# Python Programming for Scientists

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OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

NAT FAKULTÄT FÜR NATURWISSENSCHAFTEN

FOR760: Scattering Systems with Complex Dynamics

# Outline

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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)
- ...

# Outline

# Scientific *Hello, World!*

```
import sys
from math import sin, pi

def sincSquare(x):
    """Return 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 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 []!
```

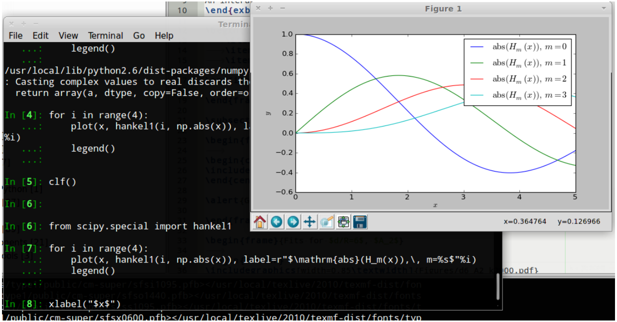
# Outline

# 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

```python
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

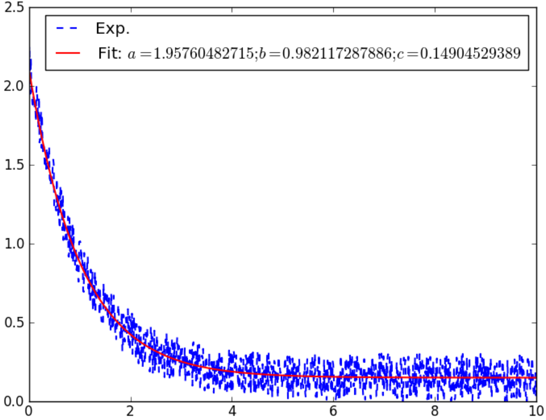
```
import numpy as np
from scipy.optimize import curve_fit
from matplotlib.pyplot import plot, show, legend

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

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

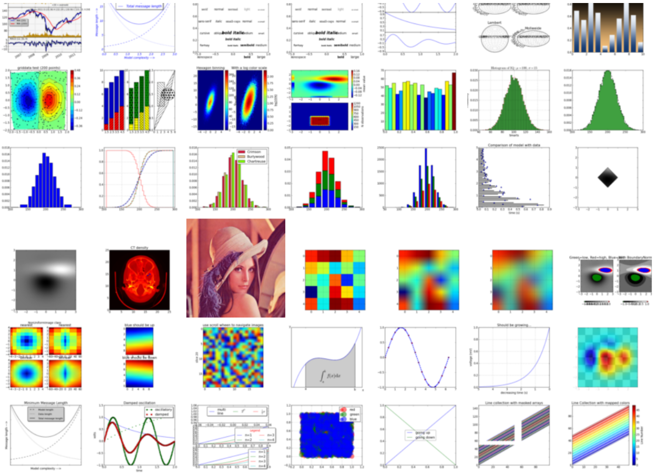
# SciPy: the example's output




Already used here: *Matplotlib*

# Matplotlib

(mostly) 2D plots



Pylab: MatLab alternative for interactive work

# Some Pylab: the logistic map

```
from matplotlib.pylab import * # some of NumPy, SciPy, MPL

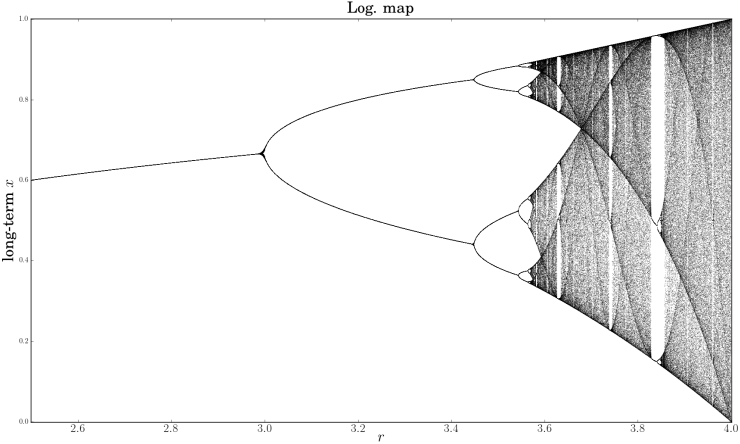
rVals = 2000; startVal = 0.5
throwAway = 300; samples = 800
vals = zeros(samples-throwAway)

for r in linspace(2.5, 4.0, rVals): # iterate r
    x = startVal
    for s in range(samples):
        x = r*x*(1-x) # logistic map
        if(s >= throwAway): vals[s-throwAway] = x
    scatter(r*ones(samples-throwAway), vals, c="k", \
            marker="o", s=0.3, lw=0) # plot

xlabel("$r$"); ylabel("$x$"); title("Log. map"); show();
```

# Some Pylab: the logistic map

The last script produces this image:



# Outline

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

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

def sincSquare(x):
    """Return the 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`

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```
import numpy as np

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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

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

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

# $\mathrm{sinc}(x)^2$ - 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 $\approx 100$!

# $\mathrm{sinc}(x)^2$ - 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 = 3.14159265358979323846264333
    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:

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

# $\mathrm{sinc}(x)^2$ - 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 $\approx 100$!

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

```fortran
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`

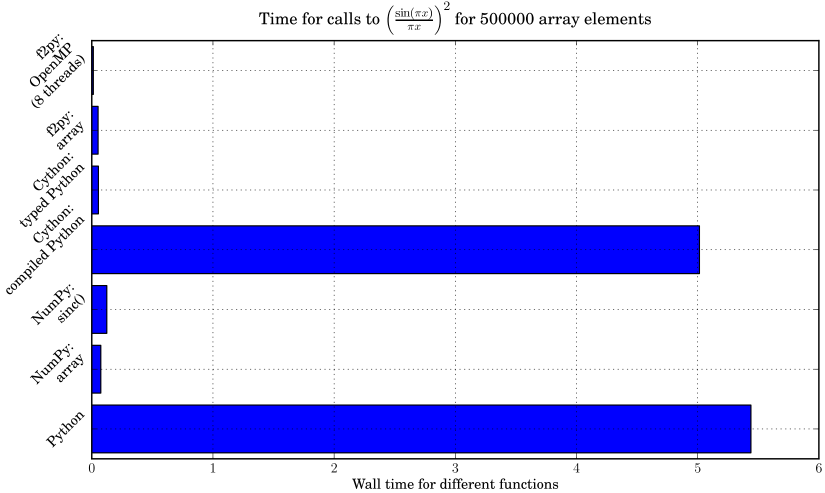
# Cheating: $\mathrm{sinc}(x)^2$ - f2py, Version 2 - OpenMP

```
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`

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

Benchmark for an Intel i7:



# 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)
```

# Outline

# Python in teaching

Python/Pylab 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, LaTeX and Python Sources available at
`http://github.com/aeberspaecher`