

# Python Programming for Scientists

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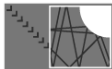
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NATURWISSENSCHAFTEN



**FOR760: Scattering Systems with Complex Dynamics**

# Outline

**1** Introduction

**2** Basics

**3** Python Modules for Science

**4** Faster Python and Glueing

**5** Summary

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# Who uses...

- We all use computers to generate or process data

Question to the audience: who uses...

- C/C++?
- Fortran?
- Ada?
- Java?
- Matlab/Octave?
- IDL?
- Perl?
- Ruby?
- **Python?**

# What is Python?

Python is/has...

- a scripting language
- general purpose
- interpreted
- easy to learn
- clean syntax
- multi-paradigm
- open-source
- available for all major platforms
- great community

# The best of all:

Python comes...

... with **batteries included!**

Libraries available for...

daily IT needs...

- networks
- OS interaction
- temporary files
- zip files
- ...

**science!**

- efficient array operations (*NumPy*)
- general numerical algorithms (*SciPy*)
- 2D visualization (*matplotlib*)
- 3D visualization (*Mayavi*)
- special problems (e.g. finite elements with FEniCS, quantum optics with QuTiP)
- symbolic math (*SageMath*, *sympy*)
- ...

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# Scientific *Hello, World!*

```
import sys
from math import sin, pi
```

```
def sincSquare(x):
    """Return  $\text{sinc}(x)^2$ .
    """
    if (x <> 0.0):
        return (sin(pi*x)/(pi*x))**2
    else:
        return 1.0
```

```
x = sys.argv[1]
y = sincSquare(float(x))
print("sinc(%s)^2 = %s"%(x, y))
```

cmp. H.-P. Langtangen,  
"Python Scripting for  
Computational Science"

run with:

python HelloWorld.py 0.0



# Control structures

```
# if statements:
```

```
if(divisor == 0):
```

```
    ...
```

```
elif(divisor > 1E20):
```

```
    ...
```

```
else:
```

```
    ...
```

```
# loops:
```

```
for i in range(10): # i = 0, 1, ..., 9
```

```
    print("i = %s"%i)
```

```
# while loops:
```

```
while(True):
```

```
    ...
```

# Functions

```
# functions:
def f(x, a=1.0, b=2.0):
    """Return a/x and a/x^b.
    """

    return a/x, a/x**b


# somewhere else:
a = 5
y1, y2 = f(x, 5.0)
y3, y4 = f(2, b=3.0)
```

# Data types

```

a = 2 # integer
b = 2.0 # float
c = "3.0" # string
d = [1, 2, "three"] # list
e = "1"

print(a*b) # valid, upcasting
print(a*c) # valid, but probably not desired: '3.03.0'
print(b*c) # invalid
print(d[1]) # prints 2
for item in d: # lists are "iterable"
    print(item)
for character in c: # strings are iterable
    print(character) # prints 3\n.\n0
f = e + c # + joins strings: f = '13.0'
g = d + [someObj, "foobar"] # + joins lists

```

# Files

```
readFile = open("infile", mode="r")
writeFile = open("outfile", mode="w")

for line in readFile: # iterate over file's lines
    xString, yString = line.split() # split the line
    x = float(xString); y = float(yString)
    print("x = %s, y = %s"%(x, y))
    writeFile.write("%s * %s = %s\n"%(x, y, x*y))

readFile.close(); writeFile.close()
```

infile:

```
1.0    2.0
3.0    4.0
```

outfile:

```
1.0 * 2.0 = 2.0
3.0 * 4.0 = 12.0
```

# Pitfalls

⚡ Common pitfalls:

- slicing: last index is *exclusive*, not *inclusive* as in e.g. Fortran

```
x = [1, 2, 3, 4]
print(x[0:2]) # prints [1, 2], not [1, 2, 3]
```

- What looks like an assignment is actually setting a reference:

```
a = []
b = a
a.append(2)
print(a) # prints [2]
print(b) # prints [2], not []!
```

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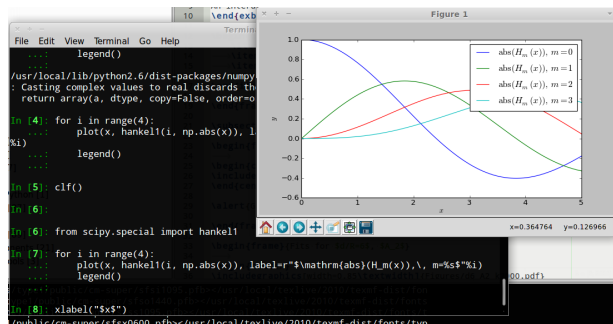
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# The IPython shell

## IPython

An interactive shell - may replace MatLab [tm] for interactive work

- Syntax highlighting
- Tab completion
- Inline documentation
- Easy profiling, timing...
- IPython ≥ 0.11: inline plots...



# NumPy: Python meets an array data type

## NumPy

Fast and convenient array operations

- Lists: + does join, not add!
- NumPy array: basic vector/matrix data type
- Convenience functions (e.g. `linspace()`, `zeros()`, `loadtxt()`...)
- Array slicing
- element-wise operations
- Code using NumPy reads and writes very similar to modern Fortran



# NumPy by examples

```
import numpy as np

a = np.array([1.0, 2.0, 3.0, 4.0])
b = np.array([4.0, 3.0, 2.0, 1.0])
for item in a: # arrays are iterable
    print(item)
c = a + b # c = [5, 5, 5, 5]
print(a[0:3:2]) # 1.0, 3.0; last element not included!
a[0:3] = b[0:-1]

print(a*b) # prints [4, 6, 6, 4], not the scalar product!
```

# SciPy

## SciPy

Numerical algorithms using NumPy arrays

Wrappers around well-established libraries

Submodules:

- `linalg`: Linear algebra (lapack)
- `sparse`: sparse matrices
- `fft`: FFT (fftpack)
- `optimize`: Optimization, Zeros (minpack)
- `integration`: Integration (quadpack, odepack)
- `special`: special functions (amos...)
- `signal`: Signal processing

# SciPy: an example

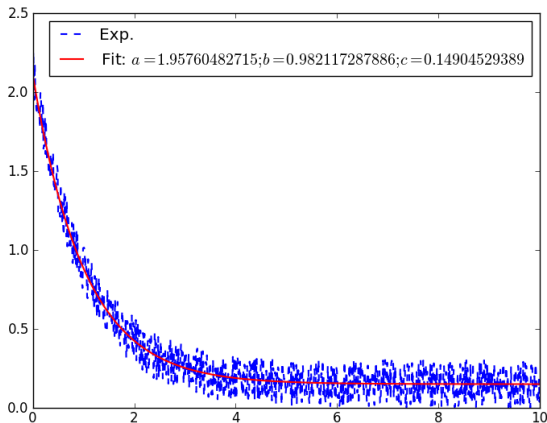
```
import numpy as np
from scipy.optimize import curve_fit
from matplotlib.pyplot import plot, show, legend

x, yExp = np.loadtxt("func.dat", unpack=True)
plot(x, yExp, ls="--", c="blue", lw="1.5", label="Exp.")

def fitFunc(x, a, b, c):
    return a*np.exp(-b*x) + c

p0pt, pCov = curve_fit(fitFunc, x, yExp)
yFit = fitFunc(x, a=p0pt[0], b=p0pt[1], c=p0pt[2])
plot(x, yFit, label="Fit: $a = %s; b = %s; c = %s$\\"
      %(p0pt[0], p0pt[1], p0pt[2]), ls="-", lw="1.5", c="r")
legend(); show()
```

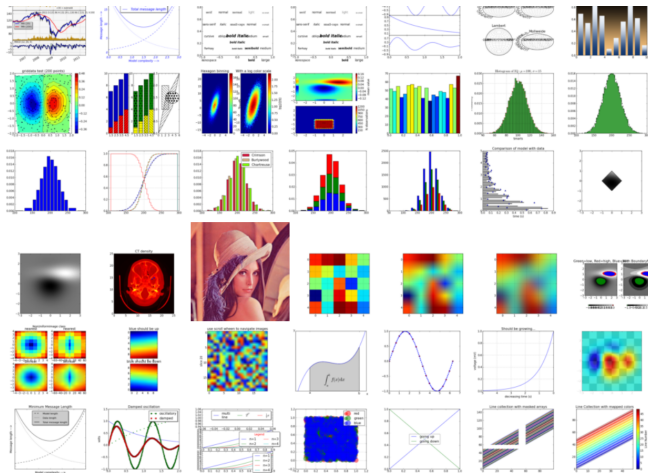
# SciPy: the example's output



Already used here: *Matplotlib*

# Matplotlib

(mostly) 2D plots



PyLab: MatLab alternative for interactive work

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# Using Python as glue

Python can wrap different different other programming languages

## Cython

compiled, *typed* Python - interface C/C++ code

## f2py

Fortran wrapper, included in NumPy

Why do that?

- Python can be *slow*
- Python loops are slow
- calling Python functions is slow
- Wrap external C/Fortran... libraries
- Happily/unfortunately (?) there is legacy code

## Problem: $\text{sinc}(x)^2$

```
import numpy as np
from math import sin, pi

def sincSquare(x):
    """Return the  $\text{sinc}(x) = (\sin(x)/x)^2$  of the array
    argument  $x$ .
    """
    retVal = np.zeros_like(x)
    for i in range(len(x)):
        retVal[i] = (sin(pi*x[i]) / (pi*x[i]))**2

    return retVal
```

$10^6$  array elements: 1 loops, best of 3: 4.91 s per loop



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    for i in range(len(x)):
        retVal[i] = (sin(pi*x[i]) / (pi*x[i]))**2

    return retVal
```

$10^6$  array elements: 1 loops, best of 3: 4.91 s per loop

# First attempt: use NumPy array operations

```
import numpy as np

def sincSquareNumPy1(x):

    return (np.sin(np.pi*x[:])/(np.pi*x[:]))**2

def sincSquareNumPy2(x):

    return np.sinc(x[:])**2
```

$10^6$  array elements: first function: 10 loops, best of 3: 73 ms  
per loop, second function: 10 loops, best of 3: 92.9 ms  
per loop4

# First attempt: use NumPy array operations

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import numpy as np

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    return (np.sin(np.pi*x[:])/(np.pi*x[:]))**2

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    return np.sinc(x[:])**2
```

$10^6$  array elements: first function: 10 loops, best of 3: 73 ms  
per loop, second function: 10 loops, best of 3: 92.9 ms  
per loop4

# How Cython works

## Cython

compiled, possibly typed Python:

`.pyx` file  $\xRightarrow{\text{Cython}}$  `.c` file  $\xRightarrow{\text{C compiler}}$  `.so/.dll` file

- various levels of typing possible
- C output and Cython's opinion on code speed can easily be inspected (optional `.html` output)
- interface C libraries

# $\text{sinc}(x)^2$ - Cython, Version 1

```
cdef extern from "math.h":
    double sin(double)
    double pow(double, int)

def sincSquareCython1(x):

    pi = 3.1415926535897932384626433
    retVal = np.zeros_like(x)

    for i in range(len(x)):
        retVal[i] = (sin(pi*x[i]) / (pi*x[i]))**2

    return retVal
```

$10^6$  array elements: 1 loops, best of 3: 4.39 s per loop

# $\text{sinc}(x)^2$ - Cython, Version 1

```
cdef extern from "math.h":
    double sin(double)
    double pow(double, int)

def sincSquareCython1(x):

    pi = 3.1415926535897932384626433
    retVal = np.zeros_like(x)

    for i in range(len(x)):
        retVal[i] = (sin(pi*x[i]) / (pi*x[i]))**2

    return retVal
```

$10^6$  array elements: 1 loops, best of 3: 4.39 s per loop

## $\text{sinc}(x)^2$ - Cython, Version 2

```
cimport numpy as np # also C-import types
```

```
cpdef np.ndarray[double] sincSquareCython2\  
    (np.ndarray[double] x):
```

```
    cdef int i
```

```
    cdef double pi = 3.1415926535897932384626433
```

```
    cdef np.ndarray[double] retVal = np.zeros_like(x)
```

```
    for i in range(len(x)):
```

```
        retVal[i] = pow(sin(pi*x[i]) / (pi*x[i]), 2)
```

$10^6$  array elements: 10 loops, best of 3: 49.1 ms per loop

That's a **speedup by a factor  $\approx 100$ !**

## $\text{sinc}(x)^2$ - Cython, Version 2

```
cimport numpy as np # also C-import types
```

```
cpdef np.ndarray[double] sincSquareCython2\  
    (np.ndarray[double] x):
```

```
    cdef int i
```

```
    cdef double pi = 3.1415926535897932384626433
```

```
    cdef np.ndarray[double] retVal = np.zeros_like(x)
```

```
    for i in range(len(x)):
```

```
        retVal[i] = pow(sin(pi*x[i]) / (pi*x[i]), 2)
```

$10^6$  array elements: 10 loops, best of 3: 49.1 ms per loop

That's a **speedup by a factor  $\approx 100$ !**



# How f2py works

## f2py

wrap Fortran code in Python:

$\text{.f/.f90 file} \xrightarrow{\text{f2py}} \text{.so/.dll file}$

- f2py is included in NumPy
- exposes NumPy arrays to Fortran code
- once 'Fortran space' is entered, you run at full Fortran speed

# $\text{sinc}(x)^2$ - f2py, Version 1

```
subroutine sincsquaref2py1(x, n, outVal)
    implicit none

    double precision, dimension(n), intent(in) :: x
    integer, intent(in) :: n
    double precision, dimension(n), intent(out) :: outVal
    double precision, parameter :: pi = 4.0d0 * atan(1.0d0)

    outVal(:) = (sin(pi*x(:)) / (pi*x(:)))*2

end subroutine sincsquaref2py1
```

$10^6$  array elements: 10 loops, best of 3: 47.4 ms per loop  
Again, a **speedup by a factor of  $\approx 100$ !**

# $\text{sinc}(x)^2$ - f2py, Version 1

```
subroutine sincsquaref2py1(x, n, outVal)
    implicit none

    double precision, dimension(n), intent(in) :: x
    integer, intent(in) :: n
    double precision, dimension(n), intent(out) :: outVal
    double precision, parameter :: pi = 4.0d0 * atan(1.0d0)

    outVal(:) = (sin(pi*x(:)) / (pi*x(:)))*2

end subroutine sincsquaref2py1
```

$10^6$  array elements: 10 loops, best of 3: 47.4 ms per loop  
Again, a **speedup by a factor of  $\approx 100$ !**

# Cheating: $\text{sinc}(x)^2$ - f2py, Version 2 - OpenMP

```
subroutine sincsquaref2py2(x, n, outVal)
  implicit none
  double precision, dimension(n), intent(in) :: x
  integer, intent(in) :: n
  double precision, dimension(n), intent(out) :: outVal
  integer :: i
  double precision, parameter :: pi = 4.0d0 * atan(1.0d0)
  !$OMP PARALLEL DO SHARED(x, outVal)
  do i = 1, n
    outVal(i) = (sin(pi*x(i)) / (pi*x(i)))**2
  end do
  !$OMP END PARALLEL DO
end subroutine sincsquaref2py2
```

$10^6$  array elements, 2 Threads: 10 loops, best of 3: 33.5 ms

# Cheating: $\text{sinc}(x)^2$ - f2py, Version 2 - OpenMP

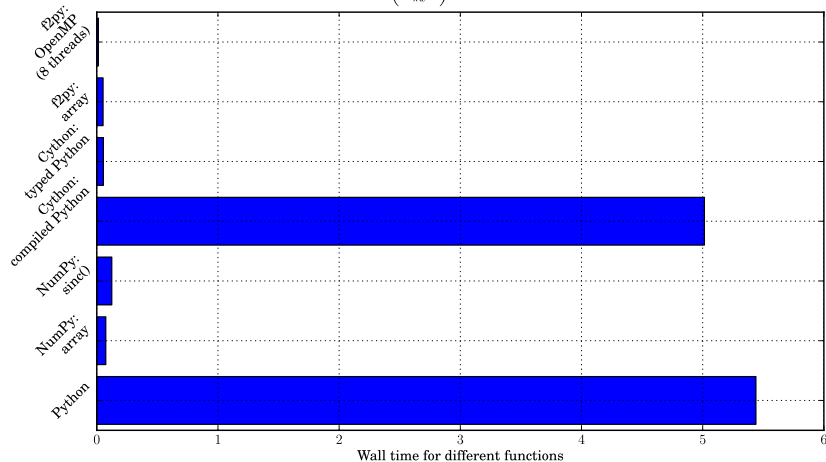
```
subroutine sincsquaref2py2(x, n, outVal)
  implicit none
  double precision, dimension(n), intent(in) :: x
  integer, intent(in) :: n
  double precision, dimension(n), intent(out) :: outVal
  integer :: i
  double precision, parameter :: pi = 4.0d0 * atan(1.0d0)
  !$OMP PARALLEL DO SHARED(x, outVal)
  do i = 1, n
    outVal(i) = (sin(pi*x(i)) / (pi*x(i)))**2
  end do
  !$OMP END PARALLEL DO
end subroutine sincsquaref2py2
```

$10^6$  array elements, 2 Threads: 10 loops, best of 3: 33.5 ms

# $\text{sinc}(x)^2$ - Overview

Benchmark for an Intel i7:

Time for calls to  $\left(\frac{\sin(\pi x)}{\pi x}\right)^2$  for 500000 array elements



# Techniques for faster Scripts

After you have written a prototype in Python with NumPy and SciPy, check if your code is already fast enough. If not,

- profile your script (IPython's `run -p` or `cProfile` module...) to find bottlenecks
- if a large numbers of function calls is the bottleneck, typing and using Cython's `cdef/cpdef` for C calling conventions speeds your code up at the cost of flexibility
- loops greatly benefit from typing, too
- consider moving heavy computations to Fortran/C completely - f2py and Cython will help you wrapping

# Slightly OffTopic: mpi4py

## mpi4py

### Interface MPI in Python

- speed-up pure Python by parallelization using MPI (OpenMPI, mpich...)
  - mpi4py also works with f2py and Cython (?)
- run the steering Python script with `mpirun...`, take care of the communicator there and use it in Fortran, too

### Alternatives:

- IPython's parallel computing facilities



# Slightly OffTopic: mpi4py

```
from mpi4py import MPI
```

```
MPIroot = 0 # define the root process
```

```
MPIcomm = MPI.COMM_WORLD # MPI communicator
```

```
MPIrank, MPIsize = MPIcomm.Get_rank(), MPIcomm.Get_size()
```

```
...
```

```
MPIcomm.Reduce(tempVals, retVal, op=MPI.SUM, root=MPIroot)
```

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# Python in teaching

Python should be used in teaching because

- it is easy...
- and yet powerful
- it may be used specialized to numerical computing...
- and also serve students as a general purpose language
- it is safe
- and best of all, it is *free*

## Take home message 1

Python is ideal for teaching

# Summary

We have...

- introduced basic Python scripting
- shown some basic modules for scientific computing
- demonstrated how to wrap other languages
- learned how to speed Python up

## Take home message 2

Python is a very valuable tool for Physicists

Slides,  $\text{\LaTeX}$  and Python Sources available at  
<http://github.com/aeberspaecher>