

Scientific programming in mathematics

Prof. Dirk Praetorius

Priv.-Doz. Giovanni Di Fratta



Institute of Analysis
and Scientific Computing

General information

- ▶ Rights & Duties
- ▶ Grading
- ▶ Course material
- ▶ Schedule

Homepages

- ▶ **TISS homepage** (login required)
 - <https://tiss.tuwien.ac.at> + search for lecture
(courseNr=101776, semester=2021S)
 - Registration
 - Lecture forum

- ▶ **TUWEL homepage** (login required)
 - <https://tuwel.tuwien.ac.at/course/view.php?id=35497>
 - Rights & Duties
 - Grading
 - Schedule & Course material
 - Weekly assignments (Download & Handing-in)

Rights & Duties

► Structure of the lecture

- Reading course
- Exercise sessions
 - * Friday, 10:15–11:45
 - * **Mandatory** attendance
 - * Start → **March 12, 2021**

► Grading

- 50% → Performance in final test
 - * **at the end of June**
- 50% → Performance in exercise sessions
 - * Number of solved exercises
 - * Active participation

► Help for students

- via Email
- Lecture forum on TISS
 - * 24/7

Exercise sessions

▶ Fridays, 10:15-11:45, via ZOOM

▶ 12 sessions

- 1: March 12, 2021
- 2: March 19, 2021
- 3: March 26, 2021

Easter Break: Monday, 29 March 2021 to Saturday, 10 April 2021

- 4: April 16, 2021
- 5: April 23, 2021
- 6: April 30, 2021
- 7: May 7, 2021

Rectors Day/dies academicus (no classes): Friday, 14 May 2021

- 8: May 21, 2021
- 9: May 28, 2021
- 10: June 4, 2021
- 11: June 11, 2021
- 12: June 18, 2021

▶ **Mandatory attendance**

▶ `lva.student.tuwien.ac.at`

Course material

- ▶ Slides (formally nothing else is necessary)

Books (optional!)

- ▶ Brian W. Kernighan, Dennis M. Ritchie
The C programming language
- ▶ Bradley L. Jones, Peter Aitken, Dean Miller
C programming in one hour a day
- ▶ Klaus Schmaranz
Softwareentwicklung in C (in German!)
- ▶ Bjarne Stroustrup
*Programming – Principles and practice using C++
The C++ programming language*
- ▶ Siddhartha Rao
C++ in one hour a day
- ▶ Klaus Schmaranz
Softwareentwicklung in C++ (in German!)

The first program in C

- ▶ Program & Algorithm
 - ▶ Source code & Executable
 - ▶ Compiler & Interpreter
 - ▶ Syntax error & Runtime error
 - ▶ How to write a program in C?
-
- ▶ `main`
 - ▶ `printf` (print text to the screen)
 - ▶ `#include <stdio.h>`

Program

- ▶ A **computer program** (or, briefly, a **program**) is a collection of statements, written in a programming language, that performs a specific task when executed by a computer
 - Statement = **declaration** or **instruction**
 - * **Declaration** = e.g., definition of variables
 - * **Instruction** = 'do something'
 - Example: Search for a phonebook entry
 - Example: Compute the value of a integral

Algorithm

- ▶ An **algorithm** is a finite sequence of unambiguous operations which specify how to solve a problem (or a class of problems)
 - **Example:** Compute the solution of a linear system of equations via Gaussian elimination
 - **Example:** Compute the zero of a quadratic polynomial using the quadratic formula
- ▶ There exist many algorithms to solve a problem
 - Not all algorithms are 'good'
 - * What does 'good' mean? (see later)

Source code

- ▶ Text of a computer program written in a programming language
- ▶ It is processed **step-by-step** while executing or compiling
- ▶ In the easiest situation: **sequentially**
 - Line-by-line
 - From the top to the bottom

Programming language

- ▶ Programming languages can be classified into **interpreted** and **compiled** languages
- ▶ The **interpreter** executes source code line-by-line during the 'translation'
 - i.e., translate and execute at the same time
 - e.g., Matlab, Java, PHP
- ▶ The **compiler** 'translates' the source code and produces a stand-alone program written in a machine-dependent object code (executable)
 - i.e., first translate, then execute
 - e.g., C, C++, Fortran
- ▶ Alternative classification:
 - **Imperative languages**, e.g., Matlab, C, Fortran
 - **Object-oriented languages**, e.g., C++, Java
 - **Functional languages**, e.g., Lisp

Be careful!

- ▶ C is a compiled programming language
- ▶ Compiled code is *system-dependent*,
 - In principle the code can run only on the system on which it has been compiled
- ▶ Source code is *system-independent*,
 - The code can be compiled also on other systems
- ▶ C compiler are not all equal
 - Before any exercise session, compile and test any program with the C compiler **gcc** on **lva.student.tuwien.ac.at**
 - Non-compiling code = bad impression and possibly also negative evaluation. . .

How to write a program in C?

- ▶ Start your favorite text editor
e.g., `nano`, `emacs`, `vim`, `gedit`, `atom`, ...
- ▶ Open a (new) file `name.c`
 - The filename extension `.c` is typical for programs in C
- ▶ Write the *source code* (= program)
- ▶ Don't forget to save the file
- ▶ Compile the code, e.g., open a shell and type `gcc name.c`
- ▶ If there are no errors, one gets the *executable* `a.out` (`a.exe` under Windows)
- ▶ This can be executed with `a.out` or `./a.out`
- ▶ Compile with `gcc name.c -o output` creates the executable `output` instead of `a.out`

The first program in C

```
1 #include <stdio.h>
2
3 main() {
4     printf("Hello World!\n");
5 }
```

- ▶ Line numbers do *not* belong to the code (included for didactic purposes)
- ▶ Every program in C has line 3 and line 5
- ▶ The execution of a program in C starts *always* from `main()`, independently of where `main()` is located in the code
- ▶ In C, curly brackets `{...}` contain so-called *blocks*
- ▶ The main program `main()` always constitutes a block
- ▶ Statements end with a *semicolon*; see line 4
- ▶ `printf` prints text to the screen (*in quotes*),
 - `\n` determines a new line
- ▶ Quotes *must* be in the same line
- ▶ Line 1: Inclusion of the C standard library for input-output (more info later)

main() vs. int main()

```
1 #include <stdio.h>
2
3 main() {
4     printf("Hello World!\n");
5 }
```

- ▶ The C programming language has evolved over the years
- ▶ `main()` { in line 3 is C89 standard
- ▶ C99 and C++ require `int main()` {

```
1 #include <stdio.h>
2
3 int main() {
4     printf("Hello World!\n");
5     return 0;
6 }
```

- ▶ Meaning:
 - `main()` communicates with the operating system
 - `main()` returns an error code via `return`
 - Return value zero = no error occurred
- ▶ In this case `return 0;` meaningful
 - More details later; see functions
- ▶ Consequence:
 - If the compiler does not accept the previous code (or gives annoying warnings), use this one!

Syntax error

- ▶ **Syntax** = Dictionary & Grammar of a language
- ▶ **Syntax error** = Wrong expression or wrong use
 - Detected by the compiler, which returns an error code

```
1 main() {  
2     printf("Hello World!\n");  
3 }
```

- ▶ Warning, inclusion of `stdio.h` missing
`wrongworld1.c:2: warning: incompatible implicit declaration of built-in function printf`
- ▶ C++ compiler gives an error due to `int main() {`
`wrongworld1.c:1: error: C++ requires a type specifier for all declarations`

```
1 #include <stdio.h>  
2  
3 main() {  
4     printf("Hello World!\n")  
5 }
```

- ▶ Error code, semicolon at the end of line 4 missing
`wrongworld2.c:5: error: syntax error before } token`

Runtime error

- ▶ Error occurring when the program is executed
 - Usually more difficult to detect
 - Should be avoided with careful programming

Variables

- ▶ What is a variable?
 - ▶ Declaration & Initialization
 - ▶ Data types int and double
 - ▶ Assignment operator =
 - ▶ Arithmetic operations + - * / %
 - ▶ Type casting
-
- ▶ int, double
 - ▶ printf (print value of a variable to the screen)
 - ▶ scanf (read value of a variable from the keyboard)

Variable

- ▶ **Variable** = symbolic name (**identifier**) of a storage location (**memory address**) containing some quantity of information (**value**)

Variable names (identifiers)

- ▶ Made of letters, digits and underscore `_`
 - Maximum length = 31
 - The first character cannot be a digit
- ▶ Variable names are case-sensitive
 - i.e. `Var`, `var`, `VAR` are three different variables
- ▶ **Convention:** `lowercase_with_underscores`

Data types

- ▶ The **data type** of a variable must be declared before using it
- ▶ Elementary data types:
 - **Floating-point numbers** for values in \mathbb{Q} , \mathbb{R} , e.g., `double`
 - **Integer** for values in \mathbb{N} , \mathbb{Z} , e.g., `int`
 - Characters (letters), e.g., `char`
- ▶ `int x;` declares a variable `x` of type `int`

Declaration

- ▶ **Declaration** = Creation of a variable
 - Assignment of a symbolic name to a storage location and specification of the data type
 - **int x;** declares a variable **x** of type **int**
 - **double var;** declares **var** of type **double**

Initialization

- ▶ Declaring a variable only assigns a storage location to it
- ▶ If no value is explicitly assigned, the value will be random
- ▶ Right after the declaration, a new value should be assigned, i.e., **initialization**
 - **int x;** (declaration)
 - **x = 0;** (initialization)
- ▶ Declaration & Initialization simultaneously
 - **int x = 0;**

A first example with int

```
1 #include <stdio.h>
2
3 main() {
4     int x = 0;
5
6     printf("Input: x=");
7     scanf("%d",&x);
8     printf("Output: x=%d\n",x);
9 }
```

- ▶ Inclusion of input-output functions (line 1)
 - **printf** prints text (e.g., the value of a variable) to the screen
 - **scanf** reads the value of a variable from the keyboard

- ▶ Percent sign % in lines 7–8 introduces a placeholder

data type	placeholder printf	placeholder scanf
int	%d	%d
double	%f	%lf

- ▶ Note the symbol & for **scanf** in line 7
 - **scanf("%d",&x)**
 - But: **printf("%d",x)**
- ▶ Forgetting & introduces a runtime error
 - The compiler does not report the error (no syntax error!)

The same example with double

```
1 #include <stdio.h>
2
3 main() {
4     double x = 0;
5
6     printf("Input: x=");
7     scanf("%lf",&x);
8     printf("Output: x=%f\n",x);
9 }
```

- ▶ Note the placeholders in lines 7–8
 - `scanf("%lf",&x)`
 - but: `printf("%f",x)`
- ▶ Use of `%f` in line 7 \Rightarrow Wrong reading!
 - Probably a runtime error!

Assignment operator

```
1 #include <stdio.h>
2
3 main() {
4     int x = 1;
5     int y = 2;
6
7     int tmp = 0;
8
9     printf("a) x=%d, y=%d, tmp=%d\n",x,y,tmp);
10
11     tmp = x;
12     x = y;
13     y = tmp;
14
15     printf("b) x=%d, y=%d, tmp=%d\n",x,y,tmp);
16 }
```

- ▶ The symbol **=** is the **assignment operator**
 - Assignment always from the left to the right
- ▶ **x = 1;** assigns the value **1** on the right-hand side to the variable **x** on the left-hand side
- ▶ **x = y;** assigns the value of the variable **y** to the variable **x**
 - In particular, x and y have the same value afterwards
 - Swapping the value of two variables usually requires an auxiliary variable
- ▶ Output:
 - a) x=1, y=2, tmp=0
 - b) x=2, y=1, tmp=1

Arithmetic operators

- ▶ The action of an operator can depend on the data type!
- ▶ Operators for integers:
 - $a=b$, $-a$ (sign)
 - $a+b$, $a-b$, $a*b$, a/b (division without remainder)
 $a\%b$ (modulus operator)
- ▶ Operators for floating point numbers:
 - $a=b$, $-a$ (sign)
 - $a+b$, $a-b$, $a*b$, a/b ('standard' division)
- ▶ Attention: $2/3$ is zero (division without remainder)
- ▶ Some notation for floating point numbers:
 - Minus sign $-$, if negative
 - Predecimal positions
 - Decimal separator (**point**)
 - Decimal positions
 - **e** or **E** with *integer* exponent
(10th power!), e.g., $2e2 = 2E2 = 2 \cdot 10^2 = 200$
- ▶ Hence: $2./3.$ is floating point division $\approx 0.\overline{6}$

Type casting

- ▶ Operators can work also with variables with different type
- ▶ Before execution the variables are converted to the same data type (**type casting**)

```
1 #include <stdio.h>
2
3 main() {
4     int x = 1;
5     double y = 2.5;
6
7     int sum_int = x+y;
8     double sum_dbl = x+y;
9
10    printf("sum_int = %d\n",sum_int);
11    printf("sum_dbl = %f\n",sum_dbl);
12 }
```

- ▶ Which data type has **x+y** in lines 7–8?
 - The ‘strongest’ data type, i.e., **double**
 - Type casting of the value of **x** to **double**
- ▶ Line 7: Type casting, from **double** to **int**
 - Truncation, no rounding!
- ▶ Output:
 sum_int = 3
 sum_dbl = 3.500000

Implicit type casting

```
1 #include <stdio.h>
2
3 main() {
4     double dbl1 = 2 / 3;
5     double dbl2 = 2 / 3.;
6     double dbl3 = 1E2;
7     int int1 = 2;
8     int int2 = 3;
9
10    printf("a) %f\n",dbl1);
11    printf("b) %f\n",dbl2);
12
13    printf("c) %f\n",dbl3 * int1 / int2);
14    printf("d) %f\n",dbl3 * (int1 / int2) );
15 }
```

► Output:

- a) 0.000000
- b) 0.666667
- c) 66.666667
- d) 0.000000

► Why the result 0 in a) and d) ?

- 2, 3 are **int** \Rightarrow **2/3** is division without remainder

► If an arithmetic operator is applied to variables of different type, type casting to the 'strongest' type

- See lines 5, 13, and 14
- 2 is **int**, 3. is **double** \Rightarrow **2/3.** is **double**

Explicit type casting

```
1 #include <stdio.h>
2
3 main() {
4     int a = 2;
5     int b = 3;
6     double dbl1 = a / b;
7     double dbl2 = (double) (a / b);
8     double dbl3 = (double) a / b;
9     double dbl4 = a / (double) b;
10
11     printf("a) %f\n",dbl1);
12     printf("b) %f\n",dbl2);
13     printf("c) %f\n",dbl3);
14     printf("d) %f\n",dbl4);
15 }
```

- ▶ It is possible to tell the compiler how to interpret a variable
 - Precede the operation with the desired data type (in brackets)
- ▶ Output:
 - a) 0.000000
 - b) 0.000000
 - c) 0.666667
 - d) 0.666667
- ▶ In lines 7–9: explicit type casting (all from **int** to **double**)
- ▶ In lines 8–9: implicit type casting

Error sources in type casting

```
1 #include <stdio.h>
2
3 main() {
4     int a = 2;
5     int b = 3;
6     double dbl = (double) a / b;
7
8     int i = dbl;
9
10    printf("a) %f\n",dbl);
11    printf("b) %f\n",dbl*b);
12    printf("c) %d\n",i);
13    printf("d) %d\n",i*b);
14 }
```

► Output:

- a) 0.666667
- b) 2.000000
- c) 0
- d) 0

► Implicit type casting should be avoided!

- i.e., use explicit type casting

► Save intermediate results of computations in the right data type!

Simple conditional statements

- ▶ Logical operators == != > >= < <=
 - ▶ Logical connectives ! && ||
 - ▶ True/false for statements
 - ▶ Conditional statements
-
- ▶ if
 - ▶ if - else

Logical operators

- ▶ Let a, b two variables (possibly of different type)
 - Comparison (e.g., `a < b`) returns `1` if true, or returns `0` if false

- ▶ Overview of comparison operators:

<code>==</code>	equality (\neq assignment operator)
<code>!=</code>	inequality
<code>></code>	strictly larger
<code>>=</code>	larger than or equal to
<code><</code>	strictly smaller
<code><=</code>	smaller than or equal to

- ▶ Advice: Put comparisons in brackets!
 - Not always necessary, but sometimes helpful!

- ▶ Logical connectives:

<code>!</code>	not
<code>&&</code>	and
<code> </code>	or

Logical concatenation

```
1 #include <stdio.h>
2
3 main() {
4     int result = 0;
5
6     int a = 3;
7     int b = 2;
8     int c = 1;
9
10    result = (a > b > c);
11    printf("a) result=%d\n",result);
12
13    result = (a > b) && (b > c);
14    printf("b) result=%d\n",result);
15 }
```

► Output:

- a) result=0
- b) result=1

► Why do line 10 return false and line 13 true?

- Evaluation from the left to the right:
 - * **a > b** is true, returns value **1**
 - * **1 > c** is false, returns value **0**
 - * Altogether **a > b > c** returns **0** (false)!
- Statement in line 10 is not properly formulated!

if-else

- ▶ Simple conditional statement: *if - then - else*
- ▶ *if* (condition) statementA *else* statementB
- ▶ After *if* there is the condition, *always in brackets*
- ▶ After the condition, *no semicolon*
- ▶ The condition is *false*, if it is 0 or if its evaluation is 0, otherwise it is *true*
 - Condition true \Rightarrow statementA is executed
 - Condition false \Rightarrow statementB is executed
- ▶ The statement consists of
 - either one line
 - or more lines in curly brackets { ... } (block)
- ▶ The *else*-part is optional
 - i.e., *else statementB* can be omitted

Example for if

```
1 #include <stdio.h>
2
3 main() {
4     int x = 0;
5
6     printf("Input x=");
7     scanf("%d",&x);
8
9     if (x < 0)
10         printf("x=%d is negative\n",x);
11
12     if (x > 0) {
13         printf("x=%d is positive\n",x);
14     }
15 }
```

- ▶ Use proper indentation (**it facilitates readability!**)
- ▶ **Attention:** non-use of blocks **{...}** is sometimes source of mistakes
- ▶ One could continue with **else** in line 11

Example for if-else

```
1 #include <stdio.h>
2
3 main() {
4     int var1 = -5;
5     double var2 = 1e-32;
6     int var3 = 5;
7
8     if (var1 >= 0) {
9         printf("var1 >= 0\n");
10    }
11    else {
12        printf("var1 < 0\n");
13    }
14
15    if (var2) {
16        printf("var2 != 0, i.e., cond. is true\n");
17    }
18    else {
19        printf("var2 == 0, i.e., cond. is false\n");
20    }
21
22    if ( (var1 < var2) && (var2 < var3) ) {
23        printf("var2 lies between the others\n");
24    }
25 }
```

- ▶ A condition is true if the value $\neq 0$
 - e.g., line 15, more explicit: `if (var2 != 0)`
- ▶ Output:
 - var1 < 0
 - var2 != 0, i.e., cond. is true
 - var2 lies between the others

Even or odd?

```
1 #include <stdio.h>
2
3 main() {
4     int x = 0;
5
6     printf("Input x=");
7     scanf("%d",&x);
8
9     if (x > 0) {
10         if (x%2 != 0) {
11             printf("x=%d is odd\n",x);
12         }
13         else {
14             printf("x=%d is even\n",x);
15         }
16     }
17     else {
18         printf("Error: Input has to be positive!\n");
19     }
20 }
```

- ▶ The program checks if a given number x is odd or even
- ▶ Conditional statements can be nested:
 - Indentation makes the code more clear
 - * Formally not needed, **but fundamental!**
 - Dependencies are emphasized

Sorting two numbers in ascending order

```
1 #include <stdio.h>
2
3 main() {
4     double x1 = 0;
5     double x2 = 0;
6     double tmp = 0;
7
8     printf("Unsorted input:\n");
9     printf(" x1=");
10    scanf("%lf",&x1);
11    printf(" x2=");
12    scanf("%lf",&x2);
13
14    if (x1 > x2) {
15        tmp = x1;
16        x1 = x2;
17        x2 = tmp;
18    }
19
20    printf("Output sorted in ascending order:\n");
21    printf(" x1=%f\n",x1);
22    printf(" x2=%f\n",x2);
23 }
```

- ▶ Input of two numbers $x_1, x_2 \in \mathbb{R}$ (possibly unsorted)
- ▶ Numbers are sorted in ascending order
 - i.e., they are swapped if needed
- ▶ Sorted numbers are printed to the screen

Inside or outside?

```
1 #include <stdio.h>
2
3 main() {
4     double r = 0;
5     double x1 = 0;
6     double x2 = 0;
7     double z1 = 0;
8     double z2 = 0;
9     double dist2 = 0;
10
11     printf("Radius of the circle r=");
12     scanf("%lf",&r);
13     printf("Center of the circle x = (x1,x2)\n");
14     printf(" x1=");
15     scanf("%lf",&x1);
16     printf(" x2=");
17     scanf("%lf",&x2);
18     printf("Point in the plane z = (z1,z2)\n");
19     printf(" z1=");
20     scanf("%lf",&z1);
21     printf(" z2=");
22     scanf("%lf",&z2);
23
24     dist2 = (x1-z1)*(x1-z1) + (x2-z2)*(x2-z2);
25     if ( dist2 < r*r ) {
26         printf("z lies inside the circle\n");
27     }
28     else {
29         if ( dist2 > r*r ) {
30             printf("z lies outside of the circle\n");
31         }
32         else {
33             printf("z lies on the boundary of the circle\n");
34         }
35     }
36 }
```

Equality vs. Assignment

- ▶ Recall: `if (a==b)` vs. `if (a=b)`
 - Both are syntactically correct!
 - `if (a==b)` checks the validity of the equality
 - * This is usually what one desires
 - But: `if (a=b)`
 - * The value of `b` is assigned to `a`
 - * Condition is true if the value of `b` is $\neq 0$
 - * It is bad programming style!
 - * Some compilers give a warning

Blocks

- ▶ Blocks {...}
- ▶ Declaration of variables
- ▶ Lifetime & Scope
- ▶ Local & global variables

Lifetime & scope

- ▶ **Lifetime** of a variable
 - = period in which a memory location is allocated to the variable
 - = period in which the variable exists
- ▶ **Scope** of a variable
 - = period in which a variable is accessible
 - = period in which the value of a variable can be read/changed
- ▶ Relation: **scope** \leq **lifetime**

Global & local variables

- ▶ **Global variables** = variables with global lifetime
 - Exist until the end of the program
 - Have possibly local scope
 - Are declared **outside** of main
- ▶ **Local variables** = variables with local lifetime
- ▶ **Convention:** Identify variables from names
 - Local variables: **lowercase_with_underscores**
 - Global variables: **underscore_also_at_the_end_**

Blocks

- ▶ Blocks are delimited by curly brackets { ... }
- ▶ Each block starts with the declaration of the additional variables needed
 - Variables *can* be declared only at the beginning of a block
- ▶ The variables declared inside a block are forgotten after the end of the block (= deleted)
 - i.e., end of their lifetime
 - They are local variables
- ▶ Nesting { ... { ... } ... }
 - Nesting is possible
 - Variables from an external block can be read or changed inside an internal block, but *not* the other way around
 - Changes remain valid, i.e., lifetime & scope are inherited only from the outside to the inside
 - If a variable *var* is declared both in an internal and in an external block, the 'external' *var* is hidden in the internal block and becomes accessible again (with the same value as before) at the end of the internal block
 - * i.e., the 'external' *var* is not in internal scope
 - * This is bad programming style!

Easy example

```
1 #include <stdio.h>
2
3 main() {
4     int x = 7;
5     printf("a) %d\n", x);
6     x = 9;
7     printf("b) %d\n", x);
8     {
9         int x = 17;
10        printf("c) %d\n", x);
11    }
12    printf("d) %d\n", x);
13 }
```

- ▶ Two different *local* variables x
 - Declaration + Initialization (lines 4 and 9)
 - Assignment (Line 6)
- ▶ Output:
 - a) 7
 - b) 9
 - c) 17
 - d) 9

More complicated example

```
1 #include <stdio.h>
2
3 int var0 = 5;
4
5 main() {
6     int var1 = 7;
7     int var2 = 9;
8
9     printf("a) %d, %d, %d\n", var0, var1, var2);
10    {
11        int var1 = 17;
12
13        printf("b) %d, %d, %d\n", var0, var1, var2);
14        var0 = 15;
15        var2 = 19;
16        printf("c) %d, %d, %d\n", var0, var1, var2);
17        {
18            int var0 = 25;
19            printf("d) %d, %d, %d\n", var0, var1, var2);
20        }
21    }
22    printf("e) %d, %d, %d\n", var0, var1, var2);
23 }
```

► Output:

- a) 5, 7, 9
- b) 5, 17, 9
- c) 15, 17, 19
- d) 25, 17, 19
- e) 15, 7, 19

- Two variables with name `var0` (line 3 and 18)
 - Name convention ignored on purpose
- Two variables with name `var1` (line 6 and 11)