Day 2:
YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

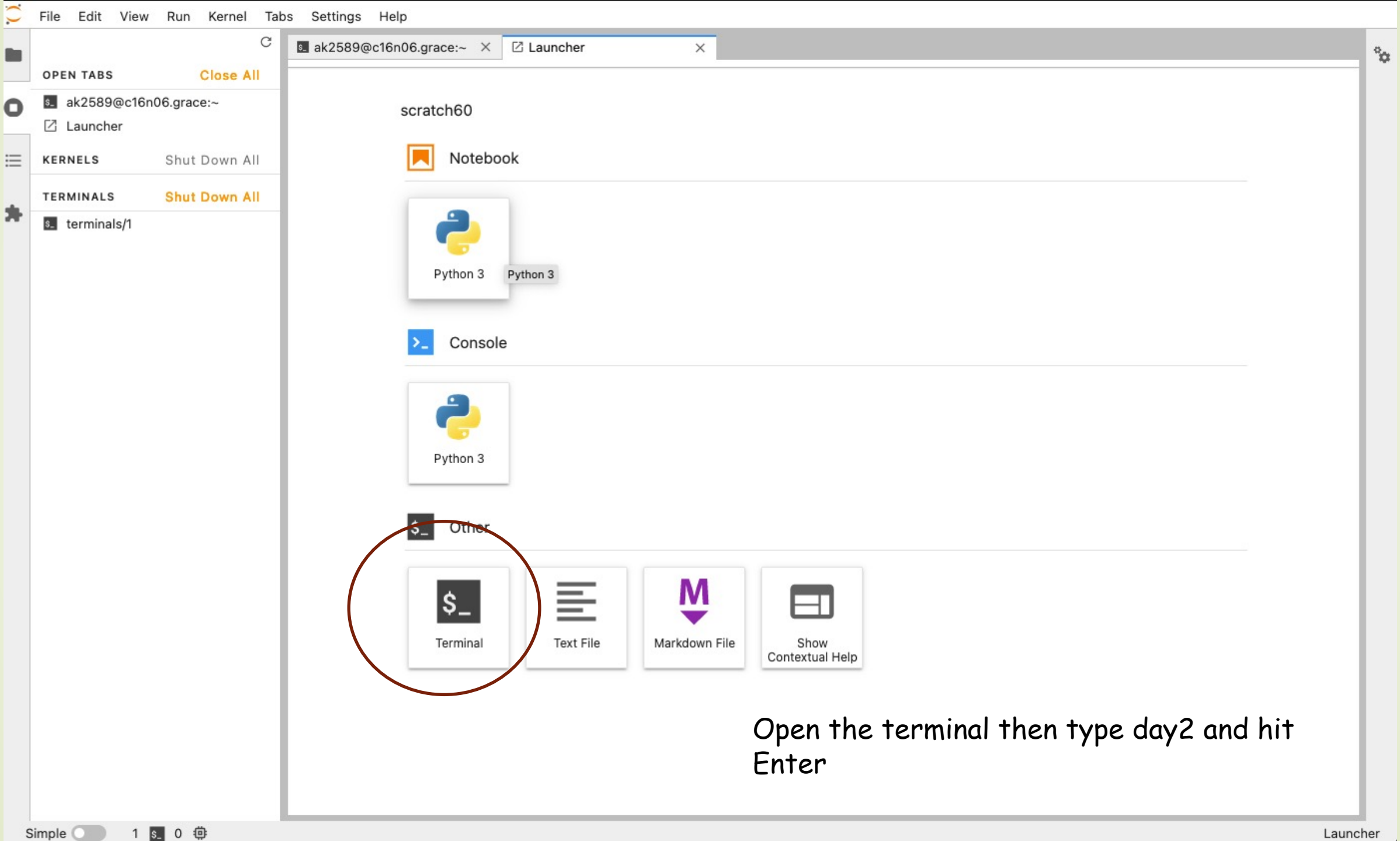
Aakash Kumar
aakash.kumar@yale.edu

Introduction to Parallel Computing: Hands-on

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

LEARNING GOALS

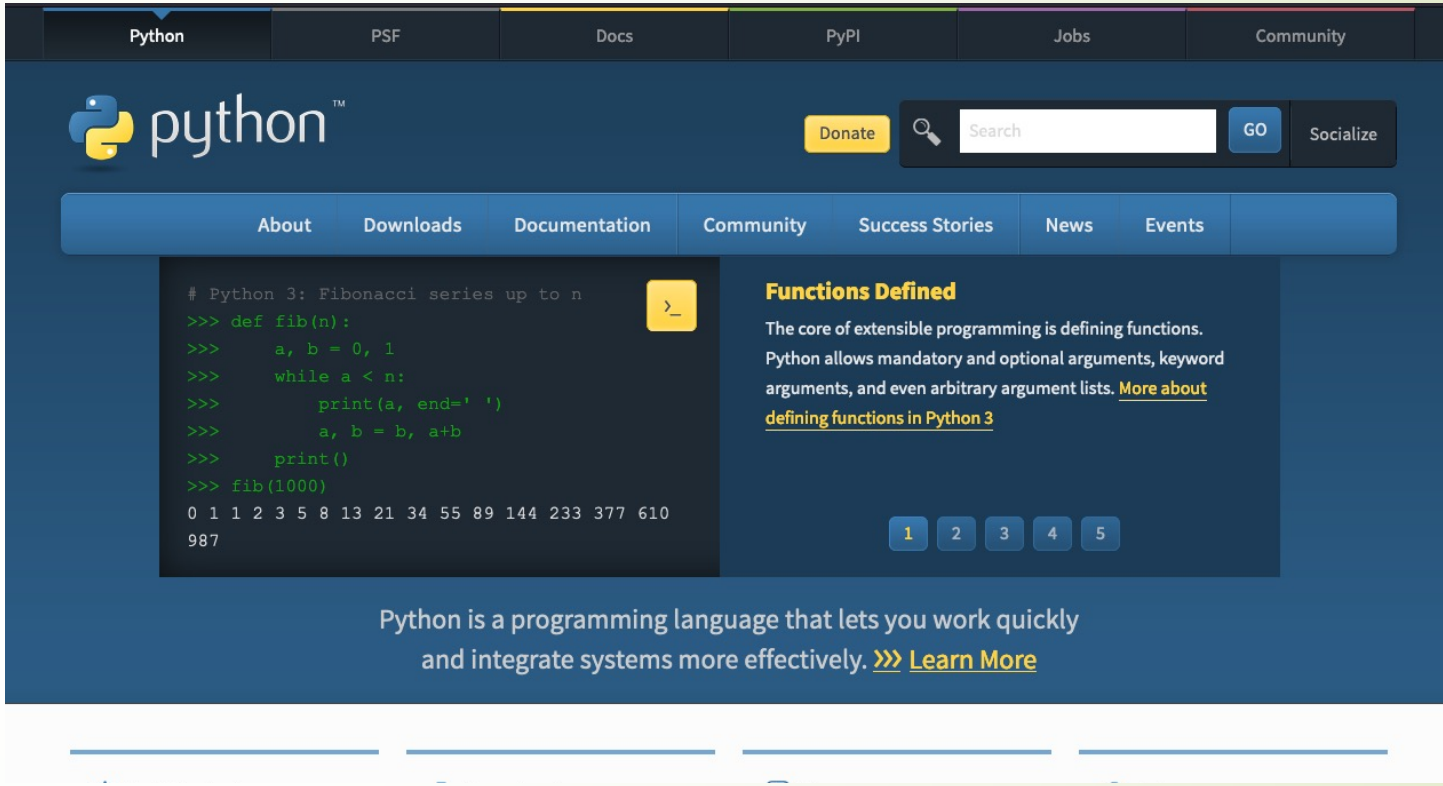
- Run basic python scripts to sum numbers and arrays
- Run parallel script to access difference cores
- Apply the ideas of broadcasting, scattering and gathering from parallel computing lecture earlier



Open the terminal then type day2 and hit Enter

PYTHON

- Scripting language
- Object-oriented
- Easy to read, friendly design




```
[Terminal] python
>>> a = 2
>>> b = 3
>>> c = a + b
>>> c
5
```

- Exit the python environment (>>>) by pressing Ctrl+D
- We can also write the above code in a file `sum.py`
- then run it as

```
[Terminal] python sum.py
```

EXERCISE 1a, 1b, 1c

- run the code in file 1a_sum.py

```
a = 2
b = 3
c = a + b
print(c)
print("The sum is", c)
```

- repeat the above with floating point numbers, so 2 is 2.0 (1b_sum_float.py)
- Use numpy module of python to define a and b as np.a, np.b and sum (1c_sum_numpy.py)

```
import numpy as np
np.a = 2
np.b = 3
np.c = np.a + np.b
print(np.c)
```

EXERCISE 1d, 1e

- Array is a list of data, represented in [], so a = [1 , 2, 3] is an array of size 3
- Its elements are a[0], a[1], a[2]
- numpy module can be used to create an array

```
np.a = np.array([1, 2, 3])
np.b = np.array([4, 5, 6])
```

- Run the following code in a file 1d_sum_array.py

```
np.c = np.a + np.b
print(np.c)
print("The sum is", np.c)
```

EXERCISE 2

- Copy the below code snippet to a file called hello.py

```
mpirun –n 6 python greetings.py
```

```
from mpi4py import MPI

comm = MPI.COMM_WORLD        # comm is the MPI object we will use
size = comm.Get_size()       # how many processes (1 on each core)
rank = comm.Get_rank()       # rank of processor (ID) 0 is head processor

print("Hello world from rank", str(rank), "of", str(size))
```

- Run the python program greetings.py on 6 cores (format is slightly different than what is shown here, notice the comm.send and comm.recv)

- Each core will print its rank and total number of cores

EXERCISE 3: BROADCAST

- broadcast data to all cores
- Code snippet:

```
if rank == 0:
    data = np.arange(4.0)

else:
    data = None

data = comm.bcast(data, root=0)

if rank == 0:
    print('Process {} broadcast data:' .format(rank), data)
else:
    print('Process {} received data:' .format(rank), data)
```

```
mpirun -n 4 python bcast.py
```

```
Process 0 broadcast data: [0. 1. 2. 3.]
Process 2 received data: [0. 1. 2. 3.]
Process 1 received data: [0. 1. 2. 3.]
Process 3 received data: [0. 1. 2. 3.]
```

EXERCISE 4: SCATTER

- scatter different data to various cores
- Code snippet:

```
if rank == 0:
    data = np.arange(4.0)

else:
    data = None

data = comm.scatter(data, root=0)

if rank == 0:
    print('Process {} broadcast data:' .format(rank), data)
else:
    print('Process {} received data:' .format(rank), data)
```

- 4b_scatter.py scatters arrays of data to all cores.

```
mpirun -n 4 python 4a_scatter.py
```

```
Process 0 has data: 0.0
Process 1 has data: 1.0
Process 2 has data: 2.0
Process 3 has data: 3.0
```

EXERCISE 5: GATHER

- Gather data from all processes/cores and Do something (SUM it up, etc.)
- Code snippet:

```
mpirun -n 4 python 5_gather.py
```

```
do something
.....
.....
.....
.....

partial_sum = comm.gather(partial_sum, root=0)

if rank == 0:
    print(Sum is {} from all data:' .format(sum(partial_sum)))
```

EXSERICSE 5:REDUCE

- reduce data from all processes/cores and sum it while collecting
- Code snippet:

```
mpirun –n 4 python 5_reduce.py
```

```
do something
.....
.....
.....
.....

total_sum = comm.reduce(partial_sum, op=MPI.SUM, root=0)

if rank == 0:
    print(Sum is {} from all data:' .format(total_sum))
```

RESOURCES

- https://hpc.llnl.gov/training/tutorials/introduction-parallel-computing-tutorial
- https://towardsdatascience.com/parallel-programming-in-python-with-message-passing-interface-mpi4py-551e3f198053
- https://www.kth.se/blogs/pdc/2019/08/parallel-programming-in-python-mpi4py-part-1/