Parallel Programming in Python:
High-level Oomph

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Overview

Introduction

Questions, questions, questions

- What is Python?

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- What is parallel?

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- What is parallel?
- How does it work?
- How to make the most of it.
- Not intended as introduction to parallel programming!

Short Snakes

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- Most versions run through C (CPython, not Cython)
- In general, slow!
- Use libraries to get real performance.

Snakes are fish now

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- No Python process can desynchronise from any other
- Efforts to remove GIL have been ongoing for years
- May finally be reaching fruition

Parallel

- What does it mean to do jobs in parallel?

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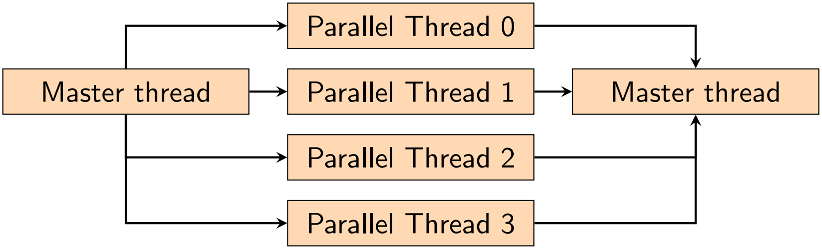
Fork-Join

- Fork-Join parallelism is temporary parallelism.



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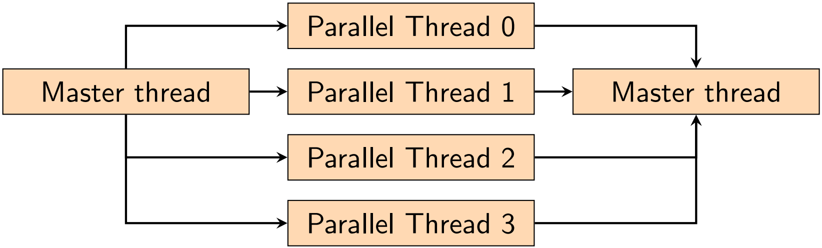

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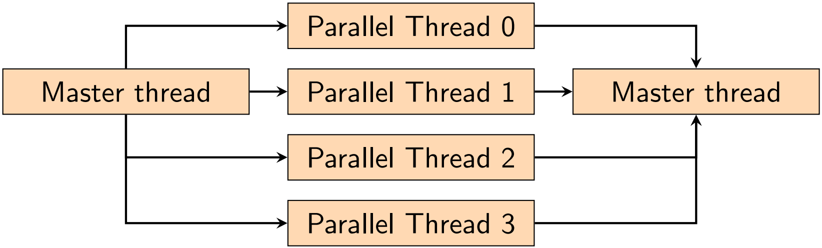

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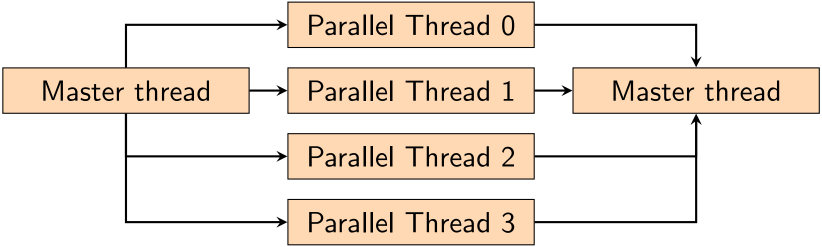
- Often less efficient.



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- Not in sync, running own copies of codes.
- Can be periodically forcibly synchronised.

Shared Memory

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- Race condition is where 2 threads try to access same memory at once

Distributed Memory

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- Need to specify which memory to transfer

Distributed Memory

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- Need to specify which memory to transfer
- Some systems allow memory windows

Basic Optimisation

Using Generators

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- Generators allow infinite loops
- Functions only calculated as needed
- Maps and filters can apply sequentially

Feeling lazy

```
def my_simple_counter(n: int = 0):
    """Count infinitely"""
    while true:
        yield n
        n = n+1

for i in my_simple_counter(15):
    print(i) # 15, 16, 17, ...
```

Using C

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- Efficient clean use of these can speed up code

Using C

- Simple comprehensions run in C
- Efficient clean use of these can speed up code
- Also implement filters and transformations

No comprende

```python
# List comprehensions
[3*x for x in range(10) if x % 2]
# Set comprehensions
{3*x for x in range(10) if x % 2}
# Dict comprehensions
{key: 3*val for key, val in zip("abcdefghij",
    range(10)) if val % 2}
# Generator comprehension
(3*x for x in range(10) if x % 2)
# Using generator comprehensions
tuple(3*x for x in range(10) if x % 2)
"\t".join(str(3*x) for x in range(10) if x % 2)
```

Vectorisation

Numpy

- Numpy provides free parallelism out of the gate

```
import numpy as np

x = np.fromiter(range(1000))
print(x + np.ones(1000))

y = np.sin(x)
```

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Numpy

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- Numpy operations on arrays vectorised in C
- Numpy ufuncs operate efficiently over arrays

```
import numpy as np

x = np.fromiter(range(1000))
print(x + np.ones(1000))

y = np.sin(x)
```

No, you func

```
import numpy as np

def add_two(x):
    "Add 2 to x"
    return x + 2

#              frompyfunc(func, nin, nout)
my_ufunc = np.frompyfunc(add_two, 1, 1)
print(my_ufunc(np.array([3, 4, 5]))) # => [5 6 7]
```

Ufunc powers

- `__call__(*args, **kwargs)`
  Call self as a function.
- `accumulate(array[, axis, dtype, out])`
  Accumulate the result of applying the operator to all elements.
- `at(a, indices[, b])`
  Performs unbuffered in place operation on operand 'a' for elements specified by 'indices'.
- `outer(A, B, /, **kwargs)`
  Apply the ufunc op to all pairs (a, b) with a in A and b in B.
- `reduce(array[, axis, dtype, out, keepdims, ...])`
  Reduces array's dimension by one, by applying ufunc along one axis.
- `reduceat(array, indices[, axis, dtype, out])`
  Performs a (local) reduce with specified slices over a single axis.

Don't vectorise

- Don't use `numpy.vectorize`
  The vectorize function is provided primarily for convenience, not for performance. The implementation is essentially a for loop.
  – Numpy Docs

https://numpy.org/doc/stable/reference/generated/numpy.vectorize.html

Threading

Threads in briefs

- Fork-join, shared memory model

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- Throttled by the GIL
- Mostly designed for background tasks where the main loop shouldn't freeze
- Think GUIs, IO operations, etc.

Threads in briefs

```python
from threading import Thread

# Declare the job and the arguments
p = Thread(target=f, args=('bob',))
# Starts a thread running the job - Fork
p.start()
# Wait until finished
p.join()
```

Threads in briefs

- In CPython, due to the Global Interpreter Lock, only one thread can execute Python code at once (even though certain performance-oriented libraries might overcome this limitation).
  – Python Docs

https://docs.python.org/3/library/threading.html

In Letters

- More like writing a note to yourself
- Do the job when the processor has free time

Be aware

- Need to be aware of “thread-safe” methods.
- Queues are useful for managing threads
- Threads are also handy for spawning other processes.

ASync

async

- In language native co-routines

async

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- Ask now, get later

async

- In language native co-routines
- Ask now, get later
- Similar to `threading`, but subtly different

async/await

- Two main keywords `async`, `await`
- Also involves the `asyncio` package.

```
import asyncio

async def sleepy():
    print("Yawn")
    asyncio.sleep(1)
    print("Awake")

# Runs in 1 second
asyncio.gather(sleepy(), sleepy(), sleepy())

# Takes all 3
for _ in range(3):
    sleepy()
```

async/await

- `async` attaches to `def`, `for` and `with`

```
async def g(x):
    return 2*x

async def f(x):
    ans = await g(x)
    return ans
```

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- `async` declares that object is to be scheduled in background.

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- `async` declares that object is to be scheduled in background.
- `await` attaches to `async` functions
- `await` says to pause execution until answer returned

```
async def g(x):
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async def f(x):
    ans = await g(x)
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```

await as gen

- Can help to think in terms of generators
- `async` declares object whose value is not computed yet
- `await` acts like `yield from` for `async`

Async objects

- Can declare object as `awaitable`
- Add `__await__` method
- Must return iterator object

```
class MyObject:
    def __init__(self):
        ...

    def __await__(self):
        ...
        return iterator_object
```

Async generator

- Like normal generators
- Can be iterated over with `async for`
- **N.B.** this is not parallelism, merely allowing other operations to borrow the processor.

```
import asyncio

async def async_generator(n=0):
    while true:
        yield n
        n = n + 1
        asyncio.sleep(1)

async for i in async_generator(3):
    print(i)
```

Multiprocessing

Finally Parallel!

- Fork-join, shared memory model

```
from multiprocessing import Process

def f(name):
    print('hello', name)

# Declare the job and the arguments
p = Process(target=f, args=('bob',))
# Starts a thread running the job
p.start()
# Wait until finished
p.join()
```

Finally Parallel!

- Fork-join, shared memory model
- Actually sidesteps the GIL – Finally parallel

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Finally Parallel!

- Fork-join, shared memory model
- Actually sidesteps the GIL – Finally parallel
- Support for task based parallelism

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Multiprocessing shared memory

- Support for shared memory processing

```
from multiprocessing import Process, Value, Array

def f(n, a):
    n.value = 3.1415927
    for i, val in enumerate(a):
        a[i] = -val

# Double
num = Value('d', 0.0)
# Integer
arr = Array('i', [4, 5, 6])
p = Process(target=f, args=(num, arr))
p.start()
p.join()
```

Swimming in threads

- Support for iterative parallelism

```
from multiprocessing import Pool

def add_two(x):
    return x + 2

# start 4 worker processes
with Pool(processes=4) as pool:

    x = pool.map(add_two, [4, 5, 6]) # 6, 7, 8
    y = pool.starmap(add, [(1, 2), (3, 4)] # 3, 7
```

Swimming in threads

- Support for iterative parallelism
- Threads are grouped into pools

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Swimming in threads

- Support for iterative parallelism
- Threads are grouped into pools
- Simplest way is to parallelise over array

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MPI4Py

MPI-ython

- MPI is a standard for parallel computing

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
size = comm.Get_size()
rank = comm.Get_rank()

print(f"Hello from process {rank} of {size}")
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- `mpi4py` is that interface to underlying C

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MPI-ython

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Hello from process 0 of 4
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- Each process has its own memory pool
- Need to send all data to other processes manually and keep track yourself.

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Communicators

- Fundamental object in MPI4py is the communicator.
- Communicator groups and labels processors.
- Enables transfer of data between them.
- `mpi4py.MPI.COMM_WORLD` is default.

```
from mpi4py import MPI

comm = MPI.COMM_WORLD

# Create new communicator for procs (1,2),(3,4)
colour = int(comm.rank < 3) # Group to be in
key = comm.rank              # Rank order on comm
new_comm = comm.split(colour, key)

# Create a 2x2 non-periodic grid of processors
comm.Create_cart([2,2], periods=[False, False])
```

What's the point(-to-point)?

- Point-to-point communications specify source and destination
- Collective communications specify source
- Collectives send/receive from all in group
- MPI4py compatible with numpy
- Cartesian communicators allow N-D destinations

```
# Send from rank -> rank + 1 (next in series)
comm.send(3, dest=(rank+1)%size)

# Split array and send equal portions to each
    processor in group
recv = np.zeros(50)
send = np.array(100)
send[0:50] = 1; send[50:] = 2;
comm.Scatter(send, recv, root=0)
```

MPI Differences

- Don't need to handle typing explicitly (uses pickle)
- Requests from asynchronous comms are objects
- `lowercase` methods transfer objects
- `Titlecase` methods transfer buffers (lower-level)

```
comm.bcast(data, root=0)
comm.Bcast((data, MPI.DOUBLE), root=0)

req = comm.isend(data, rank+1)
req.test()
req.wait()
```

MPI Features

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Tensor Computational Graph Libraries

TCGMs

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- Often include support for GPUs

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- Aesara (previously Theano)
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- Going to take a look at Aesara

Aesara

- Aesara works by defining a sequence of functions on anonymous typed arguments
- Can then dispatch those functions as needed to different backends
- Designed to be generic and able to operate generally

```
import aesara
from aesara import tensor as at

# Declare two symbolic floating-point scalars
a = at.dscalar("a")
b = at.dscalar("b")

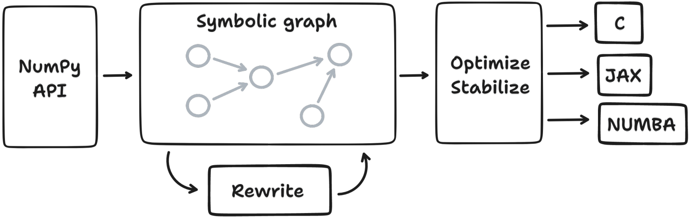
# Create a simple example expression
c = a + b

# Convert the expression into a callable object
    that takes `(a, b)`
# values as input and computes the value of `c`.
f_c = aesara.function([a, b], c)

assert f_c(1.5, 2.5) == 4.0
```

Aesara

- Builds a graph of operations
- Attempts to optimise and reduce graph
- Compiles resultant graph returning accessible function
- Compiled function dispatched to “processor”
- “Processor” may be CPU, GPU, TPU, or more



https://github.com/aesara-devs/aesara/

TCGM

- In principle saves you the work of: Optimisation, Ordering, Dispatching

```
d = a/a + (M + a).dot(v)
aesara.dprint(d)
# Elemwise{add,no_inplace} [id A] ''
#  |InplaceDimShuffle{x} [id B] ''
#  | |Elemwise{true_divide,no_inplace} [id C] ''
#  |   |a [id D]
#  |   |a [id D]
#  |dot [id E] ''
#    |Elemwise{add,no_inplace} [id F] ''
#    | |M [id G]
#    | |InplaceDimShuffle{x,x} [id H] ''
#    |   |a [id D]
#    |v [id I]
```

TCGM

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```
f_d = aesara.function([a, v, M], d)
# 'a/a' -> '1' and the dot product is replaced
    with a BLAS function
# Elemwise{Add}[(0, 1)] [id A] ''   5
#  |TensorConstant{(1,) of 1.0} [id B]
#  |CGemv{inplace} [id C] ''   4
#    |AllocEmpty{dtype='float64'} [id D] ''   3
#    | |Shape_i{0} [id E] ''   2
#    |   |M [id F]
#    |TensorConstant{1.0} [id G]
#    |Elemwise{add,no_inplace} [id H] ''   1
#    | |M [id F]
#    | |InplaceDimShuffle{x,x} [id I] ''   0
#    |   |a [id J]
#    |v [id K]
#    |TensorConstant{0.0} [id L]
```

TCGM

- Because these have access to (or are) the graph
- Can manipulate the graph constructively
- Can compute gradients or inverses

```
x = at.dmatrix('x')
# Logistic equation
s = at.sum(1 / (1 + at.exp(-x)))
gs = at.grad(s, x)

# Now have a function for derivative of logistic
dlogistic = aesara.function([x], gs)
```

Summary

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- Threading – Not parallel
- Async – Not parallel
- Multiprocessing – Parallel
- MPI4Py – Parallel
- TCGM – Maybe parallel

Worst MD

- If you want to have a play there is a really bad Python MD code available at: https://github.com/oerc0122/worst_md/blob/main/md.py