Python And Performance

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1 Introduction

- Python is interpreted: Python source code is executed by a program known as an interpreter
- In compiled languages (e.g., C/C++, Fortran), source code is compiled to an executable program
- Compiled programs generally run faster than interpreted programs
- Interpreted languages are often better for rapid prototyping and high-level program control
- Optimizing "time to science" might suggest prioritizing program development time over computational run time (or maybe vice versa)
- Python has become a popular language for scientific computing for many reasons

- How should we best use Python for applications that require numerically intensive computations?
- Can we have the best of both worlds (expressiveness and performance)?
- If there are tradeoffs, where are they and how can they be mitigated?
- As with most things in Python, there is no one answer...

2 CPython and the Python/C API

- CPython: the reference implementation of the language, and the most widely used interpreter (generally installed as "python")
- Alternative implementations/interpreters exist (e.g., IronPython, Jython, PyPy) — we will not consider these here
- IPython & Jupyter kernel are thin Python layers on top of CPython to provide additional functionality
  - but typically use python myprogram.py for long-running programs in batch
- CPython compiles Python source code to bytecodes, and then operates on those
- CPython, written in C, is accompanied by an Application Programming Interface (API) that enables communication between Python and C (and thus to basically any other language)
- Python/C API allows for compiled chunks of code to be called from Python or executed within the CPython interpreter → extension modules
- Much core functionality of the Python language and standard library are written in C

3 Extension Modules

- a compiled shared object library (.so, .dll, etc.) making use of Python/C API
  - compiled code executing operations of interest
  - wrapper/interface code consisting of calls to Python/C API and underlying compiled code
- can be imported into python interpreter just as pure Python source code can

3.1 Extension modules

[1]:
```
import math
print(math.cos(math.pi))

print(math.__file__)
```

```
-1.0
/Users/myers/anaconda3/envs/work/lib/python3.7/lib-
dynload/math.cpython-37m-darwin.so
```

[2]:
```
!nm $math.__file__
```

```
                 U _PyArg_Parse
                 U _PyArg_ParseTuple
                 U _PyArg_UnpackTuple
                 U _PyBool_FromLong
                 U _PyErr_Clear
                 U _PyErr_ExceptionMatches
                 U _PyErr_Format
                 U _PyErr_Occurred
                 U _PyErr_SetFromErrno
                 U _PyErr_SetString
                 U _PyExc_MemoryError
                 U _PyExc_OverflowError
                 U _PyExc_TypeError
                 U _PyExc_ValueError
                 U _PyFloat_AsDouble
                 U _PyFloat_FromDouble
                 U _PyFloat_Type
00000000000012f0 T _PyInit_math
                 U _PyIter_Next
                 U _PyLong_AsDouble
                 U _PyLong_AsLongAndOverflow
                 U _PyLong_FromDouble
                 U _PyLong_FromLong
                 U _PyLong_FromUnsignedLong
                 U _PyMem_Free
                 U _PyMem_Malloc
                 U _PyMem_Realloc
```

```
                 U _PyModule_AddObject
                 U _PyModule_Create2
                 U _PyNumber_Index
                 U _PyNumber_Lshift
                 U _PyNumber_Multiply
                 U _PyNumber_TrueDivide
                 U _PyObject_GetIter
                 U _PyType_IsSubtype
                 U _PyType_Ready
                 U _Py_BuildValue
0000000000006b30 s _SmallFactorials
                 U __PyArg_ParseStack
                 U __PyArg_ParseStackAndKeywords
                 U __PyArg_UnpackStack
                 U __PyLong_Frexp
                 U __PyLong_GCD
                 U __PyObject_FastCallDict
                 U __PyObject_LookupSpecial
                 U __Py_dg_infinity
                 U __Py_dg_stdnan
00000000000062d0 T __Py_log1p
                 U ___error
                 U ___memcpy_chk
                 U ___stack_chk_fail
                 U ___stack_chk_guard
                 U _abort
                 U _acos
                 U _acosh
                 U _asin
                 U _asinh
                 U _atan
                 U _atan2
                 U _atanh
                 U _ceil
                 U _copysign
                 U _cos
                 U _cosh
                 U _erf
                 U _erfc
                 U _exp
                 U _expm1
                 U _fabs
0000000000006100 t _factorial_partial_product
                 U _floor
                 U _fmod
                 U _frexp
0000000000006a70 s _gamma_integral
                 U _hypot
```

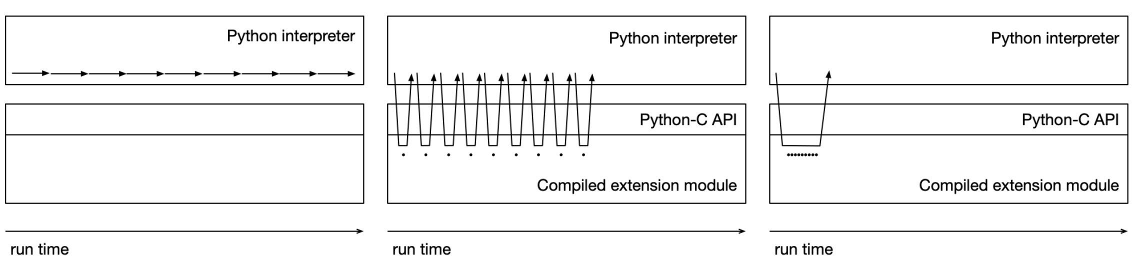
```
0000000000006a00 s _lanczos_den_coeffs
0000000000006990 s _lanczos_num_coeffs
                 U _ldexp
                 U _log
                 U _log10
                 U _log1p
                 U _log2
0000000000005d50 t _loghelper
00000000000061f0 t _m_atan2
0000000000006070 t _m_log
0000000000005fe0 t _m_log10
0000000000005cd0 t _m_log2
0000000000005980 t _m_remainder
0000000000005ea0 t _math_1
0000000000005ad0 t _math_2
00000000000013c0 t _math_acos
0000000000007960 d _math_acos_doc
0000000000001500 t _math_acosh
00000000000079b0 d _math_acosh_doc
0000000000001640 t _math_asin
0000000000007a00 d _math_asin_doc
0000000000001780 t _math_asinh
0000000000007a50 d _math_asinh_doc
00000000000018c0 t _math_atan
0000000000001a00 t _math_atan2
0000000000007af0 d _math_atan2_doc
0000000000007aa0 d _math_atan_doc
0000000000001a20 t _math_atanh
0000000000007b80 d _math_atanh_doc
0000000000001b60 t _math_ceil
0000000000008da8 d _math_ceil.PyId___ceil__
0000000000007bd0 d _math_ceil__doc__
0000000000001d10 t _math_copysign
0000000000007c40 d _math_copysign_doc
0000000000001d30 t _math_cos
0000000000007d00 d _math_cos_doc
0000000000001e70 t _math_cosh
0000000000007d50 d _math_cosh_doc
0000000000001fa0 t _math_degrees
0000000000007d90 d _math_degrees__doc__
0000000000002010 t _math_erf
0000000000007de0 d _math_erf_doc
00000000000020f0 t _math_erfc
0000000000007e10 d _math_erfc_doc
00000000000021d0 t _math_exp
0000000000007e50 d _math_exp_doc
0000000000002300 t _math_expm1
0000000000007e90 d _math_expm1_doc
```

```
0000000000002430 t _math_fabs
0000000000007f30 d _math_fabs_doc
0000000000002560 t _math_factorial
0000000000007f80 d _math_factorial__doc__
0000000000002920 t _math_floor
0000000000008d90 d _math_floor.PyId___floor__
0000000000007fe0 d _math_floor__doc__
0000000000002ad0 t _math_fmod
0000000000008050 d _math_fmod__doc__
0000000000002c60 t _math_frexp
00000000000080b0 d _math_frexp__doc__
0000000000002d10 t _math_fsum
0000000000008180 d _math_fsum__doc__
0000000000003230 t _math_gamma
0000000000008210 d _math_gamma_doc
0000000000003a50 t _math_gcd
0000000000008240 d _math_gcd__doc__
0000000000003b40 t _math_hypot
0000000000008280 d _math_hypot__doc__
0000000000003cf0 t _math_isclose
00000000000072a0 s _math_isclose._keywords
0000000000008d50 d _math_isclose._parser
00000000000082d0 d _math_isclose__doc__
0000000000003e60 t _math_isfinite
0000000000008590 d _math_isfinite__doc__
0000000000003ee0 t _math_isinf
0000000000008600 d _math_isinf__doc__
0000000000003f60 t _math_isnan
0000000000008670 d _math_isnan__doc__
0000000000003fd0 t _math_ldexp
00000000000086d0 d _math_ldexp__doc__
0000000000004210 t _math_lgamma
0000000000008730 d _math_lgamma_doc
00000000000046a0 t _math_log
0000000000004d50 t _math_log10
00000000000088b0 d _math_log10__doc__
0000000000004c00 t _math_log1p
0000000000008820 d _math_log1p_doc
0000000000004d70 t _math_log2
00000000000088f0 d _math_log2__doc__
0000000000008790 d _math_log__doc__
00000000000073a0 d _math_methods
0000000000004d90 t _math_modf
0000000000008930 d _math_modf__doc__
0000000000004e60 t _math_pow
00000000000089b0 d _math_pow__doc__
0000000000005220 t _math_radians
00000000000089f0 d _math_radians__doc__
```

```
0000000000005290 t _math_remainder
0000000000008a40 d _math_remainder_doc
00000000000052b0 t _math_sin
0000000000008b60 d _math_sin_doc
00000000000053f0 t _math_sinh
0000000000008bb0 d _math_sinh_doc
0000000000005520 t _math_sqrt
0000000000008bf0 d _math_sqrt_doc
0000000000005660 t _math_tan
0000000000008c30 d _math_tan_doc
00000000000057a0 t _math_tanh
0000000000008c80 d _math_tanh_doc
00000000000058e0 t _math_trunc
0000000000008d38 d _math_trunc.PyId___trunc__
0000000000008cc0 d _math_trunc__doc__
00000000000072d0 d _mathmodule
                 U _memcpy
                 U _modf
0000000000007340 d _module_doc
                 U _pow
                 U _round
                 U _sin
                 U _sinh
                 U _sqrt
                 U _tan
                 U _tanh
                 U dyld_stub_binder
```

4 Hybrid Codes

It is often advantageous to blend high-level languages for control with low-level languages for performance. Overall performance depends on the granularity of computations in compiled code and the overhead required to communicate between languages.



There are many different tools the support the interleaving of Python and compiled extension modules.

5 Comments and caveats about performance optimization

- Make sure you have the right algorithm for the task at hand
- Remember that "premature optimization is the root of all evil" (D. Knuth)
- Focus on performance optimization only for those pieces of code that need it
- Algorithms and computational architectures are complex: be empirical about performance

6 Outline

- Introduction
- Leveraging Compiled Code
  - Compiled Third-Party Libraries
  - Compiling Custom Code
- Leveraging Additional Computational Resources
  - Parallel Processing
- Writing Faster Python
- Performance Assessment

Material derived in part from Cornell Virtual Workshop (CVW) tutorial on "Python for High Performance", at `https://cvw.cac.cornell.edu/python` .

These slides will be available as a Jupyter notebook linked from the CVW site. Note: some code presented here is in the form of incomplete snippets to illustrate a point. This notebook will therefore not run from start to finish without errors.

7 Third-Party Libraries for Numerical & Scientific Computing

a.k.a. The Python Scientific Computing Ecosystem

- Most specific functionality for scientific computing is provided by third-party libraries, which are typically a mix of Python code and compiled extension modules
  - NumPy: multi-dimensional arrays and array operations, linear algebra, random numbers
  - SciPy: routines for integration, optimization, root-finding, interpolation, fitting, etc.
  - Pandas: Series and Dataframes to handle tabular data (e.g., from spreadsheets)
  - Scikit-learn, TensorFlow, Caffe, PyTorch, Keras: machine learning
  - NetworkX: networks
  - Matplotlib, Seaborn: plotting
  - etc.
- Bundled distributions (e.g, Anaconda) contain many of these, with tools for installing additional packages

8 NumPy

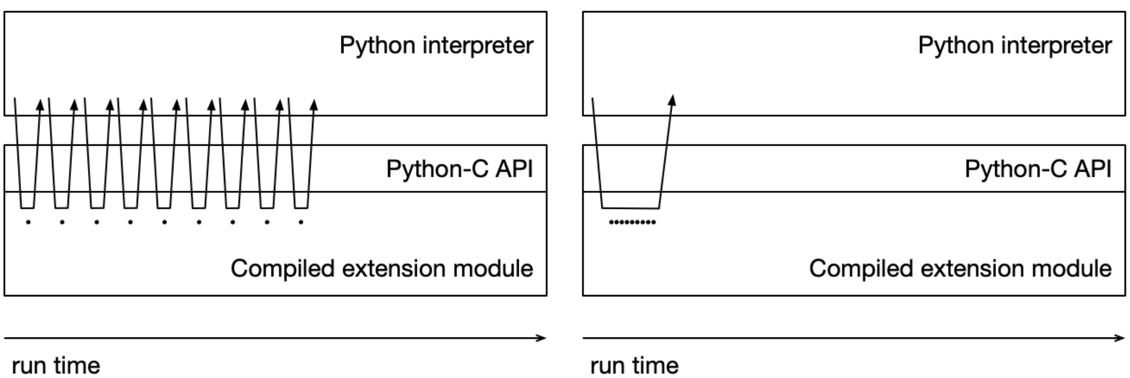
- NumPy = "Numerical Python", the cornerstone of the Python Scientific Computing Ecosystem
- largely written in C, with links to BLAS and LAPACK for linear algebra
- provides multidimensional arrays and array-level operations (a form of vectorization)

- conventional wisdom: avoid loops in Python and use array syntax
- a challenge: figuring out how to express complex operations solely using array syntax (including indexing, slicing, and broadcasting)
- a caveat: convenient syntax can disguise performance inefficiencies (e.g., temporary arrays)

9 Elementwise array operations

[ ]:
```
import numpy as np
a = np.random.random((1000,1000))
b = np.random.random((1000,1000))

log_a = np.log(a)   # an example of a ufunc

c = a + b     # throws ValueError if a and b not the same shape
```

[ ]:
```
assert(a.shape == b.shape)  # throws AssertionError if a and b not the same shape
c = np.zeros_like(a)        # prefills a zero array of the correct shape
for i in range(a.shape[0]):
    for j in range(a.shape[1]):
        c[i,j] = a[i,j] + b[i,j]
```



10 More complicated array operations

- a challenge: figuring out how to express complex operations solely using array syntax (including indexing, slicing, and broadcasting)

[ ]:
```
# numpy outer product

def outer(a,b):
    multiply(a.ravel()[:, newaxis], b.ravel()[newaxis, :], out)

# e.g., generalized outer product to compute pairwise Hamming distances between
 ↪all subsequences in a 2D array
```

```python
def Hamming_outer(a0,a1):
    return np.sum(np.bitwise_xor(a0[:,np.newaxis], a1[np.newaxis,:]), axis=2)
```

11 More complicated array operations

[ ]:
```python
# e.g., approximate Laplacian on 2D array by summing up shifted copies of array

def Del2(a, dx):
    nx, ny = a.shape
    del2a = scipy.zeros((nx, ny), float)
    del2a[1:-1, 1:-1] = (a[1:-1,2:] + a[1:-1,:-2] + \
                         a[2:,1:-1] + a[:-2,1:-1] - 4.*a[1:-1,1:-1])/(dx*dx)
    return del2a

# roughly equivalent to:

for i in range(1,nx-1):
    for j in range(1,ny-1):
        del2a[i,j] = (a[i+1,j] + a[i-1,j] + a[i,j+1] + a[i,j-1] - 4*a[i,j])/
 ↪(dx*dx)
```

12 NumPy and optimized libraries

- NumPy performance can be enhanced if linked to optimized libraries
  - `numpy.__config__.show()` to list what blas, lapack libraries numpy is linked to
- Intel MKL (Math Kernel Library) is highly optimized for Intel processors, and bundled with Anaconda Python distribution
- On multi-core architectures, optimized libraries can provide NumPy-based parallelism for free by setting environment variables appropriate for processor
  - `MKL_NUM_THREADS = N` # if using MKL
  - `OMP_NUM_THREADS = N` # if libraries support OpenMP

13 NumPy and temporary array creation

$$\frac{\partial u}{\partial t} = D\nabla^2 u + u(1-u)$$

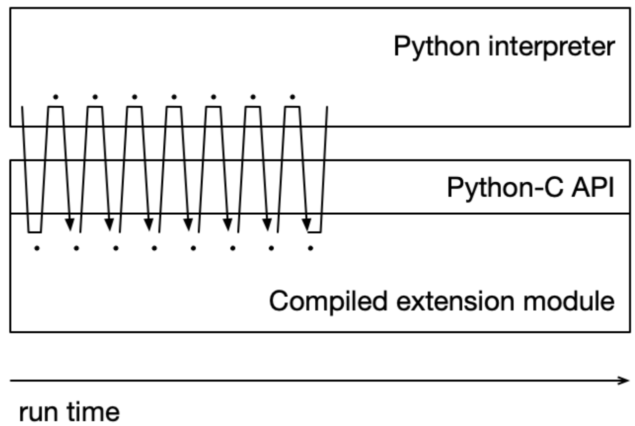
[ ]:
```python
u += dt * ( D * Del2(u) + u * (1 - u) )
```

Temporary arrays created: * Del2(u) * D * Del2(u) * 1 - u * u * (1 - u) * D * Del2(u) + u * (1 - u) * dt * (D * Del2(u) + u * (1 - u))

14 SciPy

- SciPy = “Scientific Python”
- sits on top of NumPy, wrapping many C and Fortran numerical routines, with convenient Python interface
- routines for integration, optimization, root-finding, interpolation, fitting, etc.
- Python callbacks enable ease-of-use, but with some performance penalty

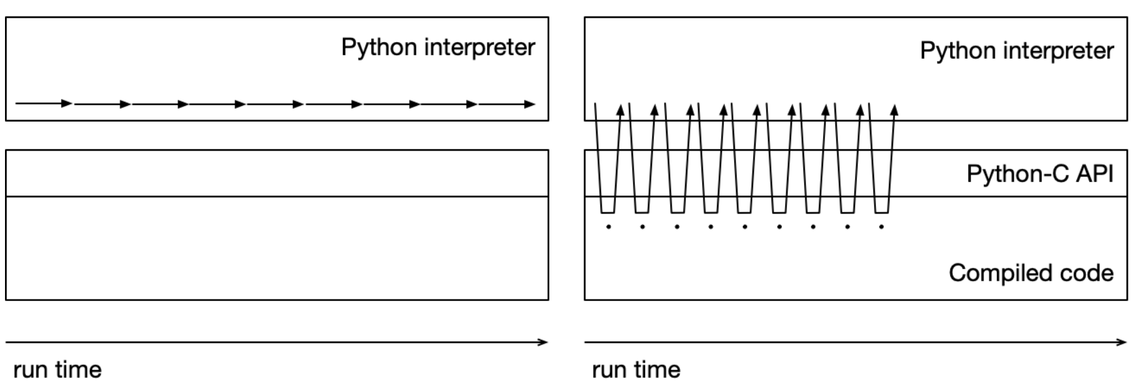
```
from scipy.integrate import solve_ivp

def func(t, y):
    dydt = …
    return dydt

# integrate dy/dt = func(t,y)
# with initial condition y=y0

sol = solve_ivp(func, trange, y0)
```



- can hack things with the help of wrapper generation tools to get compiled routines to accept a pointer to a compiled callback function
- scipy.LowLevelCallable recently introduced to work with some functions (not solve_ivp)

15 Compiling Custom Code

- Compilation frameworks
  - Numba and Cython
  - internal code generation for deep learning neural networks: Tensorflow, PyTorch, etc.
- Wrapper and interface generators



16 Numba

- a just-in-time (JIT) compiler that compiles a subset of Python and NumPy source to machine code for execution in CPython

- uses LLVM to convert Python bytecodes to intermediate representation (IR), and generates optimizes C code from that
- can be configured in more detail, but some performance improvements simply via addition of @jit decorator

17 Upending the conventional wisdom via compilation

[3]:
```
import numpy as np
from numba import jit

X = np.random.random((1000,1000))
Y = np.random.random((1000,1000))
Z = np.random.random((1000,1000))

def f1(x,y,z):
    return x + 2*y + 3*z

def f2(x,y,z):
    result = np.empty_like(x)
    for i in range(x.shape[0]):
        for j in range(x.shape[1]):
            result[i,j] = x[i,j] + 2*y[i,j] + 3*z[i,j]
    return result

@jit
def f3(x,y,z):
    result = np.empty_like(x)
    for i in range(x.shape[0]):
        for j in range(x.shape[1]):
            result[i,j] = x[i,j] + 2*y[i,j] + 3*z[i,j]
    return result
```

[4]:
```
%timeit f1(X,Y,Z)
%timeit f2(X,Y,Z)
%timeit f3(X,Y,Z)
```

```
2.96 ms ± 50.9 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
1.15 s ± 16.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
1.73 ms ± 133 µs per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

18 Cython

- a C-like superset of the Python language that adds capabilities for type declarations
- a system for converting chunks of Python/Cython code into C for compilation and exeuction within CPython

- can be used to compile extension modules ahead of time, or for on-the-fly compilation using IPython magic functions (%%cython)
- mature technology used by many packages in Python ecosystem use Cython to optimize particular functionality (Pandas, Scikit-learn, etc.)
- provides support for OpenMP-based parallelism through the cython.parallel module

[5]:
```
# Example: adapted from Cython tutorial at https://cython.readthedocs.io/en/
↪latest/src/tutorial/cython_tutorial.html#primes

def primes(nb_primes):
    if nb_primes > 1000:
        nb_primes = 1000

    p = [0]*nb_primes
    len_p = 0  # The current number of elements in p.
    n = 2
    while len_p < nb_primes:
        # Is n prime?
        for i in p[:len_p]:
            if n % i == 0:
                break

        # If no break occurred in the loop, we have a prime.
        else:
            p[len_p] = n
            len_p += 1
        n += 1

    # Let's return the result in a python list:
    result_as_list  = [prime for prime in p[:len_p]]
    return result_as_list

primes100 = primes(100)
print(primes100)
```

```
[2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41, 43, 47, 53, 59, 61, 67, 71, 73,
79, 83, 89, 97, 101, 103, 107, 109, 113, 127, 131, 137, 139, 149, 151, 157, 163,
167, 173, 179, 181, 191, 193, 197, 199, 211, 223, 227, 229, 233, 239, 241, 251,
257, 263, 269, 271, 277, 281, 283, 293, 307, 311, 313, 317, 331, 337, 347, 349,
353, 359, 367, 373, 379, 383, 389, 397, 401, 409, 419, 421, 431, 433, 439, 443,
449, 457, 461, 463, 467, 479, 487, 491, 499, 503, 509, 521, 523, 541]
```

[6]:
```
%load_ext Cython
```

[7]:
```
%%cython -a

def primes_cython(int nb_primes):
```

```
    cdef int n, i, len_p
    cdef int p[1000]
    if nb_primes > 1000:
        nb_primes = 1000

    len_p = 0  # The current number of elements in p.
    n = 2
    while len_p < nb_primes:
        # Is n prime?
        for i in p[:len_p]:
            if n % i == 0:
                break

        # If no break occurred in the loop, we have a prime.
        else:
            p[len_p] = n
            len_p += 1
        n += 1

    # Let's return the result in a python list:
    result_as_list  = [prime for prime in p[:len_p]]
    return result_as_list

cprimes100 = primes_cython(100)
print(cprimes100)
```

```
[2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41, 43, 47, 53, 59, 61, 67, 71, 73,
79, 83, 89, 97, 101, 103, 107, 109, 113, 127, 131, 137, 139, 149, 151, 157, 163,
167, 173, 179, 181, 191, 193, 197, 199, 211, 223, 227, 229, 233, 239, 241, 251,
257, 263, 269, 271, 277, 281, 283, 293, 307, 311, 313, 317, 331, 337, 347, 349,
353, 359, 367, 373, 379, 383, 389, 397, 401, 409, 419, 421, 431, 433, 439, 443,
449, 457, 461, 463, 467, 479, 487, 491, 499, 503, 509, 521, 523, 541]
```

[7]:
```
<IPython.core.display.HTML object>
Cython output in Jupyter shows annotated verson of code, which can be clicked on
 ↪to reveal injected C code
```

[8]:
```
%timeit primes(100)

%timeit primes_cython(100)
```

```
367 µs ± 1.15 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
18.8 µs ± 21.8 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

19 Wrapper and Interface Generators

Useful if you have an existing code base (C/C++, Fortran, etc.) that you would like to be able to call from Python

Typically a multi-step process:

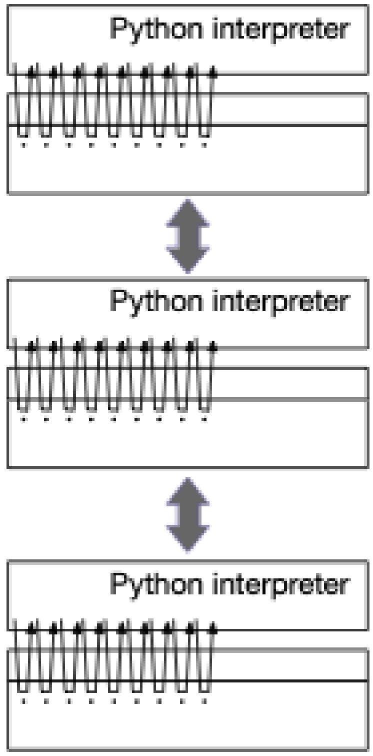
- Python/C API code generation from function and class declarations
- wrapper code compiled and linked with underlying library → .so file
- possibly some additional Python code generated

Some of the many packages available:

- CFFI and ctypes provide "foreign function interfaces", or lightweight APIs, for calling C libraries from within Python
- Boost.python helps write C++ libraries that Python can import
- SWIG reads C and C++ header files and generates a library than Python (or many other scripting languages) can import
- F2PY reads Fortran code and generates a library that Python can import
- PyCUDA and PyOpenCL provide access within Python to GPUs

20 Parallel Processing

- Parallelization: across threads, across cores, across processors
  - ...to reduce wallclock time to solution
  - ...to solve bigger problems that don't fit in a single processor
- CPython uses Global Interpreter Lock (GIL): only one thread can run at a time
- GIL does not apply to multithreaded code in compiled library (e.g., MKL)
- Multiple Python processes can run concurrently (each with their own GIL)
- (and new development is apparently underway to enable multiple interpreters within a single process)



21 Multiprocessing and concurrent.futures modules

- control of multiple processes and communication between them
- useful for multiprocessing within a multi-core, shared memory processor

[4]:
```
def f(x):
    return x*x

import multiprocessing

p = multiprocessing.Pool(processes=4)
print(p.map(f, range(10)))

# or, equivalently

import concurrent.futures

executor = concurrent.futures.ProcessPoolExecutor(max_workers=4)
print(list(executor.map(f, range(10))))
```

```
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
[0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

22 More multiprocessing (from networkx docs)

Link to networkx page

[ ]:
```
# just a subset of the code (download full example at link above to run)

def _betmap(G_normalized_weight_sources_tuple):
    return nx.betweenness_centrality_source(*G_normalized_weight_sources_tuple)

def betweenness_centrality_parallel(G, processes=None):
    """Parallel betweenness centrality  function"""
    p = Pool(processes=processes)
    node_divisor = len(p._pool) * 4
    node_chunks = list(chunks(G.nodes(), int(G.order() / node_divisor)))
    num_chunks = len(node_chunks)
    bt_sc = p.map(_betmap,
                  zip([G] * num_chunks,
                      [True] * num_chunks,
                      [None] * num_chunks,
                      node_chunks))

    # Reduce the partial solutions
    bt_c = bt_sc[0]
    for bt in bt_sc[1:]:
        for n in bt:
            bt_c[n] += bt[n]
    return bt_c
```

23 Message passing with mpi4py

- MPI = "Message Passing Interface" — a widely-used standard for parallel processing
- Many Python wrappers to MPI developed over the years; mpi4py is probably most widely used at this time
- use `mpiexec` or `ibrun` in shell to run a python program over multiple processors
  - e.g., `ibrun python myprogram.py` on Stampede2 at TACC

23.1 mpi4py

[5]:
```
from mpi4py import MPI
comm = MPI.COMM_WORLD
print(comm.Get_rank())
print(comm.Get_size())

import numpy as np
data = np.arange(1000, dtype=np.float64)
data2 = np.zeros(1000, dtype=np.float64)
print(data2[:5])
```

```
comm.Isend(data, dest=0, tag=20)
comm.Recv(data2, source=0, tag=20)
print(data2[:5])
```

```
0
1
[0. 0. 0. 0. 0.]
[0. 1. 2. 3. 4.]
```

24 Exercise: Estimating π via Monte Carlo using mpi4py

Exercise in CVW on "Python for High Performance"

25 Other Parallel Tools

- Dask
  - distributed NumPy arrays and Pandas DataFrames
  - task scheduling interface for custom workflows
- Joblib
  - lightweight pipelining with support for parallel processing
  - specific optimizations for NumPy arrays
- ipyparallel
  - parallel and distributed computing within IPython

26 Writing Faster Python

- Collections and containers
- Lazy evaluation
- Memory management

26.1 Collections and containers

Use the right data structure for the job

[1]:
```
set1 = set(range(0,1000))         # create a set with a bunch of numbers in it
set2 = set(range(500,2000))      # create another set with a bunch of numbers in
 ↪it
isec = set1 & set2                # same as isec = set1.intersection(set2)

list1 = list(range(0,1000))       # create a list with a bunch of numbers in it
list2 = list(range(500,2000))    # create another list with a bunch of numbers in
 ↪it
isec = [e1 for e1 in list1 for e2 in list2 if e1==e2]     # uses list
 ↪comprehensions
```

```
%timeit set1 & set2
%timeit [e1 for e1 in list1 for e2 in list2 if e1==e2]
```

```
14.3 µs ± 92.7 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
35.3 ms ± 610 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

26.2 Lazy evaluation

- a strategy implemented in some programming languages whereby certain objects are not produced until they are needed
- often used in conjunction with functions that produce collections of objects
- if you only need to iterate over the items in a collection, you don't need to produce that entire collection

Python provides a variety of mechanisms to support lazy evaluation:

- generators: like functions, but maintain internal state and `yield` next value when called
- dictionary views (keys and values)
- range: `for i in range(N)`
- zip: `pairs = zip(seq1, seq2)`
- enumerate: `for i, val in enumerate(seq)`
- open: `with open(filename, 'r') as f`

27 Performance Assessment

- Timing: getting timing information for particular operations
- Profiling: figuring out where time is being spent

IPython magic functions

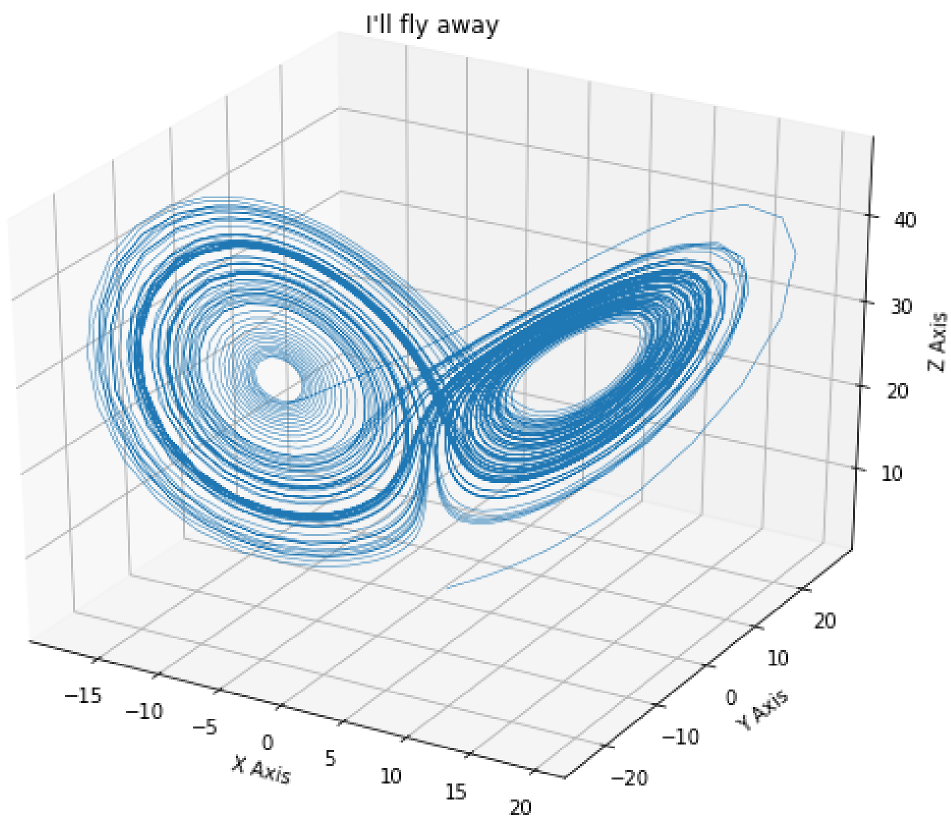
- %timeit : uses timeit module from Python Standard Library
- %prun : uses profile module from Python Standard Library

[7]:
```
from scipy.integrate import solve_ivp

sigma = 10
rho = 28
beta = 8.0/3

def lorenz(t, xyz):
    x,y,z = xyz
    xdot = sigma*(y-x)
    ydot = x*(rho-z) - y
    zdot = x*y - beta*z
    return [xdot, ydot, zdot]

def integrate_lorenz(ic=[1.,1.,1.]):
    sol = solve_ivp(lorenz, (0., 100.), ic, method='LSODA')
    return sol
```

```
%prun integrate_lorenz()
```

[5]:
```
sol = integrate_lorenz()
xs, ys, zs = sol['y']
```

[6]:
```
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
%matplotlib inline
fig = plt.figure(figsize=(10,8))
ax = fig.gca(projection='3d')

ax.plot(xs, ys, zs, lw=0.5)
ax.set_xlabel("X Axis")
ax.set_ylabel("Y Axis")
ax.set_zlabel("Z Axis")
ax.set_title("I'll fly away");
```



28 Summary

- Python and Performance together in one big tent
- There is no one answer: think about how you can best optimize "time to science"
- Make sure you have the right algorithms, do not prematurely optimize, and be empirical about performance

```
[ ]:
```