

Profiling/Optimization

Do You Want Your Code to Run Fast?

- hopefully yes!
- Algorithms can make a huge difference - FFT vs. (slow) DFT.
- Even with fast algorithm, you still win if you code it well.

What Takes Time?

- It's very useful to have an idea of how long things take.
- Floating point - AVX512 e.g. lets CPU crunch on 512 bits at a time. For 64 bit numbers, this is 8 operations per cycle. Often FMAD (fused multiply-add) does 1 multiply and 1 add in one cycle. $4 \text{ cores} * 8 \text{ FMADS/cycle} * 2 \text{ ops/FMAD} * 3 \text{ GHz} = 200 \text{ GFLOPS}$.
- This is a hard limit - we'll never go faster than this.

```

nn=[100,300,1000,3000,10000]
for n in nn:
    x=np.random.randn(n,n)
    t1=time.time()
    y=np.dot(x,x)
    t2=time.time()
    nops=2*n**3
    gflops=nops/(t2-t1)/1e9
    print("For matrix size " + repr(n) + " we have " + repr(gflops) + " GFLOPS.")

```

```

[Jonathans-MacBook-Pro:performance sievers$ python time_matrix_multiply.py
For matrix size 100 we have 10.143419588875455 GFLOPS.
For matrix size 300 we have 57.26736182048041 GFLOPS.
For matrix size 1000 we have 108.21915758240341 GFLOPS.
For matrix size 3000 we have 147.48941557071524 GFLOPS.
For matrix size 10000 we have 155.02978165356996 GFLOPS.

```

```

Processes: 505 total, 4 running, 501 sleeping, 2464 threads
Load Avg: 2.31, 1.83, 1.68 CPU usage: 24.64% user, 2.75% sys, 72.59% idle SharedLibs: 248M resident, 6
PhysMem: 31G used (4913M wired), 840M unused. VM: 2899G vsize, 1369M framework vsize, 23770976(0) swapi
Disks: 11135706/552G read, 16884444/417G written.

```

PID	COMMAND	%CPU	TIME	#TH	#WQ	#PORTS	MEM	PURG	CMPRS	PGRP	PPID	STATE	BOOSTS
37286	Python	299.9	00:11.58	3/3	0	23	1633M	0B	0B	37286	498	running	*0[1]
25139	steam_osx	100.1	04:25:19	32/1	3	1541	352M	680K	137M	25139	1	running	0[6485]
138	WindowServer	11.1	13:44:50	11	4	6544	1408M	43M+	131M-	138	1	sleeping	*0[1]
37285	top	6.1	00:01.41	1/1	0	28	10M	0B	0B	37285	442	running	*0[1]
0	kernel_task	3.8	05:51:10	226/16	0	0	679M	0B	0B	0	0	running	0[0]
37287	screen	2.4	00:00:18	2	2	57	2872K	620K	0B	310	310	sleeping	*0[1]

Only using 3 cores, so expect ~150 GFLOPS.
 Matrix multiplies can be very efficient!

Memory Bandwidth

- Another bottleneck - data has to get to and from memory to the CPU.
- A few 10s of GBs is optimistic here.
- How many numbers per second can I get to my CPU(s)?
- How many operations do I need to do while they're there to be floating-point limited?
- Say 50 GB/s, 16 bytes (2 numbers), 3 billion #'s/s. At 192 GFLOPS, need to do 64 floating point operations.

Matrix Multiply

- If I wrote matrix multiply as:
- ```
for i in range(n):
 for j in range(m):
 for ii in range(k):
 c[i,j]=c[i,j]+a[i,ii]*b[ii,j]
```
- Every element of a&b gets pulled through i times. For 10k by 10k, this is  $2 \times 10000^3 \times 8$  bytes = 16TB. At 50 GB/s, this takes  $16 \times (1000/50) = 320$ s. 30x longer than it actually took.

# Moral of the Story (so far)

- When you write code, think about operations *and* bandwidth.
- Your code will almost certainly be bandwidth-limited.

# Profiling

- There are various tools (for pretty much all languages) to tell you how long your code is taking.
- They often track which functions are called, how many times, and how long each one takes.
- `profile/cProfile` can help with this.
- Always profile before you start optimizing - it can be non-obvious which parts are slow, and effort speeding up fast code is (mostly) wasted.



```
#we can generate timing from the command line via
python3 -m cProfile -o simple_hist_timing.dat simple_hist_2d.py
```

```
import pstats
from pstats import SortKey
p=pstats.Stats('simple_hist_timing.dat')
#this prints out ALL the function calls that went on
#p.strip_dirs().sort_stats(-1).print_stats()
p.sort_stats(SortKey.TIME).print_stats(10)
```

```
Jonathans-MBP-2:performance sievers$ python3 look_at_output.py
Tue Nov 24 21:36:07 2020 simple_hist_timing.dat
```

```
67705 function calls (65534 primitive calls) in 2.629 seconds
```

```
Ordered by: internal time
```

```
List reduced from 917 to 10 due to restriction <10>
```

| ncalls  | tottime | percall | cumtime | percall | filename:lineno(function)                                    |
|---------|---------|---------|---------|---------|--------------------------------------------------------------|
| 1       | 2.407   | 2.407   | 2.442   | 2.442   | simple_hist_2d.py:4(hist_2d)                                 |
| 1       | 0.037   | 0.037   | 0.037   | 0.037   | {method 'rand' of 'numpy.random.mtrand.RandomState' objects} |
| 107     | 0.028   | 0.000   | 0.028   | 0.000   | {method 'read' of '_io.BufferedReader' objects}              |
| 31/29   | 0.024   | 0.001   | 0.026   | 0.001   | {built-in method _imp.create_dynamic}                        |
| 120     | 0.019   | 0.000   | 0.019   | 0.000   | {built-in method numpy.array}                                |
| 1       | 0.016   | 0.016   | 0.016   | 0.016   | {method 'round' of 'numpy.ndarray' objects}                  |
| 316     | 0.014   | 0.000   | 0.014   | 0.000   | {built-in method builtins.compile}                           |
| 107     | 0.010   | 0.000   | 0.010   | 0.000   | {built-in method marshal.loads}                              |
| 1       | 0.005   | 0.005   | 2.629   | 2.629   | simple_hist_2d.py:1(<module>)                                |
| 224/223 | 0.004   | 0.000   | 0.005   | 0.000   | {built-in method builtins.__build_class__}                   |

```
Jonathans-MBP-2:performance sievers$ open performance.key
```

# Performance

- Python is an interpreted language. This means things in loops are very slow!
- Look at `simple_hist_2d.py`. This is a possibly relevant case where you take a list of points and grid them into a 2D array.
- How does this speed compare with anything you might expect?
- Numpy often has vectorized code: `c=a+b` is *much* faster than `c[i]=a[i]+b[i]` looped over `i`.



# Beware...

- `scipy` ≠ `numpy`. e.g. `scipy.fft.fft` accepts optional argument “workers” which `numpy.fft.fft` doesn’t. You may wish to use `scipy` for this reason...

```
>>> x=np.random.rand(500,500,500)
>>> import time
>>> t1=time.time();y=np.fft.rfftn(x);t2=time.time();print(t2-t1)
5.877029180526733
>>> t1=time.time();y2=scipy.fft.rfftn(x);t2=time.time();print(t2-t1)
1.757699966430664
>>> t1=time.time();y2=scipy.fft.rfftn(x,workers=8);t2=time.time();print(t2-t1)
0.6568210124969482
```

# C

- Compiled code is usually much faster, at least where loops are involved.
- We can link C to python, so python can call C libraries.
- ctypes is one way to do this. There are others, but ctypes widely present and requires no setup.
- Look at `simple_hist_2d_from_c.py` and `hist2d_c.c` as an example. We win by a factor of 100.

# Numba

- We can sometimes have the best of both worlds. Numba allows real-time compilation of python into C(++?).
- `@nb.(n)jit` tells numba to try to compile code at runtime. If arg types change, it may recompile.
- Loops in Python are excruciatingly slow. Loops in Numba are fast. Often faster than vectorized code because needed memory bandwidth may decrease.
- Example - 2D stencil from Laplace solver. `np.roll` requires bringing an array through memory several times, but stencils will sit in cache in looped version.

```
@nb.njit(parallel=True)
def kernel_numba(x):
 n=x.shape[0]
 m=x.shape[1]
 y=np.empty((n,m),np.float64)
 for i in nb.prange(1,n-1):
 for j in range(1,m-1):
 y[i,j]=x[i-1,j]+x[i+1,j]+x[i,j-1]+x[i,j+1]-4*x[i,j]
 return y
```

- numba example. note code is perfectly standard python, except for @nb.njit
- note - np.empty requires tuple as size argument, not list.
- note - nb.prange will parallelize a loop for you! Make sure your loop is parallelizable first...
- look at time\_kernel.py (and laplace\_kernel.c) for smackdown for several different techniques.