

Speeding up scientific Python code using Cython

Advanced Python Summer School, Zurich



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Example Code

<https://python.g-node.org/wiki/cython>

- Example Code

Introduction

- Motivation
- Motivation (continued)
- Use Cases
- Tutorial Overview

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

Introduction

Motivation

- Example Code

Introduction

- Motivation

- Motivation (continued)

- Use Cases

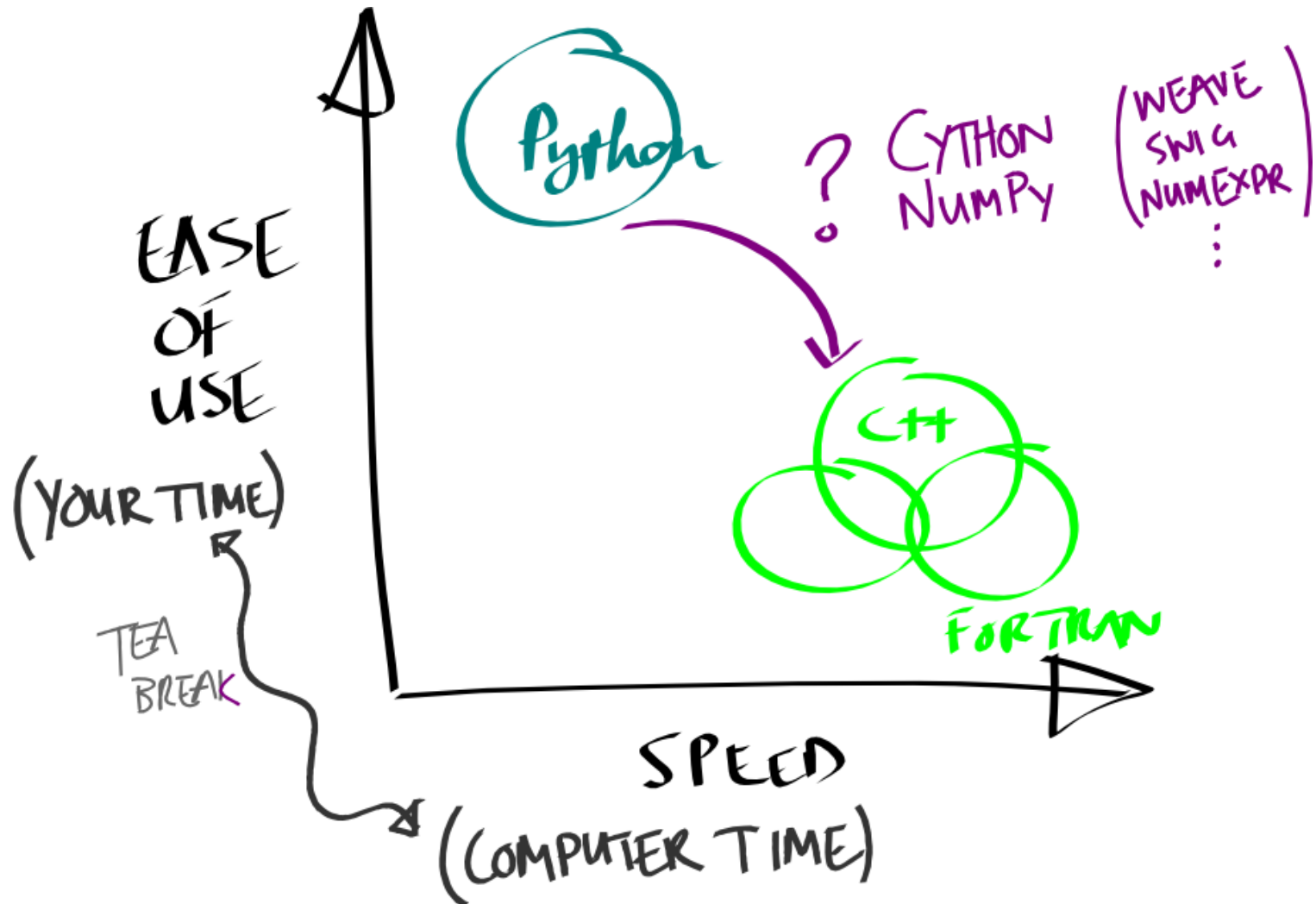
- Tutorial Overview

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries



Motivation (continued)

- Example Code

Introduction

- Motivation

- Motivation (continued)

- Use Cases

- Tutorial Overview

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Cython allows us to cross the gap
- This is good news because
 - we get to keep coding in Python (or, at least, a superset)
 - but with the speed advantage of C
- You can't have your cake and eat it. *Or can you?*
- Conditions / loops approx. 2–8x speed increase, 30% overall; with annotations: hundreds of times faster

Use Cases

- Example Code

Introduction

- Motivation
- Motivation (continued)
- Use Cases
- Tutorial Overview

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Optimize execution of Python code (profile, if possible! – demo)
- Wrap existing C and C++ code
- Breaking out of the Global Interpreter Lock; openmp
- Mixing C and Python, but without the pain of the Python C API

Tutorial Overview

- Example Code

Introduction

- Motivation
- Motivation (continued)
- Use Cases
- Tutorial Overview

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++ Libraries

For this quick introduction, we'll take the following approach:

1. Take a piece of pure Python code and benchmark (we'll find that it is too slow)
2. Run the code through Cython, compile and benchmark (we'll find that it is somewhat faster)
3. Annotate the types and benchmark (we'll find that it is much faster)

Then we'll look at how Cython allows us to

- Work with NumPy arrays
- Use multiple threads from Python
- Wrap native C libraries

- Example Code

Introduction

From Python to Cython

- Benchmark Python code
- More Segments
- Benchmark Python Code
- Compile the code with Cython

- Compile generated code
- Benchmark the new code
- Providing type information
- Benchmark
- Expense of Python

Function Calls

- The Last Bottlenecks
-
- Integrating Arbitrary Functions (callbacks)
-

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

From Python to Cython

Benchmark Python code

- Example Code

Introduction

From Python to Cython

- **Benchmark Python code**

- More Segments

- Benchmark Python Code

- Compile the code with Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary Functions (callbacks)

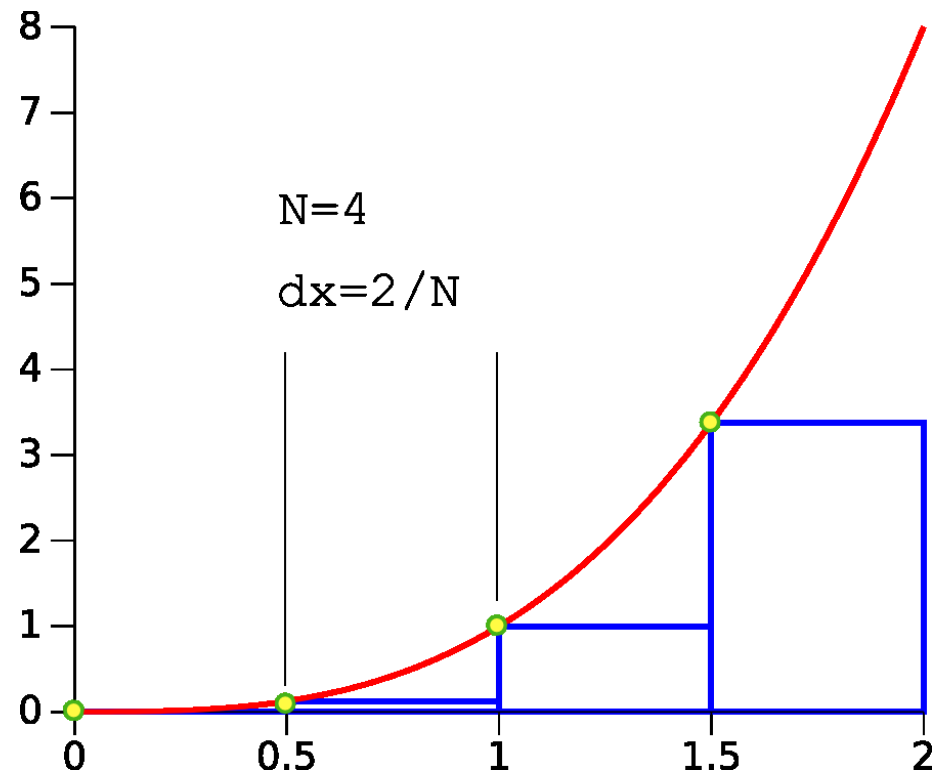
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Handling NumPy Arrays

Parallelization

Wrapping C and C++ Libraries

Our code aims to compute (an approximation of) $\int_a^b f(x)dx$



More Segments

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- **More Segments**

- Benchmark Python Code

- Compile the code with Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary Functions (callbacks)

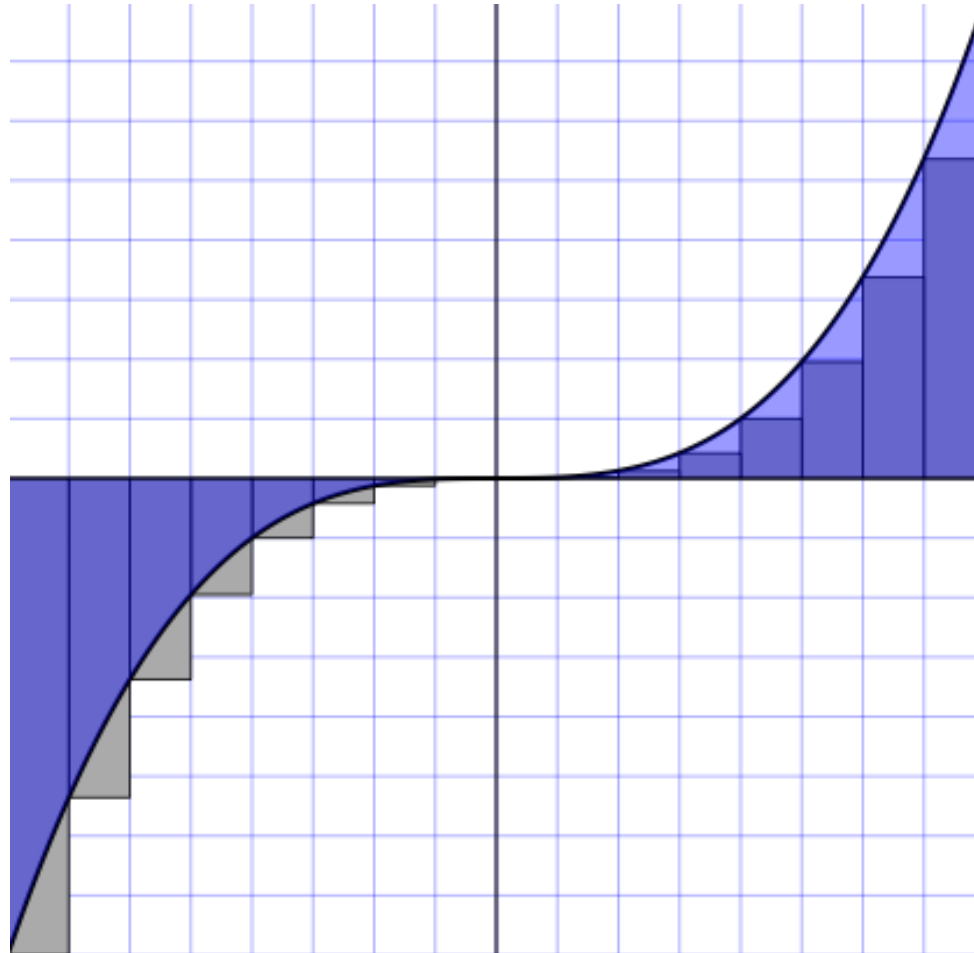
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- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries



Benchmark Python Code

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- **Benchmark Python Code**

- Compile the code with Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

```
from __future__ import division
```

```
def f(x):
```

```
    return x**4 - 3 * x
```

```
def integrate_f(a, b, N):
```

```
    """Rectangle integration of a function.
```

```
    Parameters
```

```
    -----
```

```
    a, b : int
```

```
        Interval over which to integrate.
```

```
    N : int
```

```
        Number of intervals to use in the discretisation.
```

```
    """
```

```
    s = 0
```

```
    dx = (b - a) / N
```

```
    for i in range(N):
```

```
        s += f(a + i * dx)
```

```
    return s * dx
```

Compile the code with Cython

- Example Code

Introduction

From Python to Cython

- Benchmark Python code
 - More Segments
 - Benchmark Python Code
 - Compile the code with Cython
 - Compile generated code
 - Benchmark the new code
 - Providing type information
 - Benchmark
 - Expense of Python
- ### Function Calls
- The Last Bottlenecks
 -
 - Integrating Arbitrary Functions (callbacks)
 -

Handling NumPy Arrays

Parallelization

Wrapping C and C++ Libraries

- `cython filename.[py|pyx]`
- What is happening behind the scenes? `cython -a filename.[py|pyx]`
 - Cython translates Python to C, using the Python C API (let's have a look)
- This code has some serious *bottlenecks*.

Compile generated code

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- **Compile generated code**

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary

- Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

```
$ gcc -O2 -fPIC -I/usr/include/python2.7  
-c integrate.c -o integrate_compiled.o
```

Easier yet, construct setup.py:

```
from distutils.core import setup  
from distutils.extension import Extension  
from Cython.Distutils import build_ext  
  
setup(  
    cmdclass = {'build_ext': build_ext},  
    ext_modules = [  
        Extension("integrate", ["integrate.pyx"]),  
    ])
```

Run using `python setup.py build_ext -i`. This means:
build extensions «in-place».

Benchmark the new code

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- Compile generated code

- **Benchmark the new code**

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary

- Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

- Use IPython's `%timeit` (could do this manually using `from timeit import timeit; timeit(...)`)
- Slight speed increase ($\approx 1.4\times$) probably not worth it.
- Can we help Cython to do even better?
 - Yes—by giving it some clues.
 - Cython has a basic type inferencing engine, but it is very conservative for safety reasons.
 - Why does type information allow such vast speed increases?

Providing type information

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary

- Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

```
from __future__ import division
```

```
def f(double x):  
    return x**4 - 3 * x
```

```
def integrate_f(double a, double b, int N):  
    """Rectangle integration of a function.
```

```
    ...  
    """
```

```
    cdef:
```

```
        double s = 0
```

```
        double dx = (b - a) / N
```

```
        Py_ssize_t i
```

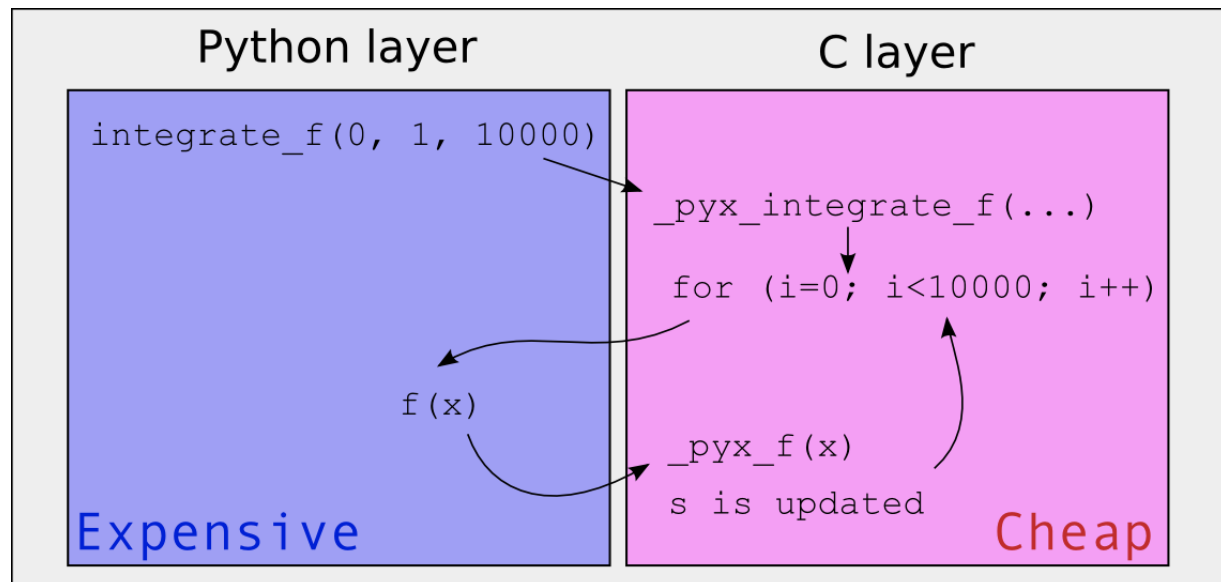
```
    for i in range(N):  
        s += f(a + i * dx)  
    return s * dx
```

Benchmark...

Expense of Python Function Calls

```
def f(double x):  
    return x**4 - 3 * x
```

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



- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary

- Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

The Last Bottlenecks

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary

- Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

```
# cython: cdivision=True
```

```
cdef double f(double x):  
    return x*x*x*x - 3 * x
```

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

Benchmark!

Integrating Arbitrary Functions (callbacks)

- Example Code

- Introduction

- From Python to Cython

- Benchmark Python code

- More Segments

- Benchmark Python Code

- Compile the code with

- Cython

- Compile generated code

- Benchmark the new code

- Providing type information

- Benchmark

- Expense of Python

- Function Calls

- The Last Bottlenecks

-

- Integrating Arbitrary Functions (callbacks)

-

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++

- Libraries

```
# cython: cdivision=True

cdef class Integrand:
    cdef double f(self, double x):
        raise NotImplementedError()

cdef class MyFunc(Integrand):
    cdef double f(self, double x):
        return x*x*x*x - 3 * x

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

Exploring Cython Further

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

- Declaring the MemoryView type
- Declaring the Numpy Array type
- Matrix Multiplication
- Our Own MatMul

Parallelization

Wrapping C and C++
Libraries

Handling NumPy Arrays

Declaring the MemoryView type

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Declaring the MemoryView type

- Declaring the Numpy Array type

- Matrix Multiplication

- Our Own MatMul

- Parallelization

- Wrapping C and C++ Libraries

```
import numpy as np

def foo( double[:, ::1] arr ):
    cdef double[:, ::1] = np.zeros_like(arr)
    cdef Py_ssize_t i, j
    for i in range( arr.shape[0] ):
        for j in range( arr.shape[1] ):
            out[i, j] = arr[i, j] * i + j

    return np.asarray( out )
```

Declaring the Numpy Array type

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Declaring the
MemoryView type

- Declaring the Numpy
Array type

- Matrix Multiplication

- Our Own MatMul

- Parallelization

- Wrapping C and C++
Libraries

An alternative to the MemoryView syntax that corresponds more closely with ndarray dtypes:

```
cimport numpy as cnp
import numpy as np

def foo( cnp.ndarray[cnp.float64, ndim=2] arr ):
    cdef cnp.ndarray[cnp.float64, ndim=2] out = np.zeros(
        arr.shape)
    cdef Py_ssize_t i, j
    for i in range(arr.shape[0]):
        for j in range(arr.shape[1]):
            arr[i, j] = i + j

    return out
```

Different types are defined in Cython/Includes/numpy.pxd.

Matrix Multiplication

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Declaring the MemoryView type

- Declaring the Numpy Array type

- Matrix Multiplication

- Our Own MatMul

- Parallelization

- Wrapping C and C++ Libraries

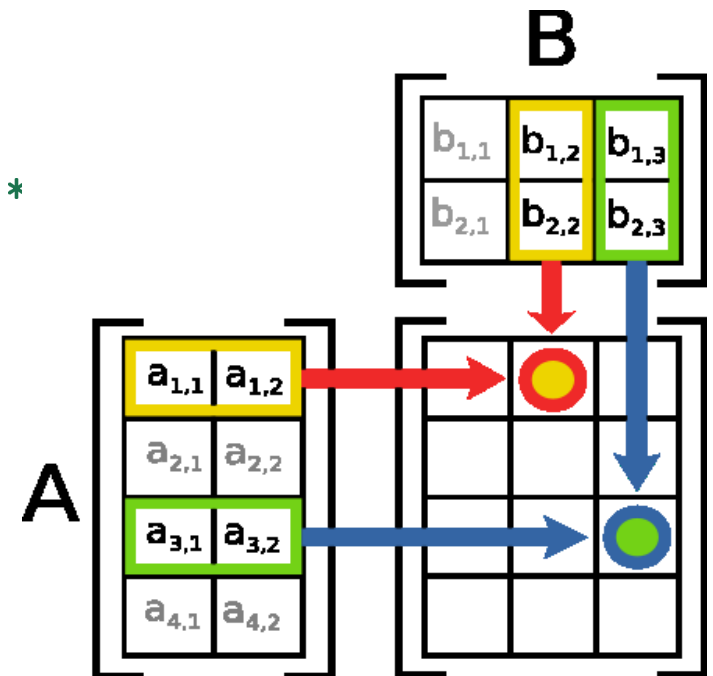
```
rows_A, cols_A = A.shape[0], A.shape[1]
rows_B, cols_B = B.shape[0], B.shape[1]
```

```
out = np.zeros(rows_A, cols_B)
```

```
# Take each row in A
for i in range(rows_A):
```

```
    # And multiply by each column in B
    for j in range(cols_B):
        s = 0
        for k in \
            range(cols_A):
            s = s + A[i, k] *
                B[k, j]
```

```
    out[i, j] = s
```



Our Own MatMul

We won't even try this in pure Python (way too slow).

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Declaring the

- MemoryView type

- Declaring the Numpy

- Array type

- Matrix Multiplication

- Our Own MatMul

- Parallelization

- Wrapping C and C++

- Libraries

```
def dot( double[:, ::1] A,
         double[:, ::1] B,
         double[:, ::1] out ):

    cdef:
        Py_ssize_t rows_A, cols_A, rows_B, cols_B
        Py_ssize_t i, j, k
        double s

    rows_A, cols_A = A.shape[0], A.shape[1]
    rows_B, cols_B = B.shape[0], B.shape[1]

    # Take each row in A
    for i in range(rows_A):
        # And multiply by every column in B
        for j in range(cols_B):
            s = 0
            for k in range(cols_A):
                s = s + A[i, k] * B[k, j]
            out[i, j] = s
```

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

- Parallel Loops with
«prange»

-

Wrapping C and C++
Libraries

Parallelization

Parallel Loops with «prange»

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Parallelization

- Parallel Loops with «prange»

-

- Wrapping C and C++ Libraries

```
@cython.boundscheck(False)
```

```
@cython.wraparound(False)
```

```
def pdot(double[:, ::1] A,
         double[:, ::1] B,
         double[:, ::1] out):
    cdef:
        Py_ssize_t rows_A, cols_A, rows_B, cols_B
        Py_ssize_t i, j, k
        double s
    rows_A, cols_A = A.shape[0], A.shape[1]
    rows_B, cols_B = B.shape[0], B.shape[1]
```

```
    with nogil:
```

```
        # Take each row in A
        for i in prange(rows_A):
            # And multiply by every column in B
            for j in range(cols_B):
                s = 0
                for k in range(cols_A):
                    s = s + A[i, k] * B[k, j]
```

```
    out[i, j] = s
```

Benchmark!

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

Wrapping C and C++ Libraries

Fortran

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Fortran

- External Definitions

- Build: Link Math Library

- C++ Class Wrapper

- C++ Class Wrapper

- C++ Class Wrapper

- C++ Class Wrapper

- In conclusion...

We won't be talking about that here, but Ondrej Certik has some excellent notes:

<http://fortran90.org/src/best-practices.html#interfacing-with-python>

External Definitions

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

Create a file, `trig.pyx`, with the following content:

```
cdef extern from "math.h":  
    double cos(double x)  
    double sin(double x)  
    double tan(double x)  
  
    double M_PI  
  
def test_trig():  
    print 'Some trig functions from C:', \  
        cos(0), cos(M_PI)
```


Build: Link Math Library

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

setup(
    cmdclass = {'build_ext': build_ext},
    ext_modules = [
        Extension("trig" ,
                  ["trig.pyx"],
                  libraries=["m"] ,
        ),
    ])
```

C++ Class Wrapper

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++
Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

```
namespace geom {  
    class Circle {  
    public:  
        Circle(double x, double y, double r);  
        ~Circle();  
        double getX();  
        double getY();  
        double getRadius();  
        double getArea();  
        void setCenter(double x, double y);  
        void setRadius(double r);  
    private:  
        double x;  
        double y;  
        double r;  
    };  
}
```

C++ Class Wrapper

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++ Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

```
cdef extern from "Circle.h" namespace "geom":  
    cdef cppclass Circle:  
        Circle(double, double, double)  
        double getX()  
        double getY()  
        double getRadius()  
        double getArea()  
        void setCenter(double, double)  
        void setRadius(double)
```

C++ Class Wrapper

- Example Code

Introduction

From Python to Cython

Handling NumPy Arrays

Parallelization

Wrapping C and C++
Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

```
cdef class PyCircle:
```

```
cdef Circle *thisptr
```

```
def __cinit__(self, double x, double y, double r):
```

```
    self.thisptr = new Circle(x, y, r)
```

```
def __dealloc__(self):
```

```
    del self.thisptr
```

```
@property
```

```
def area(self):
```

```
    return self.thisptr.getArea()
```

```
@property
```

```
def radius(self):
```

```
    return self.thisptr.getRadius()
```

```
def set_radius(self, r):
```

```
    self.thisptr.setRadius(r)
```

```
@property
```

```
def center(self):
```

```
    return (self.thisptr.getX(), self.thisptr.getY())
```

C++ Class Wrapper

- Example Code

- Introduction

- From Python to Cython

- Handling NumPy Arrays

- Parallelization

- Wrapping C and C++ Libraries

- Fortran
- External Definitions
- Build: Link Math Library
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- C++ Class Wrapper
- In conclusion...

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

setup(
    cmdclass = {'build_ext': build_ext},
    ext_modules = [
        Extension("circ", ["circ.pyx", "Circle.cpp"],
                    language="c++"),
        Extension("trig", ["trig.pyx"],
                    libraries=["m"]),
    ])
```

In conclusion...

- Build functional and tested code
- Profile
- Re-implement bottlenecks (behavior verified by tests)
- Et voilà—high-level code, low-level performance. [It's no silver bullet, but it's still pretty good.]

