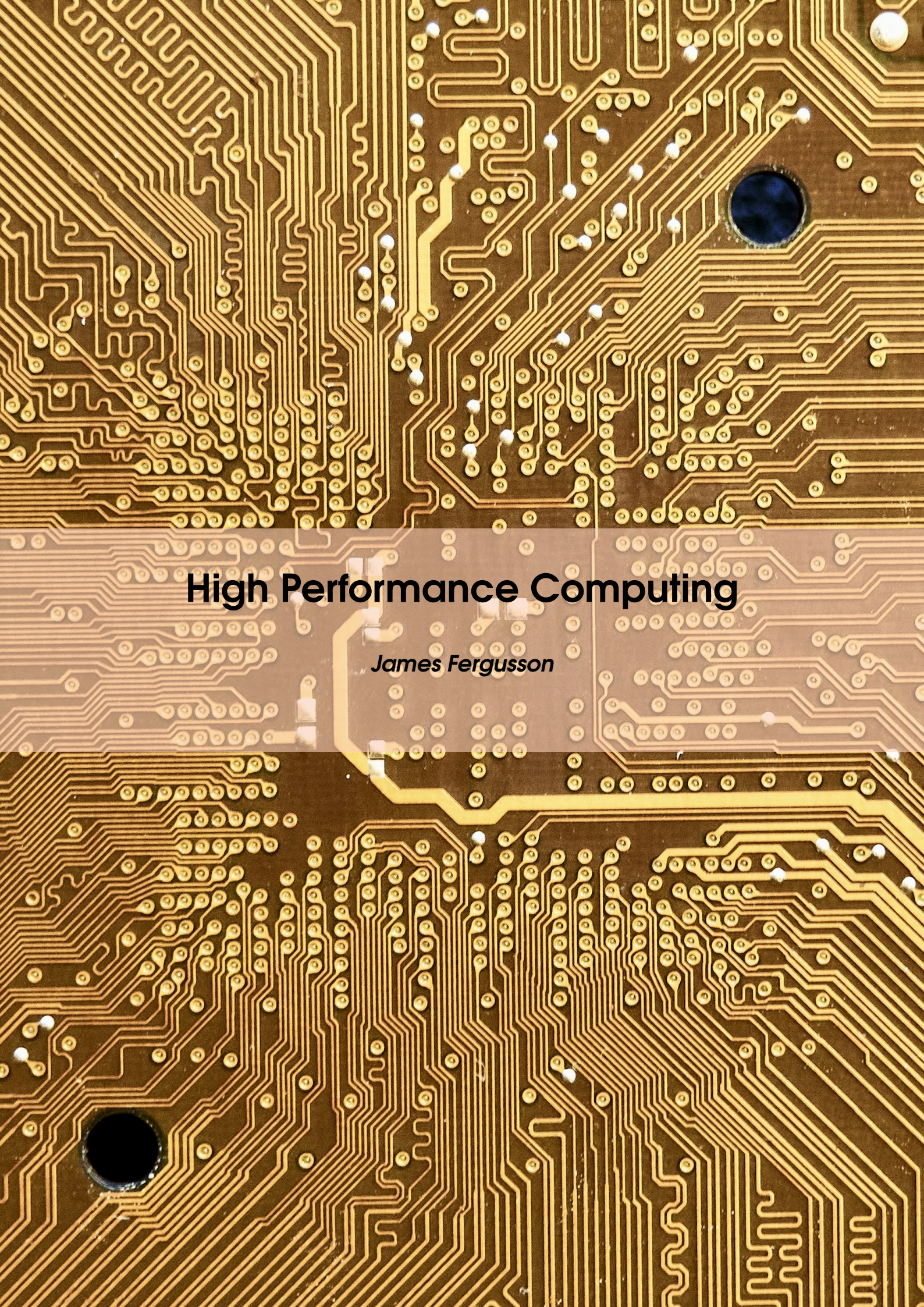

High Performance Computing

James Fergusson

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Preamble

Details:

Dr James Fergusson

Room: B1:12

J.Fergusson@DAMTP.cam.ac.uk

Textbooks:

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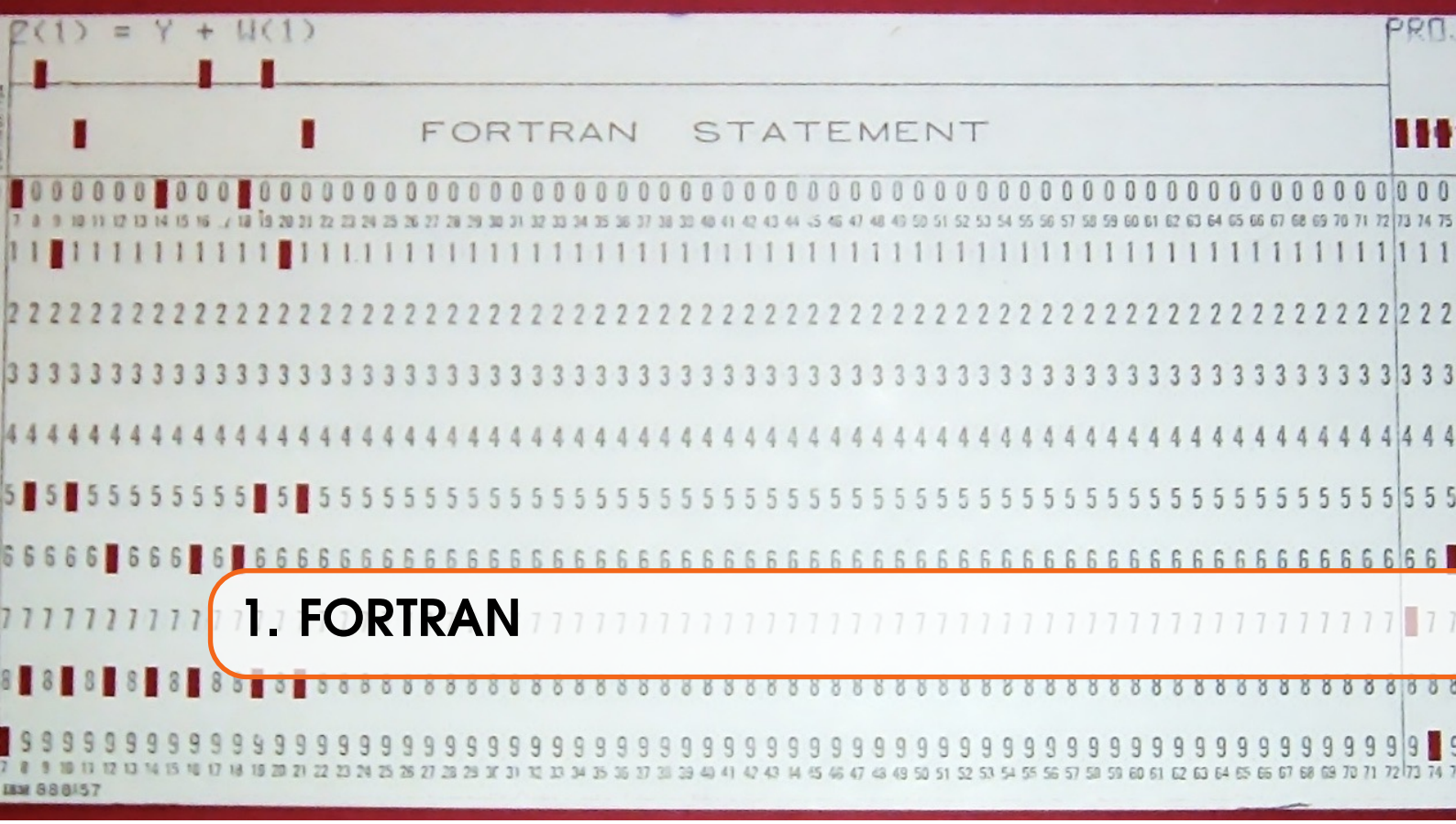

1. FORTRAN

1.1 Background

FORTRAN is one of the oldest coding languages. It was first originally developed in the 50s and was designed to work with punch cards which influences the standards created for it. So why would be want to learn about such an old fashioned language, surely we should just switch to more modern languages that are widely used like C++. Well the reason is that FORTRAN was created specificly for numerical computation (FORTRAN is a abbrevication of FORmular TRANslation) when memory and compute were very limited. This means that there is a large pool of legacy code for standard numerical tasks all of which is written in FORTRAN. In fact many standard libraries used in C++, Python and other languages are wrapped FORTRAN code (for example numpy). It is also likely that you will need to interact with FORTRAN codes in academia as many numerical codes used for scientific tasks use it. For example, while C++ dominates software development current statistics for ARCHER2 (a key supercomputer for scientific research) use are:

1. FORTRAN - 81.1%
2. C++ - 14.9%
3. Python - 2.1%
4. Other - 1.9%

so FORTRAN is still dominant in academic circles.

1.2 FORTRAN77

The first FORTRAN standard was released in 1966 but wasn't widely addopted until its revision in 1977. This standard, called FORTRAN77, became very widely used, and persisted for 13 years. It is now obselete for new development but there is a large set of legacy code still used so you may come across it occasionally. It is quite tricky as it has several features which are significantly different to modern coding languages. We will breifly review its quirks so you can recognise it when you see it (and understand why all of your edits make it crash)

Firstly, it was based on punchcards so had some very specific requirement for formating. Each line could only be 80 characters long (as this was the width of a punchcard). Each line reserved

specific purpose for each column:

1. Column 1 : Any character here indidcates the line is a comment (normal to use "C" or "*")
2. Column 2-5 : Label space, used for "GO TO" commands and "FORMAT" specifiers
3. Column 6 : Any character here indicates the line is a continuation of the previous line (normal to use "+")
4. Column 7-72 : Programming Statements
5. Column 73-80 : Sequence Number used to reorder punchcards if they were dropped

So the first issue with working with FORTRAN77 is you have to spend a bit of time counting spaces. If you acidentily put characters in the first spaces you line is ignored as a comment, in the first 5 the initial charaters are interpreted as a label. Anything in space 6 appends this line to the one above. Anything that comes after character 72 is ignored.

Here is a simple Fortran77 program (it is typical to use the extension .f or .for for FORTRAN77):

Snippets/F77/HelloWorld.f

```
1         PROGRAM main
2 c       Simple hello world program
3         WRITE(*,*) 'Hello World'
4         STOP
5         END
```

We should note the following points:

1. You start your code with the command `PROGRAM` and end them with `END`.
2. To write putput to the terminal you use `WRITE(*,*)` where the first * denotes the terminal and the second denotes upspecifed formating.
3. You have to `STOP` the program before it `END`s

To compile and run this code we use the `gfortran` compiler with the commands:

```
1 $ gfortran HelloWorld.f -o helloworld.exe
2 $ ./helloworld.exe
3 Hello World
4 $
```

Due to the limited row length, indentation is sometimes skipped which can make it hard to read. Also FORTRAN ignores all white space, which some programmes use to optimise line lenghts making this even worse.

Here are the intrinsic variables for FORTRAN77:

Snippets/F77/Intrinsics.f

```
1  PROGRAM main
2  IMPLICIT NONE
3
4  INTEGER i,j,k
5  REAL x,y,z1,z2,z3,z4
6  DOUBLE PRECISION d1, d2
7  COMPLEX c1
8  LOGICAL bool1, bool2, bool3, bool4
9  CHARACTER str*8
10 REAL arr(4,5,6)
11
12 i = 2
13 j = 3
```

```
14 x = 2.0
15 y = 3.0
16 c1 = (1,3)
17 str = 'hello'
18
19 z1 = x+y
20 z2 = x*y
21 z3 = y/x
22 z4 = y**x
23 WRITE(*,*) z1,z2,z3,z4
24
25 bool1 = i .LT. j
26 bool2 = i .GE. j
27 bool3 = i .EQ. j
28 bool4 = i .NE. j
29 WRITE(*,*) bool1,bool2,bool3,bool4
30
31 STOP
32 END
```

Firstly I have put the command `INTRINSIC NONE` (technicly not part of the 77 standard but widely supported in 77 compilers) which switched off a standard FORTRAN feature which is that all undefined variables that start with a letter i-n are automaticaly assigned as `INTEGER` and all others are assigned as `REAL`. All variable names (this includes functions and subroutines) can only be 6 characters long and must start with a letter. This is why in numerical packages you often see names like: `POTRF` for Choleski decomposition in the LAPACK numerical library (see more examples here: https://icl.utk.edu/ mgates3/docs/lapack.html).

In FORTRAN77 we only have one integer, which is 32 bit, but we have both 32 (`REAL`) and 64 (`DOUBLE PRECISION`) bit floating point numbers. We have boolians `LOGICAL` and strings with length defined by the *num part. Conveniently we have complex numbers as an intrinsic data type unlike other languages. Arrays are intrinsic, but not dynamic, in FORTRAN77. You can create multi-dimension arrays (up to 7 dimensions) simply by listing the dimension sizes in brackets when declaring them. Finally all declaration (ie assigning variables) must happen *before* any statements (code that does stuff with them). You cannot add variables halfway though some code. This means that you will ivariabley spend alot of time scrolling up and down the code when working on it.

Control flow in FORTAN77 is more limited intrinsicly but can be exteneded to any case by using `GOTO` instructions (which can make yor code very hard to read)

Snippets/F77/Controlflow.f

```
1       PROGRAM main
2       IMPLICIT NONE
3
4       INTEGER i,j,k
5       INTEGER n,m
6
7       n=0
8       m=1
9
10      IF (n .EQ. m) THEN
11          WRITE(*,*) "same"
12      ELSE IF (n .GT. m)
13          WRITE(*,*) "larger"
14      ELSE
```

```
15          WRITE(*,*) "smaller"
16      END IF
17
18      DO 99 i=1,10
19          n = n+i
20  99  CONTINUE
21      WRITE(*,*) n
22
23  88  IF(m .GT. 10) THEN
24          WRITE(*,*) m
25          m = m+1
26          GOTO 88
27      END IF
28      WRITE(*,*) m
29
30      STOP
31      END
```

Here we see the `IF` and `DO` structures plus a `IF`+`GOTO` which defines a 'while' loop. Finally, as FORTRAN does not care about spaces or case (technicaly the FORTRAN standard assumes all uppercase but most compilers don't care) `END IF` `GO TO` are identical to `endif` and `goto`. I personally always write FORTRAN instructions in caps, and variables in lower case, as I think it looks better but this choice is personal.

Fortran77 allows two subprogrammes, `FUNCTION` and `SUBROUTINE`. The first is a normal function $f(x,y,...)$ and the second takes multiple parameters and modifies them.

Snippets/F77/Subprograms.f

```
1  PROGRAM main
2  IMPLICIT NONE
3
4  INTEGER i,j,k
5  INTEGER add
6
7  i=1, j=2
8  k = add(i,j)
9  WRITE(*,*) k
10
11 CALL rotate(i,j,k)
12 WRITE(*,*) i,j,k
13
14 STOP
15 END
16
17 INTEGER FUNCTION add(i,j)
18 IMPLICIT NONE
19 INTEGER i,j
20 add = i+j
21 RETURN
22 END
23
24 SUBROUTINE rotate(i,j,k)
25 IMPLICIT NONE
26 INTEGER i,j,k,n
27 n=i
28 i=j
29 j=k
```

```
30 k=n
31 RETURN
32 END
```

Here the routines are just listed at the end after the main PROGRAM statements. If the code gets too long you can place subprograms in seperate files and add them with the statment INCLUDE filename.f which simply cuts and pastes the code from the file to this location in the main program. Key points are that the function name needs to have a type in both the main program and its declaration, also the name is the variable that you return. Subroutines operate on all variables passed to them and require a CALL statement. Remember that implicit types apply to these too if IMPLICIT NONE is not set, and the 6 character limit still applies to names.

There is quite a bit more I could put here but as you should only use FORTRAN77 if you really have to we will move onto the much more common, and modern, FORTRAN90 standard which is the most common version used today

1.3 FORTRAN90

Fortran90 was a major revision of the standard. So much so that the two standards, while backwards compatable, cannot be used in the same file with each other so a small amount of care must be taken if you wish to combine them.

The main differences between FORTRAN90 and FORTAN77 are:

1. Dropped the static formatting requirement and adopted the flexible format that all modern codes follow. Now variable names can be 31 characters long and lines 132 characters long. Comments start with, lines are continued by putting & at the end of the lihne to be continued and lower case letters are formaly allowed (but FORTRAN is still case insensitive).
2. Introduced MODULEs to replace the INCLUDE method for functions and subroutines.
3. Allowed dynamic array allocation and introduced intrinsic array functions.
4. New control structues like DO WHILE to avoid the need for GOTO and no longer require labels.

Let us look at the intrinsics again as there are some subtilties. We still have the 5 standard intrinsic types: INTEGER, REAL, COMPLEX, LOGICAL, and CHARACTER but we can control the precision of each with KIND

Snippets/F90/Intrinsics.f90

```
1  PROGRAM main
2      IMPLICIT NONE
3
4      INTEGER      :: i
5      REAL         :: x
6      COMPLEX      :: c
7      LOGICAL      :: bool
8      CHARACTER    :: a
9      CHARACTER(len=180) :: string
10
11     ! values can be assigned at creation (could do this in 77 but it was odd)
12     REAL             :: y=3.5
13     REAL, PARAMETER :: pi=3.1415927
14
15     ! change allocation size
16     INTEGER(KIND=2) :: int_short
17     INTEGER(KIND=4) :: int_normal
18     INTEGER(KIND=8) :: int_long  ! not always available
```

```
19
20      REAL(KIND=4) :: real_normal
21      REAL(KIND=8) :: real_long ! also DOUBLE PRECISION
22      REAL(KIND=16) :: real_quad ! not always available
23
24      COMPLEX(KIND=4) :: cmpx_normal
25      COMPLEX(KIND=8) :: cmpx_long
26
27  END PROGRAM
```

Arrays are where FORTRAN90 shines over C++. They are an intrinsic type and come with multiple tools for their manipulation. Python users will find this all quite familiar, numpy is a lightly wrapped version of FORTRANs native array capabilities so most of what you can do in python is available here.

Snippets/F90/arrays.f90

```
1  PROGRAM main
2      IMPLICIT NONE
3
4      ! Fixed size at compile
5      INTEGER i,j,k
6      INTEGER                  :: vector1(5)
7      INTEGER                  :: array1(5,5)
8      INTEGER, DIMENSION(5,5) :: array2
9      ! Dynamic allocation
10     INTEGER, ALLOCATABLE                    :: vector2(:)
11     INTEGER, ALLOCATABLE                    :: array3(:,:)
12     INTEGER, DIMENSION(:,:), ALLOCATABLE    :: array4
13     INTEGER, POINTER                        :: array5(:,:)
14     INTEGER, DIMENSION(:,:), POINTER        :: array6
15
16     ALLOCATE(array3(5,5))
17     IF (ALLOCATED(array3)) THEN
18         WRITE(*,*) 'Array 3 allocated'
19         WRITE(*,*) "array size", SIZE(array3,1), " X ", SIZE(array3,2)
20     END IF
21
22     ALLOCATE(array4(-5:3,0:4))  ! indicies can range from anything to anything else,
       ↪  default is 3 -> 1,2,3
23
24     ALLOCATE(array5(5,5))
25     ALLOCATE(array6(3,3))
26
27     array1 = 0 ! whole array assignment
28     array1(2,2) = 7 ! element assignment
29     vector1 = (/1,2,3,4,5/) ! all elements in one go
30     vector1 = (/(i**2,i=1,5)/) ! via a constructor rule
31     array1(1,:) = 5 ! row assignment
32     array1(3,1:5:2) = 3 ! assignment with step size -> (3,1), (3,3), (3,5) = 3
33
34     array2 = 5*array1 + 6 ! supports whole array element-wise calcuations (most
       ↪  functions too!)
35
36     array5 = 1
37     array6 = array5(2:4,2:4) ! assiging from sub-array
38
```

```
39      ! Intrinsic array operations
40
41      i = SUM(array1) ! add all elements together
42      j = PRODUCT(array1) ! multiply all elements together
43      k = MAXVAL(array1) ! find the maximum
44      k = MAXVAL(array1, MASK = (MOD(array1,2)>0)) ! find the maximum odd number
45      vector1 = MAXVAL(array1, DIM=1) ! find the maximum in each row
46      i = SIZE(SHAPE(array1))
47      ALLOCATE(vector2(i))
48      vector2 = MAXLOC(array1) ! find the location of the maximum
49
50      array5 = MATMUL(array1,array2)
51      array1 = TRANSPOSE(array1)
52
53      !  Cool syntax for conditional array modification
54      WHERE (array1/=0)
55          array1 = -array1
56      ELSEWHERE
57          array1 = 5
58      END WHERE
59
60      ! NEED TO DEALLOCATE ALLOCATABLE ARRAYS AFTER USE!!
61      DEALLOCATE(array3)
62
63  END PROGRAM
```

Some points to note are that arrays are allocatable, but this means that you need to deallocate them once you are finished to conserve memory. The pointer array is so you can pass them to functions in unallocated form. Constructors only work on 1D arrays so you need to use `RESHAPE` statement to make multi-dimension arrays from them. Not in the example above are functions like `ALL` which applies conditions to the entire array, and `SPREAD` (which is the command which allows broadcasting in python to work) copies one array to multiple dimensions of a higher dimenson array.

I/O in Fortran is handled via `READ` and `WRITE` statments. Format statments have to be specified in advance using `FORMAT` and a label which can be used in `READ` and `WRITE` statments. Files are opened and closed with labels so you can specify which file you are using.

Snippets/F90/io.f90

```
1  PROGRAM main
2      IMPLICIT NONE
3
4      INTEGER :: i
5      REAL :: x
6      INTEGER :: fileunit
7      CHARACTER(180) :: filename
8      REAL, DIMENSION(:,:), ALLOCATABLE :: array1
9
10     fileunit = 99
11
12     i = 4000
13     x = 2.45e3
14     ALLOCATE(array1(10,10))
15     array1 = 5.67
16     filename = "test.out"
17
```

```
18      90101 FORMAT('The output is: ',I5,'   ',E13.5E3)
19
20      OPEN(UNIT=fileunit, FILE=filename)
21      WRITE(UNIT=fileunit,FMT=90101) i,x
22      CLOSE(UNIT=fileunit)
23
24      ! for arrays use this:
25      OPEN(UNIT=fileunit, FILE=filename, STATUS='REPLACE', FORM='UNFORMATTED',
        ↪  ACCESS='STREAM')
26      WRITE(fileunit,*) array1
27      CLOSE(fileunit)
28
29      OPEN(UNIT=fileunit, FILE=filename, STATUS='OLD', FORM='UNFORMATTED',
        ↪  ACCESS='STREAM')
30      READ(fileunit,*) array1
31      CLOSE(fileunit)
32
33  END PROGRAM
```

The other major addiition to FORTRAN90 was the inclusions of MODULEs. This allows us ot make packages of functions and subroutines that can be used everywhere in the code. Let's create a couple of modules as an example

Snippets/F90/module1.f90

```
1  MODULE keep_count
2      IMPLICIT NONE
3
4      INTEGER, SAVE, PRIVATE :: count
5
6      PUBLIC get_count, increment
7
8      CONTAINS
9
10         FUNCTION get_count()
11             IMPLICIT NONE
12             INTEGER get_count
13             get_count = count
14         END FUNCTION get_count
15
16         SUBROUTINE increment(amount)
17             IMPLICIT NONE
18             INTEGER, INTENT(IN) :: amount
19             count = count+amount
20         END SUBROUTINE increment
21
22         SUBROUTINE reset()
23             IMPLICIT NONE
24             count = 0
25         END SUBROUTINE reset
26
27 END MODULE keep_count
```

Snippets/F90/module2.f90

```
1  MODULE constants
2      IMPLICIT NONE
3
4      SAVE
5      DOUBLE PRECISION, PARAMETER :: pi=3.1415927
6      DOUBLE PRECISION, PARAMETER :: e=2.71828
7      DOUBLE PRECISION, PARAMETER :: G=6.67430e-11
8      DOUBLE PRECISION, PARAMETER :: c=299792458
9      DOUBLE PRECISION, PARAMETER :: h=6.62607015e-34
10
11 END MODULE constants
```

Snippets/F90/usemodule.f90

```
1  PROGRAM main
2
3      USE keep_count
4      USE constants, ONLY : speed_of_light => c
5
6      IMPLICIT NONE
7
8      INTEGER :: i
9
10     CALL reset()
11
12     DO i=10,99
13         IF (MOD(i,7)==0) THEN
14             CALL increment(1)
15         END IF
16     END DO
17
18     WRITE(*,*) 'number of 2 digit numbers divisible by 7 is: ', get_count()
19     WRITE(*,*) 'speed of light is: ', speed_of_light
20
21 END PROGRAM
```

Looking at these we see that to use a module we just add it with the `USE` command at the begining and we can use the `ONLY` statment to specify which portion of the module we want to use and `=>` to rename them to avoid local name clashes. Variables declared above the `CONTAINS` statement are global to the functions and subroutines in the module and can be accessed in the main programme, unless they are specified `PRIVATE` which hides them from the main programme. All functions and subroutines must come after the contains statement. The `SAVE` statement ensures that the value of parameters are not forgoton when the module goes out of scope i.e. it could be used by routines in two different modules and we want the value to persist for all (doing this allows us to define a “global" variable in a way that is protected as it can only be accessed via the module). The other key point is that all dummy variables names in module subroutines statments should have the extra qualifier `INTENT` which can be one of `IN`, `OUT`, `INOUT`. The compiler uses these to optimise your code but they are not required. `IN` variables should be ones that the subroutine uses but does not modify, `OUT` are ones that the subroutine modifies for return without reference to their input value and `INOUT` are variables whose value is used as input and is modified for return. All other variables internal to the subroutine are private and do not require statments.

We have data structures in FORTRAN90 (which are the equivelent of structs in C). These are defined as new `TYPE`s:

Snippets/F90/types.f90

```
PROGRAM main
    IMPLICIT NONE

    TYPE :: my_type
        INTEGER :: moons
        REAL :: coord_x, coord_y
        CHARACTER(30) :: name
    END TYPE my_type

    TYPE(my_type) :: planets(8)
    REAL :: vector1(8)
    REAL :: x

    planets(1)%moons = 0
    planets(1)%name = "Mercury"
    planets(1)%coord_x = 58e6
    planets(1)%coord_y = 0e0

    planets(3) = (/1,152e6,0e0,"Earth"/)

    vector1 = planets%coord_x
    x = SUM(planets%moons)

END PROGRAM
```

We can overload operators for types we create using modules as follows:

Snippets/F90/overload.f90

```
MODULE overload
    IMPLICIT NONE

    TYPE fraction
        INTEGER :: numerator
        INTEGER :: denominator
    END TYPE fraction

    INTERFACE OPERATOR (+)
        MODULE PROCEDURE frac_add
    END INTERFACE

    CONTAINS

    SUBROUTINE reduce(frac1)
        IMPLICIT NONE
        TYPE(fraction), INTENT(INOUT) :: frac1
        INTEGER :: a,b

        a = frac1%numerator
        b = frac1%denominator

        DO WHILE (b/=0)
            a = b
            b = MOD(a,b)
        END DO

        frac1%numerator = frac1%numerator/a
```

```
29          frac1%denominator = frac1%denominator/a
30
31      END SUBROUTINE reduce
32
33      FUNCTION frac_add(frac1,frac2)
34          IMPLICIT NONE
35          TYPE(fraction), INTENT(IN) :: frac1, frac2 ! needed for overloading
36          TYPE(fraction) :: frac_add
37
38          frac_add%numerator = frac1%numerator * frac2%denominator + frac2%numerator
            ↪  * frac1%denominator
39          frac_add%denominator = frac1%denominator * frac2%denominator
40
41          CALL reduce(frac_add)
42
43      END FUNCTION frac_add
44
45  END MODULE overload
```

Modules can be compiled by the simple command we used previously

```
1 $ gfortran module1.f90 module2.f90 runmodules.f90 -o executable.exe
2 $ ./executable.exe
```

The key part is that the modules are specified in order of their dependancy. Modules deoendancies myst be strictly hierarchical, so you cannot have module1 using module2 and module2 using module1, and compiled in order from bottom to top. Compilers execute the files in order that they recieve them so putting lower modules forit ensures that the .mod files exist for later modules/programs that use them.

2. Compilation

2.1 Makefiles

Complitation of code is a bit fiddly to do from the command line every time, especially once the project becoems large with multiple source files. This has been solved by using programmes that handle the building of projects automatically. The simplest of these is to create a `Makefile`

Makefiles consist of a list of rules, usually for updating files when files they depend on change, but they can be used more generally. The rules take the form (note we need tab rather than 4 spaces for indentation):

```
target ... : dependancy ...
  commands
  ...
  ...
```

```
test :
  echo "Hello!"
```

```
test1 : test2
  echo "Hello two!"

test2 :
  echo "Hello one!"
```

This is OK but a bit verbose. Just like when writing python we are better to use variables to make the code simpler to understand. In make files variables are created with = and := signs. The values are accessed by `$(var)`. The first assignment = is implicit, which means that it doesn't expand the rhs immediately, the second := is explicit, in that it does expand it before assignment. The difference can be seen in the examples:

```
var1 = $(var2)
var2 = "hello"
echo $(var1)

var3 = "hello"
var3 := $(var3)
```

Here we don't expand var1 until we get to echo $(var1) so it doesn't matter that var2 isn't defined when we assign var1. With := this would matter as we would try to expand $(var2) when creating var1 and it wouldn't exist. Conversely for var3 if the second assignment was implicit this would create an infinite loop that can't be expanded. Here := works fine as we would expand it before assignment.

There is also ?= which assigns the variable only if it has not previously been assigned and += which will add another element to a list (which is specified just by spaces between variable names), ie:

```
var1 = one two three
var1 += four
```

We can also create pattern specific variables using:

1. % – This will match any non-empty string and can be used in any string object, but only once.
2. $@ – The filename of the target
3. $< – The first filename of the dependency
4. $^ – The filenames of all the dependencies

This allows us to set up generic rules for all files of a specific type, like object files which are always created from their c files, ie:

```
# compilers, flags and libraries
CC = gcc
CFLAGS := -g -O3 -xHost

# library packages you are useing
LIBS :=

# Directories for code objects, and librarys
OBJDIR := Objects
SRCDIR := Code
BINDIR := .

# source file(s) without suffix
CFILES = file1 file2 file3

PROGRAMS = program1 program2

#This says don't look for a file called program1 or program2
.PHONY := $(PROGRAMS)

program1 : $(CFILES:%=$(OBJDIR)/%.o) $(mainfile1:%=$(OBJDIR)/%.o)
  $(CC) $(CFLAGS) -I$(SRCDIR) $^ -o $(BINDIR)/$@ $(LIBS)

program2 : $(CFILES:%=$(OBJDIR)/%.o) $(mainfile2:%=$(OBJDIR)/%.o)
  $(CC) $(CFLAGS) -I$(SRCDIR) $^ -o $(BINDIR)/$@ $(LIBS)

# everything that ends in '.o' should be made from the same file with '.c' instead
$(OBJDIR)/%.o: $(SRCDIR)/%.c
  $(CC) $(CFLAGS) -I$(SRCDIR) -c $< -o $@

clean :
  rm $(OBJDIR)*.o
```

`Makefiles` can be a pain to create as the syntax is pretty unreadable and you generally don't create them enough to get really familiar with the process. Typically you get one that works then just cut and paste it everywhere you work then debug the inevitible issues that come up. This will allow you to automate code building and is generally ok for most small projects. However, if you move to a new system the `Makefile` will need to be updated with the correct compilers, flags and libraries etc...

2.2 CMake

The creation of `Makefiles` is sufficently difficult that there exist tools to automate the process for you. The industry standard approach is `CMake` which will generate `Makefiles` automatically from some small script files. The real benefit of using tools like `CMake` are that you can use them to automate many other build managment tasks like installing and building libraries or fetching them from git repositories, running testing frameworks and using continuous integration, and installing compiled executables.

The other main benefit is that it makes your code portable so you can jump between platforms and it will automatically discover the local compiler and libraries needed for building. It ends up working a bit like a 'package manager' for C++, like conda is for python, where it looks after all the system dependencies of your project for you and even allows you to change the generator used (`Make` by default, but there are many others) and to easily add things like parallel builds for large projects.

You will need to install `CMake` onto your system (`brew install cmake` or similar on Linux

or Windows). Once you have done this we can see a simple cmake build file for a "Hello World" program:

Snippets/CMake/HelloWorld/CMakeLists.txt

```
cmake_minimum_required(VERSION 3.15...3.26)

project(
    HelloWorld
    VERSION 1.0
    LANGUAGES CXX
)

add_executable(hello main.cpp)
```

The cmake build file must always be called `CMakeLists.txt` and exist in the project directory (wherever you would normally initialise `git`). The first line in it must always be the command `cmake_minimum_required()` which specified the minimum verson of cmake required to build the project. This is needed so as cmake commands have evolved significantly since its first release in 2000. While all scripts are backwards compatible we will be wanting to use many features form "modern" cmake which is generally anything from 3.13 on. In the above we have specified a range from 3.15 to 3.26. Next you need to give your project a name and optionally a version and language. Finally we need to specify an executable we want to build and which cpp file contains the main program to build from.

The project can be built with:

```
$ cmake -S . -B build
$ cmake --build build
```

The first builds the project from the `CMakeLists.txt` in the source directory "." and builds the project in the directory "build" (which it will create if it does not exist). The second uses the build to create the executable in the build directory.

We can add libraries simply with the following commands:

Snippets/CMake/Library/CMakeLists.txt

```
cmake_minimum_required(VERSION 3.15...3.26)

project(library_example
    VERSION 1.0
    LANGUAGES CXX
)

# This would work, but wouldn't build a library:
# add_executable(test main.cpp harmonic.cpp)
# Instead do this:

add_library(harmonic_lib
    STATIC
    harmonic.cpp
    harmonic.hpp
)

add_executable(test main.cpp)
```

```
19
20 target_link_libraries(test PRIVATE harmonic_lib)
```

Here we add the libraries with `add_libraries()` and then describe the dependance graph with the command `target_link_libraries()`. The format of cmake commands are all (target OPTIONS dependancies..) which mimics that of `Make`. We can list multiple (same level) dependancies on the same line but heiracical depencanceis should be input on multiple lines, e.g.

```
1 target_link_libraries(executable PRIVATE lib1)
2 target_link_libraries(lib1 PRIVATE lib2)
3 target_link_libraries(lib2 PRIVATE lib3)
```

We used two options to help us create our libaraies, `STATIC` and `PRIVATE`. the first is the type of library we are creating which can be `STATIC`, `SHARED`, and `MODULE`. The difference is `STATIC` are liked at compile time, `SHARED` are linked at runtime. The first will copy the library code add put it in your executable, the other is more efficent for libraries that multiple executables use as then we only need one copy. A simple rule for this is to use `STATIC` for libraries you built that only one file uses and `SHARED` for libraries that you build that multiple files use. `MODULE` is for shared libaraies that you don't link to, but instead load at runtime with a commnad like `dlopen()`. The options for linking are `PUBLIC`, `PRIVATE`, and `INTERFACE`. `PUBLIC` is for when things that link to the target need to be able to know about the dependant, `PRIVATE` is for when they don't and `INTERFACE` is for when we need to know header but not detail, for example when using header libraries, you need to specify them as `INTERFACE`. It is possible to make lib1 depend on lib2 AND lib2 depend on lib1 and cmake still work but if this happens in your code, you should have a long hard think about what you were trying to acheive.

The simple examples above are not really how you should structure your projects. It is much better to make then hieracical with the code in seperate folders. Despite what you will read in most tutorials on cmake, there is no standard way to do this (and everyone complains about it). You should just aim for something helps make you code more understandable by clearly reflecting its purpose and structure. The key difference is that you have to put `CMakeLists.txt` files in each folder. I have included my personal favourite approach as an example but you can choose others. I like to keep .ccp and .hpp files together which makes sense for most personal projects. If you are designing libraries to be used by others then you will want to split off the public .hpp files into an `include` directory. I have all code in a folder called `src` and libraries in subfolders off that. I place all binaries created in a folder called `bin`. I put the cmake commands for building libraries in the library sub directories and cmake commands for building executables in the src directory. The project folder then just have general cmake commands to set up the project. You should add both bin and build to git.ignore files. This format is fairly simple to understand but has the weakness (strength?) of being strictly heirarcical.

Cmake can do lots more. It can manage the use of external libraries like MPI or OpenMP using the `find_package()`:

```
find_package(OpenMP)
if(OpenMP_CXX_FOUND)
  target_link_libraries(MyTarget PUBLIC OpenMP::OpenMP_CXX)
endif()

find_package(MPI REQUIRED)
target_link_libraries(MyTarget PUBLIC MPI::MPI_CXX)
```

Eternal code can be included in you project with `fetch_content()`:

```
  FetchContent_Declare(contentname
      GIT_REPOSITORY https://github.com/google/content.git
      GIT_TAG        703bd9caab50b139428cea1aaff9974ebee5742e
  )
  FetchContent_MakeAvailable(contentname)
```

And, as we will see later, cmake can manage continuous integration tasks

2.3 Helper Tools

There are several useful helper tools you should use for your code to make it easier for others to use and understand. We will show the several of them Here

Doxygen

] Doxygen is a tool that creates documentation for your code automatically from the comments inside it for a wide variety of languages. First you have to install it (`brew install doxygen` or download binaries for Linux/Windows). Then you just need to create a configiration file in the project directory using

```
$ doxygen -g doxygen.config
```

This creates a long configuration file which deinfed doxygen's behaviour. To begin with you can ignore almost all of it other than changing the following:

```
PROJECT_NAME           = "Doxygen Test"
OUTPUT_DIRECTORY       = docs
EXTRACT_ALL            = YES
EXTRACT_PRIVATE        = YES
INPUT                  = src
RECURSIVE              = YES
```

Documentation is then generated by the simple command

```
$ doxygen doxygen.config
```

Which will create documentation in the `OUTPUT_DIRECTORY` in both html and latex format, with the latter having a MAKEFILE to compile the document. This will be almost blank for the example projects as I ahve not added documentation to them. This can be fixed easily by adding some comments above (or inside) each function. This is done easiest by using the Doxygen extension to VSCode. Then lyou can add comment bolcks aboce each function by typing `/**` then hitting enter which will create blocks like:

```
 /**
 * @brief
 *
 * @param x
 * @param y
 * @return
 */
double harmonic::harm_add(double x, double y)
```

To which you can add a description of the function after `@brief` and a description of each parameter after `@param`. Play with this and see how the documentation is updated.

Doxygen is very easy to add to a project being build by `CMake` with the command `doxygen_add_docs`. We will jump straight to the general case where we define a cmake module file to automate this. We need to create a directory `cmake` and include add the following file, `Doxygen.cmake`, to it:

```
function(Doxygen input output)
    find_package(Doxygen)

    if (NOT DOXYGEN_FOUND)
        add_custom_target(doxygen COMMAND false
            COMMENT "Doxygen not found!!"
        )
        return()
    endif()

    set(DOXYGEN_GENERATE_HTML YES)
    set(DOXYGEN_HTML_OUTPUT ${PROJECT_SOURCE_DIR}/${output}/html)
    set(DOXYGEN_GENERATE_LATEX YES)
    set(DOXYGEN_LATEX_OUTPUT ${PROJECT_SOURCE_DIR}/${output}/latex)
    set(DOXYGEN_EXTRACT_ALL YES)
    set(DOXYGEN_EXTRACT_PRIVATE YES)
    set(DOXYGEN_RECURSIVE YES)
    set(DOXYGEN_QUIET YES)

    doxygen_add_docs(doxygen
        ${PROJECT_SOURCE_DIR}/${input}
        COMMENT "Generating documentation"
    )

endfunction()
```

We then update our `CMakeLists.txt` to include the new function:

```
cmake_minimum_required(VERSION 3.15...3.26)

project(folder_example
  VERSION 1.0
  LANGUAGES CXX
)

list(APPEND CMAKE_MODULE_PATH "${CMAKE_SOURCE_DIR}/cmake")

set(CMAKE_RUNTIME_OUTPUT_DIRECTORY ${PROJECT_SOURCE_DIR}/bin)

include(Doxygen)
Doxygen(src docs)

add_subdirectory(src)
```

And documentation is created on the command line by specifiing the target `doxygen`

```
cmake --build build -t doxygen
```

Enforcing style

You should also add tools that help enforce formatting for your code to ensure a consistent style, and some static analysis to catch simple programming errors. `clang-format` does the former, and `clang-tidy` does the latter. These are some of the most poular tools but there are many alternatives like: `cpplint` and `cppcheck`. You can also combine these tools with other static checkers like `include-what-you-use` which removes unnessecary `include` statements.

clang-format

To use `clang_format` you just call it on the command line for whatever files you want to format:

```
lang-format -i --style=Google filename1.cpp
```

Where the `-i` means 'inplace', so re-format the file and put output to original filename, and `--style` defined the formatting style you want to use from LLVM, Google, Chromium, Mozilla, Webkit, Microsoft, GNU, custom where custom is defined by a file you create. We can automate this in `cmake` by adding a funcion like we did before. We need to include a `ClangFormat.cmake` file:

```
function(ClangFormat target directory)
    find_program(CLANG-FORMAT_PATH clang-format REQUIRED)

    # define a list of suffixes for files ot be considered
    set(EXPRESSION h hpp hh c cc cxx cpp)
    # prepend the directory to the list
    list(TRANSFORM EXPRESSION PREPEND "${directory}/*.")

    # create list of files to format recuresivly and following symboloc links
    file(GLOB_RECURSE SOURCE_FILES FOLLOW_SYMLINKS
        LIST_DIRECTORIES false ${EXPRESSION}
    )

    # Add command to run clang-format on list of files before build
    add_custom_command(TARGET ${target} PRE_BUILD COMMAND
        ${CLANG-FORMAT_PATH} -i --style=Google ${SOURCE_FILES}
    )
endfunction()
```

Then we need to add the following lines to the `CMakeLists.txt` in the `project` and `src` directorys:

```
# in project one
include(Doxygen)
include(ClangFormat)

# in src one:
add_executable(main main.cpp)
ClangFormat(main .)
```

clang-tidy

Clang tidy also works on the command line, just like clang-format, on a file by file basis:

```
$ clang-tidy filename1.cpp -options...
```

We will again automate it with `cmake` is a similar fashion. First we create a function in a `ClangTidy.cmake` file:

```
function(ClangTidy target)
    find_program(CLANG-TIDY_PATH clang-tidy REQUIRED)

    set_target_properties(${target}
        PROPERTIES CXX_CLANG_TIDY
        "${CLANG-TIDY_PATH};-checks=clang-analyzer-*,
    bugprone-*,cppcoreguidelines-*,modernize-*,readability-*"
    )
endfunction()
```

analyzer and bugprone are pretty good the next threee are a bit opinionated so can be neglected. Then we include it and add the function to the relevent `CMakeLists.txt` files (it's not recursive on libraries so you have to add it everywhere):

```
# in project one
include(Doxygen)
include(ClangFormat)
include(ClangTidy)

# in src one:
add_executable(main main.cpp)
ClangTidy(main)
ClangFormat(main .)

# in src/harmonic one:
add_library(harmonic_lib
...
)
ClangTidy(harmonic_lib)
```

You have two other options you can add, `--warnings-as-errors=*` which wil cause the build to fail if there are any warnings (for those who want to be hardcore about it) and `--fix` which will make automated fixes for issues it finds (beware this is a little buggy)