# Introduction to Programming with Scientific Applications

Gerth Stølting Brodal
Department of Computer Science
Aarhus University



#### **Course evaluation**

"The first lecture was intimidating and overwhelming"

#### Course description – kursuskatalog.au.dk/en/course/123832/

#### **Introduction to Programming with Scientific Applications**

#### **Description of qualifications**

After the course the participants will have knowledge of principles and techniques for systematic construction of programs.

At the end of the course, the participants will be able to:

- apply constructions of a common programming language,
- develop well-structured programs and perform testing and debugging of these,
- explain fundamental programming concepts and basic algorithmic techniques,
- apply standard tools for scientific applications,
- use the documentation for a programming language and available software packages.

#### **Contents**

The course gives an introduction to programming with scientific applications. Programming concepts and techniques are introduced using the **Python** programming language. The programming concepts are **illustrated in other programming languages**. The following content is included.

Basic programming constructs: Data types, operators, variables, flow of control, conditionals, loops, functions, recursion, scope, exceptions. *Object orientation*: Abstract data types, classes, inheritance, encapsulation. *Basic algorithmic techniques*: Sorting, binary search, dynamic programming. *Systematic development of programs*: Testing and debugging. File-based input/output, numerical analysis, functional programming. Scientific computing using standard packages for Python.

**ECTS** 10

Hours - weeks - periods

Lectures 2 x 2 hours/week
TA sessions 1 x 3 hours/week
Study café 3 x 1 hour/week

Language of instruction

Danish

Instructor

Gerth Stølting Brodal

**Academic prerequisites** 

(Some) Linear algebra

Exam

5 hour programming

Aid: Computer and Internet, headphones,7-point grading scale

**Prerequisites for examination participation** 

Submission and approval of 10 mandatory assignments and submission of 1 implementation project

Notes Grade reflects an overall assessment of implementation project and written examination. Project counts 20% and written exam counts 80%

#### Lecturer

| Name      | Gerth Stølting Brodal  |
|-----------|--|
| Research  | Algorithms and Data Structures (Computer Science)  |
| Teaching  |  |
| 2018 -    | BSc course on Introduction to Programming with Scientific Applications   |
| 2003 -    | BSc course on Introduction to Algorithms and Data Structures   |
| 1999 - 17 | MSc courses on Computational Geometry, Algorithm Engineering, Advanced Data Structures, External Memory Algorithms and Data Structures |
| Python    | Advanced Beginner  |

#### Question – Primary Education?

- a) Mathematics
- b) Mathematics-Economics
- c) Data Science
- d) Chemestry
- e) Physics
- f) Other Science-Technology
- g) Other

#### Question – Programming languages you know?

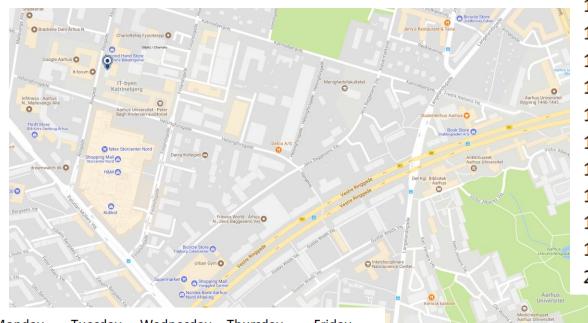
#### Question – Programming experience?

For the programming language you know best (if any) please state you proficiency level within the language.

- a) None
- b) Fundamental awareness (basic knowledge)
- c) Novice (limited experience)
- d) Intermediate (practical application)
- e) Advanced (applied theory)
- f) Expert (recognized authority)

### Some course practicalities

Primary lecture material = slides



|             | Monday     | Tuesday | Wednesday  |    | Thursday   | Friday |
|-------------|------------|---------|------------|----|------------|--------|
| 8:15-9:00   |            |         |            |    |            |        |
| 9:15-10:00  | Study cafe |         | Study cafe |    | MA1        |        |
| 10:15-11:00 | Lecture    |         | Lecture    |    |            |        |
| 11:15-12:00 | Lecture    |         |            |    |            | MA2    |
| 12:15-13:00 |            |         |            |    |            |        |
| 13:15-14:00 |            |         |            | DV |            |        |
| 14:15-15:00 |            | Mix     | KE         |    | Study cafe |        |
| 15:15-16:00 |            | MØ      | MA         |    |            |        |
| 16:15-17:00 |            | FY      | IVIA       |    |            |        |
| 17:15-18:00 |            |         |            |    |            |        |

| Veek | Monday | Tuesday     | Wednesday    | Thursday | Friday      |
|------|--------|-------------|--------------|----------|-------------|
| 5    | F1     | no TA class | F2           |          |             |
| 6    | F3     | TØ1         | TØ1 / F4     | TØ1      | TØ1         |
| 7    | F5     | TØ2         | TØ2 / F6     | TØ2      | TØ2         |
| 8    | F7     | TØ3         | TØ3 / F8     | TØ3      | TØ3         |
| 9    | F9     | TØ4         | TØ4 / F10    | TØ4      | TØ4         |
| 10   | F11    | TØ5         | TØ5 / F12    | TØ5      | TØ5         |
| 11   | F13    | TØ6         | TØ6 / F14    | TØ6      | TØ6         |
| 12   | F15    | TØ7         | TØ7 / F16    | TØ7      | TØ7         |
| 13   | F17    | TØ8         | TØ8 / F18    | TØ8      | TØ8         |
| 14   | F19    | TØ9         | TØ9 / F20    | TØ9      | TØ9         |
| 15   | F21    | TØ10        | TØ10 / F22   | TØ10     | TØ10        |
| 16   |        |             | Easter break |          |             |
| 17   |        | -           | -            | -        | Kapsejlads? |
| 18   | F23    | TØ11        | TØ11 / F24   | TØ11     | TØ11        |
| 19   | F25    | TØ12        | TØ12 / F26   | TØ12     | TØ12        |
| 20   | F27    | TØ13        | TØ13/-       | TØ13     | TØ13        |
|      |        |             |              |          |             |

#### Course page on Brightspace and GitHub

- Past exams

- Windows 11 - Mac & Linux

Python resources

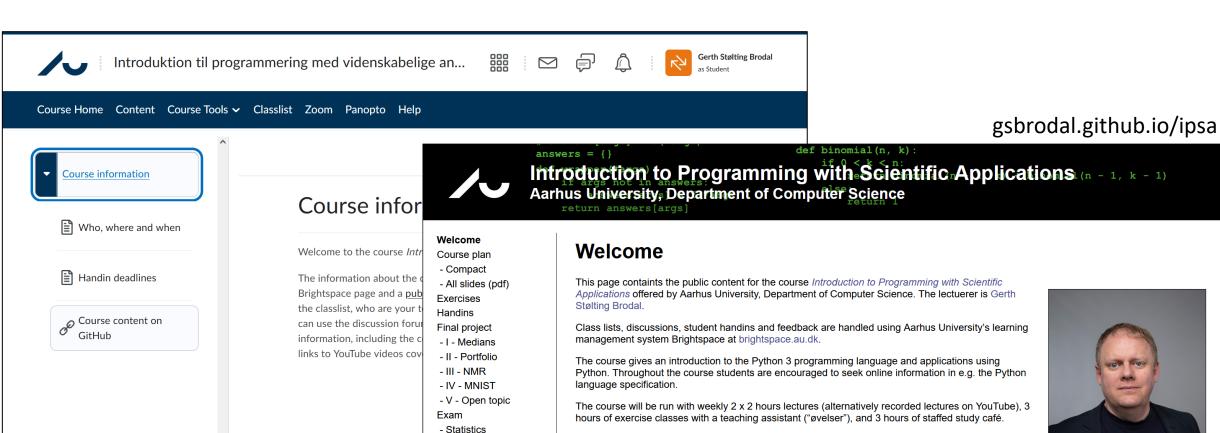
AU course description

Plagiarism

Workload

Literature Python installation

- Books - Videos



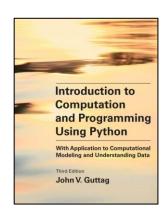
During the course students are required to hand in 10 weekly handins and one larger implementation project. Handins and the project are done in groups of up to three persons. Approval of the weekly handins is a prerequisite to attend the exam. The final exam will be a programming exam with all aids. incl. internet, and the final grade will be based on an overall evaluation of the implementation project (20%) and the programming exam (80%).

#### Course content

The course gives an introduction to programming with scientific applications. Programming concepts and techniques are introduced using the Python programming language. The programming concepts are illustrated in other programming languages. The following content is included.

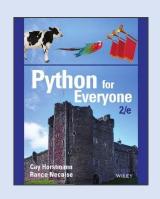
 Basic programming constructs: Data types, operators, variables, flow of control, conditionals, loops, functions, recursion, scope. exceptions.

#### Course text book – optional



John V. Guttag: Introduction to Computation and Programming Using Python, Third Edition With Application to Computational Modeling and Understanding Data. Third Edition. 664 pages. MIT Press, 2021.

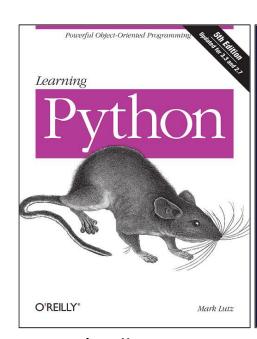
- [Guttag, 2<sup>nd</sup> Ed., page 8] "The reader should be forewarned that this book is by no means a comprehensive introduction to Python". 3<sup>rd</sup> Ed. added about 80 pages on introduction to Python.
- Covers all basic features of Python enabling you to deal with data in Chapters 1-10 (212 pages) - remaining chapters are applications
- Other resources: Google, stackoverflow, Python.org, YouTube, ...



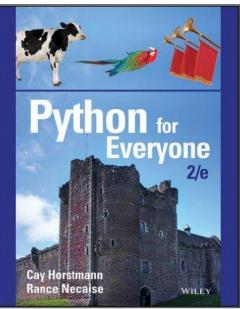
Comparison to a standard text book on the *programming language* Python by Cay Horstmann and Rance Necaise:

Topic **recursion** is covered by Guttag on page 123 (2<sup>nd</sup> edition on page 50), Horstmann and Necaise do it on page 611

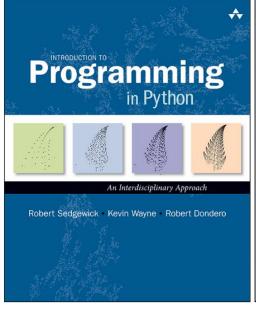
#### Some other books on Python



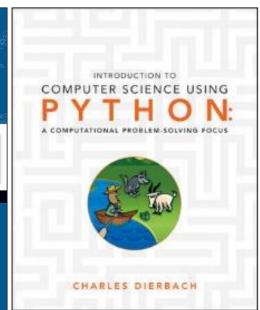
O'Reilly, 2013 1684 pages



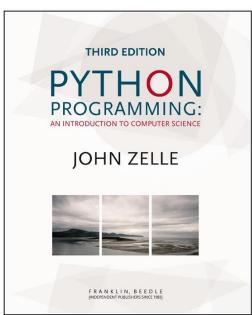
Wiley, 2016 752 pages



Addison-Wesley, 2015 794 pages



Wiley, 2013 580 pages



Franklin & Beedle, 2016 552 pages

## Two Python programs

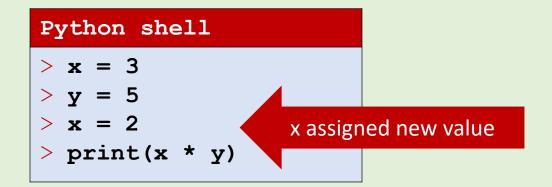
#### A Python program

```
Python shell
> x = 7
> print(x * x)
| 49
```

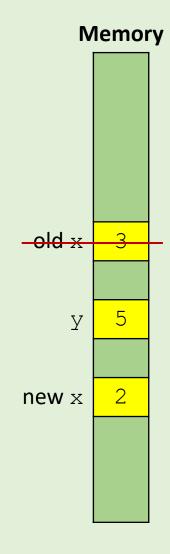
- 7 is an integer literal in Python denoted an "int"
- x is the name of a variable that can hold some value
- = is assigning a value to a variable
- \* denotes multiplication
- print is the name of a built-in function, here we call print to print the result of 7 \* 7
- A program consists of a sequence of statements, executed sequentially

Memory X

#### Question – What is the result of this program?



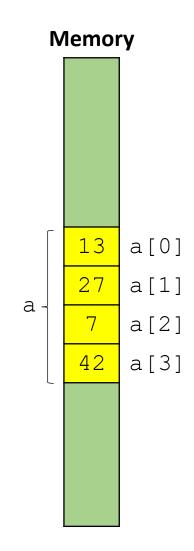
- 😬 a) 10
  - b) 15
  - c) 25
  - d) [15, 10]
  - e) Error
  - f) Don't know



#### Another Python program using lists

```
Python shell
> a = [13, 27, 7, 42]
> print(a)
| [13, 27, 7, 42]
> print(a[2])
| 7
```

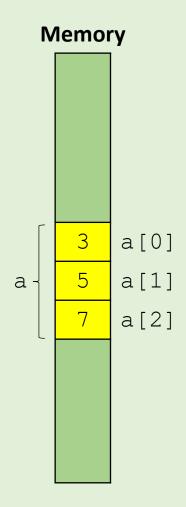
- [13, 27, 7, 42] is a *list* containing four integers
- a [2] refers to the entry in the list with index 2
   (the first element has index 0, i.e. a [2] is the 3<sup>rd</sup> element of the list)
- Note that print also can print a list



#### Question – What is the result of this program?

```
Python shell
> a = [3, 5, 7]
> print(a[1] + a[2])
```

- a) 8
- b) 10
- <u>••</u> c) 12
  - d) 15
  - e) Don't know



### Why Python?



the next slides will be technical

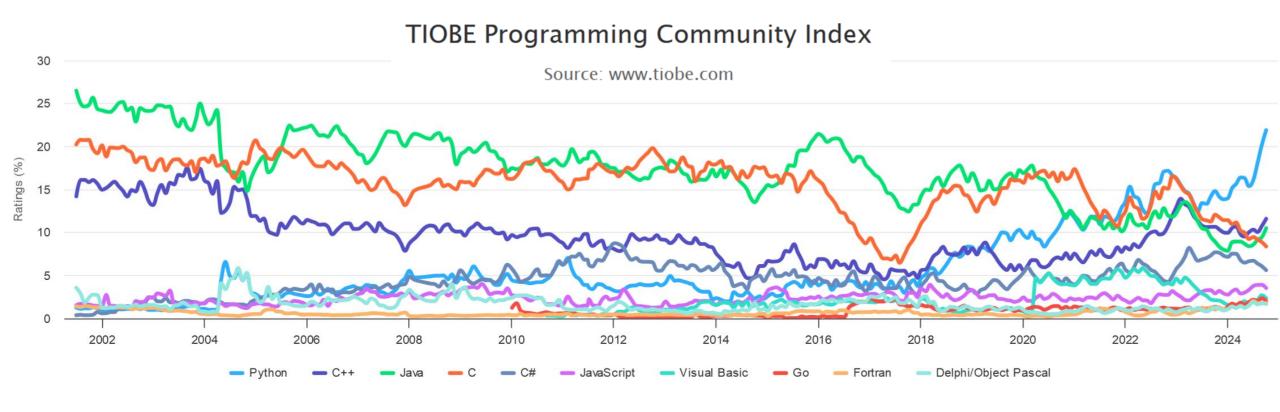
#### **TIOBE Index January 2024**

| Jan 2024 | Jan 2023 | Change   | Progra   | amming Language | Ratings | Change | Since<br>vember |
|----------|----------|----------|----------|-----------------|---------|--------|-----------------|
| 1        | 1        |          | <b>e</b> | Python          | 13.97%  |        | 2021            |
| 2        | 2        |          | 9        | С               | 11.44%  | -4.81% |                 |
| 3        | 3        |          | <b>G</b> | C++             | 9.96%   | -2.95% |                 |
| 4        | 4        |          | <u>(</u> | Java            | 7.87%   | -4.34% |                 |
| 5        | 5        |          | 8        | C#              | 7.16%   | +1.43% |                 |
| 6        | 7        | ^        | JS       | JavaScript      | 2.77%   | -0.11% |                 |
| 7        | 10       | ^        | php      | PHP             | 1.79%   | +0.40% |                 |
| 8        | 6        | •        | VB       | Visual Basic    | 1.60%   | -3.04% |                 |
| 9        | 8        | <b>~</b> | SQL      | SQL             | 1.46%   | -1.04% |                 |
| 10       | 20       | *        |          | Scratch         | 1.44%   | +0.86% |                 |

Python #1

The TIOBE Programming Community index is an indicator of the **popularity of programming languages**. The index is updated once a month. The ratings are based on the number of skilled engineers world-wide, courses and third party vendors. Popular search engines such as Google, Bing, Yahoo!, Wikipedia, Amazon, YouTube and Baidu are used to calculate the ratings. It is important to note that the TIOBE index is not about the **best** programming language or the language in which **most lines of code** have been written. www.tiobe.com

#### Popularity of programming languages



#### "Hello World"

- In Java, C, C++ a lot of "{", "}" and ";" are needed
- Java tends to have a lot of "public..." details that need to be spelled out
- Python is concise

Java

## public class HelloWorld { public static void main( String[] args ) { System.out.println( "Hello World!" ); System.exit( 0 ); } }

## #include <stdio.h> int main(int argc, char \*\*argv) { printf("Hello World"); return 0; }

```
#include <iostream>
using namespace std;

int main(int argc, char** argv) {
    cout << "Hello, World!";
    return 0;
}</pre>
```

```
Python 2
print "Hello world"
```

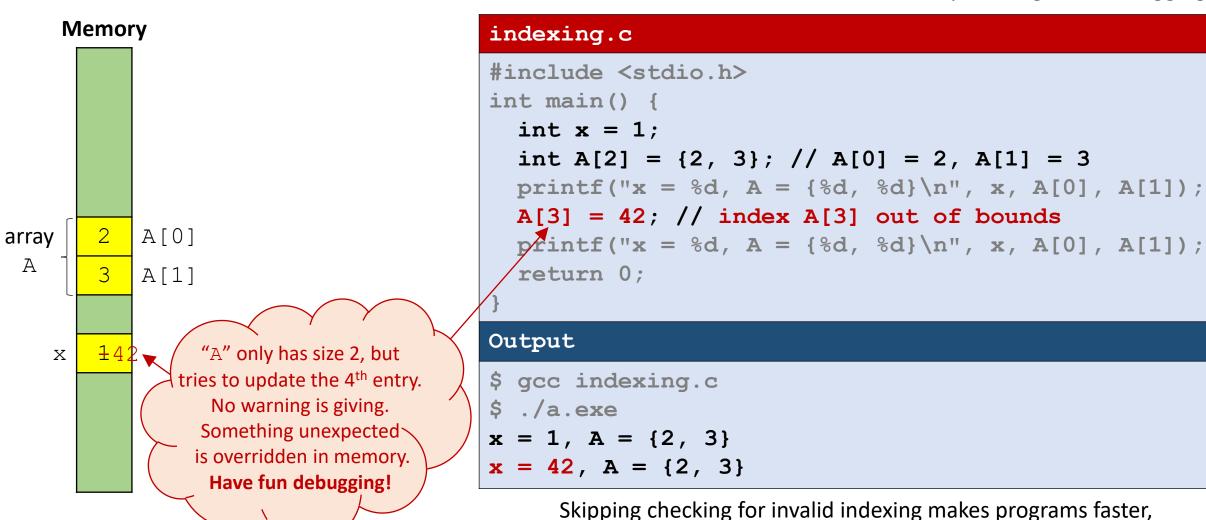
```
Python 3
print("Hello world")
```

## Why Python?

Short concise code

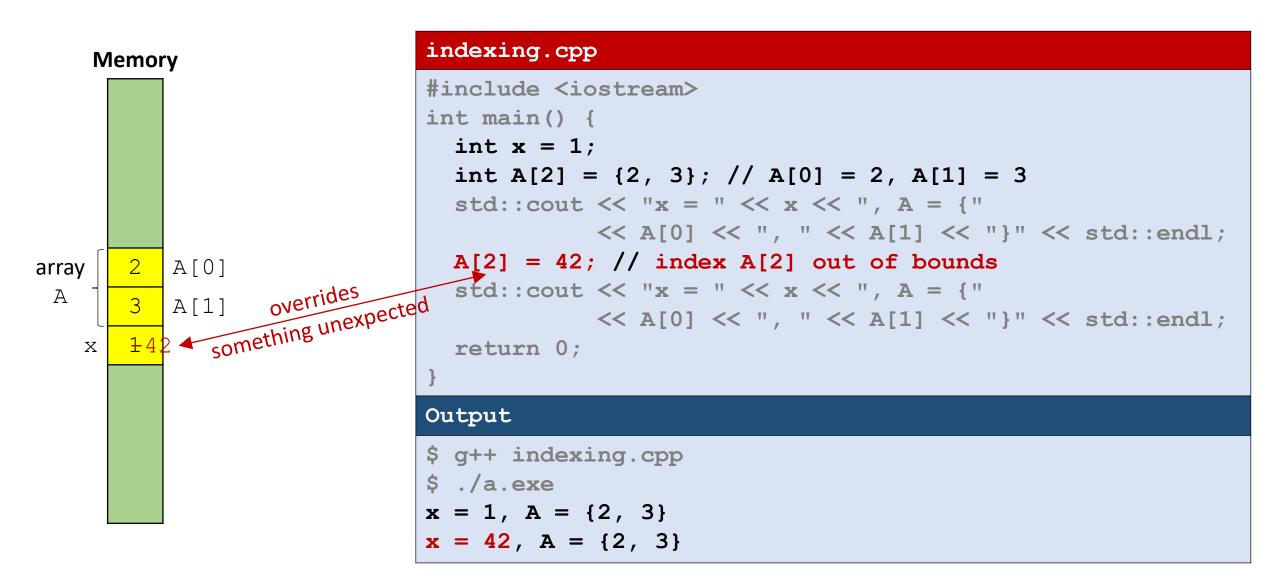
#### C index out of bounds

**Debugging** is the process of finding and resolving defects or problems within a computer program that prevent correct operation of computer software or a system. *en.wikipedia.org/wiki/Debugging* 

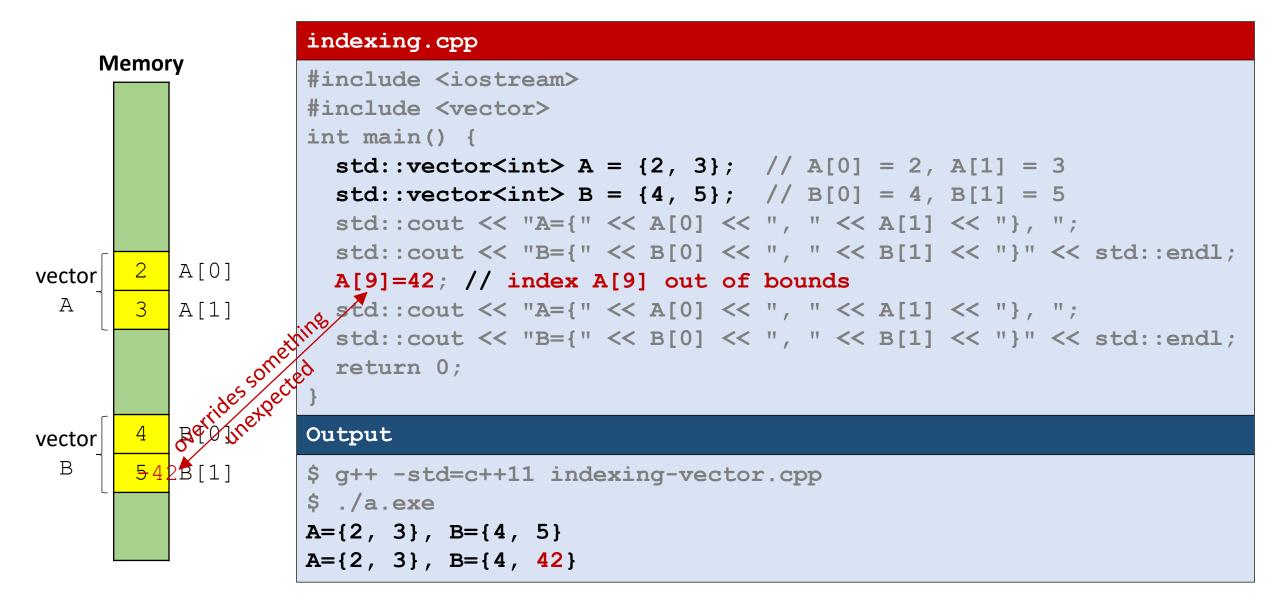


Skipping checking for invalid indexing makes programs faster but also requires disciplined programming

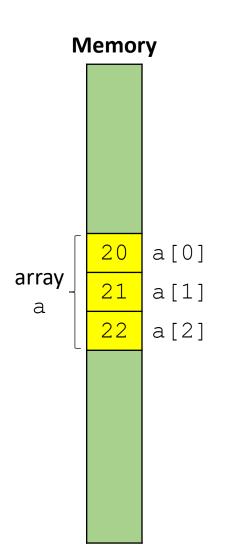
#### ... and C++ index out of bounds



#### ... and C++ vector index out of bounds

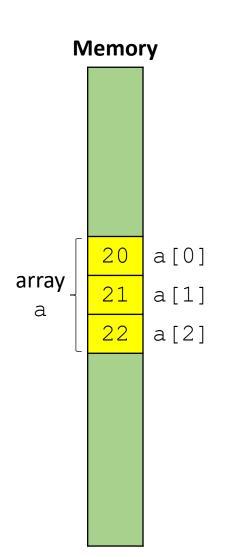


#### ... and Java index out of bounds exception



```
indexing.java
class IndexingTest{
    public static void main(String args[]) {
       int a[] = \{20, 21, 22\};
       a[5] = 42; // index a[5] out of bounds
Output
$ javac indexing.java
$ java IndexingTest
Exception in thread "main"
java.lang.ArrayIndexOutOfBoundsException: 5
        at IndexingTest.main(indexing.java:5)
     Java provides error message when running the program
```

#### ... and Python index out of bounds exception



```
indexing.py
a = [20, 21, 22]
a[5] = 42 # index a[5] out of bounds
Output
$ python indexing.py
Traceback (most recent call last):
  File "indexing.py", line 3, in <module>
    a[5] = 42
IndexError: list assignment index out of range
```

Python provides error message when running the program

#### Memory safety

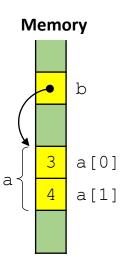
The White House 2024 | Press Release: "Future Software Should Be Memory Safe" (www.whitehouse.gov) National Security Agency 2022 | Cybersecurity Information Sheet: Software Memory Safety (media.defense.gov)

- C and C++ are flexible but memory unsafe programming languages
  - Unexpected writes to memory can be exploited by malicious cyber actors



- Python, Java, Rust are examples of memory safe languages
- Rust aims at achieving the efficiency of C by slightly restricting flexibility

```
indexing.rs
fn main() {
   let mut a = [3, 4];
   a[2] = 7; // Compile error: this operation will panic at runtime
   for i in 2..3 { a[i] = 7 } // Run-time panic: index out of bounds
   let b = &mut a;
   a[1] = 6; // Compile error: cannot use `a` because it was mutably borrowed
    (*b)[0] = 5;
   for i in 0..2 { println!("a[{}] = {}", i, a[i]) }
```



## Why Python?

- Short concise code
- Index out-of-range exceptions

#### C++ different ways to print a vector

```
vector-iterator.cpp
      #include <iostream>
      #include <vector>
      int main() {
        // Vector is part of STL (Standard Template Library)
        std::vector < int > A = \{20, 23, 26\};
        // "C" indexing - since C++98
        for (int i = 0; i < A.size(); i++)
          std::cout << A[i] << std::endl;</pre>
        // iterator - since C++98
        for (std::vector<int>::iterator it = A.begin(); it != A.end(); ++it)
          std::cout << *it << std:: endl;
        // "auto" iterator - since C++11
        for (auto it = A.begin(); it != A.end(); ++it)
          std::cout << *it << std:: endl;
        // Range-based for-loop - since C++11
elegant
        for (auto e : A)
          std::cout << e << std:: endl;</pre>
```

#### Java - different ways to print a vector

```
vector-iterator.java
    import java.util.Vector;
    import java.util.Iterator;
    class IteratorTest{
       public static void main(String[] args) {
           Vector<Integer> a = new Vector<Integer>();
           a.add(7);
           a.add(42);
           // "C" for-loop & get method
           for (int i = 0; i < a.size(); i++)
              System.out.println(a.get(i));
           // iterator
           for (Iterator it = a.iterator(); it.hasNext(); )
              System.out.println(it.next());
           // for-each loop - since Java 5
           for (Integer e : a)
elegant
              System.out.println(e);
```

## The Python way to print a list

```
print-list.py
a = [20, 23, 26]

for e in a:
    print(e)

Output

$ python print-list.py
20
23
26
```

### Why Python?

- Short concise code
- Index out of range exceptions
- Elegant for-each loop

```
cpp-error-message.cpp:7:13: error: no match for 'operator<<' (operand types are 'std::ostream {aka std::basic ostream<char>}' and 'std::vector<int>')
In file included from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/iostream:39:0,
                            from cpp-error-message.cpp:1:
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:628:5: note: candidate: std::basic ostream< CharT, Traits>& std::operator<<(std::basic ostream< CharT, Traits>&, const Tp&) [with CharT = char; Traits = std::char traits<char>; Tp = std::vector<int>] <near match>
        operator<<(basic ostream< CharT, Traits>&& os, const Tp& x)
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:628:5: note: conversion of argument 1 would be ill-formed:
cpp-error-message.cpp:7:16: error: cannot bind 'std::ostream {aka std::basic ostream<char>}' lvalue to 'std::basic ostream<char>&&'
std::cout << A << std::endl;
            operator<<(__ostream_type& (*__pf)(__ostream_type&))
/usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/ostream:108:7: note: no known conversion for argument 1 from 'std::basic_ostream<char>::_ostream_type& (*) (std::basic_ostream<char>::_ostream_type& (*) (std::basic_ostream<char>*:_ostream_type& (*) (std::basic_ostream<char>*: ostream_type& (*) (std:
 Traits>:: ostream type = std::basic ostream<char>; std::basic ostream< CharT, Traits>:: ios type = std::basic ios<char>]
            operator<<(__ios_type& (*__pf)(__ios_type&))
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:117:7: note: no known conversion for argument 1 from 'std::basic ostream<char>:: ios type& (*)(std::basic ostream<char>:: ios type& (*)(std::basic ios<char>& (*)(std::basic ios<char>&)}'
/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:127:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type& std::basic ostream
            operator<<(ios base& (* pf) (ios base&))
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:127:7: note: no known conversion for argument 1 from 'std::vector<int>' to 'std::ios base& (*) (std::ios base&)'
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:166:7: note: candidate: std::basic ostream
                                                                                                                                                                                                                                                                                                                                                                         = std::char traits<char>; std::basic ostream< CharT, Traits>:: ostream type = std::basic ostrea
                                                                                                                                                                    print-vector.cpp
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:166:7: note: no known conversion for an
/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:170:7: note: candidate: std::basic ostream:170:7: note: std::basic ostream:170:7: note: std::basic ostream:170:7: note: std::basic ostream:17
                                                                                                                                                                                                                                                                                                                                                                     r; Traits = std::char traits<char>; std::basic ostream< CharT, Traits>:: ostream type = std::bas
            operator<<(unsigned long __n)
                                                                                                                                                                    #include <iostream>
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:170:7: note: no known conversion for arg
 /usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/ostream:174:7: note: candidate: std::basic ostream
                                                                                                                                                                                                                                                                                                                                                                    std::char traits<char>; std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream<ch
                                                                                                                                                                    #include <vector>
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:174:7: note: no known conversion for arc
 In file included from /usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/ostream:638:0,
                            from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/iostream:39,
                            from cpp-error-message.cpp:1:
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/bits/ostream.tcc:91:5: note: candidate: std::basi
                                                                                                                                                                                                                                                                                                                                                                    i::char traits<char>]
        basic_ostream<_CharT, _Traits>::
                                                                                                                                                                    int main()
 /usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/bits/ostream.tcc:91:5: note: no known conversion
 In file included from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/iostream:39:0,
                            from cpp-error-message.cpp:1:
                                                                                                                                                                                std::vector < int > A = \{2, 3\};
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:181:7: note: candidate: std::basic ostream
                                                                                                                                                                                                                                                                                                                                                                    har; Traits = std::char traits<char>; std::basic ostream< CharT, Traits>:: ostream type = std::ba
            operator << (unsigned short n)
 /usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/ostream:181:7: note: no known conversion for arg
                                                                                                                                                                                std::cout << A << std::endl;</pre>
 In file included from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:638:0,
                            from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/iostream:39,
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/bits/ostream.tcc:105:5: note: candidate: std::basi
                                                                                                                                                                                                                                                                                                                                                                    ar traits<char>]
                                                                                                                                                                                return 0;
        basic_ostream<_CharT, _Traits>::
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/bits/ostream.tcc:105:5: note: no known conversion
In file included from /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/iostream:39:0,
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:192:7: note: candidate: std::basic ostrea
                                                                                                                                                                                                                                                                                                                                                                                                                                                ream< CharT, Traits>:: ostream type = std::basic os
            operator << (unsigned int n)
                                                                                                                                                                                                                                                             C++ vectors cannot be printed directly -
 /usr/lib/gcc/x86 64-pc-cvgwin/5.4.0/include/c++/ostream:192:7: note: no known conversion for argument 1 from 'std::vector<int>' to 'unsigned
/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:201:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type& std::basic
                                                                                                                                                                                                                                                                                                                                                                                                                                               tream< CharT, Traits>:: ostream type = std::basic
                                                                                                                                                                                                                                                mistake results in +200 lines of error messages
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:201:7; note: no known conversion for argument 1 from 'std::vector<int>' to 'long long
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:205:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type& std::basic
            operator<<(unsigned long long n)
/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream<220:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type std::basic ostream type std::bas
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:220:7: note: no known conversion for argument 1 from 'std::vector<int>' to 'double'
/usr/lib/qcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream<224:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream<
 /usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:224:7: note: no known conversion for argument 1 from 'std::vector<int>' to 'float'
```

/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:232:7: note: candidate: std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream< CharT, Traits>:: ostream type = std::basic ostream

/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:245:7: note: candidate: std::basic ostream type = std::basic ostre

\$ g++ -std=c++11 print-vector.cpp

cpp-error-message.cpp: In function 'int main()':

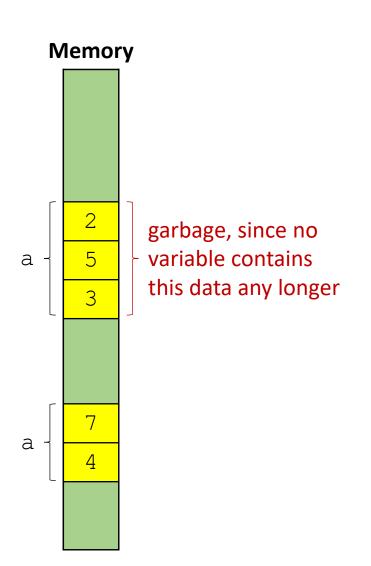
operator << (long double f)

/usr/lib/gcc/x86 64-pc-cygwin/5.4.0/include/c++/ostream:232:7: note: no known conversion for argument 1 from 'std::vector<int>' to 'long double'

#### Why Python?

- Short concise code
- Index out of range exceptions
- Elegant for-each loop
- Python hopefully better error messages than C++

#### Python and garbage collection





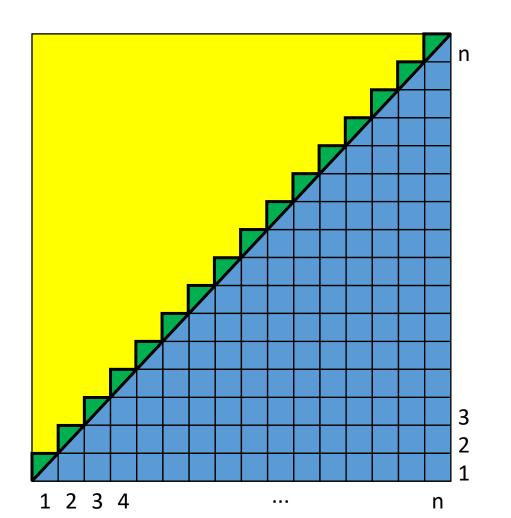
- Python and e.g. Java, C# and JavaScript have a garbage collector to automatically recycle garbage
- C and C++ garbage collection must be done explicitly by the program; forgetting to free memory again results in memory leaks – which can be really hard to find. Have fun debugging!

#### Why Python?

- Short concise code
- Index out of range exceptions
- Elegant for-each loop
- Python hopefully better error messages than C++
- Garbage collection is done automatically

## Python performance vs C, C++ and Java

Compute sum  $1 + 2 + 3 + \dots + n = n^2/2 + n/2$ 



#### $1 + 2 + \cdots + n$

```
add.py
import sys

n = int(sys.argv[1])
sum = 0
for i in range(1, n + 1):
    sum += i
print("Sum =", sum)
```

#### add.c

```
#include <stdio.h>
#include <stdlib.h>

int main(int argc, char *argv[]) {
  int n = atoi(argv[1]);
  int sum = 0;
  for (int i = 1; i <= n; i++)
     sum += i;
  printf("Sum = %d\n", sum);
}</pre>
```

#### add.cpp

```
#include <iostream>
#include <cstdlib>
using namespace std;

int main(int argc, char *argv[]) {
   int n = atoi(argv[1]);
   int sum = 0;
   for (int i = 1; i <= n; i++)
      sum += i;
   cout << "Sum = " << sum << endl;
}</pre>
```

#### add.java

## Timing results

| n               | C (gcc 9.2) | C++, int (g++ 9.2) | C++, long (g++ 9.2) | Java (12.0) | <b>CPython (3.8.1)</b> | PyPy (7.3.0) | Numba, int64 |
|-----------------|-------------|--------------------|---------------------|-------------|------------------------|--------------|--------------|
| 10 <sup>7</sup> | 0.001 sec*  | 0.001 sec*         | 0.003 sec           | 0.006 sec*  | 1.5 sec                | 0.27 sec     | 0.002 sec    |
| 10 <sup>9</sup> | 0.10 sec**  | 0.10 sec**         | 0.30 sec            | 0.40 sec**  | 145 sec                | 27 sec       | 0.2 sec      |

#### Wrong output (overflow)

- \* -2004260032 instead of 50000005000000
- \*\* -243309312 instead of 500000000500000000



- since C, C++, and Java only uses 32 bits to represent integers (and 64 bits for "long" integers)

Try Google: civilization gandhi overflow

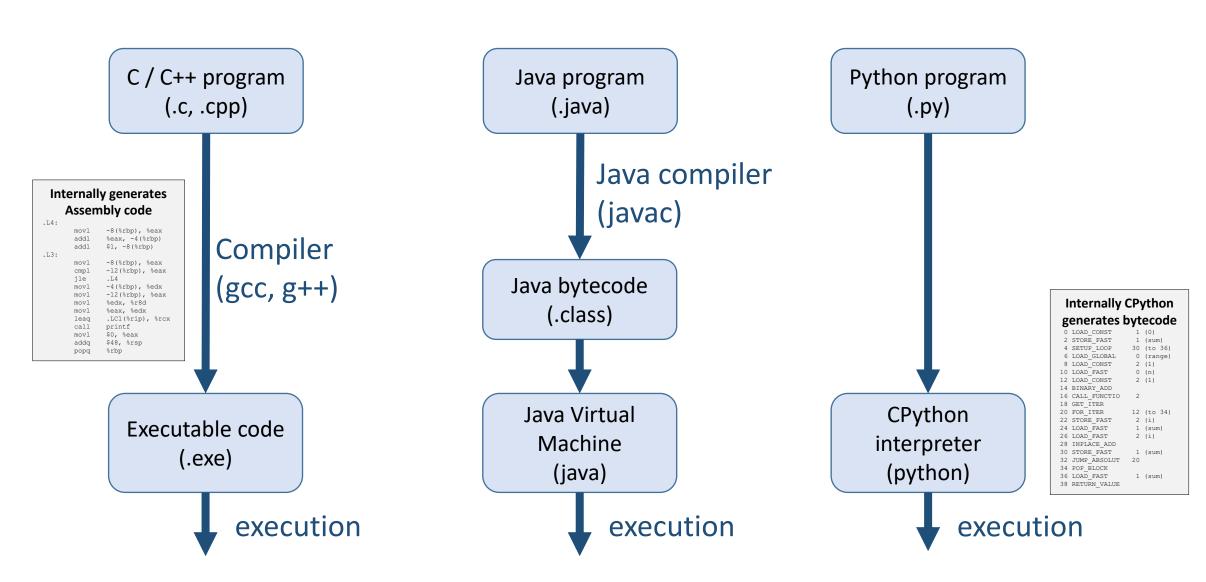
### Timing results

| n               | C (gcc 9.2) | C++, int (g++ 9.2 ) | C++, long (g++ 9.2 ) | Java (12.0) | Python (3.8.1) | РуРу (7.3.0) | Numba, int64 |
|-----------------|-------------|---------------------|----------------------|-------------|----------------|--------------|--------------|
| 10 <sup>7</sup> | 0.001 sec*  | 0.001 sec*          | 0.003 sec            | 0.006 sec*  | 1.5 sec        | 0.27 sec     | 0.002 sec    |
| 10 <sup>9</sup> | 0.10 sec**  | 0.10 sec**          | 0.30 sec             | 0.40 sec**  | 145 sec        | 27 sec       | 0.2 sec      |

Relative speed

- C, C++, Java need to care about integer overflows select integer representation carefully with sufficient number of bits (8, 16, 32, 64, 128)
- Python natively works with arbitrary long integers (as memory on your machine allows).
   Also possible in Java using the class java.math.BigInteger
- Python programs can (sometimes) run faster using PyPy
- Number crunching in Python should be delegated to specialized modules (e.g. Numpy,
   CPLEX, Numba) often written in C or C++ and requires selecting right integer representation

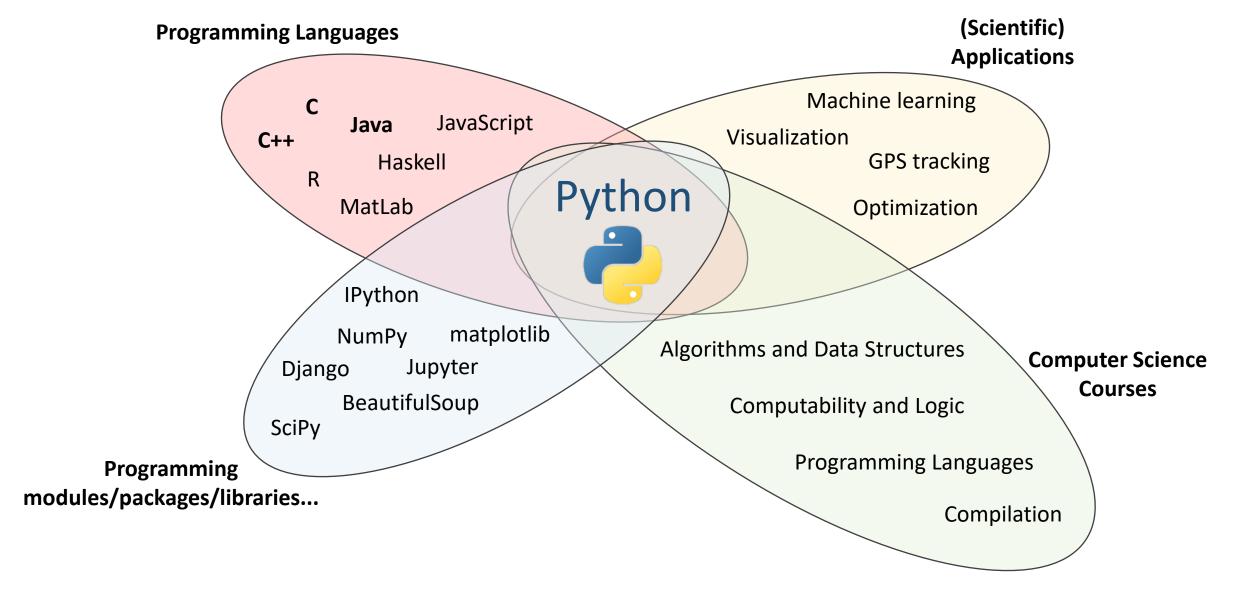
### Interpreter vs Compiler



### Why Python?

- Short concise code
- Index out of range exceptions
- Elegant for-each loop
- Python hopefully better error messages than C++
- Garbage collection is done automatically
- Exact integer arithmetic (no overflows)
- Can delegate number crunching to C, C++, ...

### This course



#### Course overview

# Basic programming Advanced / specific python Libraries & applications

| 1. Introduction to Python  | 10. Functions as objects           | 19. Linear programming              |
|----------------------------|------------------------------------|-------------------------------------|
| 2. Python basics / if      | 11. Object oriented programming    | 20. Generators, iterators, with     |
| 3. Basic operations        | 12. Class hierarchies              | 21. Modules and packages            |
| 4. Lists / while / for     | 13. Exceptions and files           | 22. Working with text               |
| 5. Tuples / comprehensions | 14. Doc, testing, debugging        | 23. Relational data                 |
| 6. Dictionaries and sets   | 15. Decorators                     | 24. Clustering                      |
| 7. Functions               | 16. Dynamic programming            | 25. Graphical user interfaces (GUI) |
| 8. Recursion               | 17. Visualization and optimization | 26. Java vs Python                  |
| 9. Recursion and Iteration | 18. Multi-dimensional data         | 27. Final lecture                   |

10 handins
1 final project (last 1 month)

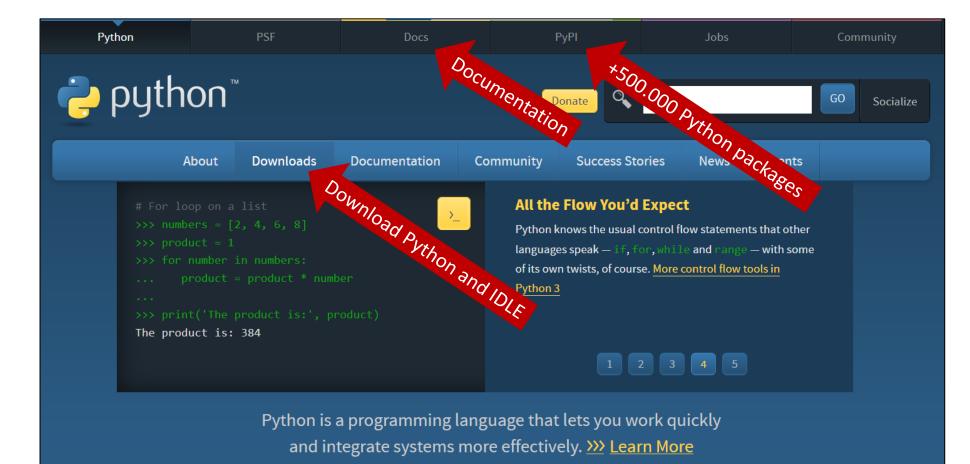
### History of Python development

- Python created by Guido van Rossum in 1989, first release 0.9.0 1991
- Python 2 

  Python 3 (clean up of Python 2 language)
  - Python 2 version 2.0 released 2000, final version 2.7 released mid-2010
  - Python 3 released 2008, current release 3.12.1
- Python 3 is not backward compatible, libraries incompatible

| Python 2                                | Python 3  |
|---|---|
| print 42                                | print(42)   |
| int = C long (32 bits)                  | int = arbitrary number of digits (= named "long" in Python 2)   |
| 7/3 → 2 returns "int"                   | 7/3 → 2.333 returns "float"                                     |
| range() returns list (memory intensive) | range() returns iterator (memory efficient; xrange in Python 2) |

# Python.org





Whether you're new to programming or an experienced developer, it's easy to learn and use Python.

Start with our Beginner's Guide



Python source code and installers are available for download for all versions!

Latest: Python 3.11.1



Documentation for Python's standard library, along with tutorials and guides, are available online.

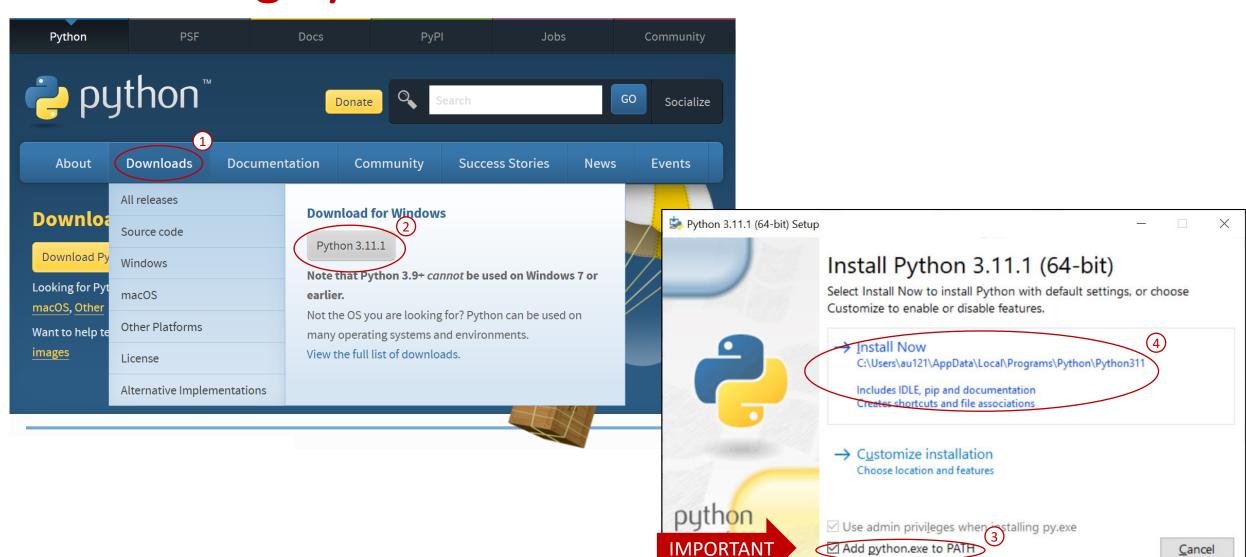
docs.python.org



Looking for work or have a Python related position that you're trying to hire for? Our **relaunched community-run job board** is the place to go.

jobs.python.org

# **Installing Python**



# Running the Python Interpreter from a terminal

- Open Command Prompt (Windows-key + cmd)
- Type "python" + return
- Start executing Python statements
- To exit shell: Ctrl-Z + return or exit() + return
- Note: Sometimes "python" is installed as "python3"

```
Command Prompt
                                                                                                                                  icrosoft Windows [Version 10.0.14393]
                   c) 2016 Microsoft Corporation. All rights reserved.
                    \Users\au121>
          Command Prompt - python
         Microsoft Windows [Version 10.0.14393]
         (c) 2016 Microsoft Corporation. All rights reserved.
          :\Users\au121>python
         Python 3.6.4 (v3.6.4:d48eceb, Dec 19 2017, 06:04:45) [MSC v.1900 32 bit (Intel)] on win32
              "help", "copyright", "credits" or "license" for more information.
Command Prompt - python
 crosoft Windows [Version 10.0.14393]
  2016 Microsoft Corporation. All rights reserved.
  hon 3.6.4 (v3.6.4:d48eceb, Dec 19 2017, 06:04:45) [MSC v.1900 32 bit (Intel)] on win32
   "help", "copyright", "credits" or "license" for more information.
  print(6*5+3*4)
```

# Installing IPython –

#### A more powerful interactive Python shell

- Open Command Prompt
- Execute:

pip install ipython

Start IPython

ipython

- pip = the Python package manager
- Note: Sometimes "pip" is installed as "pip3"

```
Command Prompt
      Microsoft Windows [Version 10.0.14393]
      (c) 2016 Microsoft Corporation. All rights reserved.
       C:\Users\au121>pip install ipython_
IPython: C:Users/au121
Microsoft Windows [Version 10.0.14393]
(c) 2016 Microsoft Corporation. All rights reserved.
C:\Users\au121>ipython
Python 3.6.4 (v3.6.4:d48eceb, Dec 19 2017, 06:04:45) [MSC v.1900 32 bit (Intel)]
Type 'copyright', 'credits' or 'license' for more information
IPython 6.2.1 -- An enhanced Interactive Python. Type '?' for help.
```

### Some other usefull packages

Try installing some more Python packages:

```
pip install numpy
pip install scipy
pip install matplotlib
pip install pylint
```

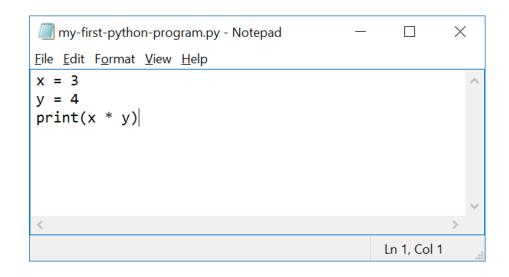
linear algebra support (N-dimensional arrays)

numerical integration and optimization

2D plotting library

Python source code analyzer enforcing a coding standard

### Creating a Python program the very basic way



- Open Notepad (or TextEdit on Mac)
  - write a simple Python program
  - save it
- Open a command prompt
  - go to folder (using cd)
  - run the program using

```
python cprogram name>.py
```

```
Command Prompt
Microsoft Windows [Version 10.0.14393]
(c) 2016 Microsoft Corporation. All rights reserved.
C:\Users\au121>cd Desktop
C:\Users\au121\Desktop>dir
 Volume in drive C is OSDisk
 Volume Serial Number is 3CDB-90D8
Directory of C:\Users\au121\Desktop
80-01-2018
                     <DIR>
                     <DIR>
                     <DIR>
                                    ipsa18
30-01-2018
                                 26 my-first-python-program.py
               1 File(s)
                                     26 bytes
               3 Dir(s) 420.462.858.240 bytes free
C:\Users\au121\Desktop>python my-first-python-program.py
C:\Users\au121\Desktop>_
```

## ... or open IDLE and run program with F5

```
enable
line numbers
under options
```

```
X
my-first-python-program.py - C:\Users\au121\Desktop\my-first-python-program.py (3.11.0)
<u>File Edit Format Run Options Window Help</u>
 x = 3
 print(x *v)
                                                                                             Ln: 4 Col: 0
IDLE Shell 3.11.0
                                                                                                  X
<u>File Edit Shell Debug Options Window Help</u>
    Python 3.11.0 (main, Oct 24 2022, 18:26:48) [MSC v.1933 64 bit (AMD64)] on win32
    Type "help", "copyright", "credits" or "license()" for more information.
>>>
    ====== RESTART: C:\Users\au121\Desktop\my-first-python-program.py ========
>>>
                                                                                             Ln: 6 Col: 0
```

- IDLE ships with Python from python.org
- Good beginner IDE (Integrated Development Environment)

### The Python Ecosystem

#### Interpreters/compiler

- CPython reference C implementation from python.org
- PyPy written in RPython (a subset of Python) faster than Cpython
- Jython written in Java and compiles to Java bytecode, runs on the JVM
- IronPython written in C#, compiles to Microsoft's Common Language Runtime (CLR) bytecode
- Cython project translating Python-ish code to C

#### Shells (IPython, IDLE, Jupyter)

#### Libraries/modules/packages

pypi.python.org/pypi (PyPI - the Python Package Index, +500.000 packages)

#### IDEs (Integrated development environment)

- IDLE comes with Python (docs.python.org/3/library/idle.html)
- Anaconda w. Spyder, IPython (www.anaconda.com/download)
- Canopy (enthought.com/product/canopy)
- Visual Studio Code (code.visualstudio.com)
- Python tools for Visual Studio (github.com/Microsoft/PTVS)
- PyCharm (www.jetbrains.com/pycharm/)
- Emacs (Python mode and ElPy mode)
- Notepad++

#### Python Style guide (PEP8)

pylint, pep8, flake8

#### Python online

• Google colab (colab.research.google.com), repl.it, sagemath.org, ...

Try to google "best ide python"



#### IDEs and Al assistants

- Some IDEs integrate Al assistants to support code suggestions, e.g. <u>GitHub Copilot in VS Code</u>
- Al assistants increase productivity if you understand their output



 Al assistants are not allowed at the exam

```
• binomial.py - Visual Studio Code  
          🕏 binomial.py 1 🔘
          C: > Users > au121 > Desktop > ♥ binomial.py > ♥ binomial
                 def binomial(n, k):
suggestion
   留
   Д
   (8)
   €$$
   ⊗1 ∆0
                   Ln 3, Col 20 Spaces: 4 UTF-8 CRLF ( Python 3.11.2 64-bit
```

Guido van Rossum, inventor of Python, on GitHub Copilot "I use it every day. It writes a lot of code for me... and usually it is slightly wrong but it still safes me typing."

Python and the Future of Programming, Guido van Rossum interviewed by Lex Fridman