scipar

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0.0.1 Accelerating Python for Scientific Computing.

Notebooks based on P. Haustin's Parallel Python Workshop.

The idea of the below code is to show you how to accelerate your code with minimal effort. You can go all the way and write in C/C++, but then you'll spend more time writing code and less solving problems.

Let's say you're solving problem Y = f(X). It took you 10 hours to implement f in pure Python. It takes 10 days to execute f. F also has a lot of hyperparameters. It runs sequentially, but you have at least 4-8 cores in a modern machine.

In this workshop I'll show you how to * accelerate sequential code * use threads and processes to accelerate even more

And I'll show you how to do this with only minimal changes to your code. If you need to learn for a week how to write threaded optimized code, then it's not worth it if your code runs in a week. If you can add a single line in 5 minutes to decrease your runtime from a week to an hour, then you might be interested.

See ./config/install.md for full list of dependencies. First, let's get all imports done.

```
In [2]: import contexttimer
        import cython
        from numba import jit
        import multiprocessing
        import threading
        from joblib import Parallel
        import logging
        import math
        import time
        import numpy as np
        from scipy.spatial.distance import euclidean
        from functools import reduce
        %load_ext Cython
        import warnings
        warnings.simplefilter('ignore') # for sqrt overflow in synthetic case
        import matplotlib.pyplot as plt
```

0.1 Overview

- Speeding up single threaded code

  - Cython
  - Numba
  - Vectorization
- Parallel Python -- Defeating the GIL
- Parallel IO & Large Datasets
- Visualization

1 0. Hello parallel world.

We define a simple N^4 function that does only computation, uses almost no memory. This example shows you how to get the code running, and what can be achieved. Later on we'll use a more realistic example.

1.0.1 Why is Python in 2018 still not parallelizable? Enter the Global Interpreter Lock.

The GIL (Global Interpreter Lock) is the main obstacle for Python threading speedup. A single bottleneck that is triggered whenever Python Objects are referenced. High performance modules such as numpy (in C) don't use Python objects, so safely can ignore the GIL. We will define 2 functions using Numba. Numba introduces decorators that will compile your function to C/C++ on the fly. It allows you to specify datatype (like in numpy) and release the GIL. Basically, you can write your own numpy-alike code, without the complexity of writing C!

Numba Numba allows you to wrap your existing code in a decorator. It will type your code, compile it to C++ on the fly and optionally release the Global Interpreter Lock.

```
In [3]: @jit('float64(int64)', nopython=True, nogil=True)
        def wait_loop_nogil(n):
            out = 0
            for m in range(n):
                for l in range(m):
                    for j in range(l):
                        for i in range(j):
                            i=i+4
                            out=i**(1/2)
                            out=out**2.
            return out

        @jit('float64(int64)', nopython=True, nogil=False)
        def wait_loop_withgil(n):
            out = 0
            for m in range(n):
                for l in range(m):
                    for j in range(l):
                        for i in range(j):
                            i=i+4
                            out=i**(1/2)
```

```
                    out=out**2.
    return out
```

Python

```
In [4]: def pure_python(n):
            out = 0
            for m in range(n):
                for l in range(m):
                    for j in range(l):
                        for i in range(j):
                            i=i+4
                            out=i**(1/2)
                            out=out**2.
            return out
```

Cython

```
In [5]: %%cython
        def cython_loop_typed(long n):
            cdef double out
            cdef long m
            cdef long l
            cdef long j
            cdef long i
            out = 0
            for m in range(n):
                for l in range(m):
                    for j in range(l):
                        for i in range(j):
                            i=i+4
                            out=i**(1/2)
                            out=out**2.
            return out
```

Defining the benchmark function.

```
In [6]: def benchmark_jitters(func, args, times):
            results = np.zeros((times, 3))
            for i in range(times):
                w, c, s = 0, 0, 0
                with  contexttimer.Timer(time.perf_counter) as wall:
                    with contexttimer.Timer(time.process_time) as cpu:
                        func(*args)
                        w = wall.elapsed
                        c = cpu.elapsed
                        s = c/w
                        results[i] = [w,c,s]
            return results
```

1.0.2 How much does Just In Time Compilation help?

Let's first look at Pure Python vs Cython. Cython gains most of its speed from typing. Typical Python interpreters generate bytecode that can't make assumptions that compiled code can (type and size of a variable in memory can change between iterations in Python).

```
In [7]: funcs = [ cython_loop_typed, pure_python]
        times = 10
        n = 200
        N = len(funcs)
        results = np.empty((N,times,3))
        finals = np.empty((N,2))
        for i,f in enumerate(funcs):
            print('Testing {}'.format(f.__name__))
            results[i] = benchmark_jitters(f, [n], times)
        for i,r in enumerate(results):
            finals[i] = np.mean(r[:,0]), np.std(r[:,1])
        M, m = [(-float('inf'), None), (float('inf'), None)]

        for f,r in zip(funcs, finals):
            M = (r[0], f.__name__) if r[0] > M[0] else M
            m = (r[0], f.__name__) if r[0] < m[0] else m
            print('Mean time for {} is \t{:.2E} with std \t{:.2E}'.format(f.__name__, *r))

        print('Worst is {} , best is {} with a speedup of {:.2E}'.format(M[1], m[1], M[0]/m[0]))
```

```
Testing cython_loop_typed
Testing pure_python
Mean time for cython_loop_typed is          8.18E+00 with std          5.86E-01
Mean time for pure_python is          2.73E+01 with std          9.50E-01
Worst is pure_python , best is cython_loop_typed with a speedup of 3.3338176178037973
```

1.0.3 Cython is clearly faster, but the compiled code generated isn't that good.

Not as fast as expected, mainly because this code is computation bound (and not memory bound).

1.0.4 JIT vs Cython.

How good is the generated code? Cython is not that easy to write (our example is trivial). Numba is more user friendly, and allows us to use objects, or if we don't, releases the GIL.

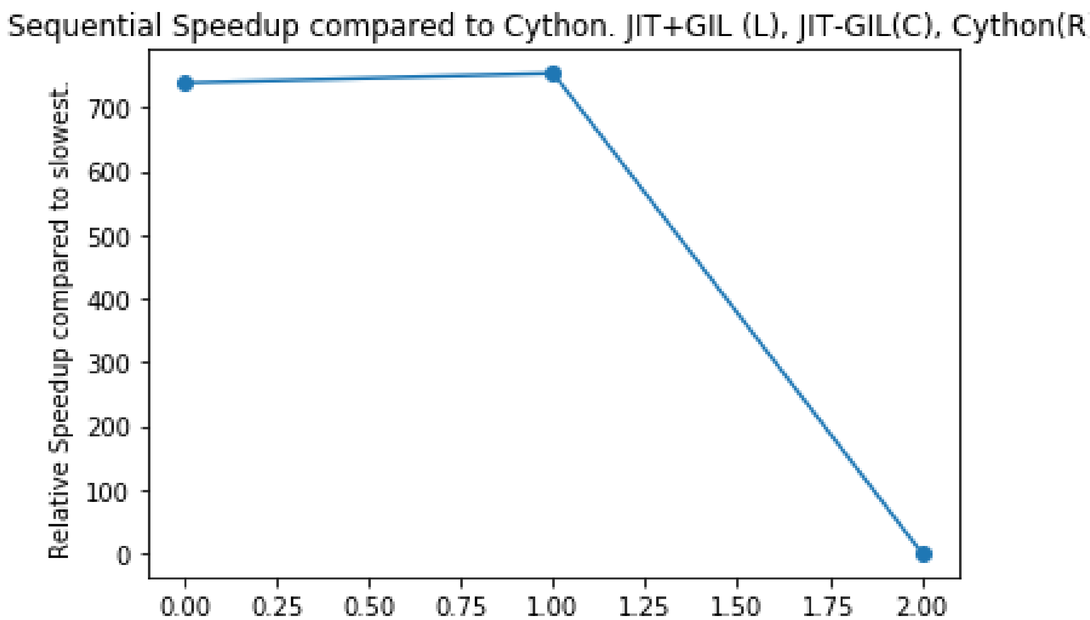
Do you expect a speedup from single threaded code *releasing* the GIL?

```
In [48]: funcs = [wait_loop_withgil, wait_loop_nogil, cython_loop_typed]
         times = 10
         n = 200
         N = len(funcs)
         results = np.empty((N,times,3))
         finals = np.empty((N,2))
```

```
         for i,f in enumerate(funcs):
             print('Testing {}'.format(f.__name__))
             results[i] = benchmark_jitters(f, [n], times)

         for i,r in enumerate(results):
             finals[i] = np.mean(r[:,0]), np.std(r[:,1])

         M, m = [(-float('inf'), None), (float('inf'), None)]

         for f,r in zip(funcs, finals):
             M = (r[0], f.__name__) if r[0] > M[0] else M
             m = (r[0], f.__name__) if r[0] < m[0] else m
             print('Mean time for {} is \t{:.2E} with std \t{:.2E}'.format(f.__name__, *r))

         print('\nWorst is {} , best is {} with a speedup of {:.2E}'.format(M[1], m[1], M[0]/m[0

         print('\nSpeedup of releasing the GIL is {:.2E}'.format(finals[0][0]/finals[1][0]))
```

```
Testing wait_loop_withgil
Testing wait_loop_nogil
Testing cython_loop_typed
Mean time for wait_loop_withgil is         1.15E-02 with std         4.36E-04
Mean time for wait_loop_nogil is         1.12E-02 with std         3.22E-04
Mean time for cython_loop_typed is         8.45E+00 with std         1.73E-01

Worst is cython_loop_typed , best is wait_loop_nogil with a speedup of 7.53E+02

Speedup of releasing the GIL is 1.02E+00
```

```
In [50]: best=M[0]
         x = [i for i in range(len(funcs))]
         means, sd = best/finals[:,0], finals[:,1]
         fig, ax0= plt.subplots(nrows=1, sharex=True)
         ax0.errorbar(x, means, yerr=sd, fmt='-o')
         ax0.set_title('Sequential Speedup compared to Cython. JIT+GIL (L), JIT-GIL(C), Cython(R
         ax0.set_ylabel('Relative Speedup compared to slowest. ')
         # ax0.set_yscale('log')
         plt.show()
```



1.0.5 JIT is *significantly* faster than Cython for our example. Releasing the GIL adds even more speed.

The reason is the generated code. Numba uses LLVM which invokes Clang with very aggresive optimizations. The quality of C++ code makes all the difference here.

1.1 Threads and processes in Python made easy with joblib.

The threshold of writing process managing code is quite high in Python (multiprocess module, MPI), high enough that it's not worth investing time in it. Joblib makes the threshold significantly lower so you can enjoy a parallel speedup.

1.1.1 A Note about Time

We're using contexttimer, which allows us to see the actual time (wall clock) and cpu time used. The distinction is *important*. * Wall time: Physical real world time * CPU time: time where the CPU is executing your code (user CPU time) or doing syscalls (system CPU).

Simply timing a function is not going to tell you much about speedup or stalls. When threads hit the GIL, they will stalls so even with 20 cores/threads your CPU time will not be more than wall time.

- **Wall < CPU** : Parallel Speedup
- **Wall = CPU** : Stalled on locks
- **Wall > CPU** : Stalled on IO/Syscalls,Scheduler

1.1.2 Processes and Threads

A process has its own memory, a thread (can) share(s) memory. If you can't afford copying data (which you need to do with processes), don't use processes. A process is heavyweight, a thread less so. Threads, however, don't scale that well, you have limited CPUs. Don't use more threads than you have cores. Don't expect 'hyperthreading' to give you a linear speedup.

```
In [40]: njobs, nprocs, nloops = 32, 16, 1000
```

Let's define a benchmark function

```
In [45]: def benchmark(func, jobs, processes, posargs=[], kwargs={}, useprocs=False):
             calc_jobs=[(func,posargs,kwargs) for i in range(jobs)]
             w, c, s = 0, 0, 0
             with  contexttimer.Timer(time.perf_counter) as wall:
                 with contexttimer.Timer(time.process_time) as cpu:
                     with Parallel(n_jobs=processes,backend='threading' if not useprocs else 'mu
                         parallel(calc_jobs)
                         w = wall.elapsed
                         c = cpu.elapsed
                         s = c/w
                     print(f'Wall time {wall.elapsed} and Cpu time {cpu.elapsed}')
             print(f'Effective Parallel Speedup (1 is None) = {cpu.elapsed/wall.elapsed}')
             return w,c,s
```

Threading With the GIL

```
In [46]: print('Threading speedup with {} jobs spread over {} threads'.format(njobs, nprocs))
         wall, cpu, speedup = benchmark(wait_loop_withgil, njobs, nprocs, [nloops], {})
         print('Speedup ratio (1 = Linear) {}'.format(speedup/nprocs))
```

```
Threading speedup with 32 jobs spread over 16 threads
Wall time 15.853111556731164 and Cpu time 15.458750341999917
Effective Parallel Speedup (1 is None) = 0.9668269277923749
Speedup ratio (1 = Linear) 0.061146780829325405
```

Without GIL

```
In [47]: print('Parallel speedup with {} jobs spread over {} threads'.format(njobs, nprocs))
         wall, cpu, speedup = benchmark(wait_loop_nogil, njobs, nprocs, [nloops], {})
         print('Speedup ratio (1 = Linear) {}'.format(speedup/nprocs))
```

```
Parallel speedup with 32 jobs spread over 16 threads
Wall time 1.2766712736338377 and Cpu time 16.184895294000057
Effective Parallel Speedup (1 is None) = 12.676078460840811
Speedup ratio (1 = Linear) 0.8317403540912072
```

With the GIL there is simply **no** way to accelerate code (unless your code does IO, calls numpy or C libs.) Without the GIL we have a **linear** speedup.

What about processes?

```
In [48]: print('Parallel speedup with {} jobs spread over {} processes'.format(njobs, nprocs))
         wall, cpu, speedup = benchmark(wait_loop_nogil, njobs, nprocs, [nloops], {}, useprocs=T
         print('Speedup ratio (1 = Linear) {}'.format(speedup/nprocs))
```

```
Parallel speedup with 32 jobs spread over 16 processes
Wall time 6.1091247741132975 and Cpu time 0.2125228639999932
Effective Parallel Speedup (1 is None) = 0.03507276574392902
Speedup ratio (1 = Linear) 0.002182622035330477
```

Processes are a *poor* choice when the compute time is short and require a copy of data. A good use case for processes is grid search, long running expensive code with almost no copying.

2 1. A more realistic Use Case: Pairwise Matching of Clusters

2 3D point clouds (R, G) each clustered into k, l clusters. Align the 'nearest' clusters. We'll use Chamfer distance, and see if we can accelerate using vectorization, threading, JIT.

A note on distance functions and speed: * You can use Ball/KD Trees to accelerate this with NlogN * You can use dot product (sklearn pairwise) but it won't be symmetric

2.0.1 Let's solve the problem itself first.

- Define Chamfer distance
  - Using pure Python
  - Using map-reduce
  - JIT'ed
- Define pairing function
  - Using map-reduce

```
In [9]: def gen_clusters(n, m, seed=0):
            # Generate N clusters of up to m 3D points per cluster with random Gaussian distribu
            np.random.seed(seed)
            meanrange = [1,10]
            sigmarange = [1,3]
            # Preallocation will fail since we don't know size of each cluster (1 < m)
            clusters = []
            for m in np.random.randint(1, m, n):
                means, sigmas = np.random.randint(*meanrange, 3), np.random.randint(*sigmarange,
                cluster = np.random.normal(loc=means, scale=sigmas, size=(m, 3))
                clusters.append(cluster)
            return clusters


        def chamfer_pure(left, right):
            '''
```

```
    Pure Python code to compute Chamfer distance between two unequal sized clusters
    '''
    lr = 0
    NL, NR = len(left), len(right)
    for li in range(NL):
        l = left[li]     # Numba doesn't implement type inference when iterating over K-
        m = float('inf')
        for ri in range(NR):
            r = right[ri]
            dlr = np.sqrt(np.dot(l, r))
            m = min(m, dlr)
        lr += m
    rl = 0
    for ri in range(NR):
        r = right[ri]
        m = float('inf')
        for li in range(NL):
            l = left[li]
            dlr = np.sqrt(np.dot(l, r))
            m = min(m, dlr)
        rl += m
    return max(lr/NL, rl/NR)
```

Going deeper with Numba Note how we now have not a simple int, but 2 2 dimensional arrays as input. Also, we want to see if builtin parallellism can be used.

Our question is, how much work does it take to write chamfer_pure in numba?

```
In [18]: @jit('float64(float64[:,:], float64[:,:])', nopython=True, nogil=True)  # cache=True ca
         def chamfer_JIT_bells_whistles(left, right):
             '''
             JIT'ed version, but with a subtle mistake crippling performance.
             I will buy the (first) person who finds the bug a (Belgian) beer.
             '''
             lr = 0
             NL, NR = len(left), len(right)
             for li in range(NL):
                 l = left[li]     # Numba doesn't implement type inference when iterating over K
                 m = np.inf
                 for ri in range(NR):
                     r = right[ri]
                     dlr = np.sqrt(np.dot(l, r))
                     m = min(m, dlr)
                 lr += m
             rl = 0
             for ri in range(NR):
                 r = right[ri]
                 m = np.inf
                 for li in range(NL):
```

```python
                l = left[li]      # Numba doesn't implement type inference when iterating ov
                dlr = np.sqrt(np.dot(l, r))
                m = min(m, dlr)
            rl += m
        return max(lr/len(left), rl/len(right))

    @jit(nopython=True, nogil=True)
    def chamfer_JIT(left, right):
        '''
        JIT'ed version
        '''
        lr = 0
        NL, NR = len(left), len(right)
        for li in range(NL):
            l = left[li]      # Numba doesn't implement type inference when iterating over K
            m = np.inf
            for ri in range(NR):
                r = right[ri]
                dlr = np.sqrt(np.dot(l, r))
                m = min(m, dlr)
            lr += m
        rl = 0
        for ri in range(NR):
            r = right[ri]
            m = np.inf
            for li in range(NL):
                l = left[li]      # Numba doesn't implement type inference when iterating ov
                dlr = np.sqrt(np.dot(l, r))
                m = min(m, dlr)
            rl += m
        return max(lr/len(left), rl/len(right))
```

2.0.2 @jit

@jit(' returntype (argument types) ', nopython=True/False, nogil=True/False, parallel=True/False, cache=True/False

- returntype: float64, int64, type[:] (single array)
- argument types: same as returntypes
- nopython: don't work with objects (classes) --> everything in Python is an Object, so a void*, and so invokes indirection, pointer chasing, runtime typing.
- nogil : Release the Global Interpreter Lock (only if you're not using objects
- parallel : use openmp to parallelize your code
- cache : store the compiled code to a file (if you run your code 10 times, instead of running a function 10 times)

2.1 So what did we need to change?

Numba 0.4 does not support for x in array if array is 2 or higher dimensional. So we need to change to code to use indices. The rest of the code is the same.

Numba will try to JIT library code, but if it fails be prepared for some deep diving into typing.

2.2 Adding Functional Programming to the mix

The above code is long, for something we can intuitively express in one sentence.

For each clusterset, find the index of the nearest cluster in the other set.

Using functional programming we can get a lot closer to our intent.

```
In [10]: def chamfer_mapreduce(left, right):
             '''
             Python's Map Reduce style of computing Chamfer
             '''
             L = sum(map(lambda l: min(map(lambda r: np.sqrt(np.dot(l,r)), right)), left))/len(l
             R = sum(map(lambda r: min(map(lambda l: np.sqrt(np.dot(l,r)), left)), right))/len(r
             return max(L, R)


         def pairs_mapreduce(left, rights, chamfer_func):
             '''
             Find index of right cluster in rights nearest to left using chamfer_func
             '''
             return min(map(lambda R: (chamfer_func(left, R[1]), R[0]), enumerate(rights)))[1]


         def solve(L, R, chamfer_func, pairfunc):
             return [pairfunc(l,R, chamfer_func) for l in L], [pairfunc(r,L,chamfer_func) for r
```

2.2.1 Understanding Map-Reduce (and when to use it)

```
map( function, iterable) -> iterable
```

Map returns a new iterable (collection, list, array, dict, ...) where each element is replaced by the result of function(element)

```
map( lambda x : x**2, [1,2,3]) == [1,4,9]
```

A lambda function is an anonymous function typically used in functional programming describing in a single expression the operation to be performed.

Why should you care? Map, Reduce, Filter, Itertools, Lambda are succinct expressions what you want to do, and they don't generate intermediate copies. Use them for streams, large data or generated data where in memory storing is too expensive. Unless you hit memory limits they will not be faster, but they **will** save memory.

Map does not 'create' a new list, it creates a generator object.

Sum of first 1e5 squares. The maximum list size is 1

```
sum(map(lambda x : x**2, (i for i in range(100000))))
```

Note (i for i in range(N))

This is a generator object, not a list. If we use [i for i in range(N)] we have a list of 1e5 numbers. Technically these are generator comprehension and list comprehension.

Note : A generator is exhausted after usage.

(i for i in range(N)) is equivalent to writing:

```
def mygenerator(N):
    n = 1
    yield n
    n += 1
```

[i for in range(N))] is equivalent to writing:

```
def mylistcomprehension(N):
    l = []
    for i in range(N)
        l.append(i)
    return l
```

Decrypting functional oneliners. Great, so how do we read:

```
return min(map(lambda R: (chamfer_func(left, R[1]), R[0]), enumerate(rights)))[1]
```

The lambda accepts R, a tuple of an index and a cluster (R[0] and R[1]). It computes the chamfer distances between 'left' and each cluster in rights. It then finds the minimum distance.

So:

- map(...) --> A: ((distance, index), (distance, index), ...)
- min(((distance, index), (distance, index), ...)) --> (mindist, corresponding cluster index)
- Finally [1] selects the index.

3 Analysis

Let's make some data.

While we do so, look at how you can use list, dictionary and * to neatly express what we want.

```
In [14]: params = {'L':{'cluster_count':50, 'max_size':35, 'seed':1},  'R':{'cluster_count':30,

         L, R = [gen_clusters(*[value for key, value in p.items()]) for _, p in params.items()]

         points = sum(sum(len(q) for q in Q) for Q in [L,R]) # double nested for loop saved.

         print('Total of {} points in L+R'.format(points))

Total of 1090 points in L+R
```

3.0.1 Pure vs Functional

In [16]:
```
# Let's define some shorthands
def solve_pure(L, R):
    return solve(L, R, chamfer_pure, pairs_mapreduce)

def solve_mapreduce(L,R):
    return solve(L, R, chamfer_mapreduce, pairs_mapreduce)

funcs = [solve_pure, solve_mapreduce]
times = 2
N = len(funcs)
results, finals = np.empty((N,times,3)), np.empty((N,2))

for i,f in enumerate(funcs):
    print('Testing {}'.format(f.__name__))
    results[i] = benchmark_jitters(f, [L,R], times)

for i,r in enumerate(results):
    finals[i] = np.mean(r[:,0]), np.std(r[:,1])

M, m = [(-float('inf'), None), (float('inf'), None)]

for f,r in zip(funcs, finals):
    M = (r[0], f.__name__) if r[0] > M[0] else M
    m = (r[0], f.__name__) if r[0] < m[0] else m
    print('Mean time for {} is \t{:.2E} with std \t{:.2E}'.format(f.__name__, *r))

print('\nWorst is {} , best is {} with a speedup of {:.2E}'.format(M[1], m[1], M[0]/m[0
```

```
Testing solve_pure
Testing solve_mapreduce
Mean time for solve_pure is         9.01E+00 with std         6.07E-02
Mean time for solve_mapreduce is         8.27E+00 with std         1.15E-01

Worst is solve_pure , best is solve_mapreduce with a speedup of 1.09E+00
```

Map Reduce doesn't improve that much in speed (small data sets, computation dominated).

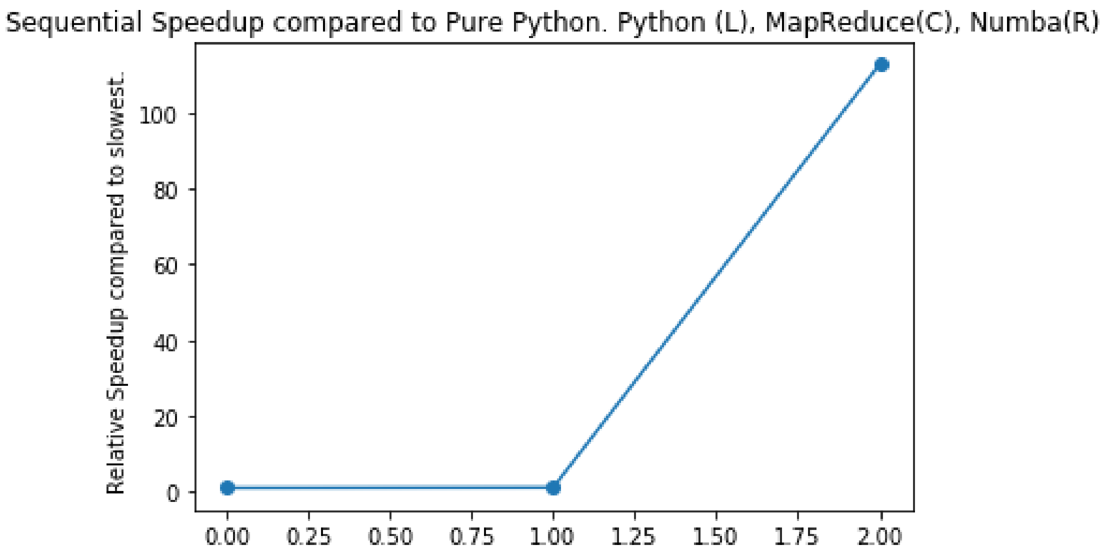
3.0.2 Pure vs JIT

In [23]:
```
def solve_pure(L, R):
    return solve(L, R, chamfer_pure, pairs_mapreduce)

def solve_mapreduce(L,R):
    return solve(L, R, chamfer_mapreduce, pairs_mapreduce)
```

```
def solve_jit(L, R):
    return solve(L, R, chamfer_JIT, pairs_mapreduce)

def solve_jitplus(L, R):
    return solve(L, R, chamfer_JIT_bells_whistles, pairs_mapreduce)

funcs = [solve_pure, solve_mapreduce, solve_jit]
times = 10
N = len(funcs)
results = np.empty((N,times,3))
finals = np.empty((N,2))
for i,f in enumerate(funcs):
    print('Testing {}'.format(f.__name__))
    results[i] = benchmark_jitters(f, [L,R], times)

for i,r in enumerate(results):
    finals[i] = np.mean(r[:,0]), np.std(r[:,1])

M, m = [(-float('inf'), None), (float('inf'), None)]

for f,r in zip(funcs, finals):
    M = (r[0], f.__name__) if r[0] > M[0] else M
    m = (r[0], f.__name__) if r[0] < m[0] else m
    print('Mean time for {} is \t{:.2E} with std \t{:.2E}'.format(f.__name__, *r))

best = m[0]
print('\nWorst is {} , best is {} with a speedup of {:.2E}'.format(M[1], m[1], M[0]/m[0
```

```
Testing solve_pure
Testing solve_mapreduce
Testing solve_jit
Mean time for solve_pure is         8.50E+00 with std         2.38E-01
Mean time for solve_mapreduce is         7.77E+00 with std         2.65E-01
Mean time for solve_jit is         7.53E-02 with std         1.63E-02

Worst is solve_pure , best is solve_jit with a speedup of 1.13E+02
```

In [47]:
```
best=M[0]
x = [i for i in range(len(funcs))]
means, sd = best/finals[:,0], finals[:,1]
fig, ax0= plt.subplots(nrows=1, sharex=True)
ax0.errorbar(x, means, yerr=sd, fmt='-o')
ax0.set_title('Sequential Speedup compared to Pure Python. Python (L), MapReduce(C), Nu
ax0.set_ylabel('Relative Speedup compared to slowest. ')
# ax0.set_yscale('log')
plt.show()
```



The explicitly typed JIT code is slower due to a mistake in the type declaration.

3.0.3 Parallell

So now we have an order of magnitude speedup. This was sequential only. We're already using numpy. Let's go parallel.

L = [l1, l2, ..., ln] R = [r1, r2, ..., rn]

So let's split the work in two (L-R and R to L) Then we split the work in l1-R, l2-R, ...

```
In [58]: # Define shorthand
         def psolve(l, R):
             pairs_mapreduce(l, R, chamfer_JIT)

         def solve(L, R, chamfer_func, pairfunc):
             return [pairfunc(l,R, chamfer_func) for l in L], [pairfunc(r,L,chamfer_func) for r


         def benchmark_solver(L, R, processes, useprocs=False):
             calc_jobs=[(psolve, [l, R],{}) for l in L] + [(psolve, [r, L],{}) for r in R]
             w, c, s = 0, 0, 0
             with  contexttimer.Timer(time.perf_counter) as wall:
                 with contexttimer.Timer(time.process_time) as cpu:
                     with Parallel(n_jobs=processes,backend='threading' if not useprocs else 'mu
                         r=parallel(calc_jobs)
                         w = wall.elapsed
                         c = cpu.elapsed
                         s = c/w
             return w,c,s
```

```
In [164]: params = {'L':{'cluster_count':400, 'max_size':200, 'seed':1},  'R':{'cluster_count':2

          L, R = [gen_clusters(*[value for key, value in p.items()]) for _, p in params.items()]

          points = sum(sum(len(q) for q in Q) for Q in [L,R]) # double nested for loop saved.

          print('Total of {} points in L+R'.format(points))
```

```
Total of 83219 points in L+R
```

3.1 Weak Scaling behaviour of Parallel Python

What happens if we have the same amount of work but throw more threads at it?

```
In [161]: procs = [2,4,8,16,32]
          times = 10
          njobs = len(L) + len(R)
          results = np.zeros((len(procs), times, 4))
          finals = np.zeros((len(procs), 2))
          for ni,nprocs in enumerate(procs):
              for t in range(times):
                  wall, cpu, speedup = benchmark_solver(L, R, nprocs, False)
                  ratio = speedup/nprocs
                  results[ni][t] = wall, cpu, speedup, ratio
              finals[ni] = np.mean(results[ni][:,2]), np.std(results[ni][:,2])

          for p,(m,s) in zip(procs, finals):
              print('Using {} threads achieves mean speedup {:.2E} +- {:.2E}'.format(p, m, s))
              print('Using {} threads achieves mean relative speedup {:.2E} +- {:.2E}'.format(p,
```

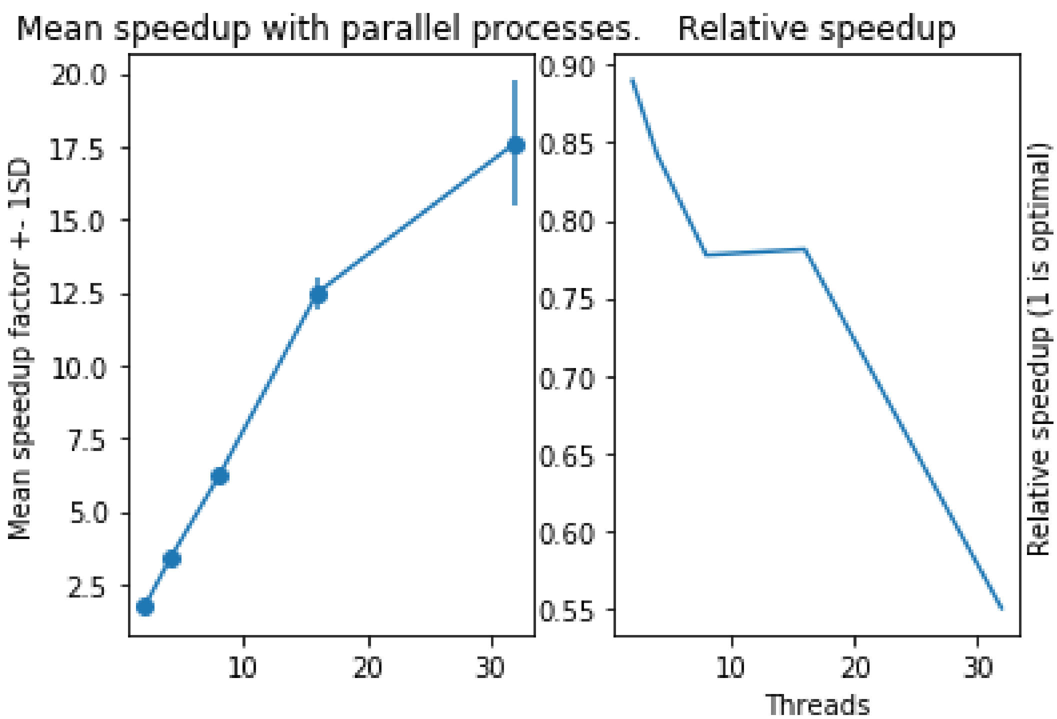
```
Wall time 165.43012145068496 and Cpu time 321.4172645919998
Effective Parallel Speedup (1 is None) = 1.939507388952666
Wall time 167.59992555342615 and Cpu time 324.21549043100003
Effective Parallel Speedup (1 is None) = 1.9322688819263387
Wall time 174.86549894604832 and Cpu time 324.05219635400044
Effective Parallel Speedup (1 is None) = 1.8504412337462075
Wall time 188.68512505758554 and Cpu time 321.3511342890006
Effective Parallel Speedup (1 is None) = 1.7016074161897083
Wall time 182.22527581453323 and Cpu time 325.06370527800027
Effective Parallel Speedup (1 is None) = 1.782608818620311
Wall time 180.87644483707845 and Cpu time 321.3229615449991
Effective Parallel Speedup (1 is None) = 1.7746769066244532
Wall time 183.85728101525456 and Cpu time 321.6588034390006
Effective Parallel Speedup (1 is None) = 1.7485367182477713
Wall time 184.30601975601166 and Cpu time 320.9943826310009
Effective Parallel Speedup (1 is None) = 1.7404760306804057
Wall time 198.5391414044425 and Cpu time 322.7628378370009
Effective Parallel Speedup (1 is None) = 1.6243623805369385
```

```
Wall time 193.74158086720854 and Cpu time 321.2103373959999
Effective Parallel Speedup (1 is None) = 1.6573436528656833
Wall time 94.98292154446244 and Cpu time 326.01713150900105
Effective Parallel Speedup (1 is None) = 3.423097209293948
Wall time 93.873236480169 and Cpu time 326.196446173999
Effective Parallel Speedup (1 is None) = 3.4725934761572437
Wall time 94.34768019896 and Cpu time 326.0148321880006
Effective Parallel Speedup (1 is None) = 3.450370585355581
Wall time 90.65048925671726 and Cpu time 324.9632003030001
Effective Parallel Speedup (1 is None) = 3.582693085808692
Wall time 95.7992107514292 and Cpu time 327.14220327399926
Effective Parallel Speedup (1 is None) = 3.4103576454306097
Wall time 99.01244391221553 and Cpu time 326.13591476000147
Effective Parallel Speedup (1 is None) = 3.2916486226852855
Wall time 102.12141093611717 and Cpu time 328.22165513099935
Effective Parallel Speedup (1 is None) = 3.211235247398652
Wall time 100.1181485131383 and Cpu time 325.43437273400014
Effective Parallel Speedup (1 is None) = 3.246868184876142
Wall time 101.13429316226393 and Cpu time 325.3837570860014
Effective Parallel Speedup (1 is None) = 3.214046836874357
Wall time 96.62403665296733 and Cpu time 326.1565405349993
Effective Parallel Speedup (1 is None) = 3.3689741503699695
Wall time 56.563270293176174 and Cpu time 361.095096346
Effective Parallel Speedup (1 is None) = 6.378201551895081
Wall time 59.388986306265 and Cpu time 360.66683780099993
Effective Parallel Speedup (1 is None) = 6.06425601383324
Wall time 58.8894515754655 and Cpu time 361.2682126609998
Effective Parallel Speedup (1 is None) = 6.1194937592052225
Wall time 60.47504727821797 and Cpu time 362.5647306690007
Effective Parallel Speedup (1 is None) = 5.988266585565126
Wall time 57.721721719019115 and Cpu time 359.2536296500002
Effective Parallel Speedup (1 is None) = 6.216009007852807
Wall time 59.53607106767595 and Cpu time 359.5980341459999
Effective Parallel Speedup (1 is None) = 6.030020019956679
Wall time 56.340928899124265 and Cpu time 360.62409026000023
Effective Parallel Speedup (1 is None) = 6.3890131758431865
Wall time 56.07378244865686 and Cpu time 361.72218607600007
Effective Parallel Speedup (1 is None) = 6.439573030110486
Wall time 59.17833804246038 and Cpu time 359.516451821999
Effective Parallel Speedup (1 is None) = 6.044426881932115
Wall time 56.115792780183256 and Cpu time 358.80947897700025
Effective Parallel Speedup (1 is None) = 6.3834802801341
Wall time 31.351583040319383 and Cpu time 384.36816634500065
Effective Parallel Speedup (1 is None) = 12.230255885884125
Wall time 30.788528186269104 and Cpu time 382.8326775409987
Effective Parallel Speedup (1 is None) = 12.369541736231907
Wall time 30.241189722903073 and Cpu time 382.90262982999775
Effective Parallel Speedup (1 is None) = 12.402689999924617
```

```
Wall time 28.965106283314526 and Cpu time 381.0180540440015
Effective Parallel Speedup (1 is None) = 13.107945642126381
Wall time 30.08530377689749 and Cpu time 382.48213656900043
Effective Parallel Speedup (1 is None) = 12.64865845473074
Wall time 28.613318433985114 and Cpu time 382.6914162799985
Effective Parallel Speedup (1 is None) = 13.296235762421578
Wall time 32.80480419378728 and Cpu time 382.90231288299765
Effective Parallel Speedup (1 is None) = 11.639595702138406
Wall time 30.66094843763858 and Cpu time 383.0774938880022
Effective Parallel Speedup (1 is None) = 12.45220801934131
Wall time 33.46978207398206 and Cpu time 384.2179893290013
Effective Parallel Speedup (1 is None) = 11.464254188789099
Wall time 30.595398145727813 and Cpu time 383.2490650730033
Effective Parallel Speedup (1 is None) = 12.50783137169629
Wall time 23.142528669908643 and Cpu time 383.6329589730012
Effective Parallel Speedup (1 is None) = 16.56883092232676
Wall time 20.77645702380687 and Cpu time 381.9824290100005
Effective Parallel Speedup (1 is None) = 17.381305262354076
Wall time 20.747365581803024 and Cpu time 383.25184483200064
Effective Parallel Speedup (1 is None) = 18.450251650880965
Wall time 21.804348956793547 and Cpu time 384.4586900860013
Effective Parallel Speedup (1 is None) = 17.62313241554302
Wall time 22.706437439657748 and Cpu time 382.9796975410027
Effective Parallel Speedup (1 is None) = 16.844680042646473
Wall time 17.772593814879656 and Cpu time 380.80055386000095
Effective Parallel Speedup (1 is None) = 21.335633629720327
Wall time 20.73494486324489 and Cpu time 383.5419308769997
Effective Parallel Speedup (1 is None) = 18.32440528594282
Wall time 22.01169817522168 and Cpu time 382.160138741001
Effective Parallel Speedup (1 is None) = 16.965774196803526
Wall time 30.976081527769566 and Cpu time 384.25858919700113
Effective Parallel Speedup (1 is None) = 12.359854157749554
Wall time 20.6696497220546 and Cpu time 382.5981622979998
Effective Parallel Speedup (1 is None) = 18.40751348614817
Using 2 threads achieves mean speedup 1.78E+00 +- 1.01E-01
Using 2 threads achieves mean relative speedup 8.89E-01 +- 1.01E-01
Using 4 threads achieves mean speedup 3.37E+00 +- 1.18E-01
Using 4 threads achieves mean relative speedup 8.43E-01 +- 1.18E-01
Using 8 threads achieves mean speedup 6.22E+00 +- 1.66E-01
Using 8 threads achieves mean relative speedup 7.78E-01 +- 1.66E-01
Using 16 threads achieves mean speedup 1.25E+01 +- 5.58E-01
Using 16 threads achieves mean relative speedup 7.81E-01 +- 5.58E-01
Using 32 threads achieves mean speedup 1.76E+01 +- 2.16E+00
Using 32 threads achieves mean relative speedup 5.51E-01 +- 2.16E+00
```

```
In [55]: x = [2,4,8,16,32]
         means, sd = [1.78, 3.37, 6.22, 12.5, 17.6], [1.01e-01, 1.18e-01, 1.166e-01, 5.58e-01, 2
```

```
rel = [m/x for (m,x) in zip(means, x)]
fig, (ax0, ax1)= plt.subplots(ncols=2, sharex=True)
ax0.errorbar(x, means, yerr=sd, fmt='-o')
ax0.set_title('Mean speedup with parallel processes.')
ax0.set_ylabel('Mean speedup factor +- 1SD')
ax1.plot(x, rel)
ax1.set_xlabel('Threads')
ax1.set_ylabel('Relative speedup (1 is optimal)')
ax1.yaxis.set_label_position("right")
ax1.set_title('Relative speedup')
plt.show()
```



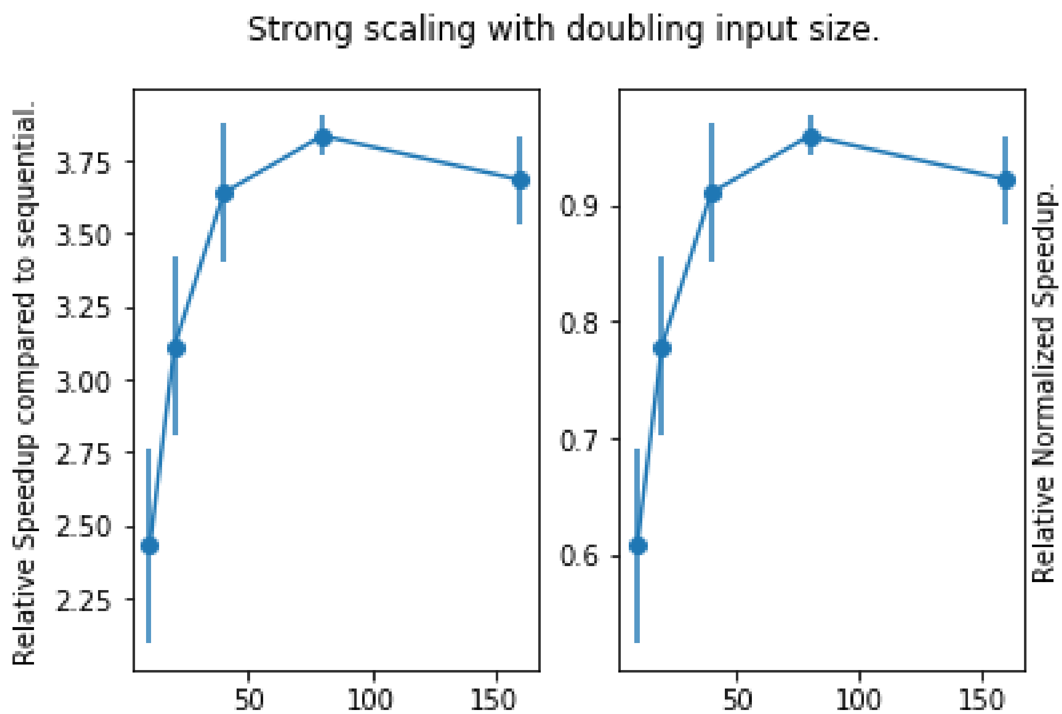
3.2 Strong Scaling: Same number of threads, but increase the load.

```
In [72]: ccounts = [10, 20, 40, 80, 160]
         nprocs = 4
         times = 10
         njobs = len(L) + len(R)
         results = np.zeros((len(ccounts), times, 4))
         finals = np.zeros((len(ccounts), 2))
         points = []
         for ni,c in enumerate(ccounts):
             print('Generating data with {}'.format(c))
             params = {'L':{'cluster_count':c+5, 'max_size':80, 'seed':1},  'R':{'cluster_count'
```

```
            L, R = [gen_clusters(*[value for key, value in p.items()]) for _, p in params.items
            points.append( sum(sum(len(q) for q in Q) for Q in [L,R]) )

            for t in range(times):
                wall, cpu, speedup = benchmark_solver(L, R, nprocs, False)
                ratio = speedup/nprocs
                results[ni][t] = wall, cpu, speedup, ratio
            finals[ni] = np.mean(results[ni][:,2]), np.std(results[ni][:,2])

        for p,(m,s),pts in zip(ccounts, finals, points):
            print('Using {} jobs achieves mean speedup {:.2E} +- {:.2E}'.format(pts, m, s))
```

```
Generating data with 10
Generating data with 20
Generating data with 40
Generating data with 80
Generating data with 160
Using 689 jobs achieves mean speedup 2.43E+00 +- 3.35E-01
Using 1219 jobs achieves mean speedup 3.11E+00 +- 3.06E-01
Using 2558 jobs achieves mean speedup 3.64E+00 +- 2.38E-01
Using 5107 jobs achieves mean speedup 3.84E+00 +- 6.84E-02
Using 10565 jobs achieves mean speedup 3.69E+00 +- 1.51E-01
```

```
In [76]: x = ccounts
         means, sd = finals[:,0], finals[:,1]
         fig, (ax0,ax1)= plt.subplots(ncols=2, sharex=True)
         ax0.errorbar(x, means, yerr=sd, fmt='-o')
         plt.suptitle('Strong scaling with doubling input size.')
         ax0.set_ylabel('Relative Speedup compared to sequential.')
         ax1.errorbar(x, means/nprocs, yerr=sd/nprocs, fmt='-o')
         ax1.set_ylabel('Relative Normalized Speedup.')
         ax1.yaxis.set_label_position("right")
         plt.show()
```



3.3 Conclusion

- Sequental Speedup: x15
- Parallel Speedup: .7 per extra thread
- Total Speedup: x15 * .7N for N threads

For our use case : x300 speedup.
Cost of adding @jit : 1s Cost of adding parallel drivers : 10 min (reusable)
Worth it if your code runs longer than 10 minutes