# Parallel Programming with Python

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# You will know

- multithreading and multiprocessing models
- commonly used strategies for parallelizing a serial Python code
- popular Python packages for parallelizing your code

# Related workshops

Parallel programming with OpenMP and MPI
(Debbie Samaddar, RCC)

Python with GPUs
(with Kris Keipert, NVIDIA)

# RCC Midway Clusters

time for you to log in to Midway3 ...

- Log in to the login node via SSH, or via ThinLinc

  ssh [your-cnetid]@midway3.rcc.uchicago.edu

- Clone the github repo for the examples

  git clone https://github.com/rcc-uchicago/parallel-python.git

- Request an interactive job

  sinteractive -N 1 --ntasks-per-node=8 --account=rcc-guest

- Load the modules and activate the environment

  module load python/anaconda-2021.05 openmpi/4.1.2+gcc-7.4.0

  source activate parallel

# Why parallelize your code?

Having repeated tasks on different datasets or input params

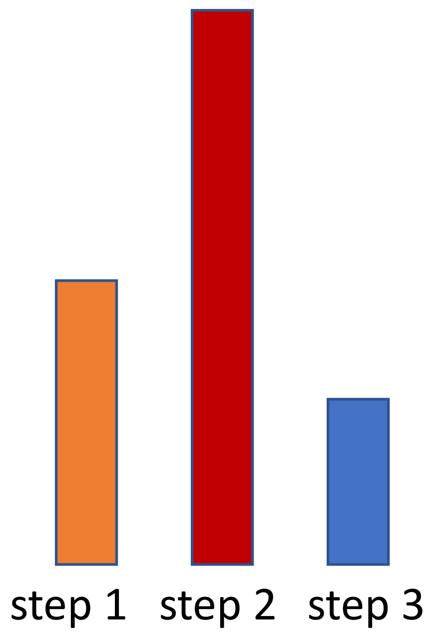
Having access to enough computing resources

Having limited time until deadlines

Curious?

# Understand your code: How can you parallelize it?

- Identify the bottlenecks in the flow chart of your program – using timers and profilers
  - How often data I/O with hard drive is performed?
  - Data layout: Are data structures arranged to memory access friendly patterns
  - Computation: Any heavy `for` loops? any external modules/packages calls in the nested inner loop?
- Can the bottleneck(s) be parallelized?
  - or, can the workload be distributed among processing units, aka "workers"?



# Amdahl's Law

- Theoretical speedup is limited by the contribution of the non-parallelized parts

$$S(N) = \frac{1}{(1-p) + \frac{p}{N}}$$

$$\lim_{N \to \infty} S(N) = \frac{1}{1-p}$$

S = theoretical speedup with N processing units

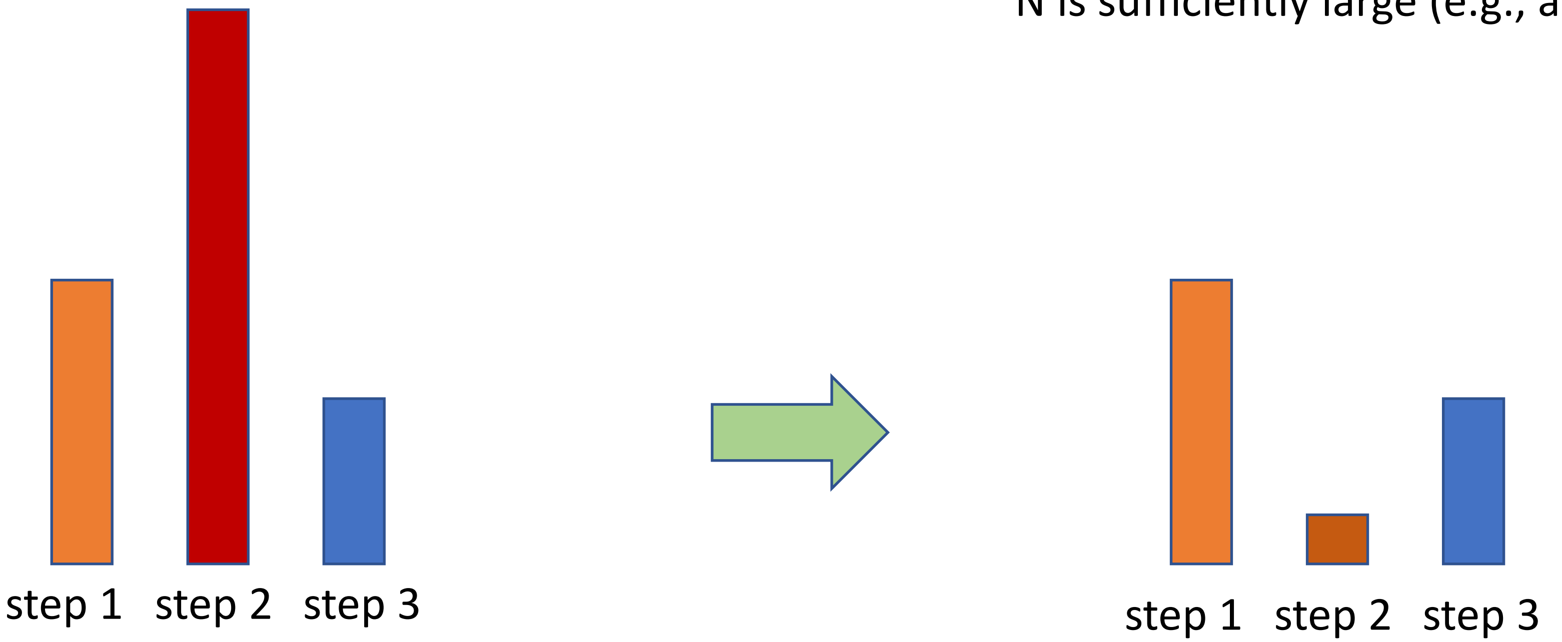
p = time percentage of the parallelized parts

N = theoretical speedup gained for the task with N processing units

# Amdahl’s Law

Serial code timings breakdown

Parallel code timings breakdown
N is sufficiently large (e.g., at breakeven)




$p = 0.5$

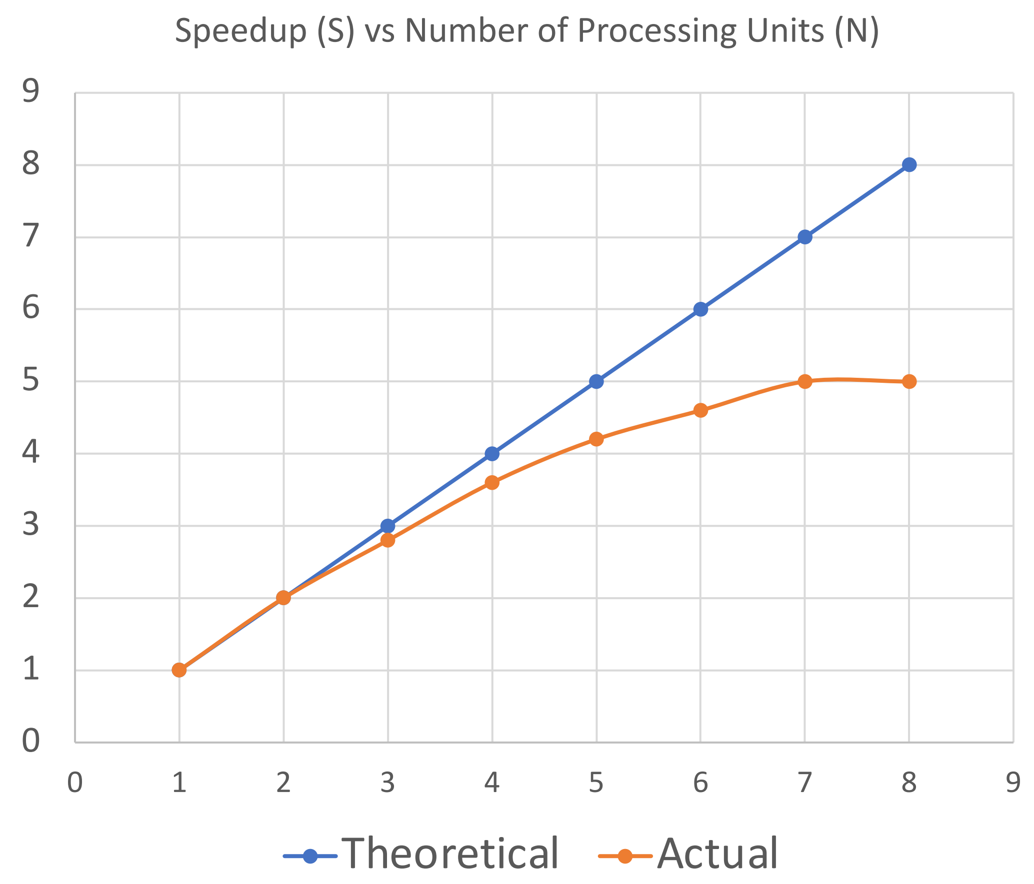
$$\lim_{N\to\infty} S(N) = \frac{1}{1-p} = \frac{1}{1-0.5} = ?$$

# Parallelization strategies: Ways to distribute workload among workers

- Process level:
  - embarrassingly parallel (multiprocessing)
  - map/reduce (multiprocessing)
- Data level:
  - data decomposition (multiprocessing, or multithreading)
- Instruction level:
  - just-in-time compilation for multi-core CPU or GPU targets (multithreading)

# Parallelization performance: Strong scaling

- Parallelization introduces overhead:
  - communication/sync between workers
- Strong scaling analysis show time to solution, or speedup, as a function of number of workers (threads, or processes)
  - linear scaling: $S_{linear} = t_1/t_N = N$
  - computation vs. communication break-even point
    - P* where speedup stops increasing with P



# Processes and threads

## A process is a program managed by the operating system (OS)

- operating on separate memory spaces
- performing a series of executions, or
- consisting of an infinite loop waiting for OS events (GUI programs)
- able to spawn/fork child processes

## A thread is a sub-process created and managed by a process

- sharing the memory space with peer threads in the same process
- able to spawn/fork child threads

## By default, Python is a program (an interpreter) with a single thread

```
python your_script.py
```

# Multithreading and Multiprocessing Programming Models

- **Multithreading**:
  - the main thread spawns/forks multiple threads
  - each thread access to the data in the shared memory pool
  - each thread executes the instructions, may sync with other threads
  - threads are terminated (joined) when done

- **Multiprocessing**:
  - create child processes, or launch peer processes (mpirun or srun)
  - each process allocates data in its memory space
  - each process executes the instructions, may send/receive among the processes
  - processes are closed (finalized) when done

# Know the hardware where your code is running

to decide which parallelization strategies would be optimal

- Single-node configuration
  - Multi-core CPUs: how many physical CPU cores? hardware threading off/on? (lscpu, /etc/cpuinfo) supporting vectorization? L1 cache size?
  - Memory
  - GPUs attached? Types? Memory size and bandwidth?
  - Storage
- Multiple-node configuration
  - Interconnect bandwidth: Infiniband?

# Midway3 Compute Nodes

to decide which parallelization strategies would be optimal

- Show the partition information:

  scontrol show partition broadwl

  sinfo –p broadwl

- Show the node information: scontrol show node midway3-xxxx
  - How many physical CPU cores?
  - Memory
  - GPUs attached?

# Profiling tools for (serial) Python codes

- **time**
- cProfile
- **pyinstrument**

Fine-grained profiling may distort actual performance.

# Profiling a python code segment with time (Exercise 1)

```
python profiling.py
```

```python
import time

start_time = time.time()
# your code segment
elapsed_time = time.time() - start_time
```

# Profiling a python code with pyinstrument

```
python profiling.py
```

```python
from pyinstrument import Profiler

profiler = Profiler()

profiler.start()
# your code segment
profiler.stop()

profiler.print()
```

# Process-based parallelization with multiprocessing Module (Exercise 2)

test-multiprocessing.py

```
from multiprocessing import Process

def func(input_args):
   (input_args)

p1 = Process(target=func, args=(args1,))
p2 = Process(target=func, args=(args2,))
p1.start()
p2.start()
p1.join()
p2.join()
```

# Communicate between processes with Queue (Exercise 3 )

`python map-reduce-pi.py`

- Each proc puts the result into a queue, and get the result

```
from multiprocessing import Process, Queue

def func(my_queue, input_args):
   my_queue.put(result)

q = Queue()
p = Process(target=func, args=(q, args,))
p.start()
res = q.get()
p.join()
```

# Map and reduce

`python map-reduce-pi.py`

- Mapping functions to process-owned data
- Reducing (tally) the results from the queues

# Map and reduce with multiprocessing Pool

```
python map-reduce-pi.py
```

```
from multiprocessing import Pool

def func(input_args):
  return result

with Pool(Ncores) as pool:
  results = pool.map(func, [args[i] for i in range(Ncores)])
np.sum(results)/Ncores
```

# Map and reduce with multiprocessing Pool

`python map-reduce-pi.py`

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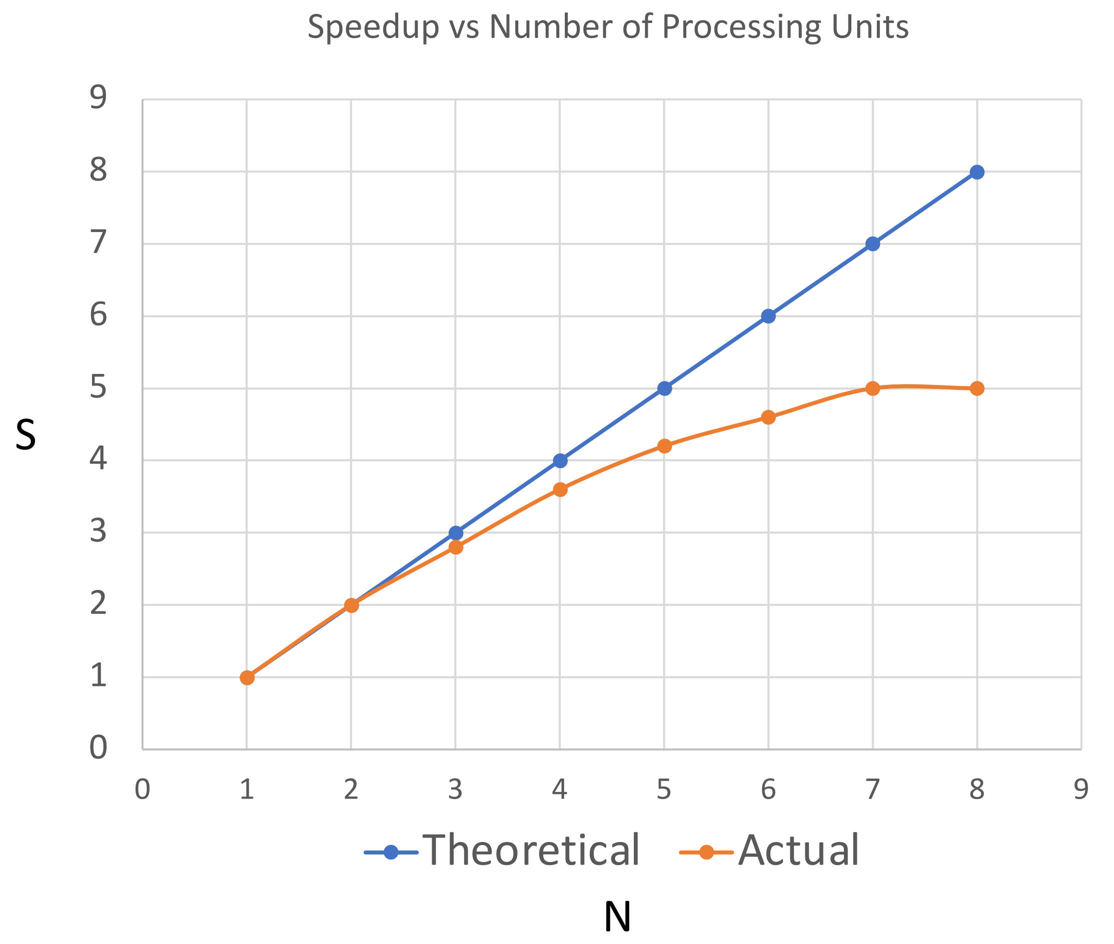
from multiprocessing import Pool

def func(input_args):
  return result

with Pool(Ncores) as pool:
  results = pool.map(func, [args[i] for i in range(Ncores)])
np.sum(results)/Ncores
```

# Parallelization efficiency: Strong scaling (Exercise 4)

`python performance.py`



# Process-level parallelization: mpi4py Module

- a wrapper for an underlying Message Passing Interface (MPI) library (OpenMPI, MPICH or Intel MPI)
- launches multiple Python instances with mpirun

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
nprocs = comm.Get_size()
my_rank = comm.Get_rank()

func(input_args, my_rank, nprocs)
```

# Communication between processes: MPI binding (Exercise 5)

```
mpirun –np 4 python mpi-comm-ops.py
```

```python
from mpi4py import MPI

comm = MPI.COMM_WORLD
nprocs = comm.Get_size()
my_rank = comm.Get_rank()

func(input_args, my_rank, nprocs)
```

From Parallel programming with MPI workshop:

- Process initialization/finalization
- Point-to-point communication
  - MPI_Send/MPI_Recv
  - MPI_Wait
- Collective communication
  - MPI_Gather/MPI_Reduce
  - MPI_Bcast/MPI_Scatter

```
Midway3: ulimit –l unlimited (if getting errors with UCX workers init)
```

# DIY: Calculate \pi with mpi4py

10 minutes

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
nprocs = comm.Get_size()
my_rank = comm.Get_rank()

local_result = calculate_pi()

comm. Allreduce(result_local, result, op=MPI.SUM)
```

# Map/reduce with mpi4py MPIPoolExecutor

analogous to `multiprocessing Pool`

```
from mpi4py.futures import MPIPoolExecutor

def func(args):
  # do smth

with MPIPoolExecutor() as executor:
   input_args_list = (input_args[i] for i in range(Nprocs))
   result = executor.map(func, input_args_list)
```

Your homework assignment!

# Data-level parallelization: multithreading

- Multithreading is generally prohibited by the Global Interpreter Lock (GIL) used by Python
  - to avoid write conflicts
  - to prevent leaked memory (object mem allocation and release)
- Module `multithreading` is useful for launching <u>I/O bound tasks</u> concurrently

# Comparing I/O bound vs CPU-bound tasks: multithreading (Exercise 6)

`python test-multithreading.py`

```
from threading import Thread

def func(input_args):
   (input_args)

t1 = Thread(target=func, args=(args1,))
t2 = Thread(target=func, args=(args2,))
t1.start()
t2.start()
t1.join()
t2.join()
```

# Common issues and Debugging Python codes

- Deadlocks during process communications:
  - Send/Recv
  - Bcast
- Write conflicts to shared variables
- Debugging tools
  - **print** on selected ranks
  - **pdb**

```
python –m pdb myscript.py
```

# Practicing with some bugs…

- Deadlocks during process communications (`mpi-comm-ops.py`)
  - Send/Recv: unmatched src/dst ranks
  - Bcast: called from some proc(s)
- Write conflicts to shared variables
- Debugging tools
  - **print** on selected ranks
  - **pdb**

```
python –m pdb myscript.py
```

# What about Python with GPU?

- Offload computation to the GPU: Single-Instruction Multiple-Threads model
- Drop-in options: **numba**, **cupy**

# Summary

- Profiling and Amdahl’s law
- Multiprocessing and multithreading models
- Popular Python modules

# Questions?

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