Using Python, multiprocessing and NumPy/SciPy for parallel numerical computing

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Modern computers have processors with multicore CPUs. To use this efficiently, programs must be written to use multiple threads or multiple processes. Because of Python's global interpreter lock (GIL), only one thread at a time can access the interpreter. Thus, Python's threads (from the `thread` or `threading` modules) cannot be used to exploit the full power of a multicore CPU, with an exception for threads that releases the GIL in extension modules. In contrast, processes do not share GIL. Python 2.6 and 3.0 have a standard module called `multiprocessing`, which allows processes to be used with approximately the same API as `threading.Thread`. Thus, `multiprocessing` can be used to let Python code take advantage of computers with multiple virtual processors, without depending on extension modules to release the GIL. There is a backport of multiprocessing to Python 2.5 that can be used together with the current versions of NumPy and SciPy.

Since processes run in isolated virtual memory spaces, objects must either be serialized and communicated using IPC (e.g. pipes or sockets) or kept in special *shared memory* segments. The `multiprocessing` package has a special `Queue` object for synchronized IPC via pipes, and special objects for allocating `ctypes` objects (and arrays of them) in shared memory: `Value`, `RawValue`, `Array` and `RawArray`. Access to `Value` and `Array` is serialized by a lock. For example, a shared memory array of 1000 double precision floating point numbers is created as follows:

```
import ctypes
import multiprocessing as mp
shmem = mp.RawArray(ctypes.c_double, 1000)
```

Processes are created with the `multiprocessing.Process` object, which has almost the same interface as `threading.Thread`. Shared memory objects must be used as initialization arguments to the `Process` object. To use them for scientific computing with NumPy and SciPy, we need to view the shared memory region as a `numpy.ndarray` object. This is a moving target as `multiprocessing`'s internals keep changing. Currently, we can do it like this:

```
def shmem_as_ndarray( raw_array ):

    _ctypes_to_numpy = {
        ctypes.c_char : numpy.int8,
        ctypes.c_wchar : numpy.int16,
        ctypes.c_byte : numpy.int8,
        ctypes.c_ubyte : numpy.uint8,
        ctypes.c_short : numpy.int16,
        ctypes.c_ushort : numpy.uint16,
        ctypes.c_int : numpy.int32,
        ctypes.c_uint : numpy.int32,
        ctypes.c_long : numpy.int32,
        ctypes.c_ulong : numpy.int32,
        ctypes.c_float : numpy.float32,
        ctypes.c_double : numpy.float64
    }
    address = raw_array._wrapper.get_address()
```

```
    size = raw_array._wrapper.get_size()
    dtype = _ctypes_to_numpy[raw_array._type_]
    class Dummy(object): pass
    d = Dummy()
    d.__array_interface__ = {
         'data' : (address, False),
         'typestr' : numpy.uint8.str,
         'descr' : numpy.uint8.descr,
         'shape' : (size,),
         'strides' : None,
         'version' : 3
    }
    return numpy.asarray(d).view( dtype=dtype )
```

The next thing to check is the number of processors on the computer. It seldom helps to have more worker processes than virtual processors:

```
def number_of_processors():
    ''' number of virtual processors on the computer '''
    # Windows
    if os.name == 'nt':
        return int(os.getenv('NUMBER_OF_PROCESSORS'))
    # Linux
    elif sys.platform == 'linux2':
        retv = 0
        with open('/proc/cpuinfo','rt') as cpuinfo:
            for line in cpuinfo:
                if line[:9] == 'processor': retv += 1
        return retv
        # Please add similar hacks for MacOSX, Solaris, Irix,
        # FreeBSD, HPUX, etc.
    else:
        raise RuntimeError, 'unknown platform'
```

To serialize access to an array in shared memory, we can use a special *scheduler* protected by an instance of `multiprocessing.Lock`. Internally, `multiprocessing.Lock` is implemented using an OS semaphore. In addition to serializing memory access, the scheduler works as a "load balancer" for the CPUs. We ideally want to keep the CPUs busy at all times, not being idle waiting for the others, and scheduling work as seldom as possible. The choice of scheduling strategy is important. With "static" scheduling, an array is split in equally sized sub-regions between the processes. This is the simplest strategy, and has the smallest scheduling overhead. In "dynamic" scheduling, an array is split into multiple small sub-arrays, many more than the number of processors, e.g. by an order of magnitude. This will be the most efficient strategy if the computations vary in duration, thus preventing some of the processors to idle for a long time while the others complete their work. This strategy can have a large scheduling overhead. A "guided" scheduler is a compromise bet**w**een dynamic and static scheduling. The chunk size is adaptively reduced until a lower limit is reached.

Here is a scheduler that is implemented as a Python iterator, and returns `slice` objects for accessing reserved sub-arrays.

```
class Scheduler(object):

    def __init__(self, ndata, nprocs, chunk=None,schedule='guided'):
        if not schedule in ['guided','dynamic','static']:
            raise ValueError, 'unknown scheduling strategy'
        self._ndata = mp.RawValue(ctypes.c_int,ndata)
        self._start = mp.RawValue(ctypes.c_int,0)
        self._lock = mp.Lock()
        self._schedule = schedule
        self._nprocs = nprocs
        if schedule == 'guided' or schedule == 'dynamic':
            min_chunk = ndata // (10*nprocs)
            if chunk:
                min_chunk = chunk
            min_chunk = 1 if min_chunk < 1 else min_chunk
            self._chunk = min_chunk
        elif schedule == 'static'
            min_chunk = ndata // nprocs
            if chunk:
                min_chunk = chunk if chunk > min_chunk else min_chunk
            min_chunk = 1 if min_chunk < 1 else min_chunk
            self._chunk = min_chunk

    def __iter__(self):
        return self

    def next(self):
        self._lock.acquire()
        ndata = self._ndata.value
        nprocs = self._nprocs
        start = self._start.value
        if self._schedule == 'guided':
            _chunk = ndata // nprocs
            chunk = max(self._chunk, _chunk)
        else:
            chunk = self._chunk
        if ndata:
            if chunk > ndata:
                s0 = start
                s1 = start + ndata
                self._ndata.value = 0
            else:
                s0 = start
                s1 = start + chunk
                self._ndata.value = ndata - chunk
                self._start.value = start + chunk
            self._lock.release()
            return slice(s0, s1)
        else:
            self._lock.release()
            raise StopIteration
```

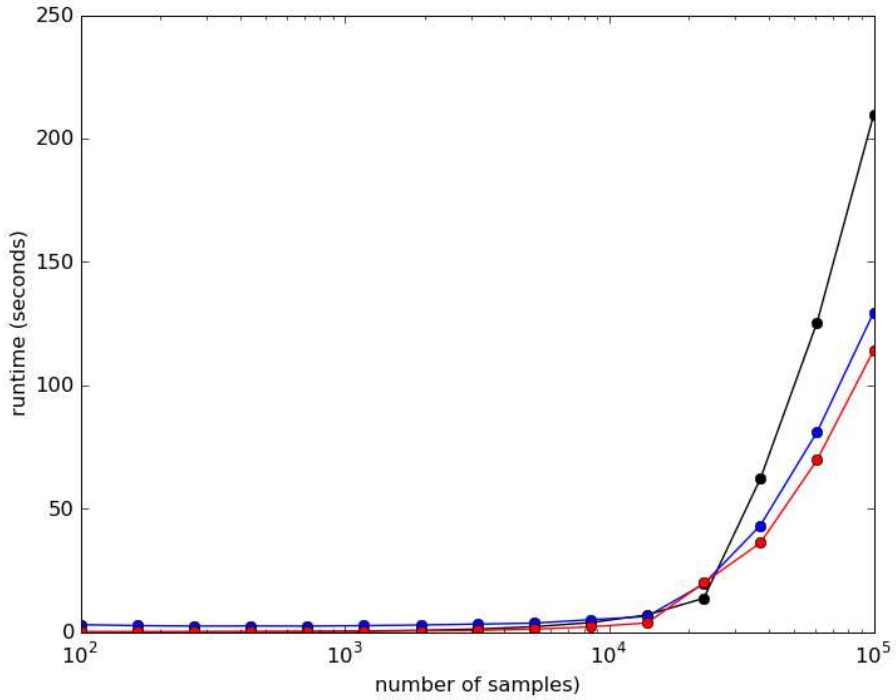
For illustration I will show you a subclass of `scipy.spatial.cKDTree` that uses `multiprocessing` for parallel queries.

```
import numpy
import scipy
import scipy.spatial
import multiprocessing as mp
import ctypes
import os
import sys
```

```
class cKDTree_MP( scipy.spatial.cKDTree ):

    ''' Multiprocessing cKDTree subclass, shared memory '''

    def __init__(self, data, leafsize=10):

        '''
        Same as cKDTree.__init__ except that an internal copy
        of data to shared memory is made.
        '''

        n, m = data.shape

        # Allocate shared memory for data
        self.shmem_data = mp.RawArray(ctypes.c_double, n*m)

        # View shared memory as ndarray, and copy over the data.
        # The RawArray objects have information about the dtype and
        # buffer size.
        _data = shmem_as_ndarray(self.shmem_data).reshape((n,m))
        _data[:,:] = data

        # Initialize parent, we must do this last because
        # cKDTree stores a reference to the data array. We pass in
        # the copy in shared memory rather than the origial data.
        self._leafsize = leafsize
        super(cKDTree_MP, self).__init__(_data, leafsize=leafsize)


    def parallel_query(self, x, k=1, eps=0, p=2,
                       distance_upper_bound=numpy.inf,
                       chunk=None, schedule='guided'):

        '''
        Same as cKDTree.query except parallelized with multiple
        processes and shared memory.

        Extra keyword arguments:

            chunk :     Minimum chunk size for the load balancer.
            schedule:   Strategy for balancing work load
                        ('static', 'dynamic' or 'guided').

        '''

        # allocate shared memory for x and result
        nx = x.shape[0]
        shmem_x = mp.RawArray(ctypes.c_double, nx*self.m)
        shmem_d = mp.RawArray(ctypes.c_double, nx*k)
        shmem_i = mp.RawArray(ctypes.c_int, nx*k)

        # view shared memory as ndarrays
        _x = shmem_as_ndarray(shmem_x).reshape((nx,self.m))
        _d = shmem_as_ndarray(shmem_d).reshape((nx,k))
        _i = shmem_as_ndarray(shmem_i).reshape((nx,k))

        # copy x to shared memory
        _x[:] = x

        # set up a scheduler to load balance the query
        nprocs = number_of_processors()
        scheduler = Scheduler(nx, nprocs, chunk=chunk, schedule=schedule)

        # return status in shared memory
        # access to these values are serialized automatically
        ierr = mp.Value(ctypes.c_int, 0)
        err_msg = mp.Array(ctypes.c_char, 1024)
```

```
        # query with multiple processes
        query_args = (scheduler,
                      self.shmem_data, self.n, self.m, self.leafsize,
                      shmem_x, nx, shmem_d, shmem_i,
                      k, eps, p, distance_upper_bound,
                      ierr)
        query_fun = _parallel_query
        pool = [mp.Process(target=query_fun, args=query_args) for n in range(nprocs)]
        for p in pool: p.start()
        for p in pool: p.join()
        if ierr.value != 0:
            raise RuntimeError, \
                  ('%d errors in worker processes. Last one reported:\n%s'
                       % (ierr.value, err_msg.value))

        # return results (private memory)
        return _d.copy(), _i.copy()



# This is executed in an external process:

def _parallel_query(scheduler,                      # scheduler for load balancing
                    data, ndata, ndim, leafsize,    # data needed to reconstruct the kd-tree
                    x, nx, d, i,                    # query data and results
                    k, eps, p, dub,                 # auxillary query parameters
                    ierr):                          # return values (0 on success)

    # Notice how this almost looks like a subroutine call in Fortran77,
    # as shapes and return arrays are passed in as arguments.

    try:
        # View shared memory as ndarrays.
        _data = shmem_as_ndarray(data).reshape((ndata,ndim))
        _x = shmem_as_ndarray(x).reshape((nx,ndim))
        _d = shmem_as_ndarray(d).reshape((nx,k))
        _i = shmem_as_ndarray(i).reshape((nx,k))

        # Reconstruct the kd-tree from the data.
        # This is relatively inexpensive.
        kdtree = scipy.spatial.cKDTree(_data, leafsize=leafsize)

        # Query for nearest neighbours, using slice ranges,
        # from the load balancer.

        for s in scheduler:
            _d[s,:],_i[s,:] = kdtree.query(_x[s,:], k=k, eps=eps, p=p,
                                           distance_upper_bound=dub)

    # An error occured, increment the return value ierr.
    # Access to ierr is serialized by multiprocessing.
    except:
        ierr.value += 1
```

Now we can benchmark the performance of this code. For comparison with multithreading in C, a version of `scipy.spatial.cKDTree` that use OpenMP was written. Kd-tree search for 5 nearest-neighbours was tested for an 8 dimensional data set of various size. The single-threaded cKDTree is marked with black, the multiprocessing sublass is blue, and the OpenMP version is red. We can now see how they perform on a computer with two processors (my dualcore laptop used to write this document):



Using `multiprocessing` incurs some overhead, in the order of a few seconds. And for data sizes below 10000 points this is worse than just using `cKDTree` with a single-thread. In comparison, the version with OpenMP was as expected the fastest. But as the number of data increases, using Python and `multiprocessing` was not much worse than multithreading in C with OpenMP.

The final thing that I will show is this tutorial is how to synchronize a pool of multiple processes. A "barrier" is a synchronization primitive often encountered in parallel numerical code. Python does not have a barrier primitive in multiprocessing, but we can easily create one using a number of `multiprocessing.Event` objects. It is so useful for numerical code that I will show how to construct one. There are many ways to construct a barrier primitive. A dissemination barrier is not the most efficient, but it is simple to program. Some overhead from using Python is expected anyway. This example also shows the other way to use `multiprocessing.Process`: subclassing and providing a custom `run()` method.

```
import multiprocessing as mp
from math import ceil, log

class PoolProcess( mp.Process ):

    def __init__(self, rank, events, numproc, lock):
        mp.Process.__init__(self)
        self.rank = rank
        self.events = events
        self.numproc = numproc
        self.lock = lock


    def barrier(self):
        if self.numproc == 1: return
```

```
        # loop log2(num_threads) times, rounding up
        for k in range(int(ceil(log(self.numproc)/log(2)))):
            # send event to thread (rank + 2**k) % numproc
            receiver = (self.rank + 2**k) % self.numproc
            evt = self.events[ self.rank * self.numproc + receiver ]
            evt.set()
            # wait for event from thread (rank - 2**k) % numproc
            sender = (self.rank - 2**k) % self.numproc
            evt = self.events[ sender * self.numproc + self.rank ]
            evt.wait()
            evt.clear()


    def run(self):

        # print the rank of this process
        # synchronize access to stdout
        self.lock.acquire()
        print 'Hello World, I am process %d' % self.rank
        self.lock.release()

        # wait for the self.numproc - 1 other processes
        # to finish printing
        self.barrier()

        # print the rank of this process
        # synchronize access to stdout
        self.lock.acquire()
        print 'Hello World again, I am process %d' % self.rank
        self.lock.release()


if __name__  == '__main__':
    numproc = 4
    lock = mp.Lock()
    events = [mp.Event() for n in range(numproc**2)]
    pool = [PoolProcess(rank, events, numproc, lock) for rank in range(numproc)]
    for p in pool: p.start()
    for p in pool: p.join()
```

When we run this code, the output becomes:

```
Hello World, I am process 2

Hello World, I am process 0

Hello World, I am process 1

Hello World, I am process 3

Hello World again, I am process 3

Hello World again, I am process 1

Hello World again, I am process 0

Hello World again, I am process 2
```

The effect of the barrier is easy to spot.

That’s all folks. Have fun multiprocessing with NumPy!