## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure ar

Control flow

statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python

Summary

# Programming in FORTRAN Advanced computational methods II

Ioannis Begleris Hao Wang

April 24, 2015

### Outline

# Programming in FORTRAN

loannis Begleris Hao Wang

#### Introduction

Variables -

statement

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

#### 1 Introduction

- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Structure and Variables

Control flow

.

Subprogram

Read and writing

Fortran to Python interface

C......

### 1 Introduction

- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

### What is all this about?

# Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Structure and Variables

Control flow statements

Array

Subprograms

Read and writing from/to file

Fortran t Python interface

Summary

#### What is FORTRAN?

- 1 Short for FORmula TRANslator
- Compiled language
- 3 Very widely used (even if you don't realise it)
- 4 60 years old, with 'minor' changes every once in a while

### Why learn FORTRAN?

- 1 Its FAST!
- 2 Well structured
- 3 Many good old codes are written in FORTRAN
- 4 Can easily be linked to high level languages like Python

# A little history

### Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Variables
Control flow

statements

C 1 .....

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

- The first FORTRAN compiler was released in 1957
- FORTRAN had many releases important ones include F77, F90 and F95
- Until F90 was released FORTRAN operated in fixed form i.e. every command had to be given after six spaces.
- There are some new FORTRAN compilers out there recently released by Intel but have not had a wide acceptance and will not be mentioned any further

# Editor and Compiler

### Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Structure and Variables

Control flow

Array

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

#### Editor

- Any editor can be used
- For the practical we will use gedit
- A FORTRAN script can saved by either .f or .f90 or .f95 depending the version its written for

### Compiler

- The gfortran compiler (comes with gcc)
- Compile for equivalent releases you want to run.
- example for FORTRAN95: compile: f95 hello.f95 -o hello run: ./hello

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

#### Structure and Variables

Variables

statemen

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summai

1 Introduction

2 Structure and Variables

3 Control flow statements

4 Arrays

5 Subprograms

6 Read and writing from/to file

7 Fortran to Python interface

8 Summary

### Structure

Programming in FORTRAN

loannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

statements

Subprogrami

Read and writing from/to file

Fortran to Python interface

Summary

### Program:structure.f90

PROGRAM Structure

[Variable declarations]

...

[code]

. . .

END PROGRAM

Every piece of code written in FORTRAN must have a main program to compile. This is equivalent to a main function in C.

Each variable used needs to be declared before use.

### Structure Example

Programming in FORTRAN

loannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

\_ .

Read and writing

Fortran to Python interface

Summar

### Program: hello.f90

```
program Hello
    ! This program says hello
    print *, "Hello World!"
end program
```

- The asterisk following the keyword print tells the computer that the programmer will not be specifying the exact format of the printed answer. The default format, also called a list-directed format, is used.
- Comments are specified with !
- Strings are given between " "

### Variable declaration

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

statements

A .....

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

### Variable types

- INTEGER
- REAL 6 digits precision
- DOUBLE PRECISION 15 digits precision
- LOGICAL -takes values TRUE or FALSE
- COMPLEX

### Implicit types

FORTRAN has types auto assigned to variables:

If the first letter is i, k, I, m or n then be default they are set to type INTEGER, Otherwise they are set to type REAL. This can get confusing and you should turn it off at the start off the program with IMPLICIT NONE

# Variable declaration Example

# Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables

stateme

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

```
Program:First program.f90
```

```
PROGRAM Define

Real :: a

INTEGER:: b

DOUBLE PRECISION :: c

READ*, a,b,c

c = a**b

print*, c

END PROGRAM
```

# Variable declaration

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summarv

### Program:First program.f90

```
PROGRAM Define
```

Real,parameter :: a=3

INTEGER,parameter:: b=4

DOUBLE PRECISION :: c

c = a\*\*b

print\*, c

END PROGRAM

# Logical expressions

Between numbers

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow statements

Arrays

Subprogram

Read and writing from/to file

Fortran t Python interface

Summary

#### A logical expression can be either TRUE or FALSE

Relation operators			
FORTRAN 77	FORTRAN 95	Equivalent	
.LT.	<	less than	
.LE.	<=	less than or equal to	
.GT.	>	greater than	
.GE.	>=	greater than or equal to	
.EQ.	==	equal to	
.NE.	/=	not equal to	

# Logical expressions Between Logicals

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

C...b.....

Read and writing

Fortran to Python interface

Summary

#### A logical expression can be either TRUE or FALSE

Relation operators			
Operator	Equivalent bool	Priority	
.AND.	and	left to right	
.OR.	or	left to right	
.NOT.	not	right to left	
.EQV.	equivalent to	left to right	
.NEQV.	not equivalent to	left to right	

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure a

Variables
Control flow

statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

- 1 Introduction
- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

# Control flow statements IF statement

# Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure a

Control flow

statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

```
IF structure

IF ('Logical expression') THEN

...

ELSE IF ('Logical expression') THEN

...

ELSE

...

END IF
```

### Control flow statements

IF statement: example

# Programming in FORTRAN

loannis Begleris Hao Wang

Introduction

Control flow

statements

Array:

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

```
sorting.f90
```

```
PROGRAM sort
   IMPLICIT NONE
   INTEGER:: a, b
   READ*, a
   READ*, b
   IF (a==b) THEN
       PRINT*, "a=b"
   ELSE IF (a>b) THEN
      PRINT*, "a>b"
   ELSE
      PRINT*, "a<b"
   END IF
END PROGRAM
```

# Control flow statements DO statement

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introductio

Structure a

Control flow

### statements

Arrays

Subprograms

Read and writing from/to file

Fortran t Python

Summary

#### DO structure

```
DO i= start,fin,step
...
END DO
```

- i will firstly take the value of start
- at each loop step will be added to i
- $\blacksquare$  until i >= end
- Equivalent to for loops

### Control flow statements

DO statement: example

```
Programming in FORTRAN
```

Ioannis Begleris Hao Wang

Introductio

Structure a

Control flow

statements

Array:

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

#### loop1.f90

```
PROGRAM loop
IMPLICIT NONE
INTEGER:: a
DO a=1,5,3 ! from 1 to 5 in steps of 3
PRINT*,"a=",a
END DO
END PROGRAM
```

This will print to the output:

a=1

a=4

# Control flow statements DO WHILE statement

# Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Structure ar

Control flow

statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python

Summary

#### DO WHILE structure

```
DO WHILE ('Logical expression')
...
END DO
```

- The statements within the loop will run untill the logical expression is false
- Equivalent to while loops

# Control flow statements

DO WHILE statement: example

```
Programming in FORTRAN
```

loannis Begleris Hao Wang

Introductio

Structure a

Control flow

statements

Allays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summai

### loop2.f90

```
PROGRAM loop_while
IMPLICIT NONE
INTEGER:: a
a=1
DO WHILE (a<=5)
PRINT*,"a=",a
a=a+3
END DO
```

This will print to the output:

END PROGRAM

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure an

Variables

Arrays

Subprogram

Supprogram

Read and writing from/to file

Fortran to Python interface

Summai

- 1 Introduction
- 2 Structure and Variables
  - 3 Control flow statements
  - 4 Arrays
  - 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

# Arrays in FORTRAN

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure an Variables

Control flow

Arrays

C...b......

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

#### Some Definitions

- FORTRAN arrays start from 1
- Support colon notation
- Like in C you should initialise the array before use

### Arrays Declare Arrays

### Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Variables

Control flow statements

#### Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

- A type declaration statement to declare the type and the number of the elements contained in the array.
- An array can be of any type: real, integer, logical, or double precision

#### Declaration statement

```
REAL, DIMENSION(16):: voltage
INTEGER, DIMENSION(2,4):: index
LOGICAL, DIMENSION(2):: temp
DOUBLE PRECISION, DIMENSION(3,2):: length
```

# Programming in FORTRAN

Begleris Hao Wang

#### Introductio

Variables

Control flow

#### Arrays

Subprograms

Read and writing

Fortran to Python interface

Summary

#### Initialise arrays with assignment statement

### Arrays Initialise Arrays

## Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introductio

Variables

Control flow statements

#### Arrays

Subprograms

Read and writing from/to file

Fortran to Python

Summarv

### Initialise arrays in type declaration statements

```
INTEGER:: i,j
```

```
REAL, DIMENSION(100) :: array1=1.
```

INTEGER, DIMENSION(5) :: array2=&

(/1, 2, 3, 4, 5 /)

INTEGER, DIMENSION(5) :: array3=(/(i, i=1, 5)/)

# Programming in FORTRAN

loannis Begleris Hao Wang

Introductio

Structure and Variables

Variables

#### Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

### Initialise Rank-2 arrays with assignment statement

```
INTEGER, DIMENSION(4, 3) :: array1
D0 i = 1.4
  D0 j = 1,3
  array1(i, j)=j
  END DO
END DO
! OR.
D0 j = 1,3
  array1(:, j)=j
END DO
!\Omega R
array1 = &
```

### Arrays 2-D or Rank-2 Arrays

# Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introductio

Variables

Control flow

#### Arrays

Subprograms

Read and writing from/to file

Fortran to Python

Summar

### Initialise Rank-2 arrays in type declaration statements

```
INTEGER, DIMENSION(4, 3) :: array1(4, 3)=&
RESHAPE((/1,1,1,1,2,2,2,2,3,3,3,3/), (/4,3/))
```

### Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure ar

Control flow

statemen

Arrays

Subprograms

Read and writing from/to file

Fortran t Python interface

Summary

If two arrays are the same shape, you can use them in ordinary arithmetic operations and the operation will be applied on an element-by-element basis.

### Whole Array Operation

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables -

.

Subprograms

Supprograms

Read and writing from/to file

Fortran to Python interface

Summar

- 1 Introduction
- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

# Subprograms Functions

### Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables

statemen

 ${\sf Subprograms}$ 

Read and writing from/to file

Fortran to Python interface

Summar

- A function takes in a number of arguments and returns one value
- The value that is returned has the name of the function.
- A function can be an INTEGER, REAL, COMPLEX, LOGICAL, DOUBLE PRECISION
- FORTRAN has some functions inbuilt, ex SIN(x)
- when a function is used, it needs to be declared in the main program as an external function Example: integer, external :: fun

# Subprograms Functions: structure

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

Arrays

Subprograms

Supprograms

Read and writing from/to file

Fortran to Python interface

Summary

### **Function**

```
'Type' FUNCTION NAME(args)
VARIABLE DECLARATIONS
```

```
...
```

name =  $\dots$ 

END FUNCTION NAME

# Subprograms Functions: Example

### Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and Variables

Control flow

Arraye

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

#### **Function**

```
PROGRAM CALCULATION
    IMPLICIT NONE
    DOUBLE PRECISION, EXTERNAL :: trig
    REAL :: x, y, z
    x=1
    \Delta = 0
    z=trig(x,y)
END PROGRAM
DOUBLE PRECISION FUNCTION trig(x,y)
    REAL x, y
    trig = sin(x) * tan(y)
END FUNCTION trig
```

# Subprograms

#### Subroutines

### Programming in FORTRAN

loannis Begleris Hao Wang

#### Introductio

Variables

statements

Array:

#### Subprograms

Read and writing from/to file

Fortran t Python interface

Summary

- A Subroutine is equivalent to void functions in C.
- Input arguments, makes calculations upon them and returns them
- Specify the intent of the arguments in the declaration part within the subroutine
- The subroutine is used by using the CALL command in the main program function
- The intent of each variable should to be stated at the subroutine's variable declarations
- these can be
  - intent(in)
  - intent(out)
  - intent(inout)

# Subprograms

Subroutine: Structure

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Variables

Control flow

Λ ........

Allays

 ${\sf Subprograms}$ 

Read and writing from/to file

Fortran to Python

Summary

#### Subroutine

SUBROUTINE NAME(args)

VARIABLE DECLARATIONS

...

END FUNCTION NAME



## Subprograms

Subroutines: Example

```
Programming in FORTRAN
```

Ioannis Begleris Hao Wang

Introductio

Structure and Variables

Control flow

.

. ... = , =

#### Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

### Subroutine

```
PROGRAM CALCULATION

IMPLICIT NONE

EXTERNAL :: trig

REAL x, y, z

x= 7; y = 9

CALL trig(x,y,z)

END PROGRAM
```

SUBROUTINE trig(x,y,z)
 IMPLICIT NONE
 REAL, INTENT(IN):: x, y
 REAL, INTENT(OUT):: z
 z = sin(x) \* tan(y)

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables

statemen

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summari

- 1 Introduction
- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

# Opening files

### Programming in FORTRAN

Ioannis Begleris Hao Wang

#### Introduction

Control flow

statements

Allays

Subprograms

Read and writing from/to file

Fortran t Python

Summar

- To read and write to/from a file it needs to be opened
- The action that is going to be taken needs to be stated
- Opening needs to have a unit associated with it
- Units can be any integer except 0,5 and 6
- The file should be closed after work is done

# Open and Read

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Variables

Control flow statements

Arravo

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

### Initialise arrays with FORTRAN READ statements

Assume a file initial.dat contains the values:

 $1\; 1\; 1\; 1\; 2\; 2\; 2\; 2\; 3\; 3\; 3\; 3$ 

```
INTEGER, DIMENSION(4,3) :: array1
OPEN (7, file='initial.dat', action='read')
READ (7, *) array1
CLOSE(7)
```

# Open and write

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Variables

Control flow statements

Statemen

C...b......

Read and writing from/to file

Fortran to Python

Summarv

### Initialise arrays with FORTRAN READ statements

Assume a file initial.dat contains the values:

1 1 1 1 2 2 2 2 3 3 3 3

```
INTEGER, DIMENSION(4,3) :: array1
OPEN (7, file='initial.dat', action='write')
WRITE (7, *) array1
CLOSE(7)
```

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables -

statemer

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

- 1 Introduction
- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

### Motivation

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introductio

Variables

Control flow statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

There are many codes that are already written in FORTRAN and may needed to be run as part of a code in a high level language.

- MEX files with Matlab (not covered)
- f2py in python

### f2py FORTRAN 2 Python interface

### Programming in FORTRAN

loannis Begleris Hao Wang

#### Introduction

Structure and Variables

### statements

Allay.

#### Subprograms

Read and writing from/to file

#### Fortran to Python interface

Summary

f2py allows the conversion of FORTRAN functions and subroutines in to python modules which can be imported and called when needed.

- Command line
- Comes with Numpy
- Allows values to be passed back to Python and called again
- Supports Numpy arrays
- runs from terminal
- can support C++ conversion

In general when the compiler is not specified f2py will try and compile FORTRAN77 failing that it will try FORTRAN90 and finally it will try C++

### How to use

### Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Control flow

Control flow statements

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summar

Suppose there is a file Process.f which contains functions and subroutines

To create the Python module:

- f2py -c process.f -m modulename
- This can then be called from python as:
  - import modulename
  - Use the functions and subroutines when needed as you would in Python
  - example: modulename.function(10.)
- There are various options and tweaks to f2py that can be found by typing f2py in terminal

### Outline

## Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Structure and

Variables

statement

Arrays

Subprograms

Read and writing from/to file

Fortran to Python interface

Summary

- 1 Introduction
- 2 Structure and Variables
- 3 Control flow statements
- 4 Arrays
- 5 Subprograms
- 6 Read and writing from/to file
- 7 Fortran to Python interface
- 8 Summary

# Summary

Programming in FORTRAN

Ioannis Begleris Hao Wang

Introduction

Control flow

Control flov statements

Array

Subprograms

Read and writing from/to file

Fortran to Python

Summary

- Structure of FORTRAN
- Variables
- Control flow statements
- Subprograms
- Reading and writing from/to a file
- FORTRAN to Python interface