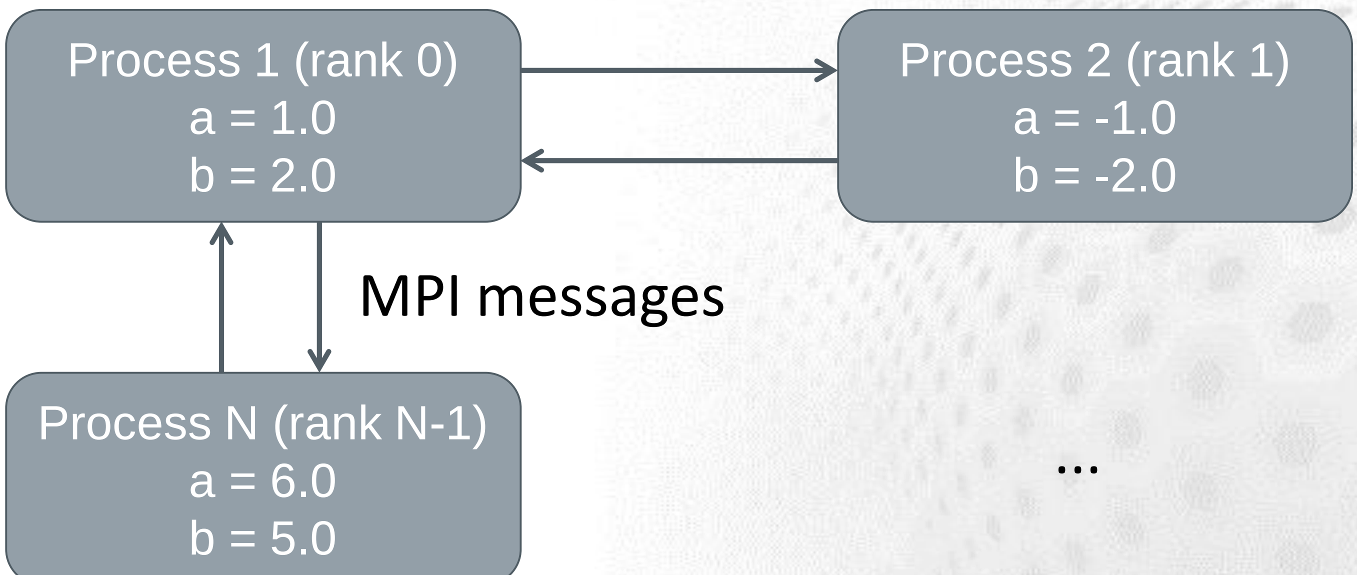
```
if (rank == 0):
    # do something
elif (rank == 1):
    # do something else
else:
    # all other processes do something different
```

MPI Concepts

- Communicator: group containing process
  - in mpi4py the basic object whose methods are called
  - **MPI_COMM_WORLD** contains all the process (MPI.COMM_WORLD in mpi4py)

Data model

- All variables and data structures are local to the process
- Processes can exchange data by sending and receiving messages



Using mpi4py

- Basic methods of communicator object
  - Get_size()
    Number of processes in communicator
  - Get_rank()
    rank of this process

mpi.py

```
from mpi4py import MPI

comm = MPI.COMM_WORLD  # communicator object containing all processes
size = comm.Get_size()
rank = comm.Get_rank()

print "I am rank %d in group of %d processes" % (rank, size)
```

Sending and receiving data

- Sending and receiving a dictionary

mpi.py

```
from mpi4py import MPI

comm = MPI.COMM_WORLD  # communicator object containing all processes
rank = comm.Get_rank()

if rank == 0:
   data = {'a': 7, 'b': 3.14}
   comm.send(data, dest=1, tag=11)
elif rank == 1:
   data = comm.recv(source=0, tag=11)
```

Sending and receiving data

- Arbitrary Python objects can be communicated with the **send** and **receive** methods of communicator
- **send(data, dest, tag)**
  - **data** Python object to send
  - **dest** destination rank
  - **tag** id given to the message
- **recv(source, tag)**
  - **source** source rank
  - **tag** id given to the message
  - data is provided as return value
- Destination and source ranks as well as tags have to match

Communicating NumPy arrays

- Arbitrary Python objects are converted to byte streams when sending
- Byte stream is converted back to Python object when receiving
- Conversions give overhead to communication
- (Contiguous) NumPy arrays can be communicated with very little overhead with upper case methods:
- **S**end(data, dest, tag)
- **R**ecv(data, source, tag)
  - Note the difference in receiving: the data array has to exist in the time of call

Communicating NumPy arrays

- Sending and receiving a NumPy array

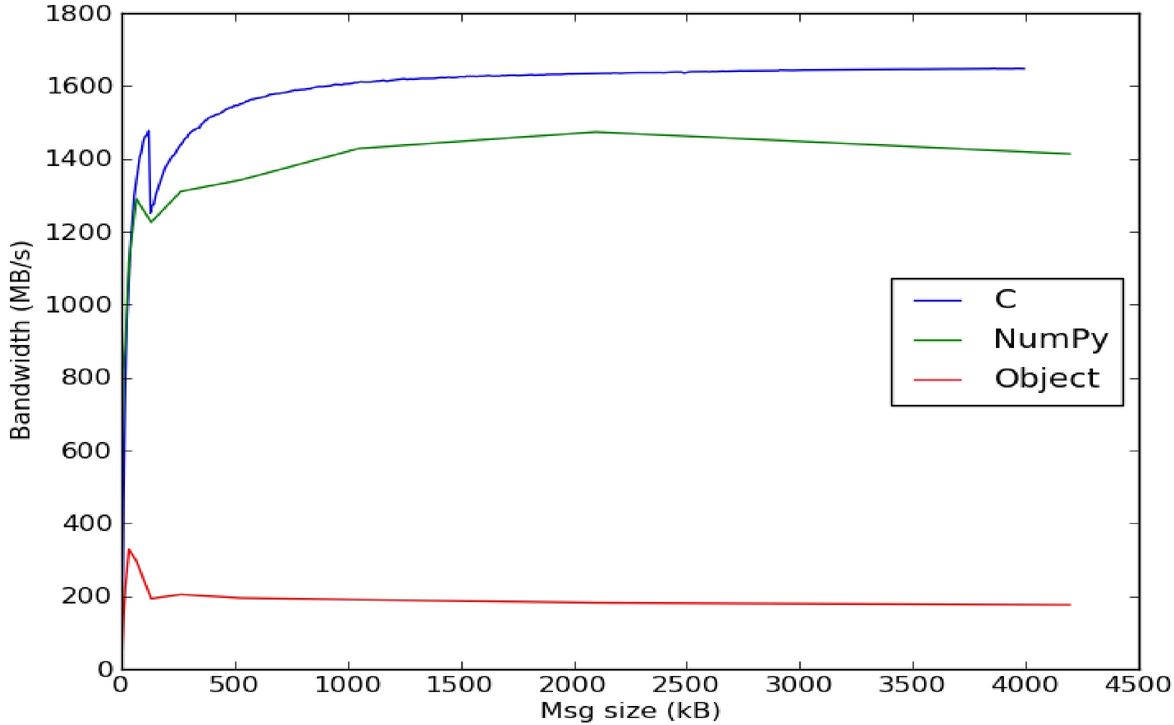
mpi.py

```
from mpi4py import MPI

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

if rank == 0:
    data = numpy.arange(100, dtype=numpy.float)
    comm.Send(data, dest=1, tag=13)
elif rank == 1:
    data = numpy.empty(100, dtype=numpy.float)
    comm.Recv(data, source=0, tag=13)
```

- Note the difference between upper/lower case!
  - send/recv: general Python objects, slow
  - Send/Recv: continuous arrays, fast

mpi4py performance

- Ping-pong test



Summary

- mpi4py provides Python interface to MPI
- MPI calls via communicator object
- Possible to communicate arbitrary Python objects
- NumPy arrays can be communicated with nearly same speed as from C/Fortran