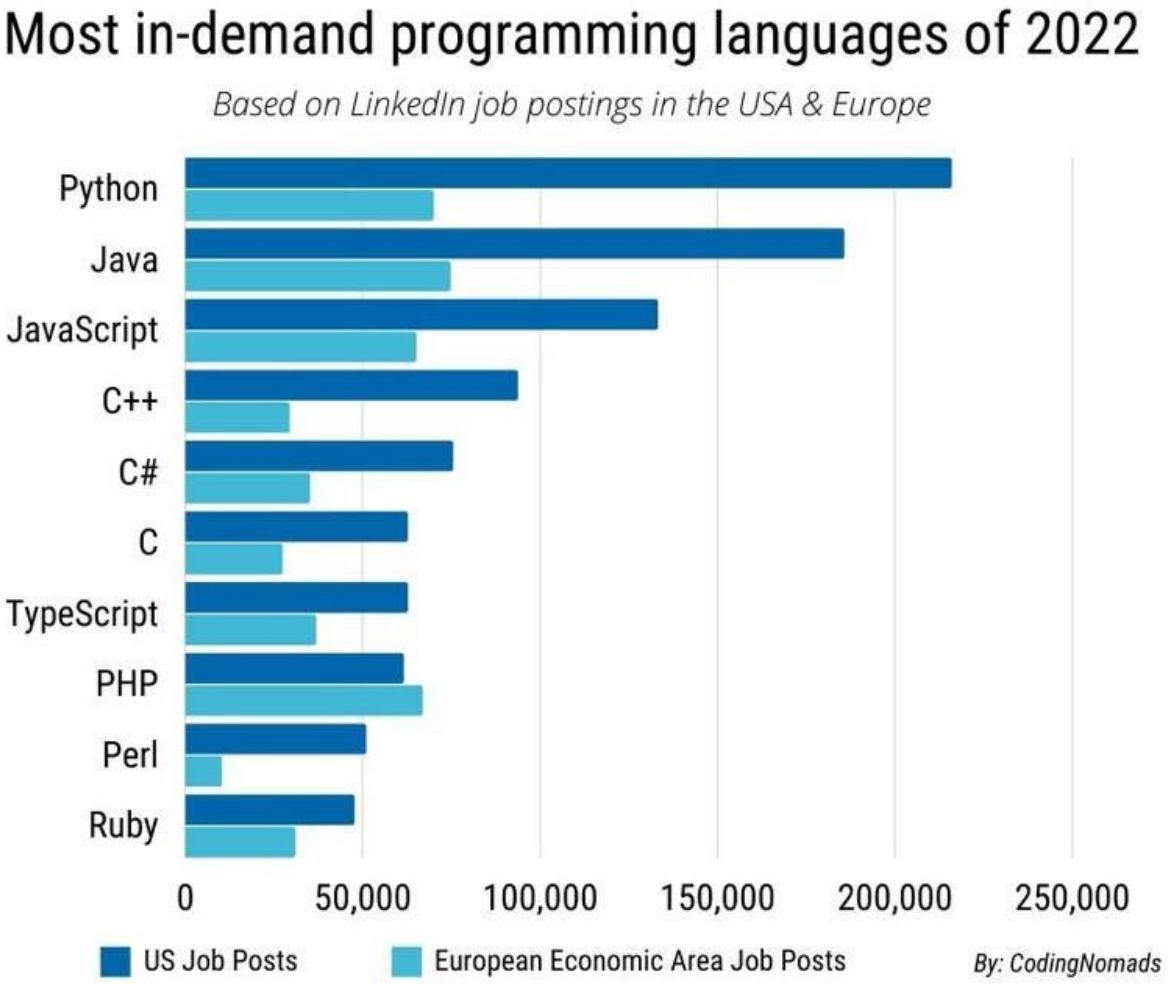
Computer modeling of physical phenomena

Lab I – Python

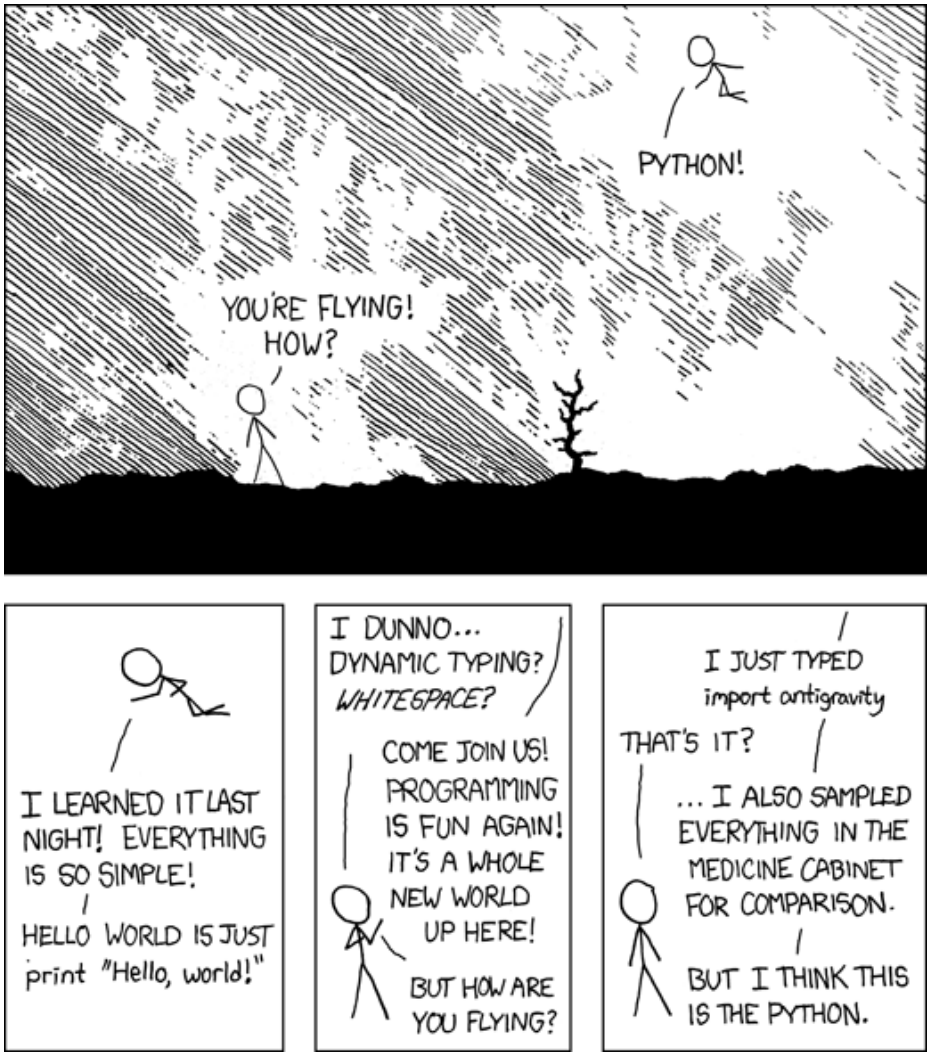
Why python?

- easy to learn, very clear syntax, readable code
- interpreter and a scripting language
- huge standard libraries, special libraries for scientific computing
- open software, good documentation, easy installation
- expandable (modules from C, C++ or Fortran can be added)

Why python?


Most in-demand programming languages of 2022
Based on LinkedIn job postings in the USA & Europe
Python
Java
JavaScript
C++
C#
C
TypeScript
PHP
Perl
Ruby
0
50,000
100,000
150,000
200,000
250,000
US Job Posts
European Economic Area Job Posts
By: CodingNomads

Freedom



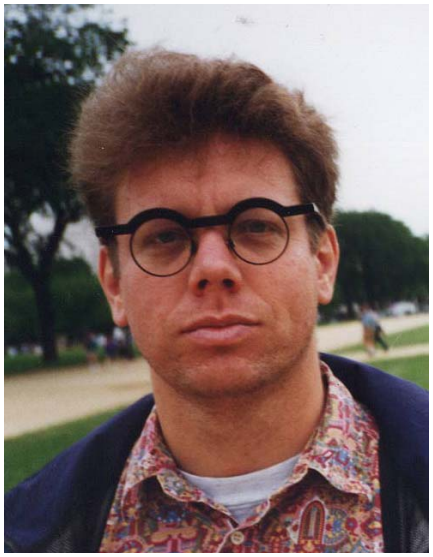
xkcd.com

PYTHON

- named after BBC show "Monty Python's Flying Circus"
- ... and has nothing to do with reptiles

Guido van Rossum

(then at the National Research Institute, Netherlands)



Over six years ago, in December 1989, I was looking for a "hobby" programming project that would keep me occupied during the week around Christmas. My office ... would be closed, but I had a home computer, and not much else on my hands. I decided to write an interpreter for the new scripting language I had been thinking about lately: a descendant of ABC that would appeal to Unix/C hackers. I chose Python as a working title for the project, being in a slightly irreverent mood (and a big fan of Monty Python's Flying Circus)

Python documentation

- http://www.python.org The major Python Web site. Contains code, documentation, and pointers to Python-related pages.
- http://docs.python.org Fast access to Python documentation.
- http://docs.python.org/tutorial/ Python Tutorial
- http://wiki.python.org/moin/ http://wiki.python.org/moin/PolishLanguage Python Wiki (also in Polish) – links to more guides

and tutorials

- “A Byte of Python” by C.H.Swaroop; good point to start (free online)
- “Python Tutorial” by Guido; a classic, sometimes too much detailed

  https://bugs.python.org/file47781/Tutorial_EDIT.pdf
- “Dive into Python”; good for consulting when we know something (free online)
- “Learning Python” by M. Lutz; long text if one prefers slower approach (our library)
- The Python Cookbook: collection of examples and useful hints

  https://d.cxcore.net/Python/Python_Cookbook_3rd_Edition.pdf
- "An introduction to Python for scientific computing" by Scott Shell

Running Python

There are different ways to use Python:

- interactive interpreter started from command line

```
>>> 2+2
4
```

- running a script

```
$ python script.py
```

- from a graphical user interface (GUI) environment; e.g. `idle`

Python identifiers

- identifier starts with a letter `A...Z` (or `a...z`),
- no `@`, `$`, and `%` within identifiers, only letters and digits
- case sensitive

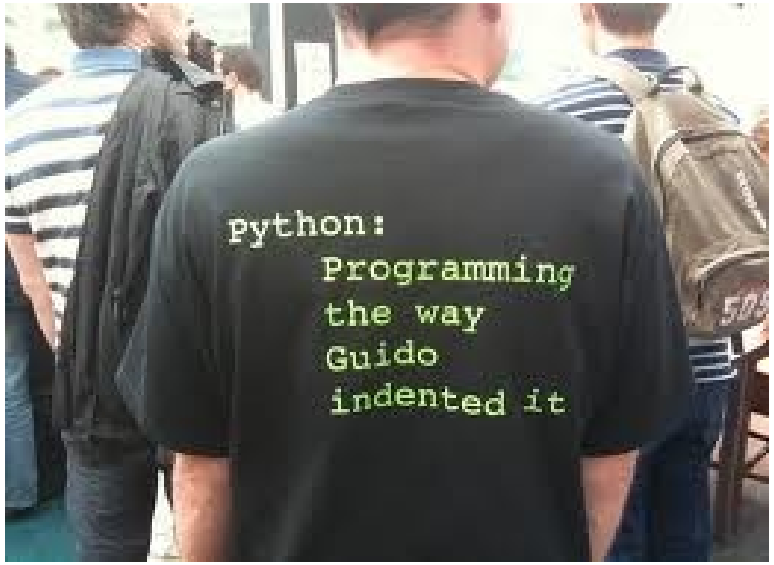
- reserved words

```
and, exec, not, assert, finally, or, break,
for,  pass, class, from, print, continue,
global, raise,  def, if, return, del, import,
try, elif, in, while,  else, is, with, except,
lambda, yield
```

Lines and indentation

- one line one statement
- blank lines encouraged for readability
- blocks of statements are denoted by indentation
  same indentation within a block

- ```
  condition = True
  if condition:
      print("True")
  else:
      print("False")
  ```


  ```

Comments

- comments follow # sign up to the line end
- string literals are contained within single ', double " or triple """ quotation marks

Variables

- the declaration happens automatically when you assign a value to a variable
- standard data types: numbers and strings

```
>>> a = 10.
>>> type(a)
<class 'float'>
>>> a = 1
>>> type(a)
<class 'int'>
>>> a = '1'
>>> type(a)
<class 'str'>
```

- numerical types: `int` = integers with unlimited precision
  `float` = C double precision
  `complex` = two floats in double precision

Lists

elements in square brackets: `['a','b','c']`,

```
>>> list = ['abcd', 786 , 2.23, 'john', 70.2]
>>> list[0]
'abcd'
>>> list[1:3]
[786, 2.23]
>>> list[3:]
['john', 70.2]
>>> list.append('eve')
['abcd', 786, 2.23, 'john', 70.2, 'eve']
```

Tuples

- Sequences similar to lists
  - elements of a tuple and its size can't be changed
  - tuples can be thought of as read-only lists
  - applications: multiple results from a function, sets of parameters

```
tup1 = (12, 34.56)
tup2 = ('abc', 'xyz')
# Following action is not valid for tuples
# tup1[0] = 100
# Let's create a new tuple as follows
tup3 = tup1 + tup2
print (tup3)
```

Type conversions

- to convert between build-in types you simply use the type name as a function

```
float(x), str(n), tuple(list)
```

- these functions return a new object representing the converted value
- in the algebraic expressions the type conversion is performed automatically (mixed types converted to a common type)

List of available operators

Python philosophy: operate on all types for which it makes sense

- assigment `=`
- more assigments `+=`, `*=`, `/=`, ...
- arithmetic: (`+` , `-` , `*` , `**` , `/` , `//` , `%`)
- logical: (`>` , `<` , `>=` , `<=` , `==` , `!=`)
- and also: (`not` , `and` , `or`)
- bit operations (`&` , `|` , `^` , `~`)

```
a=5
a+=2
a*=2
a/=7
print (a)
```

If else elif

Similar to many other languages

```
if conditions:
    statements
```

with else-elif construct

```
if expression1:
    statement(s)
elif expression2:
    statement(s)
elif expression3:
    statement(s)
else:
    statement(s)
```

While loop

Just an example:

```
running= True
while running:
    running = statements()
else:
    print "End of while loop"
```

For loop

Example 1

```
for l in "Python":
    print ("current letter :", l)
```

Example 2

```
fruits = ["banana", "apple",  "mango"]
for f in fruits:
    print ("current fruit :", f)
```

Example 3

```
n = 5
for i in range(n):
    print ("current index :", i)
```

Functions

A function is a block of organized, reusable code that is used to perform a single, related action. Functions provides better modularity for your application and a high degree of code reusability.

We can define function in any place in the code

```
def welcome():
    print ("Hello World!")

welcome()
```

There are default values for the arguments

```
def func(a, b=5, c=10):
    print ("a = ", a, "b = ", b, "c = ", c)
    return a+b+c

func(3)
func(15, c=14)
func(c=50, a=40)
```

Documenting a function

Good practice requires documenting

```
def maximum(x, y):
    """Prints the bigger of two arguments"""
    if x > y:
        print (x, "is bigger")
    else:
        print (y, "is bigger")

maximum(3, 5)
print(maximum.__doc__)
help(maximum)
maximum('ala','bob') # our code is very general!
```

What is a module?

- Module allows you to organize your Python code
- Simply, a module is a file consisting of Python code. A module can define functions, classes, and variables.
- Many most useful tools are just modules:
  NumPy, SciPy, MatPlotLib

Example on how to use a module

Import a standard system module

```
import sys

print ('The command line arguments are:')
for i in sys.argv:
    print (i)

print ('\nThe PYTHONPATH is', sys.path, '\n')
```

The code above prints arguments given at a command line

```
$ python program.py ...
```

and then the directories searched for Python modules

Warning: never name a program after a standard module name!!!

Our own module

```
# Filename: mymodule.py
def hi():
    print ("Hi, this is me, your module!")

version = "0.1"
# End of mymodule.py

-----------------------------------------------
# Filename: mymodule_demo.py
import mymodule

mymodule.hi()
print ('Version', mymodule.version)
```

Project “0”: a tutorial

there are ≈ 20 slides of a practical tutorial, illustrating all main constructs introduced during the lecture. The tutorial contains also simple examples of plots, special functions from SciPy, and some basic opperations with arrays in NumPy. Please follow this guide interactively and then write and run short scripts (as described in the text) on your own.

Interactive calculator

First task:

- install Python on your computer
- make sure you can run it in our lab

Try from the shell prompt

```
$ python -V
```

we will work with 3.x version

NUMBERS

```
$ python

>>> 2+2       # this is a comment
>>> 2/3       # floating point division (integer
              division in python 2.7)
```

Variables

```
>>> h = 20.1        # assigment
>>> h               # prints the value
>>> w = 3.2
>>> w*h

>>> w, h = 5, 6. # multiple assigment

>>> t = w, h       # composed variable
>>> t              # known as TUPLE
>>> t[0]
>>> t[1]
```

Numbers and strings

```
>>> s = "12.3"  # is a string
>>> s*2         # well, it works for the string
>>> s*0.5       # but this one doesn't

>>> float(s)*2         # this is what we mean
>>> int("2343453656") # conversion to integer type

>>> str(12.3)          # ... converting to strings
>>> str(2343453656)

>>> ss = "%.20f" % (2./3) # check what type is ss?
                          # %.20f means C formatting

>>> text = "My voltameter shows %.5f V" % (2./3)

                           # another example of formatting
```

Complex numbers

```
>>> 1j              # complex unit
>>> (1+2j)*3
>>> (1+2j)/(1+1j)
>>> z = 1.5+.5j
>>> abs(z)          # complex module
>>> z.real
>>> z.imag
```

Module *math*

```
>>> import math  # here we import a module
                 # with lots of useful math

>>> math.factorial(70)
>>> math.factorial(70)/math.factorial(69)

>>> ( math.e**(1j*math.pi) ).imag
>>> ( math.e**(1j*math.pi) ).real

>>> help(math)      # checks the documentation
                    # use q to quit
>>> help(math.tanh)
```

Module *cmath*

```
>>> z = (1+2j)*3
>>> math.cos(z)

>>> import cmath as cm    # complex numbers module
                          # we give it
                          # our own short name
>>> cm.cos(z)
>>> dir(cm)         # list of available
                    functions
>>> cm.polar(z)    # returns polar coordinates
                    # radius and angle

>>> rfi = cm.polar(z)
>>> rfi[0]              # an example how to use tuple
>>> rfi[1]
>>> r, fi = cmath.polar(z) # ... is also fine
```

Strings

```
>>> word = "Help" + "A"    # concatenation
>>> word

>>> "<" + word*5 + ">"

>>> word[0:2]              # accessing substrings
>>> "<" + word[0:2]*5 + ">"

>>> word[:2] + word[3:]
>>> len(word)              # returns length
```

Scientific computing module *SciPy*

```
>>> from scipy import constants as const
                # here we import a sub-module
>>> help(const)

>>> const.c   # speed of light
>>> const.h   # Plank's constant

>>> const.h/const.e**2 # quantum of resistance
                       # (in Ohms)

>>> from scipy import special as sp
>>> sp.jn(2,0.345)     # Bessel function Jn_2(x)

>>> help(special)      # ... many are available
```

Scripts

Set of commands can be collected into a file `*.py` and executed simply by running it `$python my_example.py`

Script “Scientific Hello World” illustrates
— how to initialize variables from the command line
— how to print numbers and text

Create a file `hello.py`

```
import sys, math          # import system module

r = float(sys.argv[1]) # reads 1-st argument
                       # from the command line
s = math.sin(r)

print ("Hello, World! sin(" + str(r) + ")=" + str(s))
```

and run using `$ python hello.py 2.3`

Editor

- use any editor which underlines Python syntax
- or use an integrated environment e.g. idle

```
$ idle &
File -> New Window  print (2+2)
Run -> Module  (or F5)
```

While loop

Write a simple script as below and run it

```
# Fibonacci sequence:
# sum of two previous elements gives the new
one
a, b = 0, 1             # multiple assigment
while b < 10 :          # !!! remember the colon
    print (b)           # !!! ... and indentation
    a, b = b, a+b

print "Done!"
```

Alternatively print results in a single line

```
while b < 10:
   print (b, end=" ")    # ... no new line
```

Lists and for loops

Run and analize (understand) what is printed in the code below:

```
# Create a list consisting of strings
b = ["Mary", "had", "a", "little", "lamb"]

print (b[3])
print (b[3][1:2])
print (len(b))
print (len(b[3]))

for i in range(len(b)):
    print (i, b[i], len(b[i]))

for x in b:
    print (b.index(x), x, len(x))
```

More list operations

Try to predict what happens in the code, then run it and check

```
# Same list as in the previous example
b = ["Mary", "had", "a", "little", "lamb"]

print (b*2)
b.append('!')
print (b)
b.reverse()
print (b)
print (b.pop(3))
print (b)
```

list.pop(i) - remove the item at the given position in the list, and return it.

Functions

We rewrite out “while loop example” using a function

```
# Define a simple function

def fib(n=3):
    a, b = 0, 1
    while a < n:
      print (a, end=" ")
      a, b = b, a+b
    print ()

fib(2000)
fib()
```

Local and global variables

Python understands that local variables do exist only within a function. Run and see what happens.

```
# Filename: func.py

def f_loc(x):
    print ('x is ', x) # print to check the value
    x = 2              # a new local variable is created
    print ('locally x is ', x)


x = 50
f_loc(x)
print ('x is still', x)
```

Local and global variables

There is a way to change a global variable within the function

```
# Filename: func.py

def f_glob():
    global x
    print ('x is', x)
    x = 2
    print ('x is now changed to ', x)


x = 50
f_glob()
print ('x in this case is ', x)
```

NumPy arrays

Run the code below, note that one-line creation of an array is more Python-like than the loop over elements.

```
import numpy as np # short name of this module

n = 7
v = np.zeros(n)     # vector is represented as numpy array

for i in range(n):
    v[i] = i/2.0    # sets elements v_i
print (v)

u = np.arange(-1.0,1.0,0.2)       # range of values
print (u)

w = np.linspace(-np.pi,np.pi,6)   # also some range,
print (w)                         # given number of points
```

Plotting with Matplotlib

Plotting is easy, check it with the example below

```
import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(-np.pi,np.pi,101)

y1 = np.cos(x)  # Numpy math functions
y2 = np.sin(x)  # operate on whole arrays

plt.plot(x, y1, color='r', linestyle='-', linewidth=2)
# plots with a red line

plt.plot(x, y2, 'g--', lw=1)
# shorter description: thinner green dashed line

plt.show()
```


PYTHON