Parallel Programming with Python

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You will know

- common strategies for parallelizing a serial Python code
- multithreading and multiprocessing models
- popular Python packages and some examples

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

RCC Midway Clusters

time for you to log in to **Midway3** ...

1. Log in to the login node via SSH, or via ThinLinc

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

2. Clone the github repo for the examples

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

3. Request an interactive job

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

4. Load the modules and activate the environment

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

   ulimit –l unlimited

   source activate parallel

No access to Midway3?

1. Clone the github repo for the examples

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

   cd parallel-python

2. Create a Python environment

   python3 –m venv parallel

3. Activate the environment and install the necessary packages

   source parallel/bin/activate

   pip install –r requirements.txt

Why parallelize your code?

Need to perform repeated tasks on different datasets or input parameters

Need to scale up your problem size or dataset

Need to meet some deadline

Curious?

Parallel programming with Python in action (1)

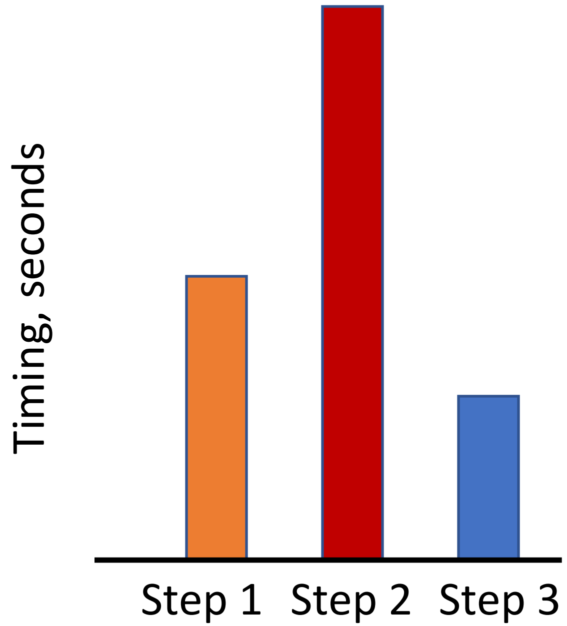
- Researcher needs to scan through thousands of input parameter sets (Help Desk Ticket #57390)
  - For each input parameter set, process input data from a set of files, and write the results to separate output files
- Proposed solution:
  - Divide the list of input parameter sets into equal-sized chunks
    - for each chunk of parameter sets, bind the Python process to a set of CPU cores on a compute node
    - combine the output files for further analysis

Parallel programming with Python in action (2)

- NSF Collaborator Affiliations Form of a principal investigator (PI)
  - Given the PI's full name, list all the coauthors within a period and their affiliations
- https://github.com/rcc-uchicago/collaborators
  - Search over Google Scholar for the list of PI's coauthors
  - Divide the list of coauthors into equal-sized chunks
    - for each chunk of coauthors, launch a process to search for the affiliation of a coauthor over Google Scholar and/or ORCID
    - combine the results into a single list

Understand your code: How can you parallelize it?

- Identify the bottlenecks in the flow chart of your program – using timers and profilers
  1. How often data I/O with hard drive is performed?
  2. Data layout: Are data structures arranged to memory access friendly patterns?
  3. 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"?



Profiling tools for (serial) Python codes

Commonly used Python modules:

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

Note: 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()
# put your code segment here
...
elapsed_time = time.time() – start_time
```

NOTE: time.perf_count() is recommended for high-resolution timings (for short events) as it relies on the CPU clock vs. time.time() using OS time() function. For long events, the diff between the two becomes negligible.

Profiling with pyinstrument (Exercise 1)

python profiling.py

```
from pyinstrument import Profiler

profiler = Profiler()

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

profiler.print()
```

Debugging your Python codes

- Follow the control flow of your code, add break points, step in and out of functions, and print out the variable values
- Debugging tools
  - **print** command
  - **pdb** module

python –m pdb my_script.py

Amdahl's Law

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

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

S = theoretical speedup with N processing units

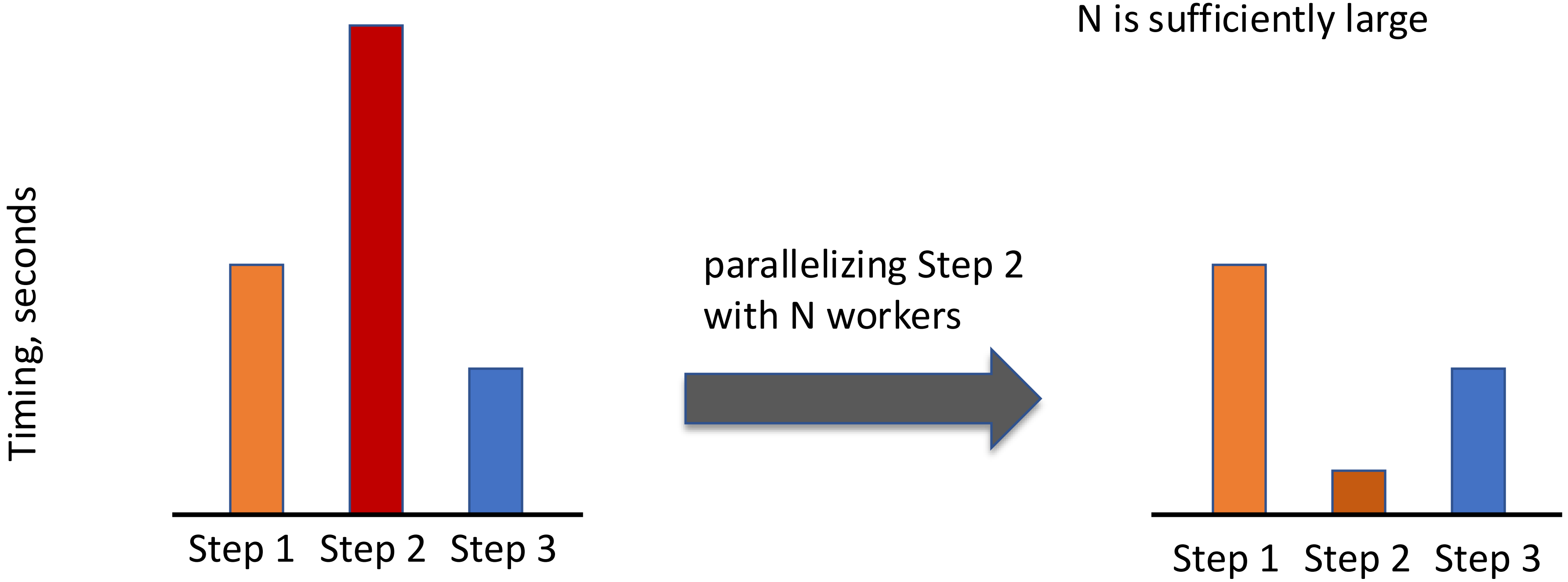
p = time percentage of the parallelized parts

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



p = 0.5

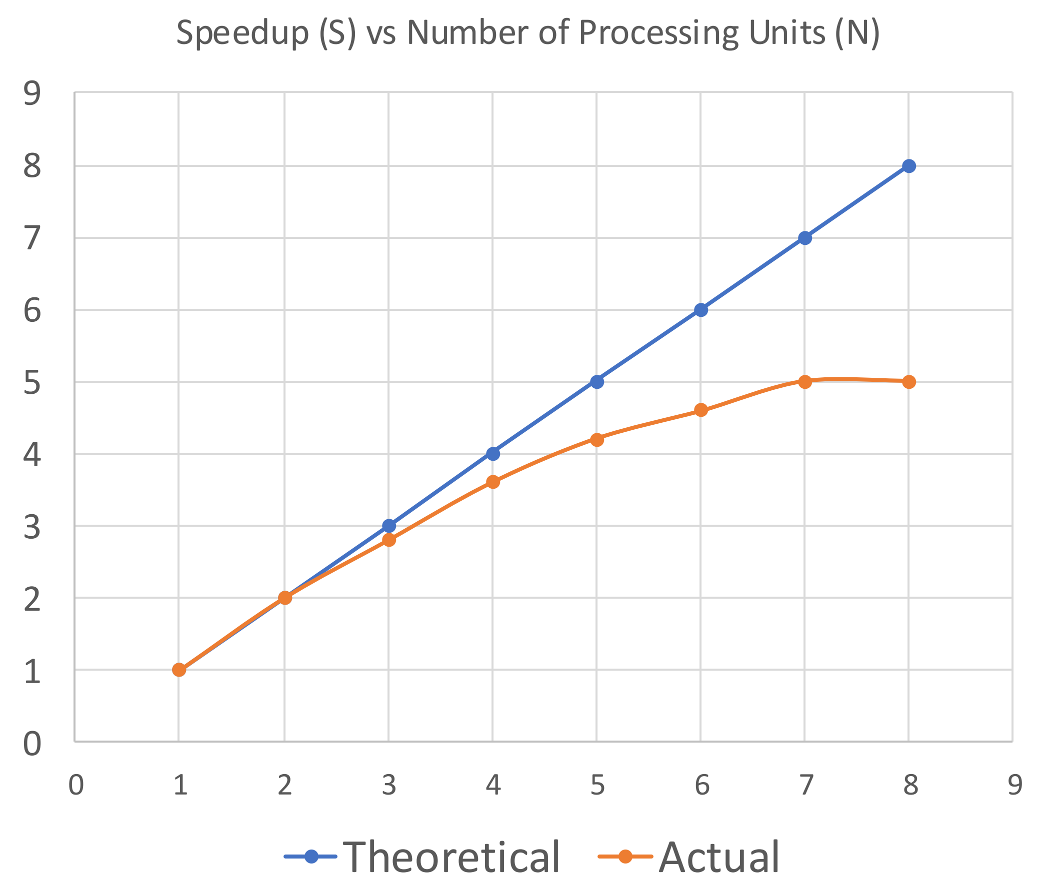
$$\lim_{N \to \infty} S(N) = \frac{1}{1-p} = \frac{1}{1-0.5} = ?$$

Parallelization strategies: Ways to distribute workload among workers

- **Application level:**
  - embarrassingly parallel
- **Process level:**
  - data decomposition
  - map and reduce
- **Instruction level:**
  - just-in-time compilation for multi-core CPU or GPU targets

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



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 (avx512)? 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 caslake

  sinfo –p caslake

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

Processes and threads

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

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

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 in order, may sync with other threads
  - threads are terminated (joined) when done

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

Multiprocessing Programming Models

- **Spawning vs Forking**
  - each forked Python process inherits all the variables and states, and modules of the parent Python process, progressing independently from the forking point.
  - each spawned process is a fresh Python process, the modules are reimported, new copies of the variables are created.

Action	fork	spawn
Create new PID for processes	yes	yes
Module-level variables and functions present	yes	yes
Each child process calls plot_function on multiple pool args	yes	yes
Child processes independently track variable state	yes	yes
Import module at start of each child process	no	yes
Variables have same id as in parent process	yes	no
Child process gets variables defined in name == main block	yes	no
Parent process variables are updated from child process state	no	no
Threads from parent process run in child processes	no	no
Threads from parent process modify child variables	no	no

https://britishgeologicalsurvey.github.io/science/python-forking-vs-spawn/

Multithreading within Python codes

- Performance gain with multithreading is generally prohibited by the Global Interpreter Lock (GIL) used by Python
  - to avoid write conflicts
  - to prevent memory leaks (object mem allocation and release)

- For launching I/O bound tasks concurrently (file reading/writing, web downloading), use the multithreading module
  - example: test-multithreading.py

Quiz

Which of the following statements INCORRECT?

A) A process can fork or spawn into multiple child processes with separate memory spaces.

B) A thread can fork or spawn into multiple threads sharing the same memory space.

C) Child processes from a parent process cannot exchange their data.

Process-level parallelization with the multiprocessing module (Exercise 2)

python3 test-multiprocessing.py

```
from multiprocessing import Process

def myfunc(arg1, arg2):
   ....
p1 = Process(target=myfunc, args=(arg11, arg12,))
p2 = Process(target=myfunc, args=(arg21, arg22,))
p1.start()
p2.start()
p1.join()
p2.join()
```

fork is the default mode of creating a new process with the multiprocessing module on Linux.

Communicate between processes with Queue (Exercise 3)

python3 map-reduce-pi.py

- Each proc puts the result into a Queue object, and get the result

```
from multiprocessing import Process, Queue

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

q = Queue()
p = Process(target=myfunc, 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 (tallying or comparing) the results across the queues
  - a common way to communicate data between processes

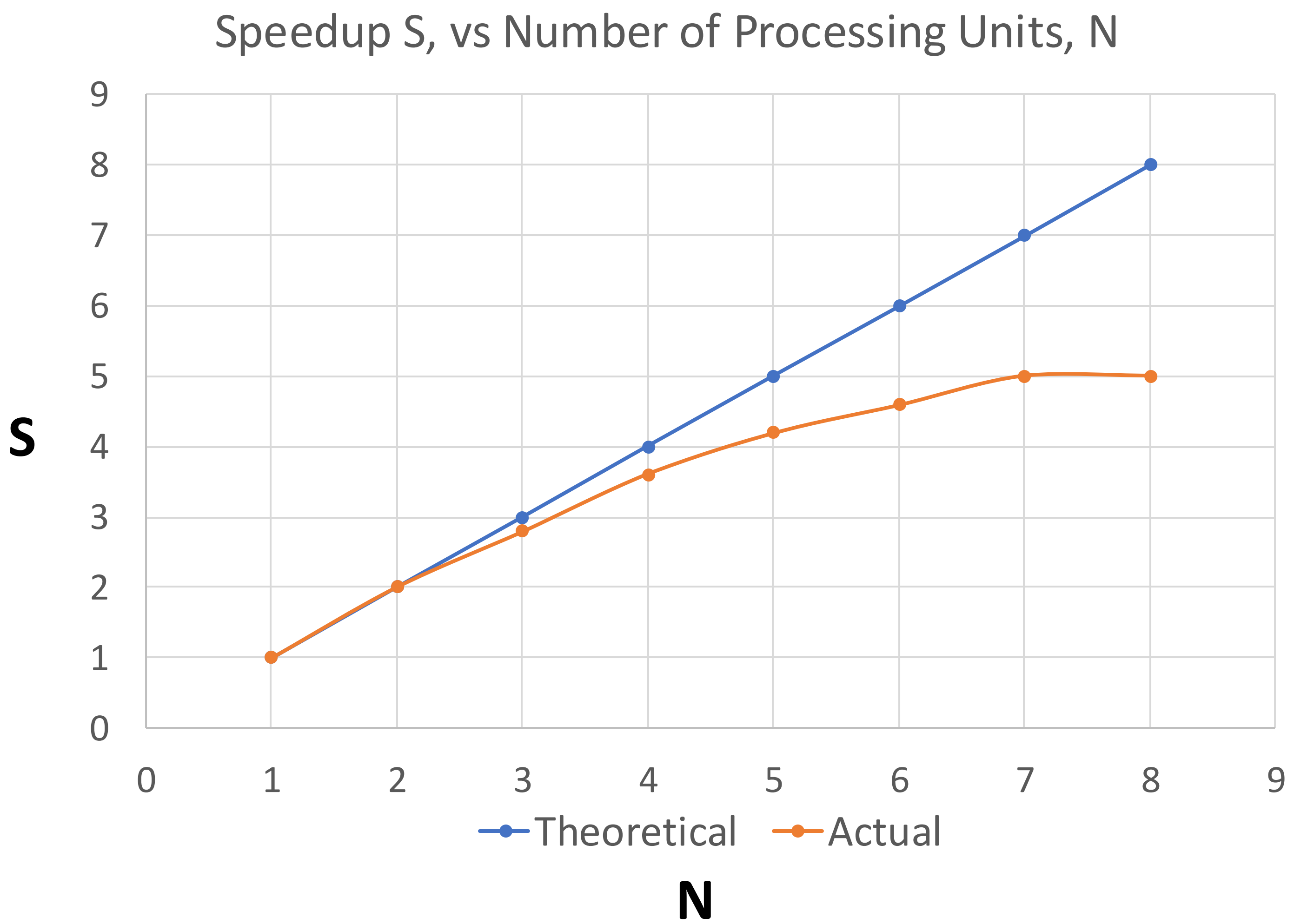
Map and reduce with multiprocessing Pool

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



Quiz

Strong scaling shows how a parallel code performs

A) given a fixed problem size per processing units (N/P) as the number of processing units (P) increases.

B) given a fixed problem size (N) as the number of processing unit (P) increases.

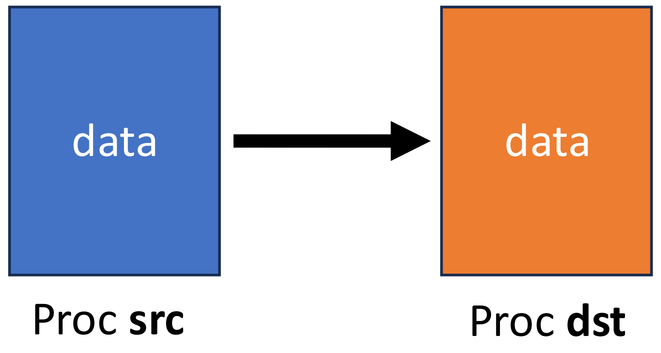
C) when there is a strong relationship between the input and output data.

Communication between processes: Message Passing Interface (MPI)Basics

- Message Passing Interface (MPI) is a specification (programming model) for exchange data between processes
  - communications: point-to-point, collective (one-to-all, all-to-all), one-sided
  - C/C++/Fortran bindings
  - Google search/ChatGPT: MPI tutorials, examples
- Different implementations (vendors): OpenMPI, Intel MPI and MPICH
  - module avail openmpi
  - module avail intelmpi
- Allow you to compile C/C++/Fortran codes with wrappers like mpicc, mpicxx, and mpifort

Communication between processes: Message Passing Interface (MPI)Basics

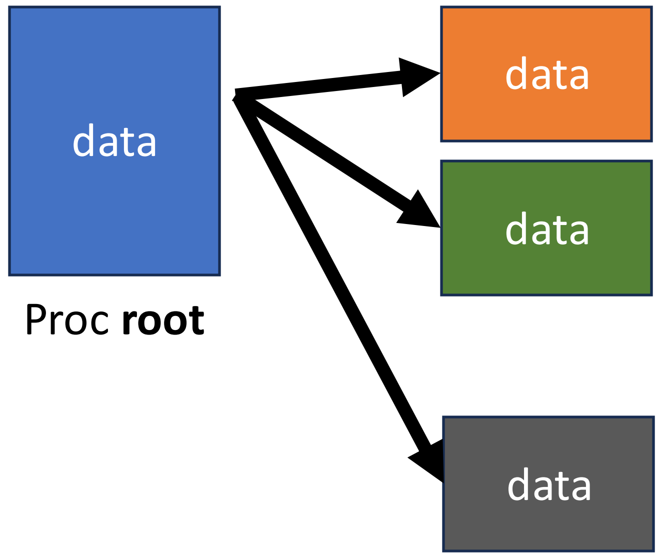
- Point-to-point communications: Send/Receive data between 2 procs
  - Non-blocking vs Blocking operations




```
if (rank == src)
  MPI_Send(&data, count, MPI_DOUBLE, dst, tag, communicator)
else if (rank == dst)
  MPI_Recv(&data, count, MPI_DOUBLE, src, tag, communicator, &status)
```

Communication between processes: Message Passing Interface (MPI)Basics

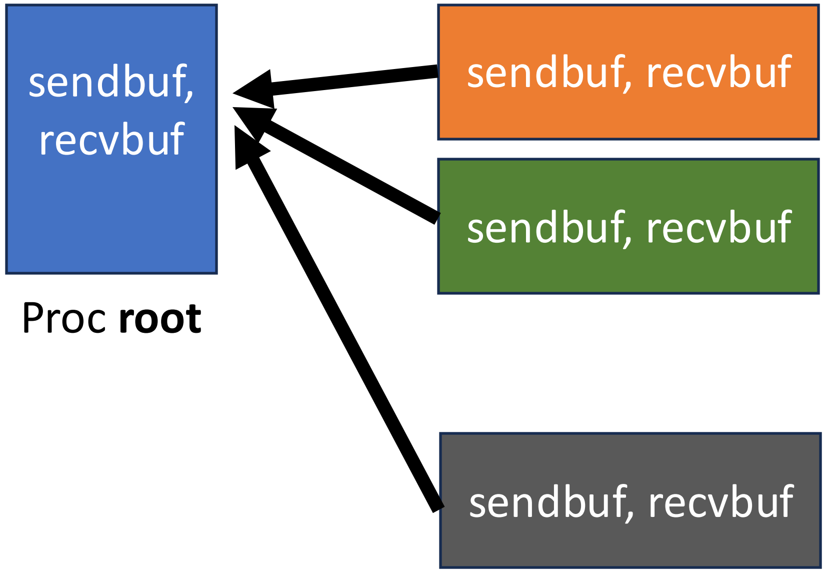
- Collective communications: Broadcast from a proc to other procs



MPI_Bcast(&**data, count, MPI_DOUBLE, root**, communicator)

Communication between processes: Message Passing Interface (MPI)Basics

- Collective communications: Reduce (tally) from other procs to a proc



MPI_Reduce(&**sendbuf, &recvbuf, count, MPI_DOUBLE, MPI_SUM, root,** communicator)

Process-level parallelization with the mpi4py module

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

```
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)
```

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

Communication between processes: MPI binding (Exercise 5)

mpirun –np 4 python mpi-comm-ops.py

- Point-to-point communication
  - blocking: MPI_Send/MPI_Recv
  - non-blocking: MPI_Isend/MPI_Irecv
  - MPI_Wait

```
# non-blocking send, and receive
if rank == 0:
  data = {'a': 7, 'b': 3.14}
  comm.isend(data, dest=1, tag=11)
elif rank == 1:
  req = comm.irecv(source=0, tag=11)
  data = req.wait()
  print(data)
```

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

Communication between processes: MPI binding (Exercise 5)

mpirun –np 4 python3 mpi-comm-ops.py

- Collective communication
  - MPI_Gather/MPI_Reduce
  - MPI_Bcast/MPI_Scatter

```
# Bcast
# allocate array properly on all procs
if rank == 0:
  data = np.arange(100, dtype='i')
else:
  data = np.empty(100, dtype='i')

comm.Bcast(data, root=0)
for i in range(100):
  assert data[i] == i
```

Calculating π with mpi4py (Exercise 6)

mpi-calculate-pi.py

```
from mpi4py import MPI

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

local_result = calculate_pi()

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

DIY: Create a new function, e.g. get_max_rand(), and return the maximum value returned from all the procs

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 still useful for launching <u>I/O bound tasks</u> concurrently

Comparing I/O bound vs CPU-bound tasks: multithreading (Exercise 7)

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 parallel 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
mpirun -np 4 xterm -e python -m pdb your_script.py

Quiz

To parallelize a serial Python code, you can start

A) given a fixed problem size (N) as the number of processing unit (P) increases.

B) given a fixed problem size per processing units (N/P) as the number of processing units (P) increases.

C) when there is a strong relationship between the input and output data

What about Python with GPU acceleration?

- Offload computation to the GPU (Single-Instruction Multiple-Threads model) via Just-In-Time compilation
- Need a GPU node to run your code
- Options:
  - **numba** (https://numba.pydata.org/): open source (needs a CUDA backend for NVIDIA GPUs, or a ROCm backend for AMD GPUs)
  - **cupy** (https://cupy.dev/): open source, relies on the NVIDIA CUDA toolkit
  - **JAX** (https://github.com/jax-ml/jax): open source
  - **PyTorch** (https://github.com/pytorch/pytorch): open source, for matrix operations

Summary

- Common strategies for parallelizing Python codes
  - Multiprocessing and multithreading models
- Popular Python modules
  - multiprocessing
  - mpi4py
  - multithreading
- Some examples

Questions?

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