

Hands on Fortran

GOD is REAL (unless declared INTEGER)

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Todays Menu

Starter

About Myself

Main Course

Fortran

Dessert

GnuPlot



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What is Fortran ??

Programming language suited to numeric computation and scientific computing

Developer: John Backus and IBM

First appeared in 1957 65 years ago

Latest is Fortran 2018

Open source compilers

GNU Fortran Compiler (gfortran)

LLVM Flang

Commercial compilers

Intel / NVIDIA HPC SDK /IBM® XL Fortran

AMD Optimizing C/C++ Compiler (AOCC) compiler

Isnt it obsolete in todays world ???

NO NOT YET !!

Used in the following area

computational physics

numerical weather prediction

computational fluid dynamics

geophysics

computational chemistry

And the list goes on

Benchmark and rank the world's fastest supercomputers

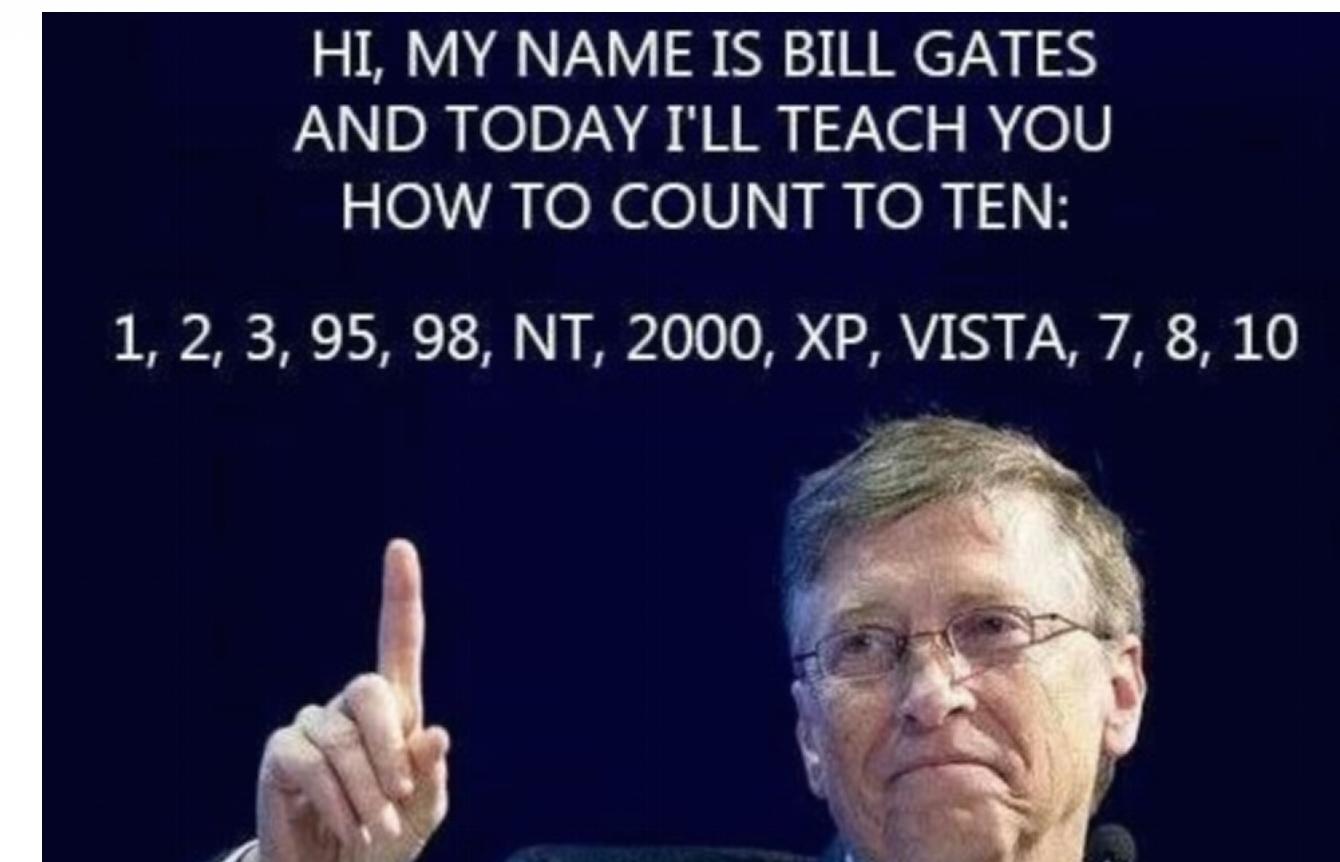
LINPACK Benchmarks

Eugene Loh (18 June 2010). "The Ideal HPC Programming Language". Queue. 8 (6).

HPL – A Portable Implementation of the High-Performance Linpack Benchmark for Distributed-Memory Computers". Retrieved 21 February 2015

The Operating Systems

Windows



The Operating Systems

Linux

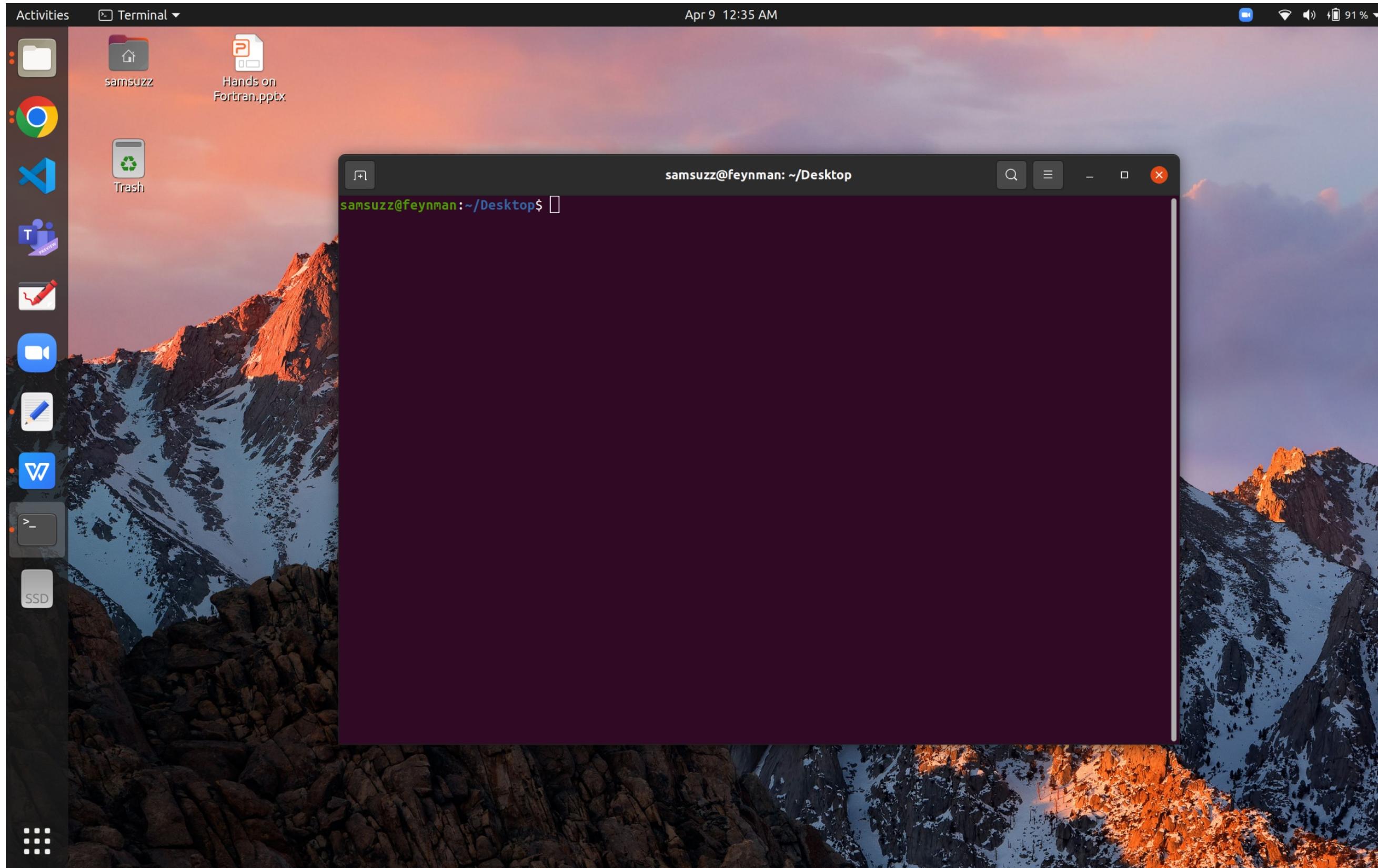


ubuntu



CentOS

The Terminal (Where the hell it is?????)



Text Editor

In Windows we have ==> MS WORD ,Notepad

In ubuntu/ cent os we have **gedit**

Step 1

- Create a folder with your name (msc_fortran)
- Keep all files in it
- Let us create a new file (gedit example1.f90)



Now type the following in the gedit (example1.f90)

```
!~~~~~
```

```
! Program to add two numbers
```

```
!~~~~~
```

```
program abc
```

```
implicit none
```

```
integer :: a,b,c
```

```
a = 2
```

```
b = 3
```

```
c = a + b
```

```
write(*,*) c
```

```
end program abc
```

- How to run a fortran code

The screenshot shows a Linux desktop environment with a dark theme. On the left is a vertical dock containing icons for various applications like a file manager, browser, VS Code, and terminal. The main window is a terminal titled "Terminal" with the command line "samsuzz@feynman: ~/Research/Basic_FORTRAN_codes". The terminal window displays the following session:

```
samsuzz@feynman:~/Research/Basic_FORTRAN_codes$ gfortran example1.f90
samsuzz@feynman:~/Research/Basic_FORTRAN_codes$ ./a.out
5
samsuzz@feynman:~/Research/Basic_FORTRAN_codes$ gfortran -o program_to_add example1.f90
samsuzz@feynman:~/Research/Basic_FORTRAN_codes$ ./program_to_add
5
samsuzz@feynman:~/Research/Basic_FORTRAN_codes$
```

All the codes for this session can be found in the following site

https://github.com/SoftMatterCode/Basic_FORTRAN_Codes/tree/main/Hands_on_FORTRAN

How to take user input (example2.f90)

!~~~~~

! Program to add two numbers by taking user input

!~~~~~

program abc

implicit none

integer :: a,b,c

write(*,*)"Please enter the value for a"

read(*,*)a

write(*,*)"Please enter the value for b"

read(*,*)b

c = a + b

write(*,*) "The sum of a & b is =", c

end program abc

How to save it in a file (example3.f90)

```
!~~~~~
```

```
! Program to add two numbers by taking user input and saving it in a file
```

```
!~~~~~
```

```
program abc
```

```
implicit none
```

```
real :: a,b,c
```

```
open(unit=1,file="addition.txt")
```

```
write(*,*)"Please enter the value for a"
```

```
read(*,*)a
```

```
write(*,*)"Please enter the value for b"
```

```
read(*,*)b
```

```
c = a + b
```

```
write(unit=1,fmt=*)"The sum of a & b is = ", c
```

```
end program abc
```

Format specifier in fortran

- For integer

rIw.m (w = total digits, m = minimum)

- For real

rFw.d (w = total digits, d = total digits to the right of decimal places)

- For Character

rAw

- For space use **nX**

Lets check with example in **example4.f90**



Functions and subroutines in fortran

- A function is a procedure that returns a single quantity.
should not modify its arguments.

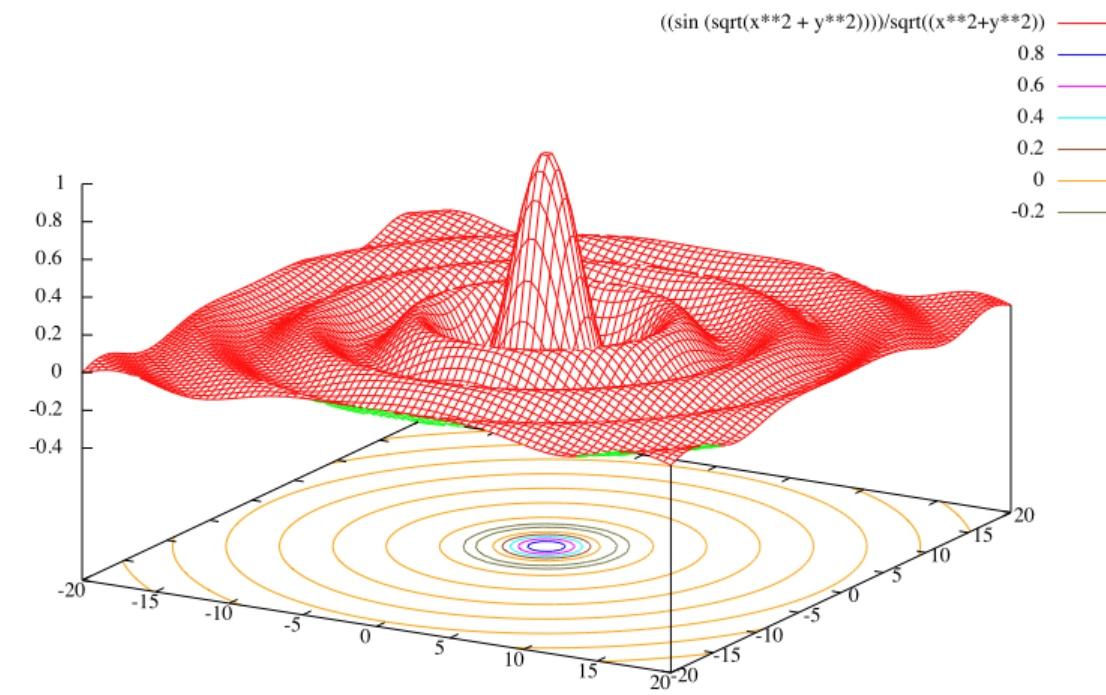
Lets test it with **example5.f90**

- A subroutine does not return a value, however it can modify its arguments.

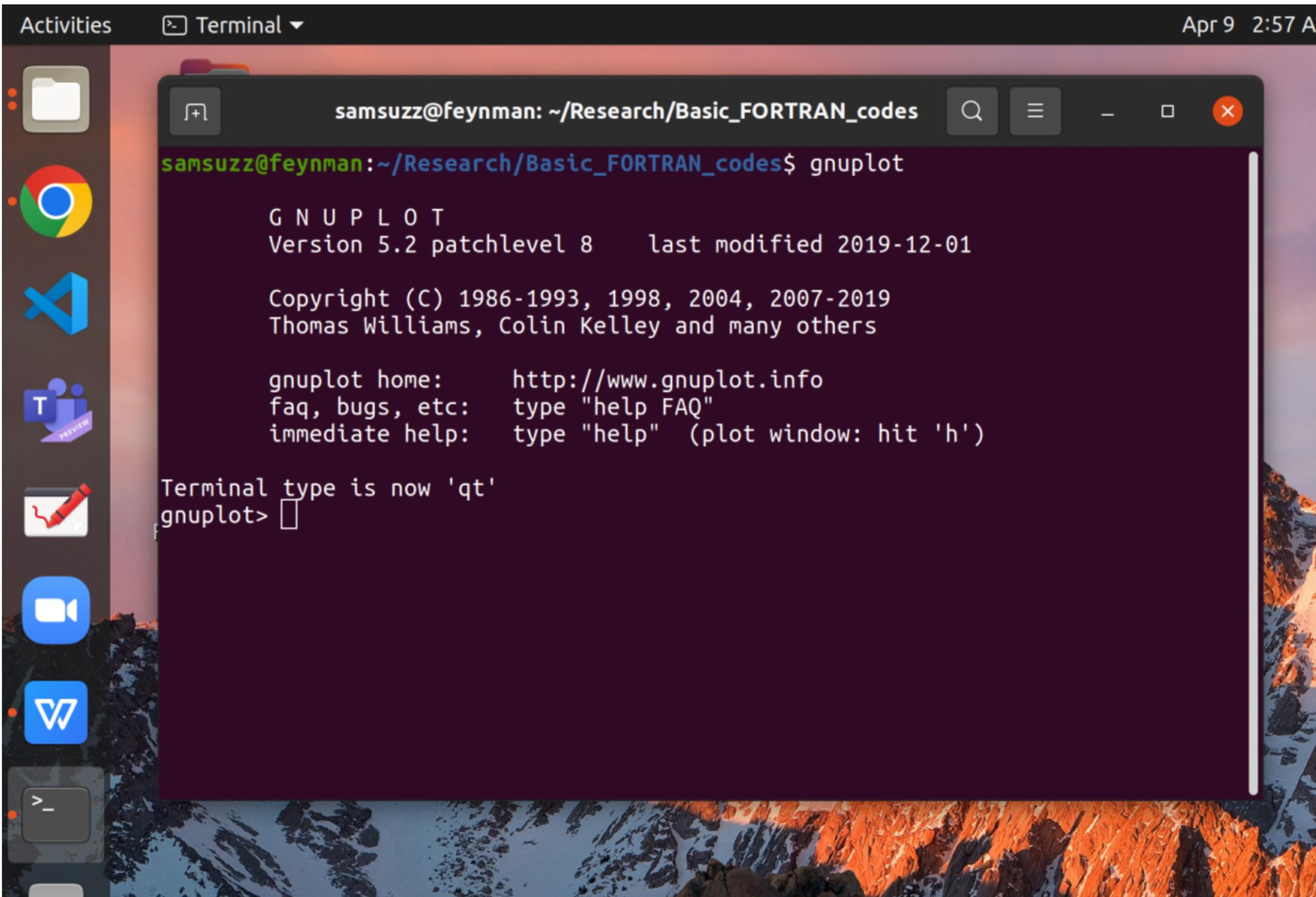
Lets test it with **example6.f90**

GnuPlot

- Gnuplot is a portable command-line driven graphing utility for Linux, OS/2, MS Windows, OSX, VMS, and many other platforms.
- It was originally created to allow scientists and students to visualize mathematical functions and data interactively, but has grown to support many non-interactive uses such as web scripting.



- To open gnuplot , simply type **gnuplot** in terminal

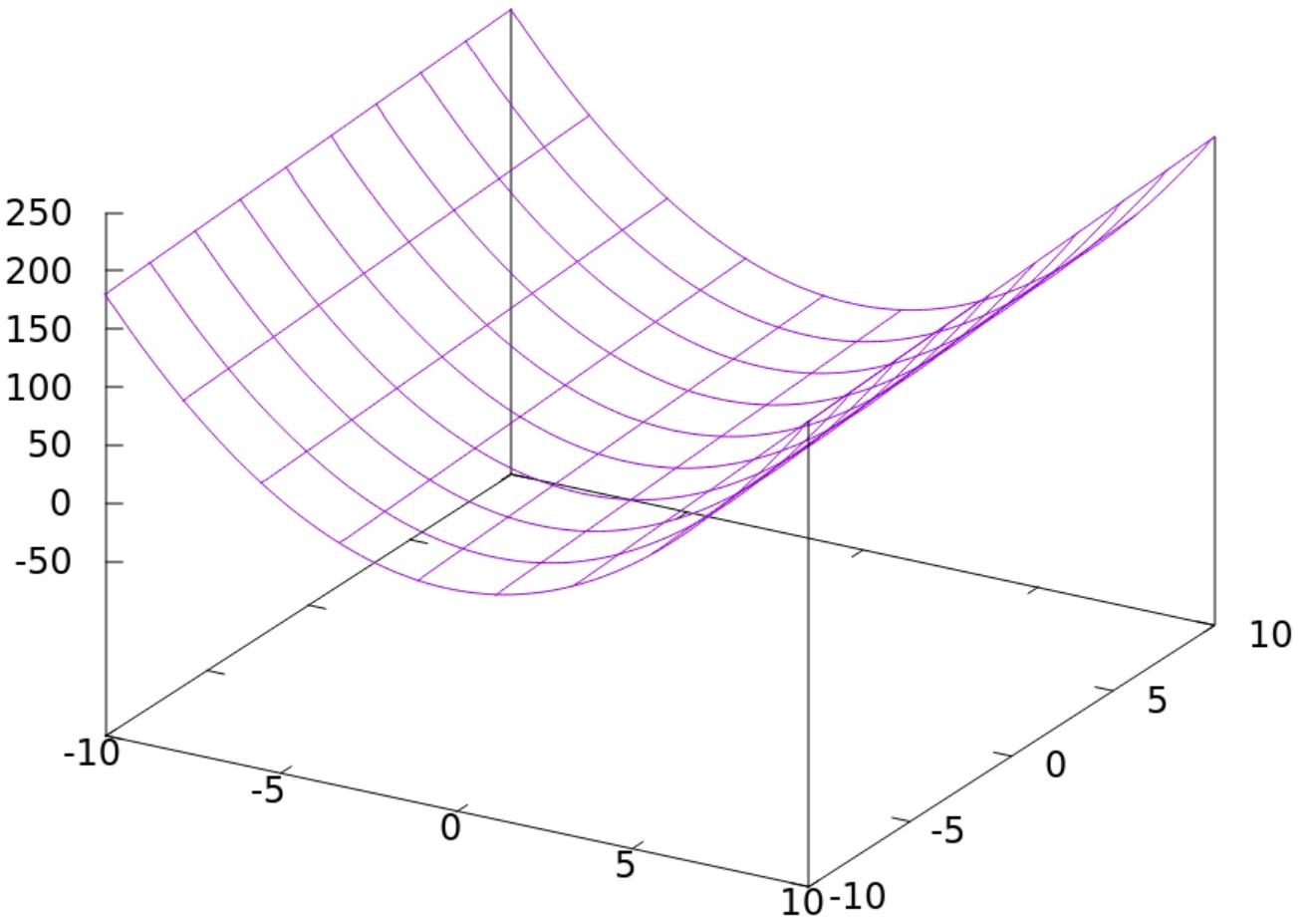
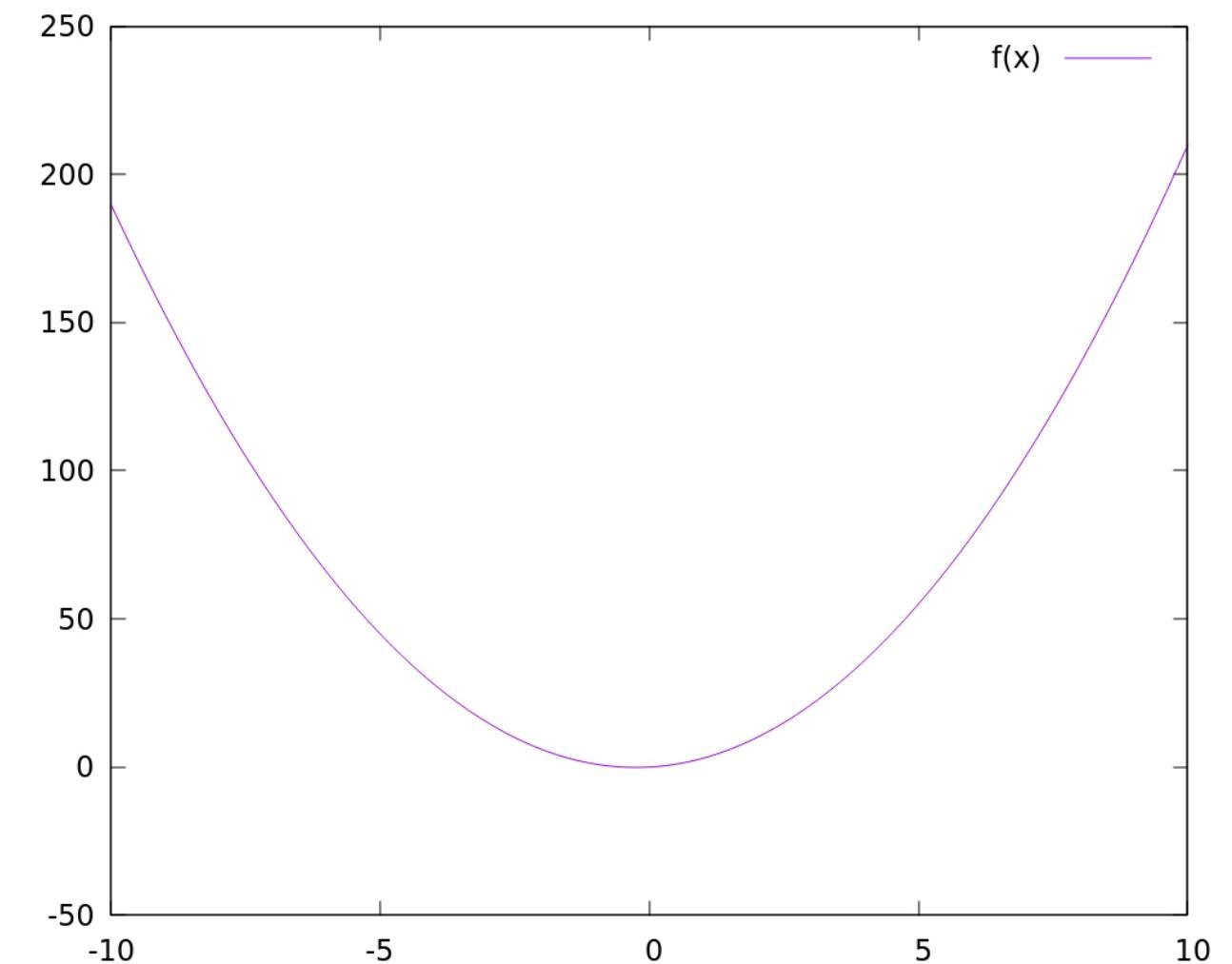


A screenshot of an Ubuntu desktop environment. On the left, there's a vertical dock with icons for File Explorer, Google Chrome, Visual Studio Code, Microsoft Teams (Preview), Paint, Camera, and WPS Office. The main area shows a terminal window titled "Terminal" with the command "gnuplot" entered. The terminal output is as follows:

```
samsuzz@feynman: ~/Research/Basic_FORTRAN_codes$ gnuplot
G N U P L O T
Version 5.2 patchlevel 8      last modified 2019-12-01
Copyright (C) 1986-1993, 1998, 2004, 2007-2019
Thomas Williams, Colin Kelley and many others
gnuplot home:      http://www.gnuplot.info
faq, bugs, etc:    type "help FAQ"
immediate help:   type "help"  (plot window: hit 'h')
Terminal type is now 'qt'
gnuplot>
```

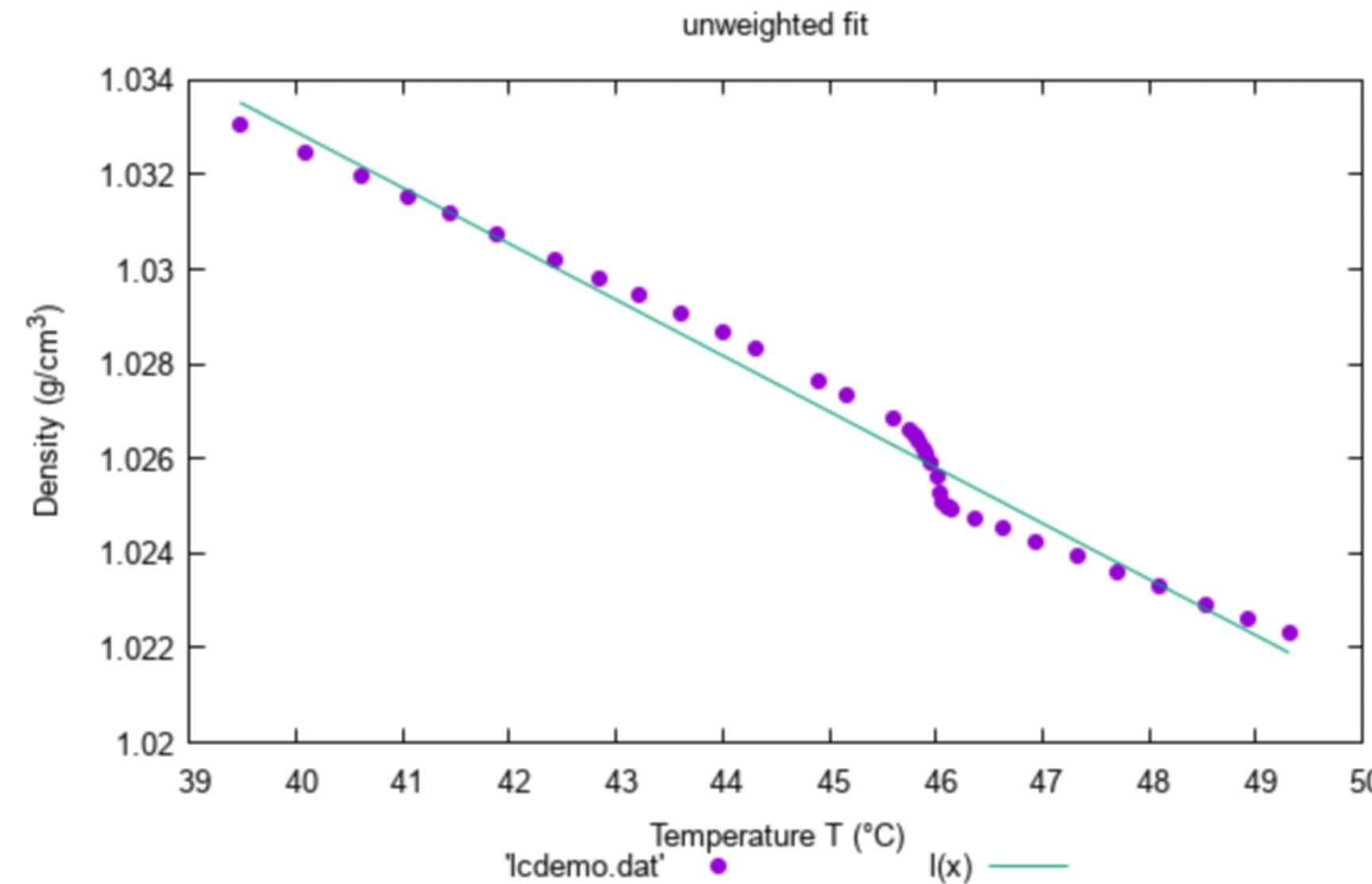
Lets Plot

- plot $\sin(x)$
- $f(x) = 2*x*x + x$
plot $f(x)$
- $f(x,y) = 2*x*x + x + y$
splot $f(x,y)$

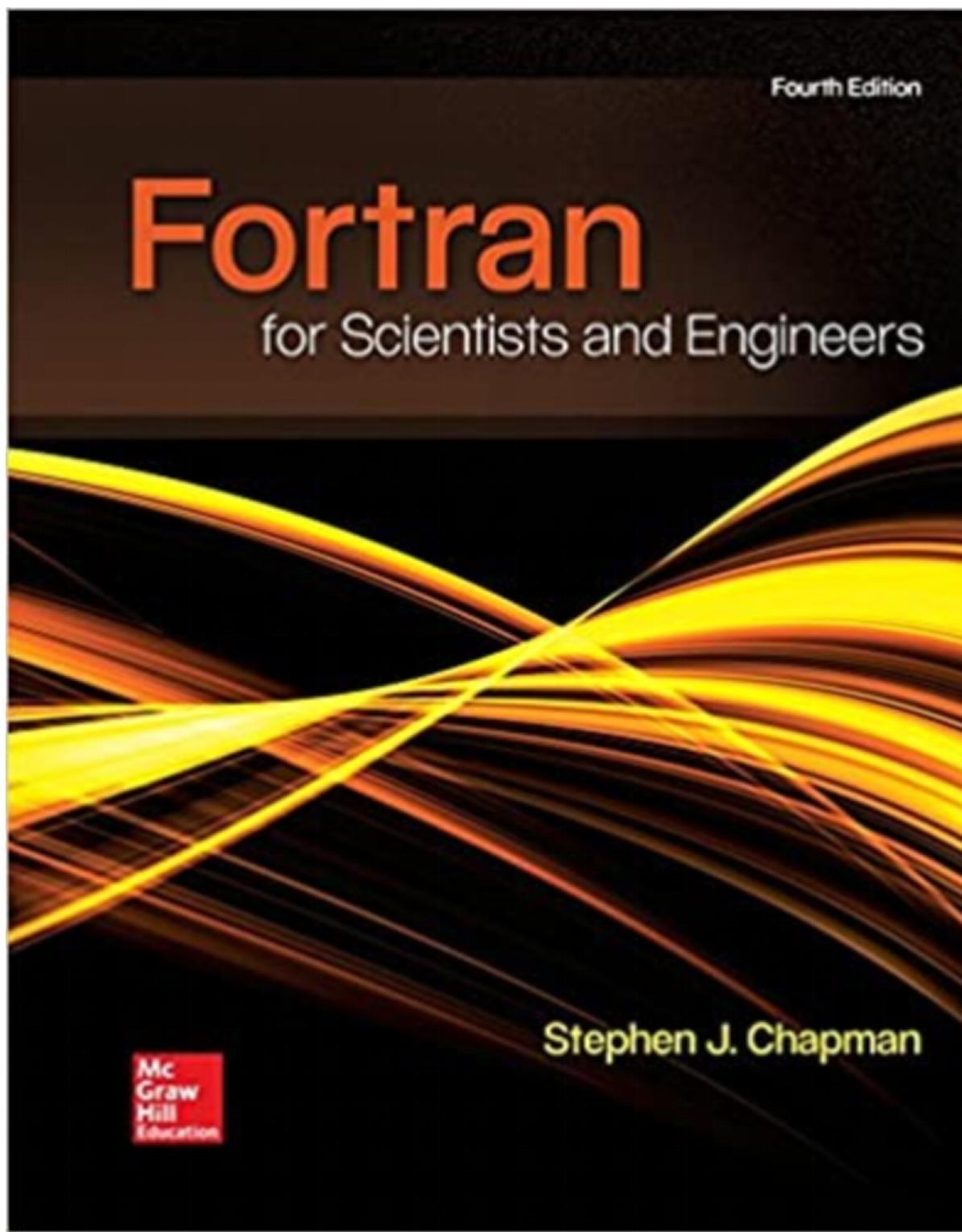


Curve Fittings

- **Curve fitting is the process of constructing a curve, or mathematical function, that has the best fit to a series of data points**
- lets try an example gnuplot_1.p load ‘gnuplot_1.p’



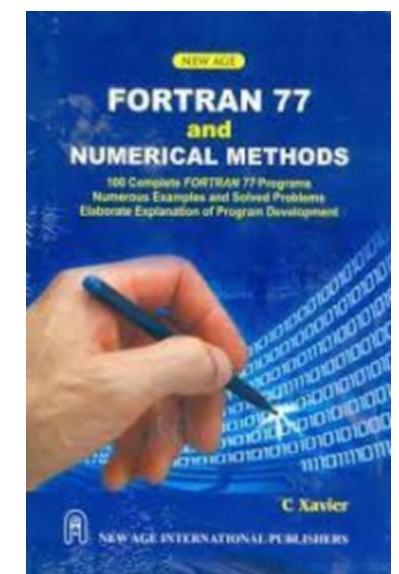
- <https://people.duke.edu/~hpgavin/gnuplot.html>



NUMERICAL RECIPES in Fortran 77

Second Edition

The Art of Scientific Computing





THANK
YOU :)