Introduction to Programming with Scientific Applications

Gerth Stølting Brodal Department of Computer Science Aarhus University



Course evaluation

"The first lecture was intimidating and overwhelming"

Lecturer

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

Course description – kursuskatalog.au.dk/en/course/130939/

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, no AI 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%

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?

+750 listed on en.wikipedia.org/wiki/List_of_programming_languages

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	Wedn	esday	Thursday	Friday
8:15-9:00	TA meeting					
9:15-10:00	Study cafe		Study	/ cafe	MA1 (1Y)	
10:15-11:00	Locturo		Loct			
11:15-12:00	Lecture		Lecture			MA2 (1Y)
12:15-13:00						
13:15-14:00				DV		
14:15-15:00		MA3 (2Y)	MOL		Study cafe	Hold 2
15:15-16:00		FY	MØD			
16:15-17:00		Hold 1	IVIQ2			
17:15-18:00						

Week	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	ТØЗ	TØ3 / F8	ТØЗ	ТØЗ
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



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, 2nd Ed., page 8] "The reader should be forewarned that this book is by no means a comprehensive introduction to Python". 3rd 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, Als...



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 (2nd edition on page 50), Horstmann and Necaise do it on page 611

Some other books on Python



... numerous online introduction texts/courses/videos on Python

Two Python programs

A Python program

Python shell	
<pre>> x = 7 > print(x * x) 49</pre>	

- 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

Х

Question – What is the result of this program?



<u>•</u> 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]						
<pre>> print(a[2])</pre>						
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 3rd 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])	
> princ(a[i] · a[2])	

- a) 8
- **b)** 10

- **d)** 15
- e) Don't know



Why Python ?



TIOBE Index January 2025

Python #1 Since

November

Jan 2025	Jan 2024	Change	Program	ming Language	Ratings	2021
1	1		0	Python	23.28%	+9.32%
2	3	^	0	C++	10.29%	+0.33%
3	4	^	(i) (i)	Java	10.15%	+2.28%
4	2	~	C	С	8.86%	-2.59%
5	5		0	C#	4.45%	-2.71%
6	6		JS	JavaScript	4.20%	+1.43%
7	11	*	-60	Go	2.61%	+1.24%
8	9	^	SQL	SQL	2.41%	+0.95%
9	8	~	VB	Visual Basic	2.37%	+0.77%
10	12	*	F	Fortran	2.04%	+0.94%

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

TIOBE Programming Community Index

Source: www.tiobe.com



Most Popular Programming Languages 1958 – 2025 (YouTube)

"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 );
}
```

С

#include <stdio.h>

int main(int argc, char **argv) {
 printf("Hello World");
 return 0;

C++

}

}

#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 developed by Dennis Ritchie 1969-73)

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*



indexing.c	
<pre>#include <stdio.h></stdio.h></pre>	
<pre>int main() {</pre>	
int x = 1;	
int $A[2] = \{2, 3\}; // A[0]$	D] = 2, A[1] = 3
$printf("x = %d, A = \{ %d, $	%d}\n", x, A[0], A[1]);
A[3] = 42; // index A[3]	out of bounds
$printf("x = %d, A = {%d,$	%d}\n", x, A[0], A[1]);
return 0;	

Output

```
$ gcc indexing.c
$ ./a.exe
x = 1, A = {2, 3}
x = 42, A = {2, 3}
```

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

(C++ was developed by Bjarne Stroustrup 1985)

... and C++ index out of bounds



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

indexing.cpp



(Java was developed by James Gosling 1995)

... and Java index out of bounds exception

Memory



indexing.java class IndexingTest{ public static void main(String args[]) { int a[] = {20, 21, 22}; a[5] = 42; // index a[5] out of boundsOutput \$ 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

(Python first release by Guido van Rossum 1991)

... 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" (<u>www.whitehouse.gov</u>) National Security Agency 2022 | Cybersecurity Information Sheet: Software Memory Safety (<u>media.defense.gov</u>)

- C and C++ are flexible but memory unsafe programming languages
 - Unintended writes or reads 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

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++)</pre>
           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;</pre>
        // "auto" iterator - since C++11
        for (auto it = A.begin(); it != A.end(); ++it)
           std::cout << *it << std:: endl;</pre>
        // 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

prin	t-list.py
a =	[20, 23, 26]
for	e in a: print(e)
Outp	ut
\$ py 20	thon print-list.py

Why Python ?

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

<pre>\$ g++ -std=c++11 print-vector.cpp cpp=error=message.cpp: In function 'int main()': cpp=error=message.cpp:713: error: no match for 'operator<<' (operand types are 'std::ostream {aka std::cout << A << std::endl;</pre>	<pre>std::basic_ostream<char>}' and `std::vector<i:< pre=""></i:<></char></pre>	nt>')				
<pre>In file included from /usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/iostream:39:0,</pre>	<_CharT, _Traits>& std::operator<<(std::basic_	ostream<_CharT, _I	Fraits>&&, const _Tp&) [with _C	harT = char; _Traits = st	d::char_traits <char>; _Tp = std::vector<int>] <near match=""></near></int></char>	
<pre>/usr/lib/gcc/x86_64-pc-cygwin/5.4.0/include/c++/ostream:628:5: note: conversion of argument 1 wo cpp-error-message.cpp:7:16: error: cannot bind `std::ostream {aka std::basic_ostream<char>}' lvalu std::cout << A << std::endl;</char></pre>	uld be ill-formed: e to `std::basic_ostream <char>&&'</char>		• •			
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<pre>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::basic basic_ostream<_CharT,Traits>::</pre>					:::char_traits <char>]</char>	
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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!
- Automatic garbage collection increases memory safety

Why Python ?

- Short concise code
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- 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 + ••• + 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

```
class Add{
   public static void main(String args[]){
      int n = Integer.parseInt(args[0]);
      int sum = 0;
      for (int i = 1; i <= n; i++)
          sum += i;
      System.out.println("Sum = " + sum);
   }
</pre>
```

Timing results

Python

n	C (gcc 9.2)	C++, int (g++ 9.2)	C++, long (g++ 9.2)	Java (12.0)	CPython (3.8.1)	РуРу (7.3.0)	Numba, int64
107	0.001 sec*	0.001 sec*	0.003 sec	0.006 sec*	1.5 sec	0.27 sec	0.002 sec
10 ⁹	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 5000000050000000



Bit position	66666666665 98765432109	55555555555555555555555555555555555555
bin(10**9)		111011100110101010100000000
bin(500000050000 bin(-2004260032-	000) +2**32)	101101011110011000100010010010101101010000
bin(500000000500 bin(-243309312+2	000000) 2**32)	1101111000001011011010110011111000101111

Try Google: civilization gandhi overflow

Have fun

debugging!

Timing results

Python

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Relative speed

$C \approx C++ > Java >> Python$

- 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 \rightarrow 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 3.13.1
- 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)
$7/3 \rightarrow 2$ returns "int"	7/3 → 2.333 returns "float"
range() returns list (memory intensive)	range() returns iterator (memory efficient; xrange in Python 2)

100th episode of Talk Python To Me: Python past, present, and future with Guido van Rossum

Python.org



Python is a programming language that lets you work quickly and integrate systems more effectively. <u>>>> Learn More</u>

🕛 Get Started

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

Start with our Beginner's Guide

🕹 Download

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

Latest: Python 3.11.1

🚺 Docs

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

docs.python.org

🚔 Jobs

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"



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"



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 optimization2D and 3D plotting libraryPython source code analyzer enforcing a coding standard

Creating a Python program the very basic way

my-first-python-program.py - Notepad	_		\times
<u>F</u> ile <u>E</u> dit F <u>o</u> rmat <u>V</u> iew <u>H</u> elp			
x = 3 y = 4 print(x * y)			~
			\sim
<			>
		Ln 1, Col 1	.:

- 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 <program name>.py



... or open IDLE and run program with F5

	🕞 my-first-python-program.py - C:\Users\au121\Desktop\my-first-python-program.py (3.11.0) —		\times
	<u>F</u> ile <u>E</u> dit F <u>o</u> rmat <u>R</u> un <u>O</u> ptions <u>W</u> indow <u>H</u> elp		
	1 x = 3		~
	$\begin{vmatrix} 2 \\ y \end{vmatrix} = 4$		
	al		
enable			\sim
line numbers		Ln: 4	Col: 0
under options			
	PIDLE Shell 3.11.0		\times
	<u>F</u> ile <u>E</u> dit She <u>l</u> l <u>D</u> ebug <u>O</u> ptions <u>W</u> indow <u>H</u> elp		
	Python 3.11.0 (main, Oct 24 2022, 18:26:48) [MSC v.1933 64 bit (AMD64)]	on wir	n32 🔺
	Type "help", "copyright", "credits" or "license()" for more information	ı.	
	>>>		
	12		
			\sim
		Ln: 6	Col: 0

IDLE ships with Python from python.org

under

Good beginner IDE (Integrated Development Environment)

The Python Ecosystem

Interpreters/compiler

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- 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, ...



"Visual Studio Code is used by more than twice as many developers than its nearest alternative", <u>Stack overflow survey 2024</u>

Try to google "best ide python"



IDEs and AI assistants

- Some IDEs integrate AI assistants to support code suggestions, e.g. <u>GitHub Copilot</u> in <u>VS Code</u>
- Al assistants increase productivity if you understand their output
- Interacting with an AI assistant can be a great programming tutor
- Al assistants are not allowed at the exam



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