# scipar

July 19, 2018

#### 0.0.1 Accelerating Python for Scientific Computing.

Synthetic Use Case 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 [78]: 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
         import vtk
```

```
The Cython extension is already loaded. To reload it, use:
  %reload_ext Cython
```

### 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.

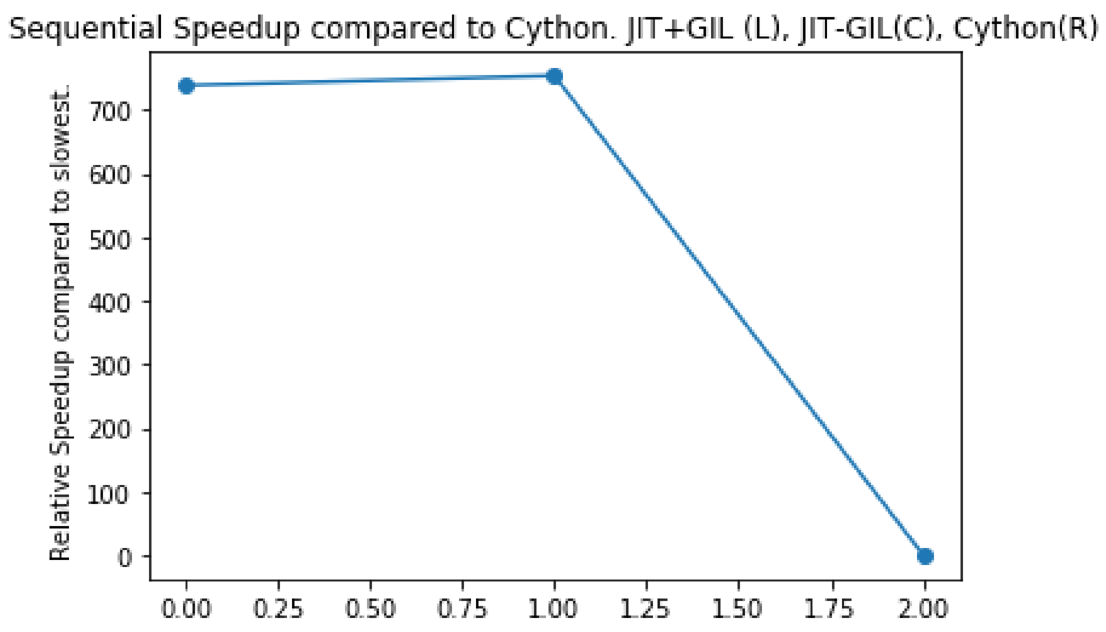
Do you expect a speedup from single threaded code *releasing* the GIL?

```
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) 0.06114678082932540 5
```

#### 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):
```

```
            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
```

### 3.1 Visualizing the Data with VTK/Paraview.

```
In [108]: class VtuWriter(object):
              def __init__(self, filename, points, values):
                  '''
                  Appends .vtu to filename
                  '''
                  self._points= vtk.vtkPoints()
                  self._grid = vtk.vtkUnstructuredGrid()
                  self._values = vtk.vtkDoubleArray()
                  self._values.SetName('point_values_array')
                  self._grid.SetPoints(self._points)
                  self._grid.GetPointData().SetScalars(self._values)
                  self._loadPoints(points, values)
                  self._write("{}.vtu".format(filename))

              def _loadPoints(self, points, values):
                  poly = vtk.vtkPolyVertex()
                  poly.GetPointIds().SetNumberOfIds(points.shape[0])
                  for i, (point, value) in enumerate(zip(points, values)):
                      poly.GetPointIds().SetId(i, self._points.InsertNextPoint(point))
                      self._values.InsertNextValue(value) # fix arbitrary data
                  self._grid.InsertNextCell(poly.GetCellType(), poly.GetPointIds())

              def _write(self, filename):
                  writer = vtk.vtkXMLUnstructuredGridWriter()
                  writer.SetFileName(filename)
                  writer.SetInputData(self._grid)
                  writer.Write()


          def concatenateArrays(points):
              rows = [p.shape[0] for p in points]
              result = np.empty((sum(rows), points[0].shape[1]))
              values = np.zeros((sum(rows), 1))
              rownr = 0
              for index,p in enumerate(points):
                  result[rownr:rownr+rows[index]] = p
                  rownr += rows[index]
                  values[rownr:rownr+rows[index]] = index
              return result, values

          def writeClustersMerged(C):
              for i,c in enumerate(C):
                  merged = concatenateArrays(c)
                  print('Writing {}'.format(len(merged[0])))
                  VtuWriter('cluster_{}'.format(i), *merged)

In [109]: writeClustersMerged([L,R])
```