

PH302 - Computing Skills

Introduction to Programming

Convenor: Dr. Jingqi Miao
Lecturer: Dr. Dean Sayle

Timothy Kinnear
tk218@kent.ac.uk
Room 104 Ingram

Demonstrators:
Paul Cornwall Ricky Hibbert
Chrysa Avdellidou Jimmel Stewart

Aims

- To gain a familiarity with Unix based Operating Systems (Linux)
- To learn the Fortran 90 programming language to a basic level
- To appreciate some of the uses of programming within the context of science and data analysis
- To understand some of the principles of how computers work behind GUIs/etc

What are Programming Languages For?

- Need to be able to tell a computer what to do
- Computer operates in machine language, direct binary instructions
- Programming languages provide a level between human understanding, and machine instructions
- Each language has a specific *syntax*
- Then use a *compiler* to convert the language text into an executable program

How are Programming Languages Used?

- Code written in standard ASCII text file (.f90)
- Compiler is run on the file
- An *object* file created (.o)
- Object file is *linked* to relevant libraries (.a/.so/.dll)
- Executable Binary is created

What Can You Do With Programming?

- Data processing
- Interaction/visualisation of data
- Computation solutions to analytical/mathematical problems ('Numerical Methods/Analysis')
- Computational Simulation
 - Video - '*AREPO*' Fluid Dynamics Code¹;
Kelvin-Helmholtz Instability and Rayleigh-Taylor Instability.
 - Kelvin-Helmholtz cloud image².
 - Jupiter atmosphere animation³.
 - Video - In-house Astrophysics Fluid Dynamics Code⁴;
Fragmentation of a Molecular Hydrogen Cloud at an HII Boundary Region.

¹Springel, V. 2010, MNRAS, 401, 791

²John Bennett, <http://cloudappreciationsociety.org/gallery/photo-07739/>, accessed 07/12/12

³NASA Multimedia, credit: University of Arizona

⁴Code Described in Miao, J. et al, 2006, MNRAS, 369, 143

Weekly Topics - First Half

- Week 13 - The *PCSPS07* Server, Unix and Your First Programs
- Week 14 - Using Input and Output in Programs
- Week 15 - Conditional Logic and **IF**/**CASE** Statements
- Week 16 - Loops and the **DO** Statement
- Week 17 - Arrays
- Week 18 - Arrays/Subroutines and Functions

Weekly Topics - Second Half

- Week 19 - Class Test + Subroutines and Functions
- Week 20 - Characters, Strings and Formatting
- Week 21 - Advanced Functionalities and Concepts of Fortran
- Week 22 - Introduction to Scientific Programming and Numerical Methods
- Week 23 - Mini-project
- Week 24 - Class Test

Workshop Sessions

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00-10:00		Group 2 Weeks 13-18 & 20-23 ECT1 CA			
10:00-11:00		Group 1 Weeks 13-18 & 20-23 ECT1 CA			
11:00-12:00		Class Tests Week 19 : Eliot Hall Week 24 : Sports Hall Check Email/Moodle	Group 3 Weeks 13-18 & 20-23 ECT1 CA		
12:00-13:00				Group 3 Weeks 13-24 ECT1 PC	
13:00-14:00					
14:00-15:00					Group 3 Weeks 13-24 ECT1 RH, JS
15:00-16:00				Group 1 Weeks 13-24 ECT1 PC	Group 1 Weeks 13-24 ECT1 RH, JS
16:00-17:00					Group 2 Weeks 13-24 ECT1 RH, JS
17:00-18:00	Lecture Week 13 RLT1 All			Group 2 Weeks 13-24 ECT1 PC	

Assessment

Week		Programs	Questions	Date due in
Uni	Course			
13	1	0	No	
14	2	2	Yes	Friday (31/01/13)
15	3	2	Yes	Friday (07/02/13)
16	4	2	Yes	Friday (14/02/13)
17	5	2	Yes	Thursday (27/02/13, week 18)
18	6	0	No	
19	7	2	Yes	Friday (07/03/13)
20	8	1	Yes	Friday (14/03/13)
21	9	2	Yes	Friday (21/03/13)
22	10	2	Yes	Friday (28/03/13)
23	11	1	No	Friday (11/04/13, week 24)
24	12	0	No	

Assessment

- Mid-term class test:
Tuesday, 4th March, 11:00-12:00, Eliot Hall
- End of term class test:
Tuesday, 8th April, 11:00-12:00, Sports Hall

Creating Your Account

- Use 'Putty' to ssh to the server 'PCSPS07.kent.ac.uk'
- Log in with your ITS username and initial password
'[ITS username]_[university number]' (remember your student card!)
- e.g. for ITS username 'aa000' and student number '987654321', password would be:
aa000_987654321
- Follow instructions presented to reset your password
- Putty will close after this is done, your password will be set to whatever you selected, and your account will be ready for subsequent logins

Using PCSPS07 via Xming

- Run the 'Xming X Launch Wizard' application (search within Start menu)
- Select 'One Window' mode
- Select 'Open session via XDMCP'
- Enter 'PCSPS07.kent.ac.uk' as the server
- If desired, save the configuration to create a shortcut to do the above automatically in future
- Enter username and password to log in

Exiting Xming

- **Do not** exit Xming by selecting a 'log out' or 'exit' option within the virtual desktop
- **Do** close Xming directly using the 'x' close window icon in the upper right, or the Alt-F4 keyboard shortcut

Some Terms

- *Terminal* - The bit you type in
- *Shell* - The language and 'interface' between actions in the terminal, and what is performed by the computer
- '*Bash*' - The shell which you will be using for this course; '**B**ourne **A**gain **S**hell'
- '*ssh*' - **S**ecure **S**hell, protocol which lets you interact with a Unix machine remotely
- '*X*' or '*X11*' - The set of instructions with which graphics are displayed on screen in most Unix versions
- *Directory* - Equivalent to 'folder' on Windows machines

Structure of Terminal Commands

- `command [-o|-p] [argument1] [argument2] [argument3]`
- `ls` → lists contents of current directory
- `ls ./mysubdir/` → lists contents of the sub directory 'mysubdir'
- `ls -l` → lists contents of current directory in 'long' mode
- `ls -l ./mysubdir/` → lists contents of the sub directory 'mysubdir' in 'long' mode
- `ls -l -a` → lists contents of current directory in 'long' mode, including 'hidden' files

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 - produces → myinputfile.out

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- Additional option '-o' to specify what the output name should be
- **command** -o myoutputfile myinputfile
 - produces → myoutputfile

Structure of Terminal Commands

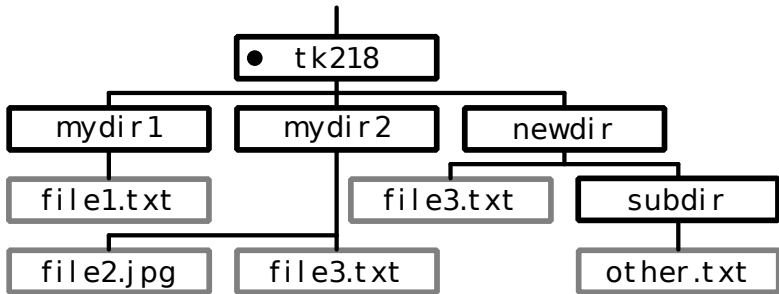
- **command** myinputfile
 - produces → myinputfile.out
- Additional option '-o' to specify what the output name should be
- **command** -o myoutputfile myinputfile
 - produces → myoutputfile
- **command** [-a] [-b [option_argument]] [command_argument]

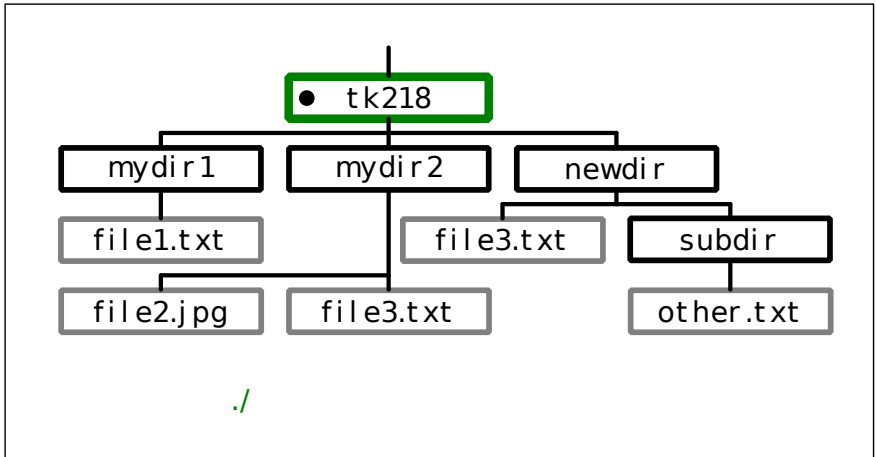
Structure of Terminal Commands

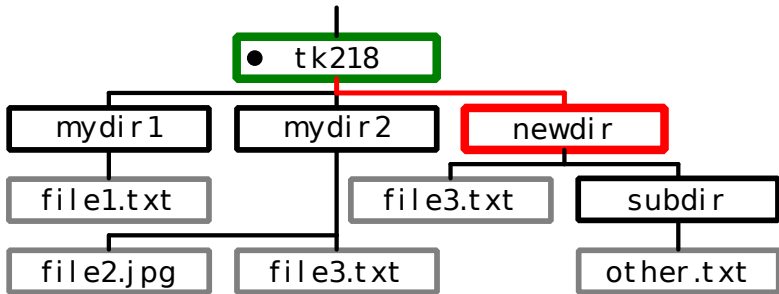
- **command** myinputfile
 - produces \rightarrow myinputfile.out
- Additional option '**-o**' to specify what the output name should be
- **command** **-o** myoutputfile myinputfile
 - produces \rightarrow myoutputfile
- **command** [**-a**] [**-b** [option_argument]] [command_argument]
- Like mathematical functions:
 - $f(x, g(y), z)$
 - Command(**a**, **b**(optarg), comarg)

Important Commands

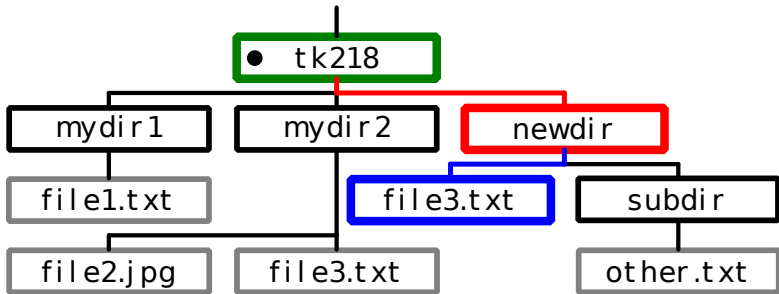
- `man` commandname → **MAN**ual page for the command 'commandname'
- `ls` → **LiSt**, lists contents of a directory
- `cd` targetdir → **C**hange **D**irectory, moves to directory specified by 'targetdir'
- `mkdir` dirname → **MaKe DIR**ectory, makes a directory named 'dirname'
- `cp` from to → **CoPy**, copies the file 'from' to the location/name 'to'
- `mv` from to → **MoVe**, moves the file 'from' to the location/name 'to'
- `rm` filename → **ReMove**, deletes the file 'filename'
- `rm -r` dirname → '**R**ecursive' option, deletes the directory 'dirname'



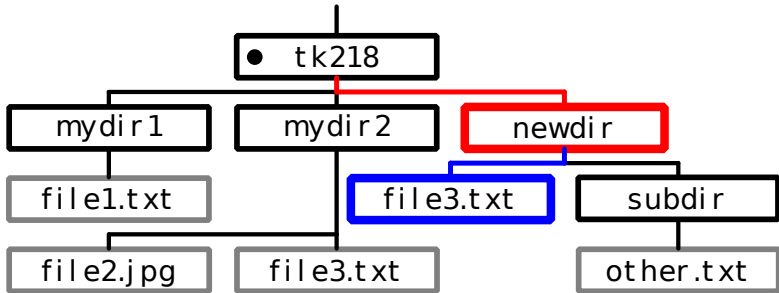




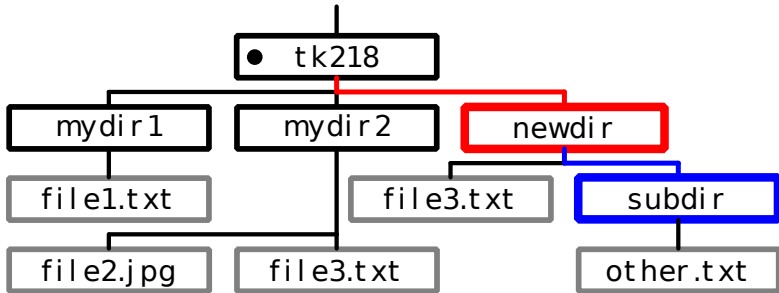
`./newdir/`



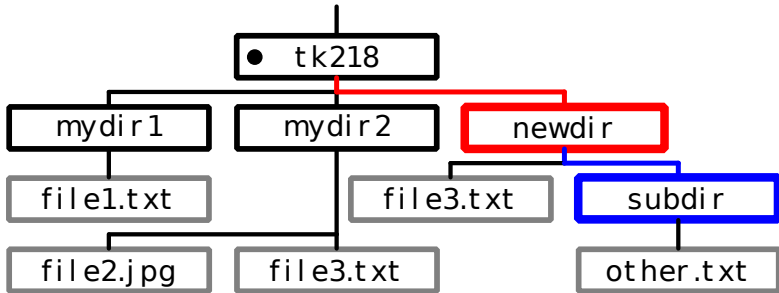
`./newdir/file3.txt`



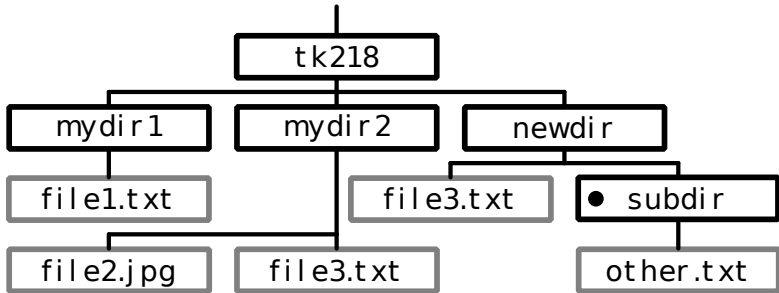
newdir/file3.txt

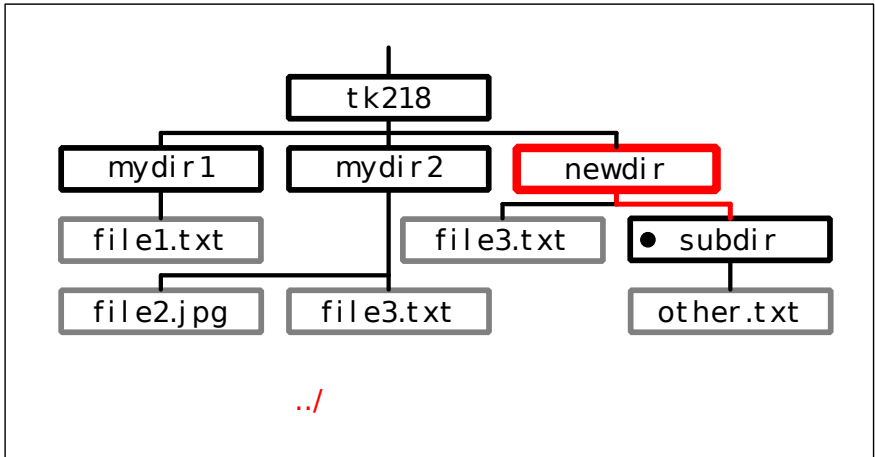


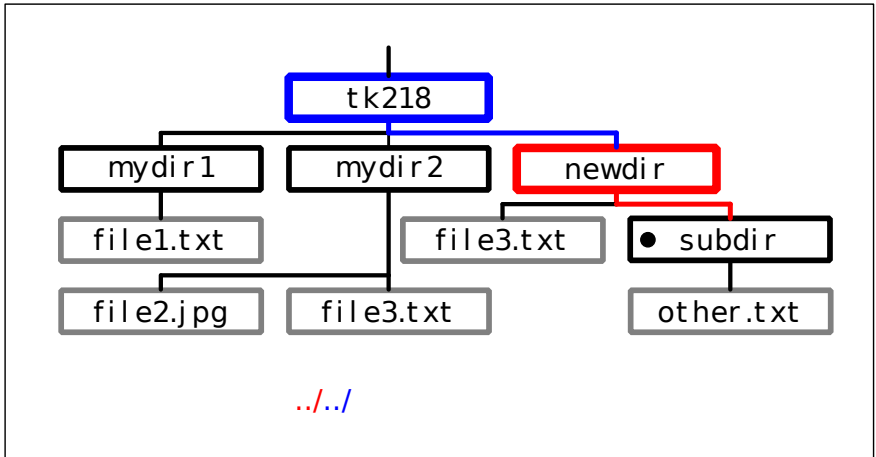
newdir/subdir/

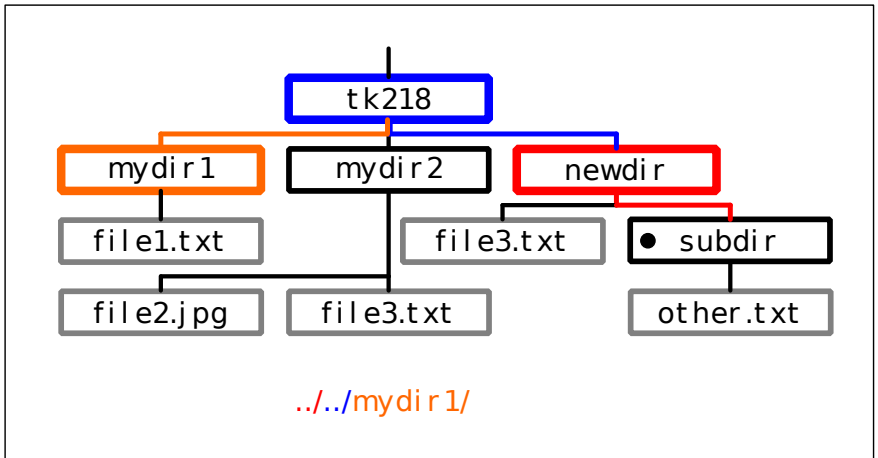


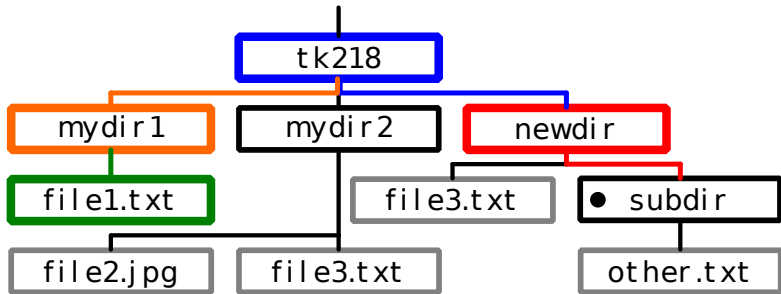
cd newdir/subdir/



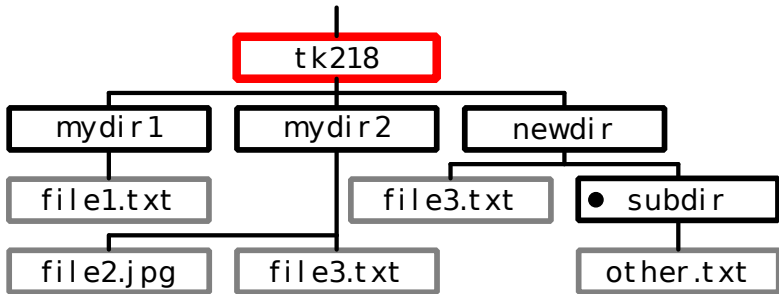




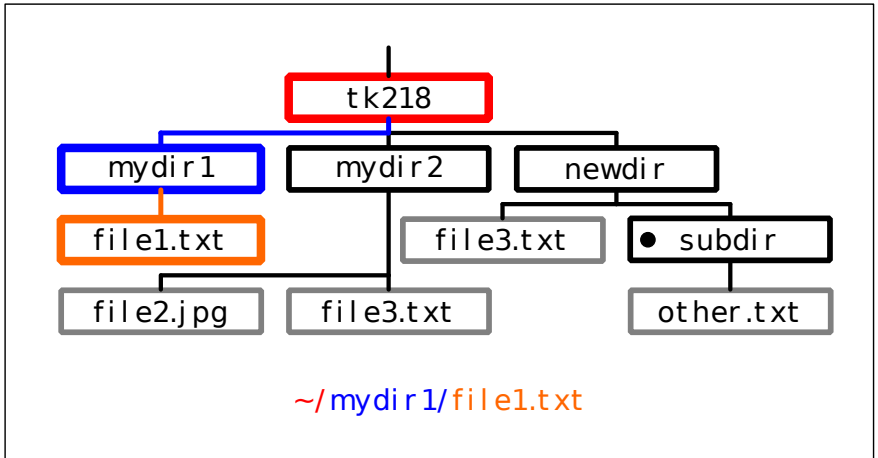


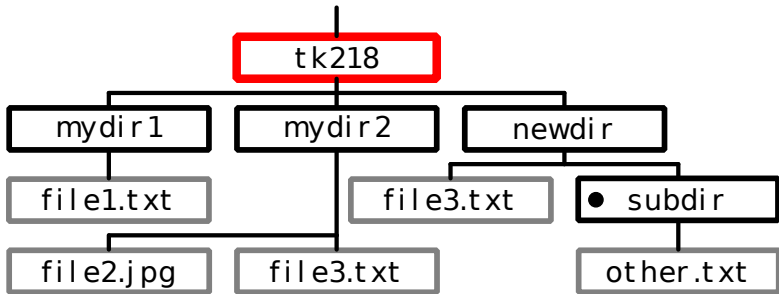


../.. / mydir1 / file1.txt

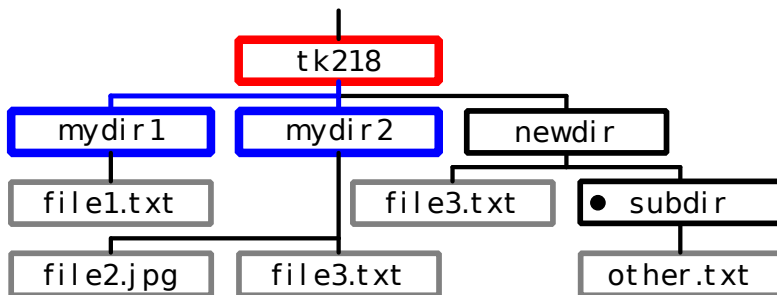


~/





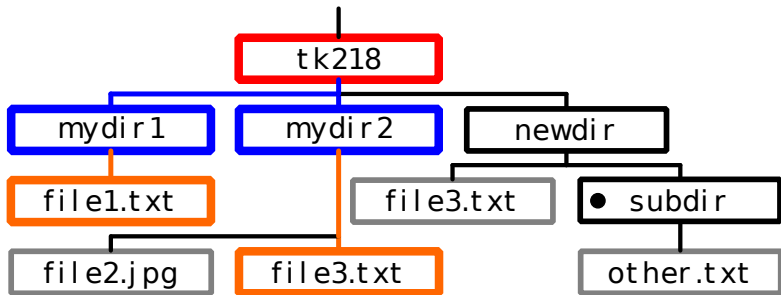
~/



~/my*/

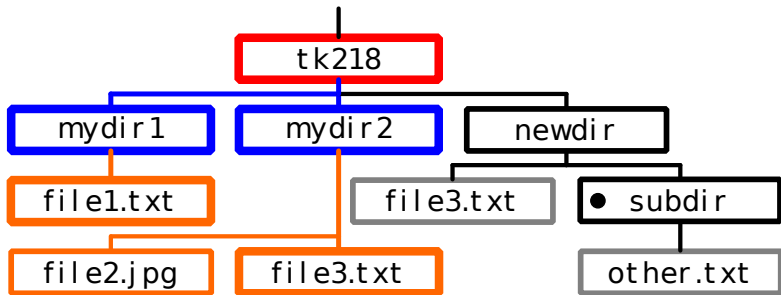
~/mydir1/

~/mydir2/



~/my*/*.txt

~/mydir1/file3.txt ~/mydir2/file1.txt



~/my*/file*

~/mydir1/file3.txt

~/mydir2/file2.jpg

~/mydir2/file1.txt

What is Fortran?

- 1957, First Version of FORTRAN
- 1962, FORTRAN IV
- 1966, FORTRAN 66
- 1977/1980, FORTRAN 77
- 1991, Fortran 90
 - Many modernised features
 - 'free form'
 - Still fully backwards compatible with F77
- 1997, Fortran 95
 - Minor changes to F90
 - Some obsolete features removed permanently - not fully back-compatible with F77
- 2004, Fortran 2003
 - Still propriatory - No free compilers
- 2010, Fortran '2008'
 - Minor changes, similar to F90 → F95

Hello World Code

```
PROGRAM helloworld  
  IMPLICIT NONE  
  !print out the phrase "hello world" to the terminal  
  WRITE(*,*) 'Hello World'  
END PROGRAM helloworld
```

Compiling and Running Code

Compiling: `:> gfortran -o helloworld helloworld.f90`

(Compiling: `:> gfortran [-o (helloworld)] [helloworld.f90])`

Running: `:> ./helloworld`

Output: Hello World

Empty Prompt: `:> _`

References

Using GNU Fortran; for GCC version 4.5.0. Free Software Foundation, 2008.

Springel, V. 2010, MNRAS, 401, 791

John Bennett, <http://cloudappreciationsociety.org/gallery/photo-07739/> accessed 07/12/12

Animation of Jupiter, NASA Multimedia, University of Arizona

Miao, J. et al, 2006, MNRAS, 369, 143

Standards Documents. <http://gcc.gnu.org/wiki/GFortranStandards>

Any Questions?