Introduction to MPI with Python

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Python Bindings for MPI Calls

- The mpi4py Python module provides wrappers for calling MPI library functions from Python
- Two types of data supported:
  - “Native” Python types → pickle, send, unpickle
    => function names start with lower case character
  - NumPy arrays/buffers → send directly
    => function names start with upper case character
- Object oriented approach using “communicator objects” → MPI calls become member functions
- Many functions have default arguments

Computing Pi in Python

```
#!/usr/bin/env python
from math import pi
from time import time


tstart = time()
num = 1000000
sum = 0.0
width = 1.0/num


for i in range(0,num):
    x = (float(i) + 0.5) * width
    f_x = 4.0 / (1.0 + x*x)
    sum += f_x
tend = time()


print("Pi is approximately ", sum*width, " versus ", pi)
print("              Error ", (sum*width) - pi)
print("              Time  ", tend – tstart)
```

Computing Pi in Parallel Python (1)

```
#!/usr/bin/env python
from mpi4py import MPI   # MPI_Init() called during import
from math import pi
from time import time

comm = MPI.COMM_WORLD
size = comm.Get_size()   # MPI_Comm_get_size()
rank = comm.Get_rank()   # MPI_Comm_get_rank()


tstart = time()
num = 1000000
sum = 0.0
width = 1.0/num

for i in range(rank, num, size):
    x = (float(i) + 0.5) * width
    f_x = 4.0 / (1.0 + x*x)
    sum += f_x
```

Computing Pi in Parallel Python (2)

```
[...]

tend = time()

tot_sum = comm.reduce(sum, MPI.SUM)  # defaults: root=0, tag=0

if rank == 0:
    print("Pi is approximately ", tot_sum*width, " versus ", pi)
    print("                    Error ", (tot_sum*width) - pi)
    print("                    Time  ", tend – tstart)
```

- Call to MPI_Finalize() automatic during exit
- mpi4py docs at: https://mpi4py.readthedocs.io/
- Installation with: python -m pip install mpi4py