

Introduction to Programming and Computational Physics

Presentation of the course

PD Dr. Akitaka Ariga

Bern, February 18th, 2020

Description of the course

The course is aimed to provide students with a basic knowledge of the **C programming** language and of its employment to address **physics-related questions** such as numerical integration, solving of differential equations and the Monte Carlo method for simulations of physical processes.

The students are not expected to have any background in programming.

Program

Part I: Introduction to Programming

Algorithms

Operating systems

Introduction to C language

- Variables and data types
- Arithmetical and logical operators
- Functions
- Selection
- Iteration
- Arrays
- Data I/O
- Pointers
- Dynamic memory allocation
- Strings
- Structures

Histograms and functions plotting

Program

Part II: Computational Physics

Root finding in one dimension

Numerical integration:

- Trapezoidal rule
- Simpson rule

Ordinary differential equation:

- Second order Runge-Kutta method

Monte Carlo method:

- Random numbers
- Monte Carlo integration
- Simulation of physical processes

Suggested books and learning material

Programming:

Lectures slides (+ any C online manual)

B. W. Kernighan, D. M. Ritchie
The C programming language

Computational physics:

W. H. Press, B. P. Flannery, S.A. Teukolsky, W. V. Wetterling
Numerical recipes in C, the art of scientific computing
<http://www.nrbook.com/a/bookcpdf.php>

J. E. Gentle
Random Number Generation and Monte Carlo Method

Where we are

Dr. Akitaka Ariga

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web repository

<http://www.physik.unibe.ch> → Studium → Bachelorprogramm

→ Introduction to Programming and Computational Physics (4)

Organization of the course

Frühjahrssemester 2020 17.02.2020 - 29.05.2020
Ferien ab Karfreitag 10.04.2020 - 19.04.2020

Theory: Tuesday 14-15 in **B6**, Exercises: Friday 10-12 in **A95**

Next Friday only: 1 hour theory (in B1) and 1 hour exercises

Exam

Proposed date: June 26th, 09:00-12:00 in A95 (To be confirmed)

Written exam, solving 2-3 exercises and handing in source code

Must use the terminals in A95. No laptop.

Open books

No internet access, no smartphones (Skype/Messenger/Whatsapp/ ...)

Evaluation criteria

The source codes should be *compiled* and *return* the correct results.

A program is well-written, so that it

- optimizes the usage of CPU time and memory
- can be easily understood and extended by the author (one year later...) or other programmers
- exploits the appropriate resources provided by the language

Access to terminal room

Rooms A95 is reserved for you on Friday 10-12

You can use them at any time (if not reserved)

Your campus accounts are valid to log in but you're not allowed to use the printers and you don't have a permanent home directory (→ **save your files to a USB drive**)

If you would like to have a permanent home and use the printers, please contact Mr. Peppo Brambilla. (brambi@iam.unibe.ch)

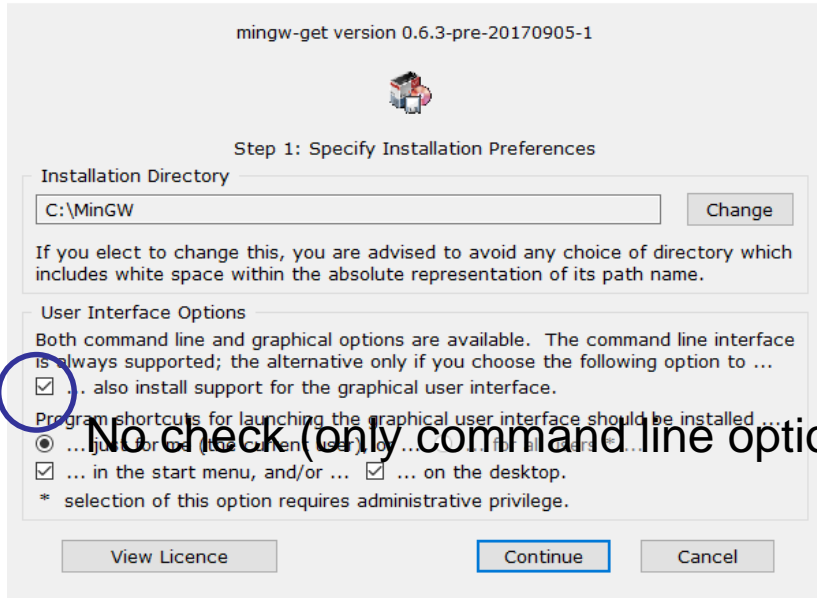
All you need is...

- A **computer** (A95 terminal room with Linux/Unix OS or your laptop)
- An **editor** (emacs or kate or jedit on Linux/UNIX OS, Notepad++ on Windows OS)
<http://notepad-plus-plus.org/>
- A **compiler** (We will use gcc, which is probably the most universal one)

GCC installation on Windows

- Download and install (mingw-get-setup.exe)
- <https://sourceforge.net/projects/mingw/files/Installer/>
- Open "Command prompt" (cmd.exe)
- type `c:\MinGW\bin\mingw-get.exe install gcc`

MinGW Installation Manager Setup Tool



Command Prompt

```
C:\Users\User>
C:\Users\User>
C:\Users\User> c:\MinGW\bin\mingw-get.exe install gcc
```

If gcc is correctly installed, you will have this message

```
C:\Users\User> \MinGW\bin\gcc.exe
gcc.exe: fatal error: no input files
compilation terminated.
```

No check (only command line option)

Setting environment variable on Windows 10

1. Open setting → search "Environment variables"
 2. System Properties → Advanced → Environment Variables
 3. Edit "Path" variable, click "new" and add "c:\MinGW\bin"
- NB: This operation is dangerous...be careful !!!
 - Then you can use gcc without writing full path

```
C:\Users\User\Documents>gcc  
gcc: fatal error: no input files  
compilation terminated.
```

Linux users: gcc is already installed !

Installation of gcc for Mac users

1. Open the App Store
2. Search for Xcode
3. Click on Install

It should be possible to install gcc without full Xcode installation → ask an expert

FAQ

Can I use my own laptop at the exam?

No, you can't

Should I hand in all my solutions to the exercises?

No, exercises are meant only to learn programming

Is the attendance to the lessons mandatory?

No, it isn't

I'm already a good C programmer, what would you suggest me?

You can skip the first lessons on programming, but you better attend the lessons on computational physics

I don't know C but I know other program languages, may I use them at the exam?

No, only C is allowed (C++ could be an exception)

Can I use another compiler?

It's not forbidden but you should ensure yourself that it has a *high compatibility* with gcc

UNIX/Linux commands

The general syntax of a UNIX command can be summarized as:

```
command [-option] [arguments]
```

Example: obtain the list of the files stored in the /home/pistillo directory

```
> ls -l -h /home/pistillo
```



prompt: it says to the user that the shell is ready to receive commands (sometimes used "\$")

Many other options available. Try the command:

```
> man ls
```

Files and directories

A *file system* is a method for storing and organizing computer files and the data they contain to make it easy to find and access them.

Directories are organized in a tree structure and the command to move inside is `cd`

```
> cd /home/pistillo/data/MC/numuCC/run20/
```

Basics commands for file manipulations are:

<code>cp</code>	(copy)
<code>mv</code>	(transfer or rename)
<code>rm</code>	(delete)
<code>less / more</code>	(show the content)
<code>mkdir</code>	(create a directory)
<code>rmdir</code>	(delete a directory)

Other commands

passwd	(change password)
whoami	(says who is the current user)
pwd	(current folder)
top	(running processes and CPU/memory usage)
ps	(running processes)
kill	(kill a process)
clear	(clean up the terminal)

Installation of gcc for Windows users

Download the software : “gcc installer” and execute it
(you need to have a network access to download packages during installation)

You could get this message from Windows Firewall:
gcc_installer.exe is not commonly downloaded and could harm your computer **Actions->More options->Run anyway**

Leave all the settings as they are...

Then try
you should get the answer

```
C:\MinGW\bin\gcc.exe  
gcc.exe: no input files
```

How to set an environment variable (Windows 7/10)

If you don't want to be forced to give the full path `C:\MinGW\bin\gcc.exe` you need to set an *environment variable*.

Open

Control Panel -> System and Security -> System -> Advanced system settings -> Environment variables

Among **System variables** select **Path** and then click **Edit**

Leave the content as it is and add at the end **;C:\MinGW\bin** and then click **OK**

Then you should be able to start gcc simply typing `gcc.exe`

NB: This operation is dangerous...be careful !!!