Scientific computing using Cython: Best of both worlds!

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About me

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What this talk is about?

What is Cython?

Unleash Cython superpowers.

Build your first cython module.

Cython and NumPy

Unleash more superpowers.

Project demo: Cyvlfeat

What is Cython?

Optimising static compiler for both the Python and Cython

It makes writing C extensions for Python as easy as Python itself.

Unleash superpowers.

- Write Python code that calls back and forth from and to C or C++ code natively at any point.

- ➔ Easily tune readable Python code into plain C performance by adding static type declarations.

Pure Python code:

```python
def f(x):
    return x**2-x

def integrate_f(a, b, N):
    s = 0
    dx = (b-a)/N
    for i in range(N):
        s += f(a+i*dx)
    return s * dx
```

With additional Static Type declarations: 4 times speedup

```
def f(double x):
    return x**2-x

def integrate_f(double a, double
b, int N):
    cdef int i
    cdef double s, dx
    s = 0
    dx = (b-a)/N
    for i in range(N):
        s += f(a+i*dx)
    return s * dx
```

Def

def - Basically, it's Python

def is used for code that will be:

- Called directly from Python code with Python objects as arguments.
- Returns a Python object

Cdef

cdef - Basically, it’s C

cdef is used:

- Where Cython functions are intended to be pure ‘C’ functions.
- All types *must* be declared.
- The generated code is about as fast as you can get though.

Cpdef

cpdef - It's both

cpdef combines both def and cdef by creating two functions; a cdef for C types and a def for Python types.

- Uses early binding when using C fundamental types
- Uses dynamic binding when Python objects are passed

➔ It can call C/C++ libraries directly using cimport

```
In [11]: %%cython -a
         # libc math functions
         from libc cimport math

         print( math.sin(math.M_PI / 2) )

         1.0

Out[11]:
         Generated by Cython 0.23.beta1

         Yellow lines hint at Python interaction.
         Click on a line that starts with a "+" to see the C code that Cython generated for it.
          1: # libc math functions
          2: from libc cimport math
          3:
         +4: print( math.sin(math.M_PI / 2) )
```

→ Integrate natively with existing code.


The force is strong with this one.

Where’s the magic?

Motivation

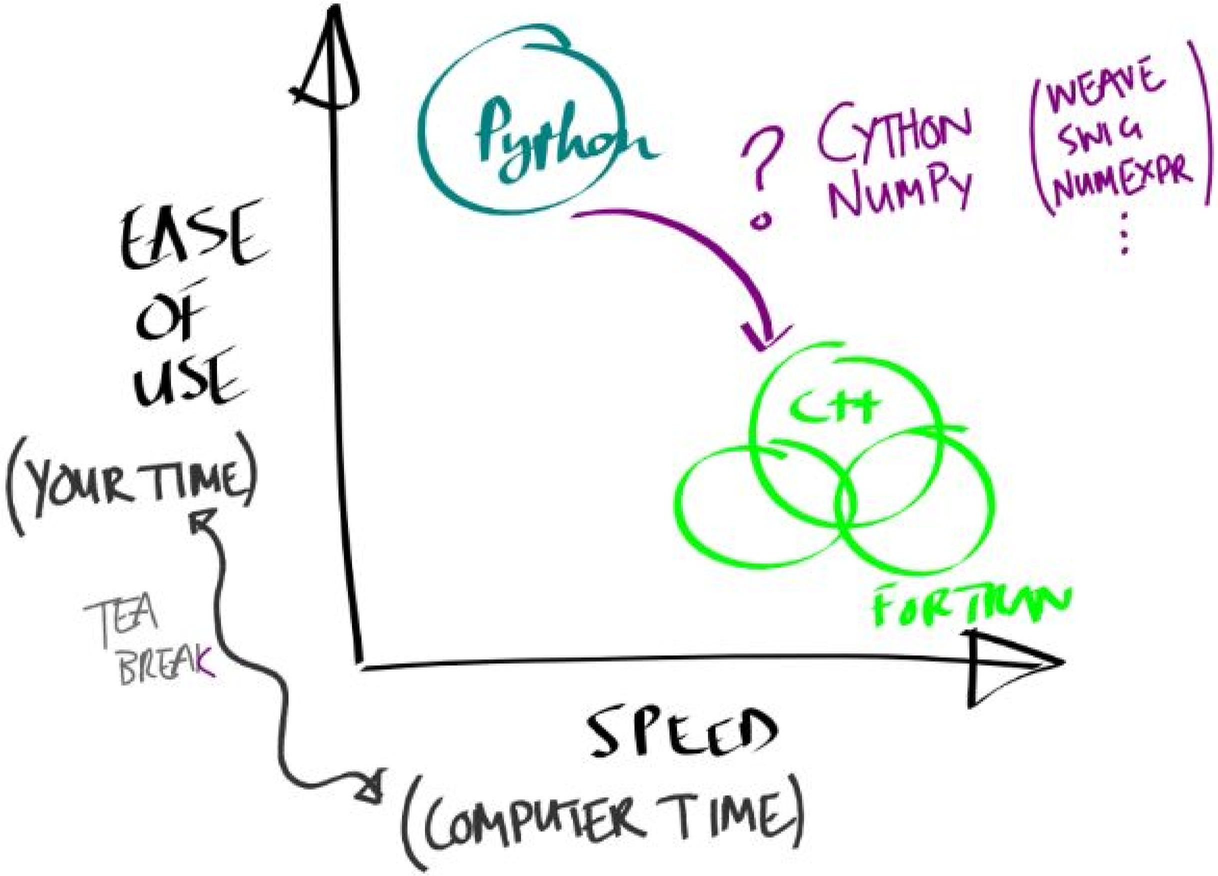


Illustration borrowed from: Stéfan van der Walt's presentation at Advanced Python Summer School, Kiel 2012.

Cython by example

Python 1x

```
def fib(n):
    a,b = 1,1
    for i in range(n):
        a, b = a+b, a
    return a
```

C/C++ 100x

```
int fib(int n)
{
    int tmp, i, a, b;
    a = b = 1;
    for(i=0; i<n; i++){
    tmp = a;
    a += b;
    b = tmp;
    }
}
```

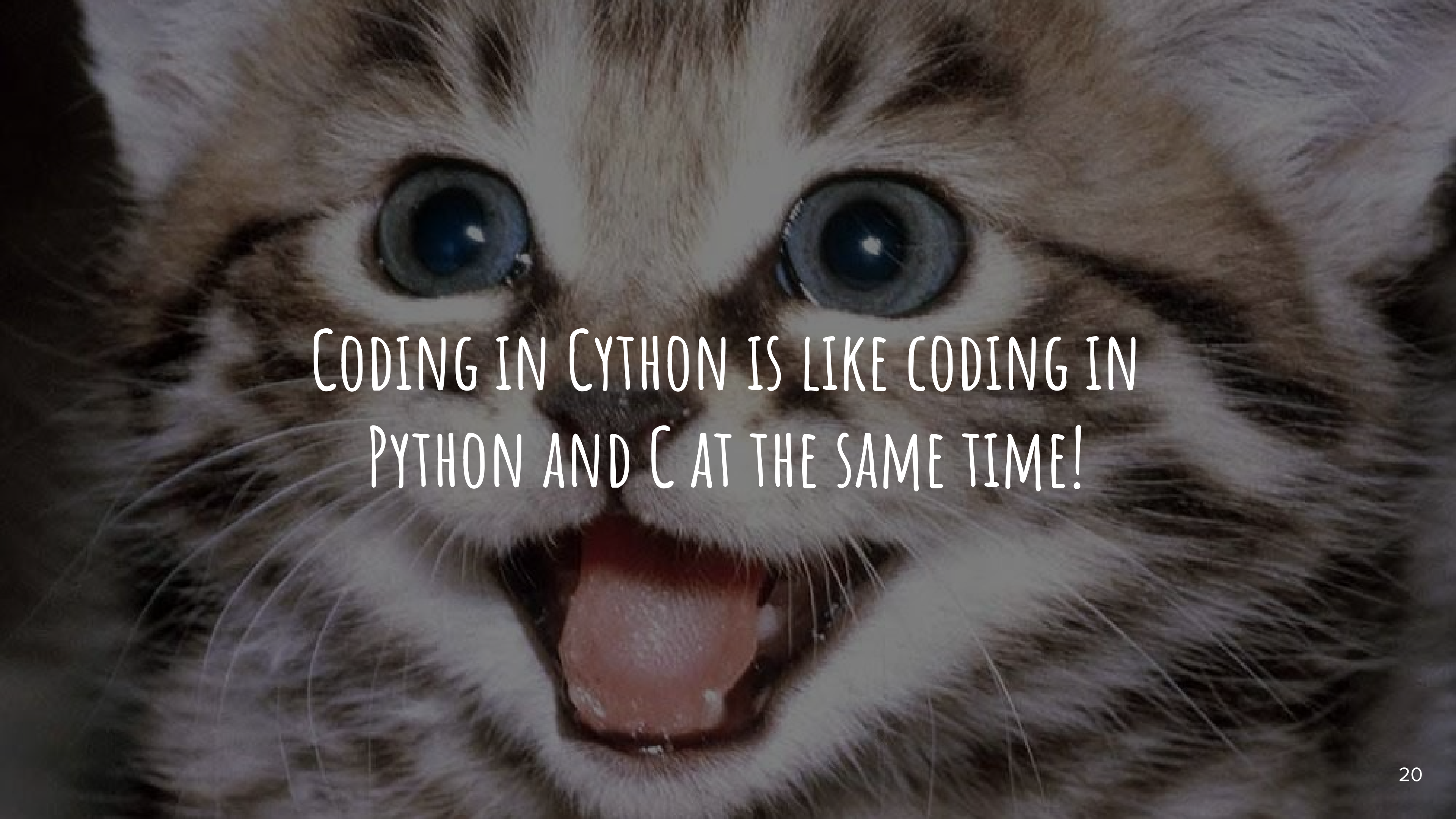
Cython 80x

```
def fib(int n):
    cdef int i, a, b
    a, b = 1,1
    for i in range(n):
        a, b = a+b, a
    return a
```

Cython in wild

Project	Cython files	Cython SLOC
sage	761	477,000
numpy	14	5,000
scipy	28	24,000
pandas	21	27,000
lxml	12	22,000
scikits-learn	35	15,000
scikits-image	48	11,000
mpi4py	48	12,000
yt	45	18,000

Projects master branches as of November 2014


Coding in Cython is like coding in Python and C at the same time!

Use Case 1: Library Wrapping

Cython is a popular choice for writing Python interface modules for C libraries

Use Case 2: Performance-critical code

- Python
- High-level
- Slow
- No variables typed

- C/C++/Fortran
- Lower-level
- Fast
- All variables typed

Common procedure: Where speed is needed, use a compiled language, then wrap the code for use from Python.

Use Case 3: Breaking out of the GIL

Cython As a few of you might know, C Python has an infamous Global Interpreter Lock (GIL)

- It limits thread performance

The Unwritten Rules of Python

- You do not talk about the GIL.
- You do NOT talk about the GIL.

Don't even mention the GIL.
No seriously...

Consider this simple script, that runs twice, sequentially, a busy_sleep, i.e. a function that simulate a CPU intensive task:

```
from def busy_sleep(n):
    while n > 0:
        n -= 1
N = 99999999
busy_sleep(N)
    busy_sleep(N)
```

This takes 6.7 seconds to run.

Now consider the threaded version:

```
from threading import Thread
def busy_sleep(n):
   while n > 0:
       n -= 1
N = 99999999
t1 = Thread(target=busy_sleep, args=(N, ))
t2 = Thread(target=busy_sleep, args=(N, ))
t1.start()
t2.start()
t1.join()
t2.join()
```

This takes 11.1 seconds to run. What?

Cython offers a wonderful context manager to run instructions without the GIL: *with nogil*.

Demo

With Nogil

```
def busy_sleep(int n):
    _busy_sleep(n)

def busy_sleep_nogil(int n):
    with nogil:
        _busy_sleep(n)

cdef inline void _busy_sleep(int n) nogil:
    cdef double tmp = 0.0
    while n > 0:
        tmp = (n ** 0.5) ** 0.5
        n -= 1
```

Building Cython code

Building Cython code

Cython code must, unlike Python, be compiled. This happens in two stages:

- A .pyx file is compiled by Cython to a .c file, containing the code of a Python extension module
- The .c file is compiled by a C compiler into a .so file (or .pyd on Windows) which can be imported directly into a Python session.

Building Cython code

There are several ways to build Cython code:

- Write a distutils setup.py.
- Use pyximport, importing Cython .pyx files as if they were .py files (using distutils to compile and build in the background).
- Use the Jupyter notebook or the Sage notebook, both of which allow Cython code inline.

Building Cython modules using distutils

Imagine a simple “hello world” script in a file hello.pyx:

```
def say_hello_to(name):
    print("Hello %s!" % name)
```

The following could be a corresponding setup.py script:

```
from distutils.core import setup
from Cython.Build import cythonize

setup(
  name = 'Hello world app',
  ext_modules = cythonize("hello.pyx"),
)
```

Building Cython modules using distutils

To use this to build your Cython file use the command line options:

```
$ python setup.py build_ext --inplace
```

It leaves a file in your local directory called helloworld.so (unix) or helloworld.pyd (Windows).

```
>>> import helloworld
Hello World
```

pyximport: Cython Compilation the Easy Way

To load .pyx files directly on import, without having to write a setup.py file.

```
>>> import pyximport; pyximport.install()
>>> import hello
Hello World
```

Build with Jupyter

Load the cython magic extension

```
In [1]: %load_ext cython
```

Then simply use the cython magic function to start writing cython code

```
In [2]: %%cython

        cdef int a = 0
        for i in range(10):
            a += i
        print(a)

        45
```

Build with Jupyter

Add --annotation or -a for showing the code analysis of the compiled code

In [3]:
```
%%cython --annotate

cdef int a = 0
for i in range(10):
    a += i
print(a)
```

```
45
```

Out[3]:

Generated by Cython 0.25.2

Yellow lines hint at Python interaction.
Click on a line that starts with a "+" to see the C code that Cython generated for it.

```
 1:
+2: cdef int a = 0
+3: for i in range(10):
+4:     a += i
+5: print(a)
```

C arrays

In [21]:

```
%%cython -a
def carrays():
    cdef int[10] a, b
    a[:5] = [1,2,3,4,5]
    b = a
    b[5:] = [6,7,8,9,10]

    for i in b[:3]:
        print(i+1)

    return b
```

Out[21]:

Generated by Cython 0.23.beta1

Yellow lines hint at Python interaction.
Click on a line that starts with a "+" to see the C code that Cython generated for it.

```
+01: def carrays():
 02:     cdef int[10] a, b
+03:     a[:5] = [1,2,3,4,5]
+04:     b = a
+05:     b[5:] = [6,7,8,9,10]
 06:
+07:     for i in b[:3]:
+08:         print(i+1)
 09:
+10:     return b
```

The conclusions:

1. Naive Cython does speed things up, but not by much (x1.8)
2. Optimised Cython is fairly effortless (in this case) and worthwhile (x2.5)
3. cpdef gives a good improvement over def
4. cdef is really valuable (x72)
5. Cython’s cdef is insignificantly different from the more complicated C extension that is our best attempt

NumPy and Cython

Provides fast access to NumPy arrays

It has a C-level type -> *typed memoryview*

Similar to NumPy array buffer support.

Allows us to work with buffers without having to know the details.

Example: Typed Memoryviews

The double[:] foo syntax declares foo to be a typed memoryview.

```
def sum_arg(double[:] foo):
    """Sums its argument's contents."""
    cdef double i, total = 0.0
    for i in foo:
        total += i
    return total
```

Providing C-Level access to Typed Memoryview data

```
def sum_arg(double[:] foo):
    """Sums its argument's contents."""
    cdef:
        double total = 0.0
        int j, length
        length = foo.shape[0]
    for j in range(length):
        total += foo[j]
    return total
```

Trading Safety for performance

Trading Safety for performance

```
from cython cimport boundscheck, wraparound
def sum_arg(double[:] foo):
    ...
    ...

    with boundscheck(False), wraparound(False)
        for j in range(length):
        ...
```

Trading Safety for performance

```
from cython cimport boundscheck, wraparound
@boundscheck(False)
@wraparound(False)

def sum_arg(double[:] foo):
    ...
    ...

    with boundscheck(False), wraparound(False)
        for j in range(length):
        ...
```

Trading Safety for performance

```
# cython: boundscheck = False
# cython: wraparound = False

def sum_arg(double[:] foo):
    ...
    ...

    with boundscheck(False), wraparound(False)
        for j in range(length):
        ...
```

So what have we learned?

Project demo
Cyvlfeat
Google summer of code 2016
@ Portland State University

A cython/python wrapper for VLFeat

What is Vlfeat?

What is CYVlfeat?

github.com/menpo/cyvlfeat

Contributions are welcome!

github.com/simmimourya1/cyvlfeat

Features which need more work

1. Binsum
2. Kdtree module

github.com/simmimourya1/pycon_india_17

Thank you