

# A Hands-on Introduction to MPI Python Programming

Sung Bae, Ph.D

New Zealand eScience Infrastructure

## 1 INTRODUCTION: PYTHON IS SLOW

---

### 1.1.1 Example: Computing the value of $\pi=3.14159...$

For

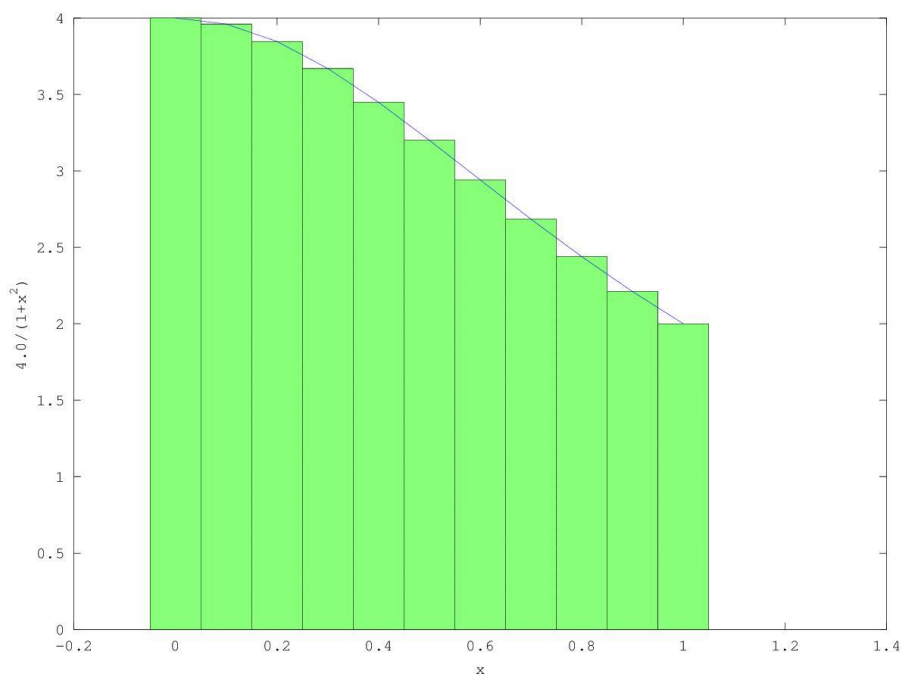
$$F(x) = \frac{4.0}{(1+x^2)}$$

it is known that the value of  $\pi$  can be computed by the numerical integration

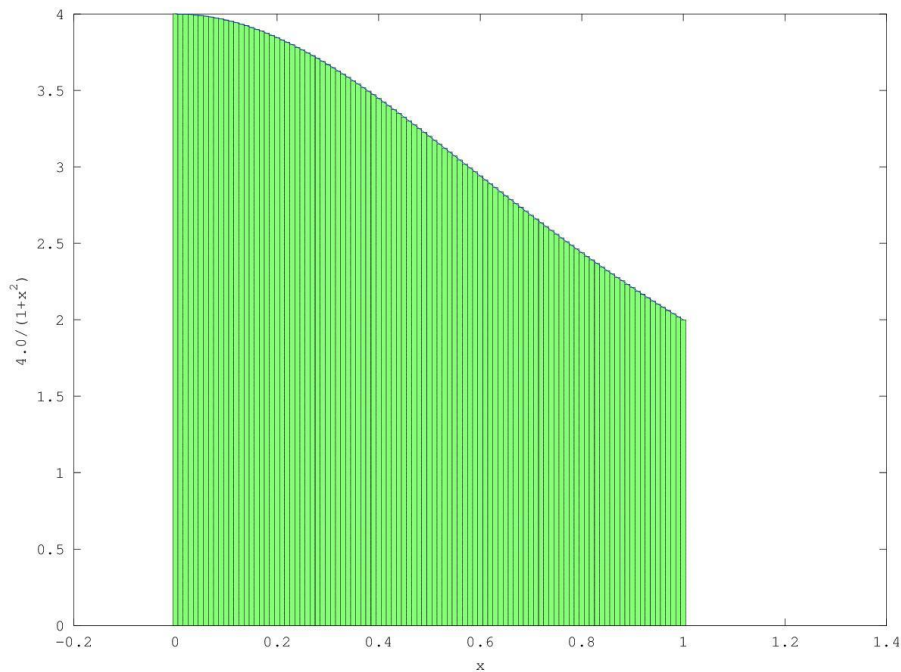
$$\int_0^1 F(x)dx = \pi$$

This can be approximated by

$$\sum_{i=0}^N F(x_i)\Delta x \approx \pi$$



By increasing the number of steps (ie. smaller  $\Delta x$ ), the approximation gets more precise.



We can design the following C and Python programs.

#### EXAMPLE

<pre>import time  def Pi(num_steps):      start = time.time()     step = 1.0/num_steps     sum = 0     for i in xrange(num_steps):         x = (i+0.5)*step         sum = sum + 4.0/(1.0+x*x)      pi = step * sum     end = time.time()     print "Pi with %d steps is %f in %f secs" %(num_steps, pi, end-start)  if __name__ == '__main__':     Pi(100000000)</pre>	<pre>#include &lt;stdio.h&gt; #include &lt;time.h&gt; void Pi(int num_steps) {     double start, end, pi, step, x, sum;     int i;     start = clock();     step = 1.0/(double)num_steps;     sum = 0;     for (i=0;i&lt;num_steps;i++) {         x = (i+0.5)*step;         sum = sum + 4.0/(1.0+x*x);     }     pi = step * sum;     end= clock();     printf("Pi with %d steps is %f in %f secs\n", num_steps, pi,(float)(end- begin)/CLOCKS_PER_SEC);  int main() {     Pi(100000000);     return 0; }</pre>
--	---

#### HANDS ON

- Go to examples directory
1. Compile pi.c (gcc pi.c -o pi -O3) and run by **interactive -A uoa00243 -c 1 -e “./pi”**
  2. Run pi.py by **interactive -A uoa00243 -c 1 -e “python pi.py”**

## DISCUSS

Why is Python code slow?  
How can we speed it up?

## 2 FASTER PYTHON CODE

### 2.1 SPEED-UP OPTIONS



### 2.2 PROFILING

- Find what is slowing you down
  - Line-by-line profiling is often useful [http://pythonhosted.org/line\\_profiler](http://pythonhosted.org/line_profiler)
  - Not part of standard python. Needs separate installation (already installed)
- Put @profile above the function that you're interested in

#### EXAMPLE

```
...
@profile
def Pi(num_steps):
    start = time.time()
    step = 1.0/num_steps
    sum = 0
    for i in xrange(num_steps):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    ....
```

#### HANDS ON

1. Go to “examples/profiling” subdirectory.
2. Open pi.py
3. Add @profile to the function Pi
4. This will take some time. Update the last line of pi.py : Pi(100000000) → Pi(1000000)
5. Run **interactive -A uoa00243 -c 1 -e "python kernprof.py -l -v pi.py"**

#### OUTPUT

Pi with 1000000 steps is 3.14159265358976425020 in 13.541438 secs  
Wrote profile results to pi.py.lprof  
Timer unit: 1e-06 s

File: pi.py  
Function: Pi at line 8  
Total time: 6.54915 s

Line #	Hits	Time	Per Hit	% Time	Line Contents
8					@profile
9					def Pi(num_steps):
10	1	5	5.0	0.0	start = time.time()
11	1	4	4.0	0.0	step = 1.0/num_steps
12					
13	1	2	2.0	0.0	sum = 0
14	1000001	1986655	2.0	30.3	for i in range(num_steps):
15	1000000	2189274	2.2	33.4	x= (i+0.5)*step
16	1000000	2373071	2.4	36.2	sum = sum + 4.0/(1.0+x*x)
17					
18	1	5	5.0	0.0	pi = step * sum
19					
20	1	6	6.0	0.0	end = time.time()
21	1	128	128.0	0.0	print "Pi with %d steps is %.20f in %f secs" %(num_steps, pi, end-start)

## DISCUSS

Identify the bottleneck of this program

## 2.3 NUMBA

Numba (<http://numba.pydata.org/>) is a just-in-time compiler and produces optimized native code from Python code.

### HANDS ON

Open “examples/pi\_numba.py”

#### STEP 1. SEPARATE THE BOTTLENECK

```
# pi_numba.py
import time

def Pi(num_steps):
    start = time.time()
    step = 1.0/num_steps
    sum = 0
    for i in xrange(num_steps):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    pi = step * sum
    end = time.time()
    print "Pi with %d steps is %f in %f secs" %(num_steps, pi, end-start)
if __name__ == '__main__':
    Pi(100000000)
```

## STEP 2. MAKE A FUNCTION THAT CONTAINS THE BOTTLENECK

```
# pi_numba.py
import time

def loop(num_steps):
    step = 1.0/num_steps
    sum = 0
    for i in xrange(num_steps):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    return sum

def Pi(num_steps ):
    start = time.time()
    sum = loop(num_steps)
    pi = sum/num_steps
    end = time.time()
    print "Pi with %d steps is %f in %f secs" %(num_steps, pi, end-start)
if __name__ == '__main__':
    Pi(100000000)
```

## STEP 3. IMPORT NUMBA AND ADD A DECORATOR

```
# pi_numba.py
import time
from numba import jit
@jit
def loop(num_steps):
    step = 1.0/num_steps
    sum = 0
    for i in xrange(num_steps):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    return sum

def Pi(num_steps ):
    start = time.time()
    sum = loop(num_steps)
    pi = sum/num_steps
    end = time.time()
    print "Pi with %d steps is %f in %f secs" %(num_steps, pi, end-start)
if __name__ == '__main__':
    Pi(100000000)
```

## DISCUSS

1. Execute pi\_numba.py by **interactive -A uoa00243 -c 1 -e "python pi\_numba.py"**
2. Compare its performance. Is it adequately improved?
3. Try num\_steps=1,000,000,000 (add another 0) and see how long it takes

## 3 PARALLEL PROGRAMMING

---

Once all the options in “serial (or sequential) processing” paradigm have been exhausted, and if we still need further speed-up, “parallel processing” is the next step.

### 3.1 PARALLEL PROGRAMMING IN PYTHON

#### 3.1.1 Distributed Memory – mpi4Py

Each processor (CPU or core) accesses its own memory and processes a job. If a processor needs to access data resident in the memory owned by another processor, these two processors need to exchange “messages”. Python supports MPI (Message Passing Interface) through mpi4py module.

#### 3.1.2 Shared Memory - multiprocessing

Processors share the access to the same memory. OpenMP is a typical example. OpenMP enables concurrently running multiple threads, with the runtime environment allocating threads to different processors. Python has Global Interpreter Lock (GIL), which prevents multiple native threads from executing Python bytecodes at once<sup>1</sup>, and as a result, there is no OpenMP package for Python.<sup>2</sup>

Python’s standard “multiprocessing” module

(<http://docs.python.org/2/library/multiprocessing.html>) may be considered as an alternative option.

#### 3.1.3 GPGPU – PyCUDA, PyOpenCL

General-purpose computing on graphics processing units (GPGPU) utilizes GPU as an array of parallel processors. Python supports NVidia’s proprietary CUDA and open standard OpenCL. Ideal for applications having large data sets, high parallelism, and minimal dependency between data elements.

---

<sup>1</sup> This statement is only true for CPython, which is the default, most-widely used implementation of Python. Other implementations like IronPython, Jython and IPython do not have GIL.  
<http://wiki.python.org/moin/GlobalInterpreterLock>

<sup>2</sup> Recent development combined OpenMP with Cython and demonstrated how to use OpenMP from Python  
<http://archive.euroscipy.org/talk/6857>

## 3.2 BASICS MPI4PY PROGRAMMING

Go to “parallel” subdirectory.

### EXAMPLE 1. MPI HELLO WORLD

Write hello\_mpi.py as follows.

```
#hello_mpi.py
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()
print "hello world from process %d/%d" %(rank,size)
```

MPI program is executed by the following command

```
$interactive -A uoa00243 -c 4 -e "python ./hello_mpi.py"
```

where “-c 4” means the number of parallel processes.

### OUTPUT

```
hello world from process 0/4
hello world from process 1/4
hello world from process 3/4
hello world from process 2/4
```

### EXERCISE 1. EMBARRASSINGLY PARALLEL PHOTO PROCESSING

The following program “exercises/exercise1/denoise\_serial.py” applies a de-noise algorithm to the list of photos.

```
import numpy as np
from skimage import data, img_as_float
from skimage.filter import denoise_bilateral
import skimage.io
import os.path
import time

curPath = os.path.abspath(os.path.curdir)
noisyDir = os.path.join(curPath,'noisy')
denoisedDir = os.path.join(curPath,'denoised')

def loop(imgFiles):
    for f in imgFiles:
        img = img_as_float(data.load(os.path.join(noisyDir,f)))
        startTime = time.time()
        img = denoise_bilateral(img, sigma_range=0.1, sigma_spatial=3),
        skimage.io.imsave(os.path.join(denoisedDir,f), img)
        print("Took %f seconds for %s" %(time.time() - startTime, f))

def serial():
    total_start_time = time.time()
    imgFiles = os.listdir(noisyDir)
```

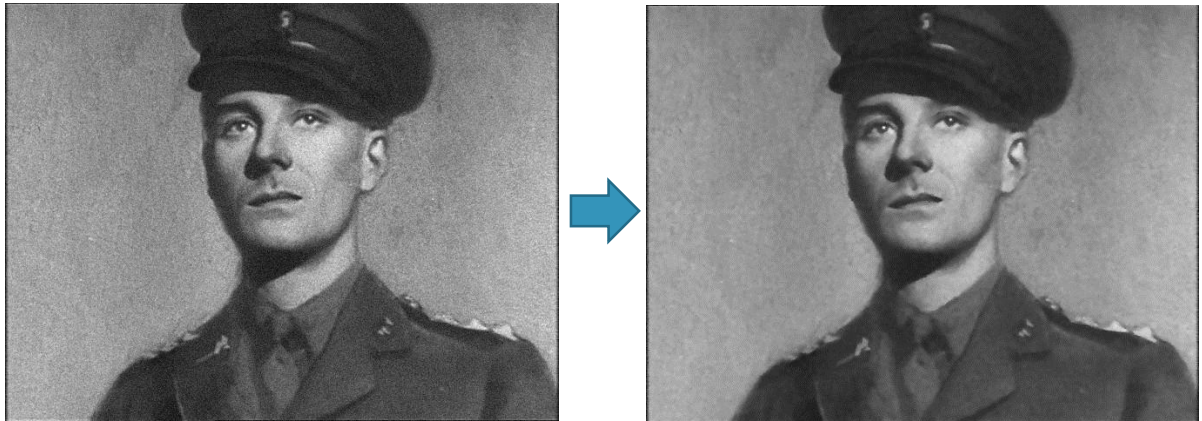
```

imgFiles=[x for x in imgFiles if '.jpg' in x]
imgFiles.sort()
loop(imgFiles)
print("Total time %f seconds" %(time.time() - total_start_time))

if __name__=='__main__':
    serial()

```

A noisy photo will look less grainy.



(Image obtained from The Alfred Hitchcock Wiki ([www.hitchcockwiki.com](http://www.hitchcockwiki.com)) – *Secret Agent* (1936))

## DISCUSS

How long does it take to process 100 photos?  
Can we use Numba to speed-up?

## HANDS ON

Complete the parallel version “`exercises/exercise1/denoise_parallel.py`”, using MPI such that 100 photos can be processed in parallel

```

import numpy as np

from skimage import data, img_as_float
from skimage.filter import denoise_tv_chambolle, denoise_bilateral, denoise_tv_bregman
import skimage.io

import os.path
import time
from mpi4py import MPI
from numba import jit

curPath = os.path.abspath(os.path.curdir)
noisyDir = os.path.join(curPath, 'noisy')
denoisedDir = os.path.join(curPath, 'denoised')

@jit
def loop(imgFiles, rank):
    for f in imgFiles:

```



```

        img = img_as_float(data.load(os.path.join(noisyDir,f)))
        startTime = time.time()
        img = denoise_bilateral(img, sigma_range=0.1, sigma_spatial=3),
        skimage.io.imsave(os.path.join(denoisedDir,f), img)
        print ("Process %d: Took %f seconds for %s" %(rank, time.time() - startTime, f))

def parallel():
    comm = MPI.COMM_WORLD
    rank = comm.Get_rank()
    size = comm.Get_size()

    totalStartTime = time.time()
    imgFiles = os.listdir(noisyDir)
    imgFiles=[x for x in imgFiles if '.jpg' in x]
    imgFiles.sort()
    numFiles = len(imgFiles)/size #number of files this process will handle
    imgFiles = imgFiles[rank*numFiles:(rank+1)*numFiles] #list of files this process will handle
    loop(imgFiles,rank)

    print "Total time %f seconds" %(time.time() - totalStartTime)

if __name__=='__main__':
    parallel()

```

Let's test this parallel version. Don't forget to run it with "interactive" command. Test with 4 cores.

```
$ interactive -A uoa00243 -c 4 -e "python ./denoise_parallel.py"
```

## EXAMPLE 2 POINT-TO-POINT COMMUNICATION

The following example "examples/hello\_p2p.py" shows the basic point-to-point communication, send and recv.

```

#hello_p2p.py
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()
if rank == 0:
    for i in range(1, size):
        sendMsg = "Hello, Rank %d" %i
        comm.send(sendMsg, dest=i)
else:
    recvMsg = comm.recv(source=0)
    print recvMsg

```

Execute this program by the following command

```
$interactive -A uoa00243 -c 4 -e "python hello_p2p.py"
```

This will launch 4 parallel processes, rank 0...rank 3, and produce output similar to:

## OUTPUT

```
Hello, Rank 1  
Hello, Rank 2  
Hello, Rank 3
```

### EXAMPLE 3. COLLECTIVE COMMUNICATION – BROADCAST

```
#hello_bcast.py  
from mpi4py import MPI  
comm = MPI.COMM_WORLD  
rank = comm.Get_rank()  
size = comm.Get_size()  
if rank == 0:  
    comm.bcast("Hello from Rank 0", root=0)  
else:  
    msg=comm.bcast(root=0)  
    print "Rank %d received: %s" %(rank, msg)
```

Execute this program by the following command

```
$interactive -A uoa00243 -c 4 -e "python hello_bcast.py"
```

This will launch 4 parallel processes, rank 0...rank 3, and produce output similar to:

## OUTPUT

```
Rank 2 received: Hello from Rank 0  
Rank 1 received: Hello from Rank 0  
Rank 3 received: Hello from Rank 0
```

### EXAMPLE 4. P2P VS COLLECTIVE – REDUCE

Consider the following example code.

```
#sum_p2p.py  
from mpi4py import MPI  
comm = MPI.COMM_WORLD  
rank=comm.Get_rank()  
size=comm.Get_size()  
val = (rank+1)*10  
print "Rank %d has value %d" %(rank, val)  
if rank == 0:  
    sum = val  
    for i in range(1,size):  
        sum += comm.recv(source=i)  
    print "Rank 0 worked out the total %d" %sum
```

```
else:  
    comm.send(val, dest=0)
```

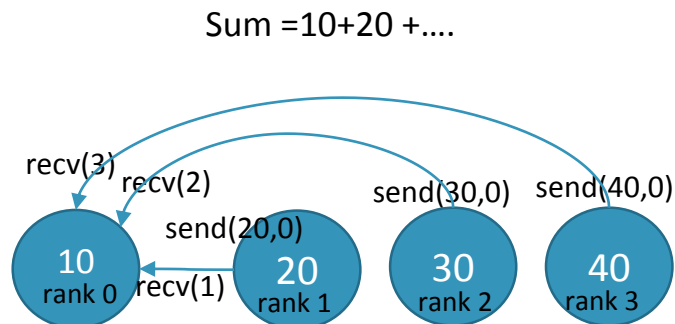


Figure 1. Computing Sum at Rank 0: Values received from Rank 1,2 and 3

Each process sends a value to Rank 0 – Rank 1 sends 20 etc. Rank 0 doesn't need to send to itself.

Rank 0 collects all values and computes the sum, and produces an output like

#### OUTPUT

```
Rank 0 worked out the total 100
```

Note that Rank 0 “receives” from Rank 1, Rank2 and Rank 3 **in sequence**. Each process starts to “send” as soon as the process gets executed, but the “send” only completes when the corresponding “recv” is called by Rank 0.

Having this “sequential” routine in parallel code is not ideal. With only 4 processes, this may not sound like a big deal, but this can be very inefficient when we have, say, 1000 processes. Sending values sequentially defeats the purpose of parallel programming.

Now, consider the following code.

```
from mpi4py import MPI  
comm = MPI.COMM_WORLD  
rank = comm.Get_rank()  
size = comm.Get_size()  
val = (rank+1)*10  
print "Rank %d has value %d" %(rank, val)  
sum = comm.reduce(val, op=MPI.SUM, root=0)  
if rank==0:  
    print "Rank 0 worked out the total %d" %sum
```

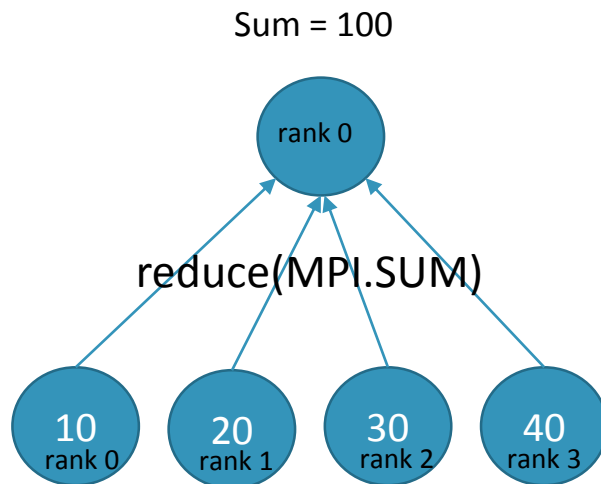


Figure 2. Computing Sum at Rank 0: All values collected and computed by "reduce"

This program produces the same result, but uses a collective call "reduce". This function causes the value in "val" in every process to be sent to the root process (Rank 0 in this case), and applies "SUM"<sup>3</sup> operation on all values. As a result, multiple values are *reduced* to one value.

## EXERCISE 2 PARALLEL COMPUTATION OF PI

Let's revisit pi\_numba.py

We have identified the "for" loop was the bottleneck and used NUMBA to make it fast

```

#pi_numba.py
import time
from numba import jit
@jit
def loop(num_steps):
    step = 1.0/num_steps
    sum = 0
    for i in xrange(num_steps):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    return sum

def Pi(num_steps ):
    start = time.time()
    sum = loop(num_steps)
    pi = step * sum
    end = time.time()
    print "Pi with %d steps is %f in %f secs" %(num_steps, pi, end-start)
if __name__ == '__main__':
    Pi(100000000)
  
```

<sup>3</sup> Other available operations are MAX, MIN, PRODUCT, Logical AND, Logical OR etc.

[http://www.open-mpi.org/doc/v1.4/man3/MPI\\_Reduce.3.php](http://www.open-mpi.org/doc/v1.4/man3/MPI_Reduce.3.php)

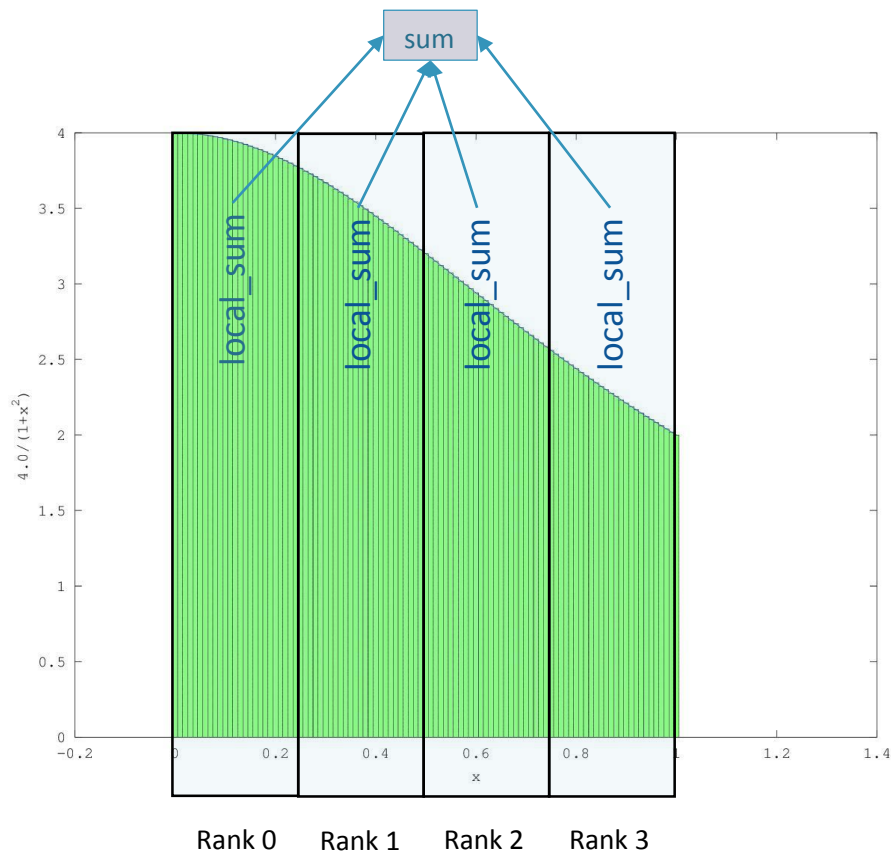


Figure 3 Computing total sum from local\_sum's computed by processes

Here,  $num\_steps=100000000$ , and the function loop will run  $num\_steps$  iterations.

Suppose we wish to parallelize this with 4 processes. We will allocate " $num\_steps/4$ " steps to each process, such that

- Steps  $[0..num\_steps/4]$  allocated to Rank 0
- Steps  $[num\_steps/4..2*num\_steps/4]$  allocated to Rank 1
- Steps  $[2*num\_steps/4..3*num\_steps/4]$  allocated to Rank 2
- Steps  $[3*num\_steps/4..num\_steps]$  allocated to Rank 3

Let's complete `pi_numba_mpi_reduce.py` to accommodate this idea.

## HANDS ON

### STEP 1: MODIFY FUNCTION LOOP() TO SPECIFY BEGIN AND END STEPS

```
@jit
def loop(num_steps, begin, end):
    step = 1.0/num_steps
    sum = 0
    for i in xrange(begin, end):
        x= (i+0.5)*step
        sum = sum + 4.0/(1.0+x*x)
    return sum
```

## STEP 2. ADD MPI

```
from mpi4py import MPI
...
def Pi(num_steps):
    comm = MPI.COMM_WORLD
    rank = comm.Get_rank()
    size = comm.Get_size()
    ...
```

## STEP 4. DECOMPOSE THE PROBLEM

```
def Pi(num_steps):
    comm = MPI.COMM_WORLD
    rank = comm.Get_rank()
    size = comm.Get_size()
    start = time.time()
    num_steps2 = num_steps/size
    local_sum = (num_steps, ??????, ??????)
    ##(to be continued)
```

The modified code above makes each process compute “local\_sum” from the allocated steps.

These “local\_sum”s from processes will need to be collected and added up to get the total “sum”.

## STEP 4. COLLECT RESULTS

In Example 3, two techniques that compute sum of values were demonstrated.

Complete the remaining of the function “Pi” such that local\_sum’s from processes are collected and the total “sum” is computed at Rank 0.

You may choose either approach – “send/recv” or “reduce”, it is advisable to use “reduce”. It is simpler, more efficient and it scales better.

```
##(continued)
sum = ??????
end = time.time()

if rank == 0:
    pi = sum / num_steps
    print "Pi with %d steps is %.20f in %f secs" %(num_steps, pi, end-start)
```

## STEP 5. EXECUTE THE PROGRAM

```
$interactive -A uoa00243 -c 4 -e "python pi_numba_mpi_reduce.py"
```

## DISCUSS

Try -c 2,4,8,16. How does it scale?

## 4 ADVANCED TOPICS

---

This tutorial presented some basic techniques that can boost the speed of Python programs.

Numba is a very simple Just-in-time compiler to boost the speed of a Python program. See [1] for more examples. Numba produces a native code automatically, but you can use Cython for more control. See [2] and [3] for more information on Cython. Some performance comparison was made and the difference appears to be very little [4].

MPI is very powerful and complex framework. We didn't discuss advanced features in MPI. For more information, see [5] for more advanced tutorial and examples. for references. MPI4py API documentation [6] is not very actively maintained. See 6 Appendix : Basic MPI functions for basic reference or see [7] for information on MPI in general.

While not covered in this tutorial, NumPy is one of the most important Python modules for scientific programming. A very nice tutorial is available online [8].

NumPy can be used in conjunction with Cython. See [2] for more info. NumPy depends on BLAS ([Basic Linear Algebra Subprograms](#)) library, and if BLAS is built with multithreading support, it will automatically utilize multi-core CPU and do parallel computing for certain linear algebra calculations such as matrix multiplication<sup>4</sup>. If you identify that matrix multiplication is the bottleneck of the program, replacing BLAS library can give you a simple solution for parallel computing.

## 5 REFERENCES

---

- [1] "Numba Examples," [Online]. Available: <http://numba.pydata.org/numba-doc/dev/examples.html>.
- [2] S. Behnel, R. Bradshaw, W. Stein, G. Furnish, D. Seljebotn, G. Ewing and G. Gellner, "Cython Tutorial Release 0.15pre," November 2012. [Online]. Available: <http://115.127.33.6/software/Python/Cython/cython.pdf>.
- [3] M. Perry, "A quick Cython introduction," 19 April 2008. [Online]. Available: <http://blog.perrygeo.net/2008/04/19/a-quick-cython-introduction/>.
- [4] J. V. d. Plas, "Pythonic Perambulations," 15 6 2013. [Online]. Available: <http://jakevdp.github.io/blog/2013/06/15/numba-vs-cython-take-2/>. [Accessed 25 4 2014].
- [5] J. Bejarano, "A Python Introduction to Parallel Programming with MPI¶," 2012. [Online]. Available: <http://jeremybejarano.zzl.org/MPIwithPython/>.
- [6] L. Dalcin, "MPI for Python v1.3 documentation," 20 Jan 2012. [Online]. Available: <http://mpi4py.scipy.org/docs/usrman/index.html>.
- [7] Open MPI, "Open MPI v1.6.4 documentation," 21 February 2013. [Online]. Available: <http://www.open-mpi.org/doc/v1.6/>.

---

<sup>4</sup> <http://stackoverflow.com/questions/5260068/multithreaded-blas-in-python-numpy>

[8] SciPy.org, “Tentative NumPy Tutorial,” [Online]. Available:  
[http://wiki.scipy.org/Tentative\\_NumPy\\_Tutorial](http://wiki.scipy.org/Tentative_NumPy_Tutorial).

---

## 6 APPENDIX : BASIC MPI FUNCTIONS

---

### 6.1 POINT-TO-POINT COMMUNICATIONS

```
send(self, obj, dest=0, tag=0)
```

```
recv(self, obj, source=0, tag=0, status=None)
```

```
comm.send([1,2,3], dest=2, tag=0)
```

Sends a list of [1,2,3] to rank 2, with message tag 0

```
x=comm.recv(source=0,tag=0)
```

Receives a message from rank 0 with tag 0 and store it to x

If you wish to monitor the status,

```
st=MPI.Status()
```

```
x=comm.recv(source=0,tag=0, status=st)
```

```
print "%s (error=%d)" %(x, st.Get_error()) #error = 0 is success
```

### 6.2 COLLECTIVE COMMUNICATIONS

```
bcast(self, obj, root=0)
```

```
reduce(self, obj, op=SUM, root=0) # op : MAX, MIN, LOR, LXOR, LAND BOR, BXOR, BAND,MAXLOC,MINLOC
```

```
scatter(self, obj, root=0)
```

```
gather(self, obj, root=0)
```

```
sum = comm.reduce(val, op=MPI.SUM, root=0)
```

Each process send its “val” variable to rank 0 and rank 0 does “SUM” operation with all collected “val”s, and stores into “sum”.

Example of scatter and gather (examples/scatter\_gather.py)

```
from mpi4py import MPI  
comm = MPI.COMM_WORLD  
rank = comm.Get_rank()  
size = comm.Get_size()
```



```

# scatter assumes a list at root to have EXACTLY "size" elements.

l=[]
if rank == 0:
    l = range(size) #l is [0,1,2,3] at rank 0 if size = 4
x=comm.scatter(l, root=0) #rank 0 scatters l and each process gets one element from l.
print "Rank %d received a scattered int "%rank +str(x)

x = x*10 #each process updates the value

l2 = comm.gather(x,root=0) #rank 0 collects x from all processes into a new list l2.
if rank == 0:
    print "Rank %d collected a list " %rank + str(l2)
    #l2 is None at other ranks
...

```

When executed with 4 processes, your output will look like this:

```

Rank 0 received a scattered int 0
Rank 1 received a scattered int 1
Rank 2 received a scattered int 2
Rank 3 received a scattered int 3
Rank 0 collected a list [0, 10, 20, 30]

```

Note that “scatter” requires the root has the list of exactly “size” elements. One element from the list will be distributed to each process. If you wish to distribute items in different way, you will have to restructure the list. For example, if you have 4 processes, (ie. size=4), 8 elements (0,1,2,3,4,5,6,7) and you wish to distribute 2 elements to each process, you have to have to package the list like:

```
l=[ [0,1],[2,3],[4,5],[6,7] ]
```