

Need for Speed – Python meets C/C++

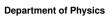
Scientific Programming with Python Christian Elsasser

Based partially on a talk by Stéfan van der Walt



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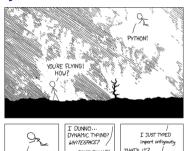
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[xkcd]

Python is nice, but by construction slow ...









Speed/Complexity

Department of Physics

... why not therefore interfacing it with C/C++

(or something similar, e.g. if you don't feel too young to use Fortran)

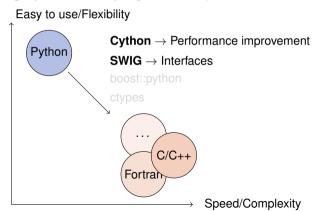
Easy to use/Flexibility Python . . . Fortra





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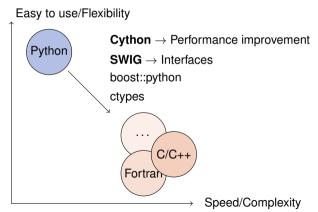






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 - Standard Template Library
 - Exceptions
 - Classes
- SWIG (and other wrappers)





C++ on one Slide

www.cplusplus.com and www.learncpp.com

- ► C++ is an (if not the) object-oriented programming language (like Python)
- ▶ including inheritance (like Python does in a slightly different way)
- ► ... operator overloading (like Python)
- ► It has a rich variety of libraries (like Python)
- ► It can raise exceptions (like Python)
- ► It requires declaration of variables (not like Python)
- ► It is (usually) a compiled language! (not like Python)
- ⇒ C++ and Python share a lot of similarities!

C is just the non-object-oriented version of C++ (minus some other missing features, e.g. exceptions)





A Few Words of Warning



Bad code stays bad code! – Better clean it up than trying to overpaint it!



Do not expect miracles! - You have to master two languages!





C keeps Python running ...

- ► CPython is the standard implementation of the Python interpreter written in C.
- ► The Python C API (application programming interface) allows to build C libraries that can be imported into Python (https://docs.python.org/3/c-api/)...
- ▶ ... and looks like this:

Pure Python

```
>>> a = [1,2,3,4,5,6,7,8]
>>> sum(a)
36
```





... but takes a lot of the fun out of Python

Python C can understand

```
sum_list(PyObject *list) {
   int i. n:
  long total = 0;
  PyObject *item;
  n = PyList_Size(list);
  if (n < 0)
    return -1: /* Not a list */
  for (i = 0; i < n; i++) {
    item = PyList_GetItem(list, i); /* Can't fail */
    if (!PyInt_Check(item)) continue; /* Skip non-integers */
    total += PvInt AsLong(item):
  return total:
```





C/C++ in Python: Not a New Thing

NumPy's C API

```
ndarray typedef struct PyArrayObject {
    PyObject_HEAD
    char *data;
    int nd;
    npy_intp *dimensions;
    npy_intp *strides;
    PyObject *base;
    PyArray_Descr *descr;
    int flags;
    PyObject *weakreflist;
} PyArrayObject;
```

⇒ Several Python "standard" libraries are using C/C++ to speed things up





Cython – An easy way to get C-enhanced compiled Python code

(http://cython.org)

- ► Hybrid programming language combining Python and an interface for using C/C++ routines.
- ... or a static compiler for Python allowing to write C/C++ extensions for Python and heavily optimising this code.
- ▶ It is a successor of the Pyrex language.
- ⇒ Every valid Python statement is also valid when using cython.
- \Rightarrow Code needs to be compiled \rightarrow Time!
 - ▶ Translates you "C-enhanced" Python code into C/C++ code using the C API

Cython (v0.29.1) understands Python 3, and also most of the features of C++11





Requirements: Cython package and a C compiler

cython The latest version can be downloaded from http://cython.org.

► C/C++ compiler, e.q. gcc/g++/clang (or for Windows: mingw)

Mille viae ducunt hominem per saecula ad compilorem!

Linux: usually already installed

(Ubuntu/Debian: sudo apt-get install build-essential)

MacOS X: XCode command line tools

Windows: Download of MinGW from http:// mingw.org and install it





Benchmark One: Fibonacci series

Fibonacci (Pure Python)

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





Benchmark One: Fibonacci series

Fibonacci (Cython)

```
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
```

► Type declaration (cdef) ⇒ Python/Cython knows what to expect





Benchmark One: Fibonacci series

```
Fibonacci (Cython)

def fib(int n):
    cdef int i,a,b
    a,b = 1,1
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```

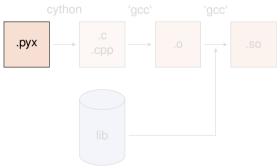
- ► Type declaration (cdef) ⇒ Python/Cython knows what to expect
- ▶ A few (simple) modifications can easily change the CPU time by a factor of $\mathcal{O}(100)$

a,b = a+b,a





Compiling Cython Code (The hard way)

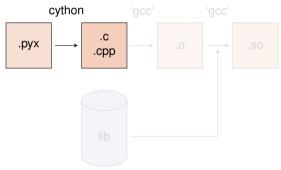


- Compile Cython code to C/C++ code cython/cython3 -3 <name>.pyx
- 2. Create object files
 gcc -02 -fPIC
 -I<path_to_python_include> <name>.c -o <name>.o
- 3. Compile shared object (i.e. library gcc [options]
 -L<path_to_python_library>
 <name>.o -o <name>.so
 - If using C++ code, cython needs the option -+ and gcc → g++
 - options are for MacOS X -bundle -undefined dynamic_lookup and for Debian -shared





Compiling Cython Code (The hard way)



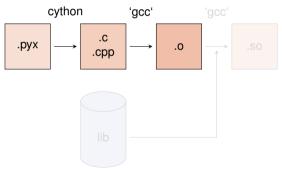
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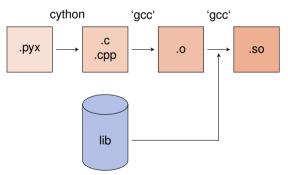
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Compiling Cython Code (The hard way)



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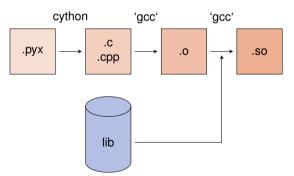
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Compiling Cython Code (The hard way)



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Compiling Cython Code (The easy way)

Support via the distutils (distribution utilities) package in building and installing Python modules ⇒ applicable for cython

Command python setup.py build_ext --inplace creates for each .pyx file a .c/.cpp file, compiles it to an executable (in the build directory of the corresponding OS/architecture/Python version) and compiles a .so file (or a .pxd if you are using Windows)

Further options for cythonize via help explorable





How Performant is My Code?

cython -3 -a/--annotate <name>.pxy \rightarrow additional HTML file

- ▶ bad performance → yellow marking
- allows to investigate code and to learn about performance tuning

▶ Not every yellow part can be improved!

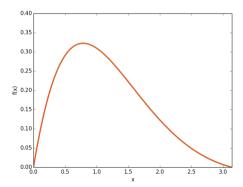




Benchmark Two: Numerical Integration

Integral of $f(x) = \sin x \cdot e^{-x}$ between 0 and π

 \Rightarrow Exact result: $(e^{-\pi} + 1)/2 = 0.521607$





Benchmark Two: Numerical Integration

```
Integral of f(x) = \sin x \cdot e^{-x} between 0 and \pi

\Rightarrow Exact result: (e^{-\pi} + 1)/2 = 0.521607
```

Integrate

```
from math import sin,exp

def f(double x):
    return sin(x)*exp(-x)

def integrate(double a,double b,int N):
    cdef double dx,s
    cdef int i
    dx = (b-a)/N
    s = 0.0
    for i in range(N):
        s += f(a+(i+0.5)*dx)
    return s*dx
```





Benchmark Two: Numerical Integration

Integral of $f(x) = \sin x \cdot e^{-x}$ between 0 and π \Rightarrow Exact result: $(e^{-\pi} + 1)/2 = 0.521607$

Python layer (expensive)	C layer (cheap)
integrate(a,b,N)	
f(x)	'_pyx_integrate'(a,b,N) for (i=0; i <n; i++)<="" th=""></n;>
	'_pyx_f'(x) sum updated





Benchmark Two: Numerical Integration

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Integral of f(x) = \sin x \cdot e^{-x} between 0 and \pi

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Benchmark Two: Numerical Integration

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Integrate

```
from libc.math cimport sin,exp

cpdef double f(double x):
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Benchmark Two: Numerical Integration

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```

Integrate

```
from libc.math cimport sin,exp

cpdef double f(double x):
    return sin(x)*exp(-x)

def integrate(double a,double b,int N):
    cdef double dx,s
    cdef Py_ssize_t i
    dx = (b-a)/N
    s = 0.0
    for i in range(N):
        s += f(a+(i+0.5)*dx)
    return s*dx
```



Benchmark Two: Numerical Integration

Integral of $f(x) = \sin x \cdot e^{-x}$ between 0 and π \Rightarrow Exact result: $(e^{-\pi} + 1)/2 = 0.521607$

- ► Return values of function can be specified via the key word cdef
- ► cpdef ⇒ function also transparent to Python itself (no performance penalty)
- ► C/C++ library can be imported via from libc/libcpp.<module> cimport <name> (see later)
- ▶ Using C++ functions can lead to a huge speed-up
- ► Try to do as much as you can in the C-layer
- ► Already huge speed-up when levaraging numpy and its vectorisation





You are here!







STL Containers

An often used feature of C++ are the Standard Template Library containters (e.g. std::vector, std::map, etc.)

Object holders with specific memory access structure, e.g.

- ▶ std::vector allows to access any element
- std::list only allows to access elements via iteration
- ▶ std::map represents an associative container with a key and a mapped values





STL Containers

An often used feature of C++ are the Standard Template Library containters (e.g. std::vector, std::map, etc.)

... and Cython knows how to treat them!

```
Python \longrightarrow C++ \longrightarrow Python
               iterable
                                                      list
                                 std::vector
               iterable
                                  std::list
                                                      list
               iterable
                         → std::set
                                                      set
     iterable (len 2) \rightarrow
                                  std::pair
                                                 \rightarrow tuple (len 2)
                                  std::map
                   dict. \rightarrow
                                                      dict.
```







STL Containers

An often used feature of C++ are the Standard Template Library containters (e.g. std::vector, std::map, etc.)

A few remarks!

- ▶ iterators (e.g. it) can be used ⇒ dereferencing with dereference(it) and incrementing/decrementing with preincrement (i.e. ++it), postincrement (i.e. it++), predecrement (i.e. --it) and postdecrement (i.e. it--) from cython.operator
- ► Be careful with performance! ⇒ performance lost due to shuffling of data
- More indepth information can be found directly in the corresponding sections of the cython code https://github.com/cython/cython/tree/master/Cython/Includes/libcpp
- ► C++11 containters (like std::unordered_map) are partially implemented





Exceptions/Errors

In terms of exception and error handling three different cases need to be considered:

- ► Raising of a Python error in cython code ⇒ return values make it impossible to raise properly Python errors (Warning message, but continuing)
- ► Handling of error codes from pure C functions
- ► Raising of a C++ exception in C++ code used in cython ⇒ C++ exception terminates if not caught – program





Errors in Python

Python Error

```
cpdef int raiseError():
    raise RuntimeError("A problem")
    return 1
```

⇒ Just prints a warning (and worse gives an ambigious return value)





Errors in Python

Python Error

```
cpdef int raiseError():
    raise RuntimeError("A problem")
    return 1
```

⇒ Just prints a warning (and worse gives an ambigious return value)

Python Error

```
cpdef int raiseError() except *:
    raise RuntimeError("A problem")
    return 1
```

⇒ Propagates the RuntimeError





Errors in C

C does not know exceptions like Python or C++. If errors should be caught, it is usually done via dedicated return values of functions which cannot appear in a regular function call.

Use the except statement to tell cython about this value

C Error

```
cpdef int raiseException() except -1:
    return -1
```

 \Rightarrow allows to indicate error codes from C \Rightarrow raises SystemError



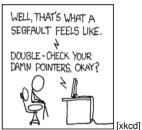


Exceptions in C++









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In cython this is also true for C++ exceptions!

Cython is not able to deal with C++ exceptions in a try'n'except clause!

⇒ But caption in cython and translation to Python exceptions/errors is possible!

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Exceptions in C++

... and how to tackle them!

- ► cdef <C++ function>() except + ⇒ translates a C++ exception into a Python error according to the right-hand scheme
- ► cdef <C++ function>() except
 +<Python Error> e.g. MemoryError ⇒
 translates every thrown C++ exception into
 a MemoryError
- ► cdef <C++ function>() except +<function raising Python error> ⇒ runs the indicated function if the C++ function throws any exception. If <function raising Python error> does not raise an error, a RuntimeError will be raised.

$C++ \longrightarrow Pvthon$ bad alloc MemoryError \rightarrow bad cast TypeError domain_error ValueError invalid_argument ValueError \rightarrow ios base::failure IOError \rightarrow out_of_range IndexError overflow error OverflowError ArithmeticError range_error underflow error ArithmeticError \rightarrow (all others) RuntimeError \rightarrow





Classes

Classes are a common feature of Python and C++

There are two aspects when dealing with cython:

- ► Defining classes containing C++ code in cython
- ► C++ classes integrated into Python

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Defining Classes in Cython

Let's go back to the integration examples

Integrate with classes

```
cdef class Integrand:
    cpdef double evaluate(self,double x) except *:
        raise NotImplementedError()

cdef class SinExpFunction(Integrand):
    cpdef double evaluate(self,double x):
        return sin(x)*exp(-x)

def integrate(Integrand f,double a,double b,int N):
    ...
    s += f.evaluate(a+(i+0.5)*dx)
    ...
```

Cython does not know @abstractmethod from the module abc!





Defining Classes in Cython

Let's go back to the integration examples

Integrate with classes

```
class Poly(Integrand):
    def evaluate(self,double x):
        return x*x-3*x

integrate(Poly(),0.0,2.0,1000)
```

⇒ Speed lost with respect to definition in cython, but still faster than a pure Python implementation





Integration of C++ Classes in Cython – Possible but cumbersome

Starting point: .cpp/.h file for class Rectangle defined in a namespace shapes

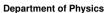
- 1. Expose it to Cython by delaring the class structure and method signatures
- 2. Integrating it into Cython either via direct usage or by defining a wrapper class

rect.pyx (File to expose C++ class to cython)

```
# distutils: language = c++
# distutils: sources = Rectangle.cpp

cdef extern from "Rectangle.h" namespace "shapes":
    cdef cppclass Rectangle:
        Rectangle(int, int, int, int) except +
        int x0, y0, x1, y1
        int getLength()
        int getHeight()
        int getArea()
        void move(int, int)
```





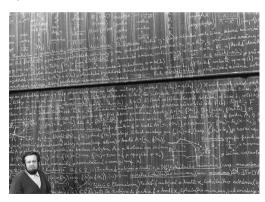


Automatic Wrappers

... since not everybody likes to write lines of error-prone code

- ► SWIG
- boost::python
- ▶ ctypes
- ▶ ...

Goal: creating compilable C/C++ code based on the Python C API







SWIG

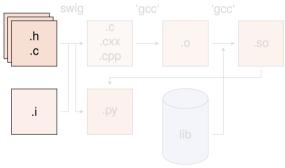
SWIG: Simplified Wrapper and Interface Generator

- ► Generic Wrapper for C/C++ to script-like languages
 - ▶ R
 - Perl
 - Ruby
 - ► Tcl
 - ► PHP5
 - Java
 - ...and Python
- ► Pretty old created in 1995 by Dave Beazley
- ► Current version is 3.0.12





SWIG - in a Nutshell



Moduel (<name>.py) can be imported into Python with $import\ name \Rightarrow$ Shared object needs different name

 Create python wrapper and necessary C files
 swig -c++ -python <name>.i

- Create object files based on output from the wrapper plus native C/C++ code
- 3. Compile shared object (i.e. library)

 Normally step 2 and 3 can be

 combined with via Distutils setup.py

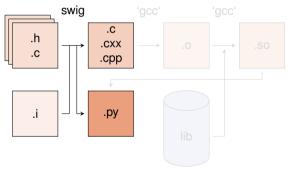
 python setup.py build_ext

 --inplace





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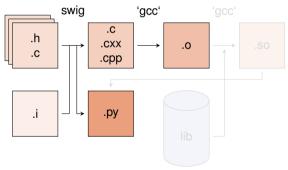
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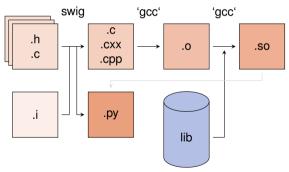
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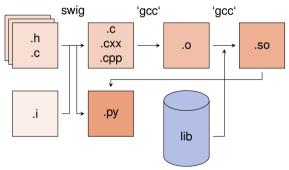
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 Normally step 2 and 3 can be combined with via Distutils setup.py python setup.py build_ext --inplace





SWIG - The interface file

Main configuration with interface (.i) files

- ▶ tells which (header) file(s) contains the C/C++ code to wrap
- defines some special data types (e.g. std::vector<...>)
- ► handles some additional configuration (e.g. exception/error translation)

Interface file

```
%module geom // name of the module
...
// things swig should know about
%include "Shape.h"
%include "Rectangle.h"
...
// things that should be put into the
header of the wrapper file (.c/.cxx)
%{
#include "Shape.h"
#include "Rectangle.h"
%}
```





SWIG - The Distutils file

- ► To be build extension needs a different name than the module set up by switch ⇒ Avoid name conflicts
- ► Language option only for C++
- ▶ python setup.py build_ext --inplace

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A Few Remarks about SWIG

- ► SWIG ≈ performance loss with respect to cython
- ► If SWIG works: ②
- ► If it does not: ②
- ▶ ... and therefore you can lose a lot of time with special problems
- ► It is not always optimal to expose the whole class to Python





Conclusion

- Interfacing Python with C/C++ is or better - can be a way to create powerful code
- cython and SWIG are two nice tools to do so
- ... but always make the interfacing maintainable/useful/etc. i.e. not a British train door
- ► And it's all about finding the sweet spot!

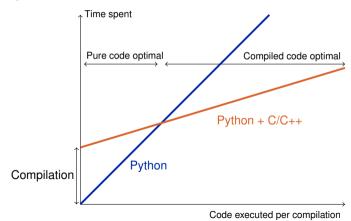


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The Sweet Spot!

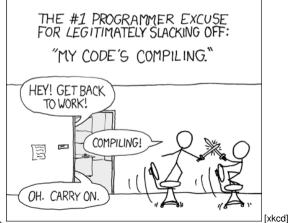


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The End!



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References

- 1. Stéfan van der Walt, *Speeding up scientific Python code using Cython*, Advanced Scientific Programming in Python, 2013 (Zurich) & 2014 (Split)
- 2. Stefan Behnel et al., *Cython tutorial*, Proceedings of the 8th Python in Science Conference (SciPy 2009) ⇒ based on older cython version, but the main reference of cython
- 3. Dave Beazley, Swig Master Class, PyCon'2008
- 4. http://docs.cython.org/src/tutorial/
- 5. http://www.swig.org





Backup





Fortran meets Python

The f2py compiler (http://docs.scipy.org/doc/numpy-dev/f2py/) offers – in a similar way as cython – the possibility to generate extension modules for Python from Fortran code.

f2py -c -m <module name> <fortran file>.f/.f90 -I<path to python header file> builds from the code in <fortran file>.f/.f90 a importable module (i.e. shared object) <module name>.so

Fortran modules and subroutines are exposed to Python on time of the import of the built module.

The compilation can also be split into a first step generating a signature file, which is in a second step compiled into the extension module





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 1

```
cdef extern from 'except_cy.h'
    cdef void raiseException() except +
def tryIt():
    try:
       raiseException()
    except RuntimeError as e:
       print(e)
```

 \Rightarrow OK as raiseException() throws a std::exception \rightarrow RuntimeError





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 2

```
cdef extern from 'except_cy.h'
    cdef void raiseException() except +MemoryError
def tryIt():
    try:
       raiseException()
    except RuntimeError as e:
       print(e)
```

 \Rightarrow Not OK as raiseException() throws a std::exception which is explicitly transformed into a MemoryError





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 3

```
cdef extern from 'except_cy.h'
    cdef void raiseBadAlloc() except +
def tryIt():
    try:
       raiseBadAlloc()
    except RuntimeError as e:
       print(e)
```

 \Rightarrow Not OK as raiseBadAlloc() throws a std::bad_alloc which is transformed into a MemoryError





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 4

```
cdef extern from 'except_cy.h'
    cdef void raiseBadAlloc() except +
def tryIt():
    try:
       raiseBadAlloc()
    except MemoryError as e:
       print(e)
```

⇒ OK as raiseBadAlloc() throws a std::bad_alloc which is transformed into a MemoryError





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 5

```
cdef void raise_py_error() except *:
    raise MemoryError("Problem")

cdef extern from 'except_cy.h':
    cdef void raiseBadAlloc() except +raise_py_error

def tryIt():
    try:
        raiseBadAlloc()
    except MemoryError as e:
        print(e)
```

 \Rightarrow OK as raise_py_error() throws an error





Exceptions in C++

Examples

Two C++ functions void raiseException() and void raiseBadAlloc() defined in except_cy.h

Exception Example 6

```
cdef void raise_py_error() except *:
    pass

cdef extern from 'except_cy.h':
    cdef void raiseBadAlloc() except +raise_py_error

def tryIt():
    try:
        raiseBadAlloc()
    except MemoryError as e:
        print(e)
```

⇒ Not OK as no error is thrown by raise_py_error()





Integration of C++ Classes

Assuming a C++ class Rectangle

```
Rectangle.h

namespace shapes {
    class Rectangle {
    public:
        int x0, y0, x1, y1;
        Rectangle(int x0, int y0, int x1, int y1);
        ~Rectangle(); // destructor
        int getLength();
        int getHeight();
        int getArea();
        void move(int dx, int dy);
    };
}
```





Integration of C++ Classes

Assuming a C++ class Rectangle

```
Rectangle.cpp
#include "Rectangle.h"
#include <iostream>
using namespace shapes:
Rectangle::Rectangle(int XO, int YO, int X1, int Y1) {
   x0 = X0:
   yO = YO;
   x1 = X1:
   v1 = Y1:
   std::cout « "Here I am" « std::endl;}
Rectangle::~Rectangle() {
    std::cout « "Byebye" « std::endl;}
. . .
```





Integration of C++ Classes

Now exposing it to cython

```
# distutils: language = c++
# distutils: sources = Rectangle.cpp

cdef extern from "Rectangle.h" namespace "shapes":
    cdef cppclass Rectangle:
        Rectangle(int, int, int, int) except +
        int x0, y0, x1, y1
        int getLength()
        int getHeight()
        int getArea()
        void move(int, int)
```





Integration of C++ Classes

... and using it!

Either in further cython code!

rect.pyx def tryIt(): cdef Rectangle* r try: r = new Rectangle(1,2,3,4) print("My length is: %f"%r.getLength()) print("My first x-coordinate is: %f"%r.x0) finally: del r





Integration of C++ Classes

... and using it!

Or for creating a Python (wrapper) class!

```
rect.pyx

cdef class PyRectangle:
    cdef Rectangle *thisptr
    def __cinit__(self, int x0, int y0, int x1, int y1):
        self.thisptr = new Rectangle(x0, y0, x1, y1)

def __dealloc__(self):
    del self.thisptr
    def getLength(self):
        return self.thisptr.getLength()
    def getHeight(self):
        return self.thisptr.getHeight()

...
```





Special features: STL Stuff with SWIG

- ► Dedicated interface files need to be integrated when running SWIG
- ... and templates for each containers + each content need to be defined

```
Interface file
...
%include "std_vector.i"
%include "std_string.i"
...
%template(dVector) std::vector<double>;
%template(rectVector) std::vector<Rectangle*>;
...
```



Special features: Exceptions with SWIG

```
Interface file
%include "exception.i"
. . .
%exceptionclass ShapeError;
%exception *::whine {
  try {
    $action
  } catch(ShapeError & e) {
    ShapeError *ecopy = new ShapeError(e);
    PyObject *err = SWIG_NewPointerObj(ecopy, SWIGTYPE_p_ShapeError, 1);
    PyErr_SetObject(SWIG_Python_ExceptionType(SWIGTYPE_p_ShapeError), err);
    SWIG fail:
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```





Special features: Overloading

Cython deals the usual way with overloaded methods in C++:

but it cannot happen in a Python wrapper class:

```
rect.pyx does not work

cdef class PyRectangle:
    ...
    def move(self,dx,dy):
        return self.thisptr.move(dx,dy)
    def move(self,d):
        return self.thisptr.move(d)
```





Special features: Inheritance

As in Python C++ classes can inherit from parent classes including overriding of methods

C++ classes

```
class Shape {
public:
    ...
    void virtual printInfo(); // Prints "Shape"
};
class Rectangle : public Shape {
public:
    ...
    void printInfo(); // Prints "Rectangle"
};
```





Special features: Inheritance

Cython can also deal with this feature, but there are two points to keep in mind:

1. If parent class is also exposed to cython, no redefinition of overridden methods is required (and also allow → mis-interpreted as overloading)

```
C++ classes
cdef extern from "Rectangle.h" namespace "shapes":
    cdef cppclass Shape:
        Shape() except +
        void printInfo()

cdef cppclass Rectangle(Shape):
        Rectangle(int, int, int, int) except +
        ...
    void printInfo() # causes problems
    ...
```





Special features: Inheritance

2. The inheritance can only be transported into wrapper classes if child classes have the same set of methods as the mother class

```
C++ classes
```

```
cdef class PyObject:
    cdef Object* thisptr
    def __cinit__(self):
        self.thisptr = new Object()
    def __dealloc__(self):
        del self.thisptr
    def printInfo(self):
        self.thisptr.printInfo()

cdef class PyRectangle(PyObject):
    def __cinit__(self,int x0,int y0,int x1,int y1):
        self.thisptr = new Rectangle(x0,y0,x1,y1)
```

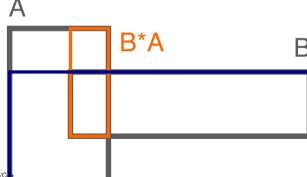




Special features: Operator Overloading

C++ as well as Python offers the potential to define operators for objects.

Example with Rectangles:







Special features: Operator Overloading

C++ code

```
Rectangle operator*(Rectangle& rhs){
    return Rectangle(x0,y0,rhs.x1,rhs.y1);
};
```

rect.pyx

```
# to expose it to cython
Rectangle operator*(Rectangle)

# in the wrapper class
def __mul__(PyRectangle lhs,PyRectangle rhs):
    res = PyRectangle(0,0,0,0)
    res.thisptr[0] = lhs.thisptr[0]*rhs.thisptr[0] # ptr deref
    return res
```

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Arrays

Arrays in cython are usually treated via typed memoryviews (e.g. double[:,:] means a two-dimensional array of doubles, i.e. compatible with e.g. np.ones((3,4)))

Further you can specify which is the fastest changing index by :1, e.g.

- ▶ double[::1,:,:] is a F-contiguous three-dimensional array
- ▶ double[:,:,::1] is a C-contiguous three-dimensional array
- ▶ double[:,::1,:] is neither F- nor C-contiguous

For example a variable double[:,::1] a has as NumPy arrays variables like shape and size and the elements can be accessed by a[i,j]

But be aware: NumPy is already heavily optimised, so do not to reinvent the wheel!