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 Samadar, 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

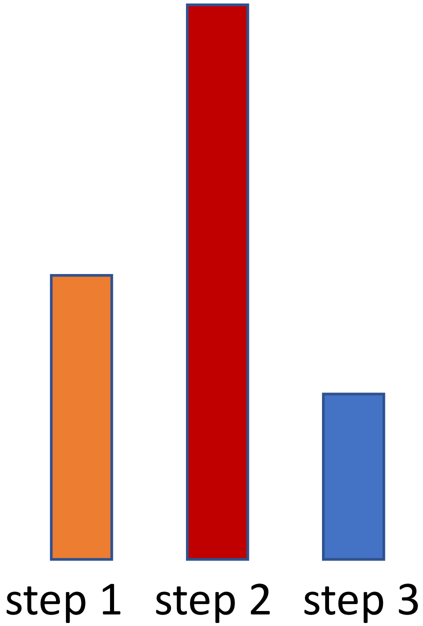
Having access to enough computing resources

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

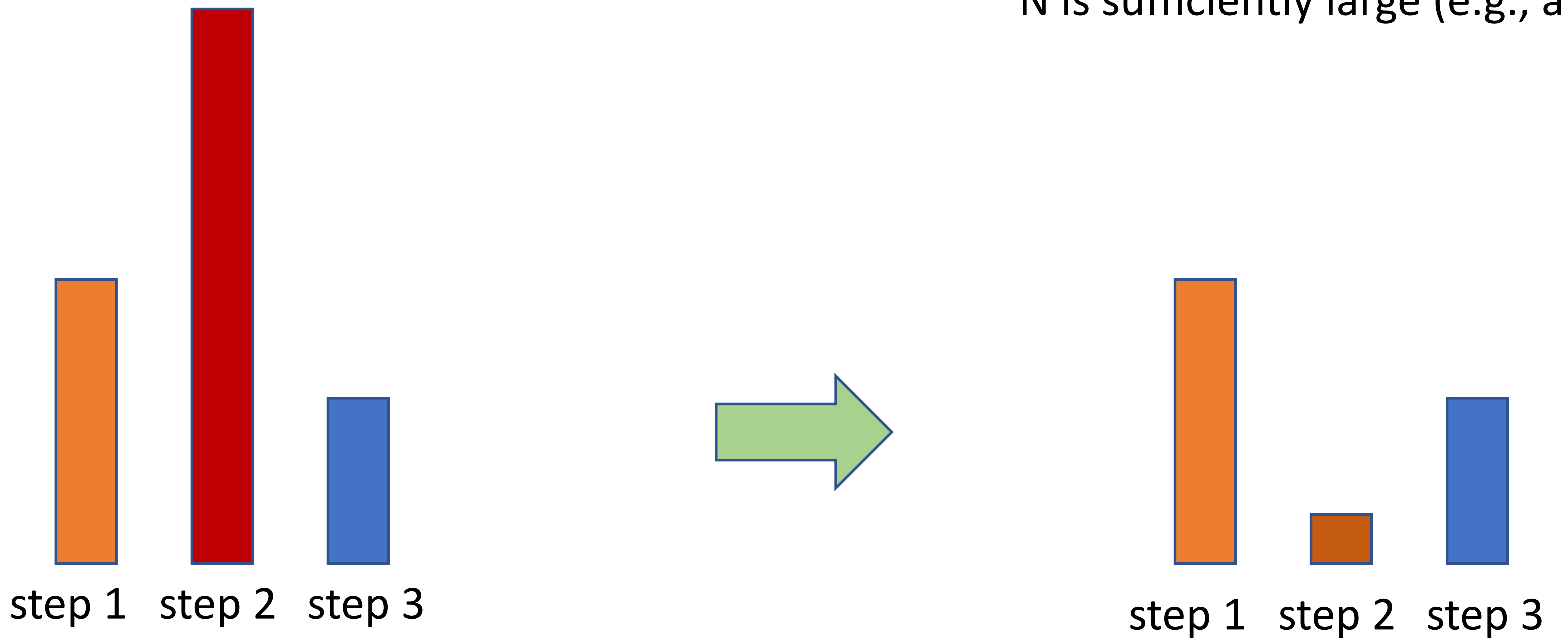
p = time percentage of the parallelized task

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

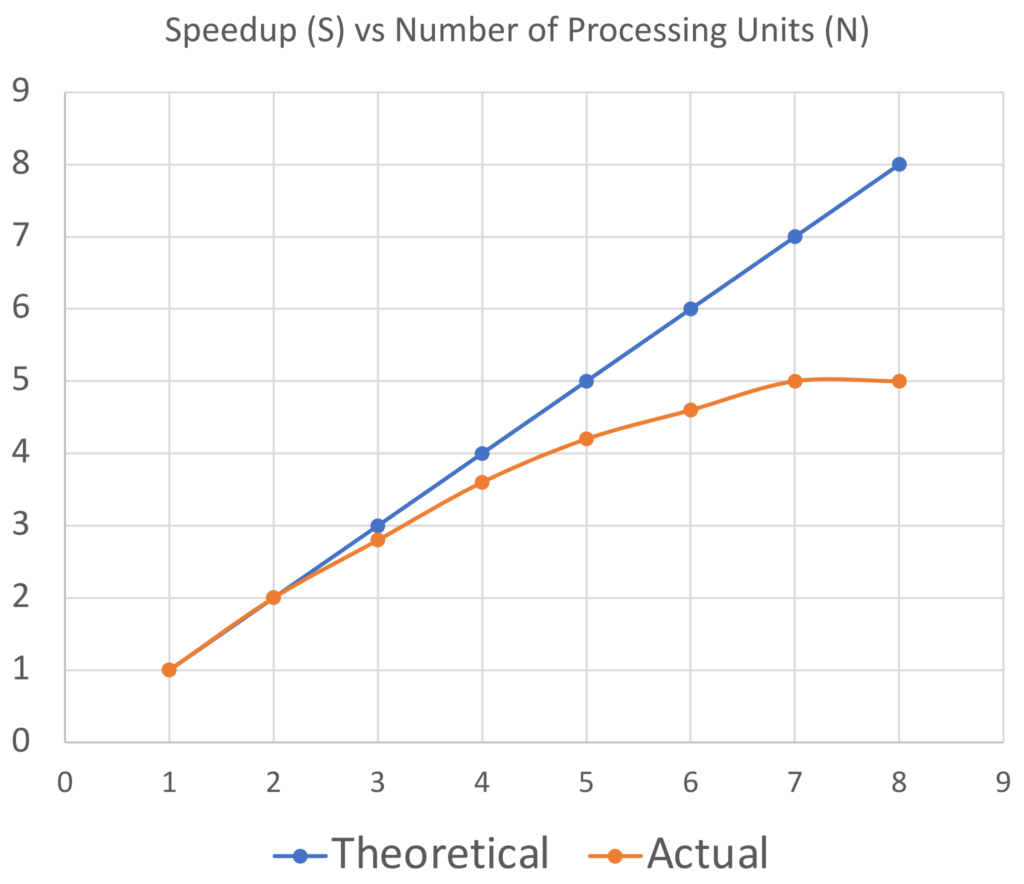
$$\lim_{N \to \infty} S(N) = \frac{1}{1-p} = \frac{1}{1-0.5} = ?$$

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
```

```
import time

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

Profiling a python code with pyinstrument

```
python profiling.py
```

```
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
```

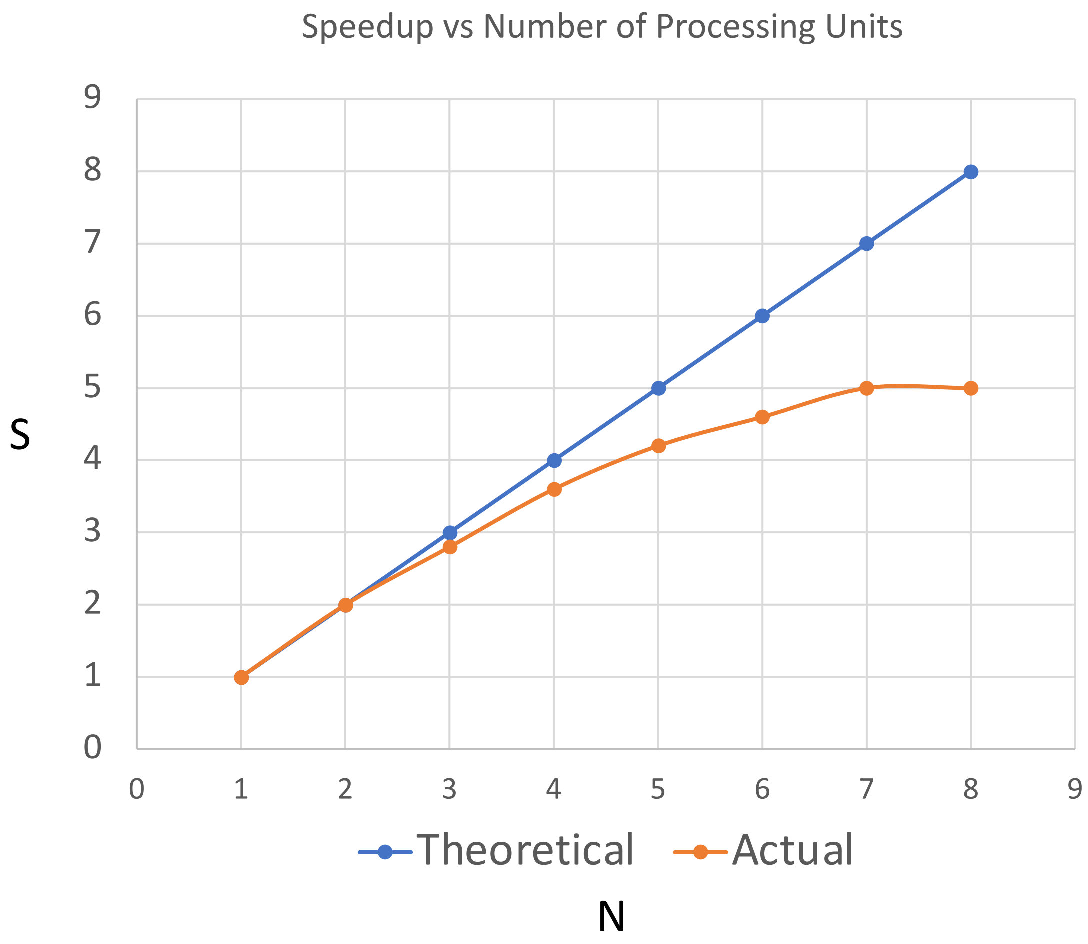
```
from multiprocessing import Pool

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
```

```
from mpi4py import MPI

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

func(input_args, my_rank, nprocs)
```

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(input_args):
  # do smth

with MPIPoolExecutor() as executor:
   iterable =
   result = executor.map(func, input_args)
```

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 I/O bound tasks

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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