Introduction to Fortran 90

Abishek Gopal

TAMU Oceanography & HPRC

Texas A&M HPRC Short Course

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Slides adapted from Jian Tao’s Spring 21 Fortran course
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Section 1

Introduction
Hello World in Fortran

Source code helloworld.f90

```fortran
program hello
    print *, 'Hello World!'
end program hello
```

Compile and run

```
gfortran -o helloworld helloworld.f90
./helloworld
Hello World!
```
What is Fortran?

- Fortran (formerly FORTRAN, derived from FORMula TRANslation) is a general-purpose, imperative programming language that is especially suited to numeric computation and scientific computing.
- Originally developed by IBM in the 1950s for scientific and engineering applications.
- Widely used in computationally intensive areas such as numerical weather prediction, finite element analysis, etc.
- It has been a popular language for high-performance computing and is used for programs that benchmark and rank the world’s fastest supercomputers.
Why still learn Fortran?

- Well suited for scientific computing - A majority of scientific codes use Fortran.
- Second to none in terms of execution speed. Performance comparable to C.
- Very convenient array handling for scientific codes
- Actively supported by Intel, GNU, PGI, etc
- Optimized numerical libraries available for Fast Fourier Transforms, Linear Algebra, etc
- Can scale on hundreds of thousands of cores with MPI + OpenMP parallelization
Section 2

Basics of Fortran 90 Language
Compiler - from Wikipedia

A compiler is a computer program (or a set of programs) that transforms source code written in a programming language (the source language) into another computer language (the target language), with the latter often having a binary form known as object code. The most common reason for converting source code is to create an executable program.

The FORTRAN team led by John Backus at IBM introduced the first unambiguously complete compiler in 1957.

Some popular Fortran compilers

GNU Fortran(gfortran), Intel Fortran(ifort), G95(g95), IBM(xlf90), Cray(ftn), Portland Group Fortran (pgf90)
Typical Fortran program structure

```
PROGRAM program-name
IMPLICIT NONE
[specification part]
[execution part]
[subprogram part]
END PROGRAM program-name
```

The **PROGRAM** statement (optional) gives a name to the program. The first character of the name must be a letter. Use the **IMPLICIT NONE** statement to avoid implicit typing rules. The **END** statement terminates the program and returns control to the computer’s operating system.
A Basic Fortran Example

Square of a number

```
PROGRAM square
!
 IMPLICIT NONE
 REAL :: x, x_sq

WRITE (* ,*) 'Enter the value of x:'
READ (* ,*) x

y = x**2
WRITE (* ,*) 'The square of x is:', y

END PROGRAM square
```
Fortran 90 and later versions support free format source code.

- Fortran source code is in ASCII text and can be written in any text editor.

- Fortran source code is case **insensitive**. PROGRAM is the same as Program and pRoGrAm.

- Use whatever convention you are comfortable with and be consistent throughout.

- Comments in Fortran 90 source code start with an exclamation mark (!) except in a character string. Comments help to enhance the readability of your code.
A statement is a complete instruction. Statements may be classified into two types: executable and non-executable.

- Executable statements are those which are executed at runtime.
- Non-executable statements provide information to compilers.
- If a statement is too long, it may be continued by the ending the line with an **ampersand (*)&.**
- Max number of characters (including spaces) in a line is 132 though it’s standard practice to have a line with up to 80
- Multiple statements can be written on the same line provided the statements are separated by a semicolon.
Variables

Variables are the fundamental building blocks of any program

- A variable name may consist of up to 31 alphanumeric characters and underscores, of which the first character must be a letter.
- There are no reserved words in Fortran.
- Variable names must begin with a letter and should not contain a space.
Variable Types

Intrinsic data types

- INTEGER: exact whole numbers
- REAL: real, fractional numbers
- COMPLEX: complex, fractional numbers
- LOGICAL: boolean values
- CHARACTER: strings

Users can define additional types.

- REAL is a single-precision floating-point number.
- FORTRAN provides DOUBLE PRECISION data type for double precision REAL. This is obsolete but is still found in many programs.
Basics of Fortran 90 Language

Contants - I

Integer

242, -2341, 290223

Real (single precision)

1.03, 3.51e23, -8.201

Real (double precision)

1.03d0, 3.51d23, -8.201d0
Constants - II

Complex (single precision)

\((1.0, 0.0), (-2.5e-5, 3.0e-6)\)

Complex (double precision)

\((1.0d0, 0.0d0), (-2.5d-5, 3.0d-6)\)

Logical

\. True ., . False .

Character

"Hello World!", "Is pi 3.1415926?"
Implicit typing of variables

**IMPLICIT DOUBLE PRECISION (a-h,o-z)**

- it is highly recommended to explicitly declare all variable and avoid implicit typing using the statement.

**IMPLICIT NONE**

- the IMPLICIT statement must precede all variable declarations.
Numerical variables

```
INTEGER :: i, j = 2
REAL :: a, b = 4.d0
COMPLEX :: x, y
```

Constant variables

```
INTEGER, PARAMETER :: j = 2
REAL, PARAMETER :: pi = 3.14159265
COMPLEX, PARAMETER :: ci = (0.d0,1.d0)
```
Logical variables

LOGICAL :: l, flag=.true.

Character variables

The length of a character variable is set with LEN, which is the maximum number of characters (including space) the variable will store. By default, LEN=1 thus only the first character is saved in memory if LEN is not specified.

CHARACTER (LEN=10) :: a
CHARACTER :: ans = 'yes' ! stored as ans='y'
Operators

Arithmetic Operators

+ , −, *, /, **

Relational Operators

==, <, <=, >, >=, /=

Logical Operators

.AND., .OR., .NOT., .EQV., .NEQV.

Character Concatenation Operator

//
Expressions

An expression is a combination of one or more operands, zero or more operators, and zero or more pairs of parentheses.

**Arithmetic expressions**

\[ y + 1.0 - x, \sin(x) + y \]

**Relational expressions**

\[ a \ .\ and\ .\ b, c \ .\ neqv\ .\ d \]

**Character expressions**

\[ 'hello' \ // \ 'world', 'ab' \ // \ 'xy' \]
Operator Precedence

- All operator evaluations on variables is carried out from left-to-right.
- Arithmetic operators have a highest precedence while logical operators have the lowest precedence.
- The order of operator precedence can be changed using parenthesis, '()' and ')
- Users can define their own operators.
- Extra parenthesis could be added to enhance readability and avoid mistakes.
Fortran provides many commonly used functions, called intrinsic functions.

**Numerical functions**

```fortran
ABS(A), CEILING(A), FLOOR(A), MAX(A,B),
MIN(A,B), MOD(I,J), SQRT(A), EXP(A), LOG(A),
LOG10(A), INT(A), REAL(A), DBLE(A),
CMPLX(A[,B]), AIMAG(A)
```

**Math functions**

```fortran
SIN(A), COS(A), TAN(A), ASIN(A),
ACOS(A), ATAN(A), ATAN2(A,B), SINH(A),
COSH(A), TANH(A)
```
Character functions

LEN(S), LEN_TRIM(S), LGE(S1,S2), LGT(S1,S2),
LLE(S1,S2), LLT(S1,S2), ADJUSTL(S),
ADJUSTR(S), REPEAT(S, N), SCAN(S, C), TRIM(S)

Array functions

SIZE(A[,N]), SUM(A[,N]), PRODUCT(A[,N]),
TRNSPOSE(A), DOT_PRODUCT(A,B), MATMUL(A,B),
CONJG(X)
Exercise

Write a short Fortran program to convert 10 Celsius to Fahrenheit, and 40 Fahrenheit to Celsius.

The expressions to convert between the two are given below:

\[ T(F) = \frac{9}{5} T(C) + 32 \]

\[ T(C) = \frac{5}{9} (T(F) - 32) \]
Section 3

Control Structures
A Fortran program is executed sequentially. Control Constructs change the sequential execution order of the program.

- **Conditionals:** `IF`, `IF-THEN-ELSE`
- **Switches:** `SELECT/CASE`
- **Loops:** `DO`
- **Branches:** `GOTO` (obsolete in Fortran 95/2003, use `CASE` instead)
IF construct

if ( expression ) statement

IF THEN ELSE construct

if ( expression 1 ) then
    executable statements
else if ( expression 2 ) then
    executable statements
else
    executable statements
end if
**Conditionals - IF Example**

**IF construct**

```java
if (value < 0) value = 0
```

- When the if statement is executed, the logical expression is evaluated.
- If the result is true, the statement following the logical expression is executed; otherwise, it is not executed.
- The statement following the logical expression cannot be another if statement. Use the if-then-else construct instead.
Conditionals - IF-THEN-ELSE Example

IF THEN ELSE construct

```java
if ( x < 50 ) then
    GRADE = 'F'
else if ( x >= 50 .and. x < 60 ) then
    GRADE = 'D'
else if ( x >= 60 .and. x < 70 ) then
    GRADE = 'C'
else if ( x >= 70 .and. x < 80 ) then
    GRADE = 'B'
else
    GRADE = 'A'
end if
```
Exercise

The roots of a quadratic equation \( ax^2 + bx + c = 0 \) are given by:

\[
q_1 = \frac{1}{2a} (-b + \sqrt{b^2 - 4ac})
\]

\[
q_2 = \frac{1}{2a} (-b - \sqrt{b^2 - 4ac})
\]

Write a Fortran program to read in (or assume) the coefficients \( a, b \) and \( c \), and then compute the roots of the corresponding equation. Using an if clause, check that the discriminant \( b^2 - 4 \times a \times c \) is positive before doing the computation, otherwise print that the roots are complex and exit.
SELECT CASE construct

```plaintext
[case_name:] select case ( expression )
  case ( selector )
    executable statement
  case ( selector )
    executable statement
  case default
    executable statement
end select [case_name]
```

The value of the expression in the select case should be an integer or a character string. The case name is optional.
Character case selector

```plaintext
select case ( traffic_light )
    case ( "red" )
        print *, "Stop"
    case ( "yellow" )
        print *, "Caution"
    case ( "green" )
        print *, "Go"
    case default
        print *, "Illegal value: ", traffic_light
end select
```
Integer case selector

```
select case ( score )
    case ( 50 : 59 )
        GRADE = "D"
    case ( 60 : 69 )
        GRADE = "C"
    case ( 70 : 79 )
        GRADE = "B"
    case ( 80 : )
        GRADE = "A"
    case default
        GRADE = "F"
end select
```
DO construct

\[
[\text{do name:}] \text{ do loop_control} \\text{ execution statements} \\text{end do [do name]}
\]

The do loop name is optional. To exit the do loop, use the **EXIT** or **CYCLE** statement.

- The **EXIT** statement causes termination of execution of a loop.
- The **CYCLE** statement causes termination of the execution of one iteration of a loop.
Factorial with DO construct

```plaintext
program factorial1
  implicit none
  integer(KIND=8) :: i, factorial, n=6
  factorial = n
  do i = n-1, 1, -1
    factorial = factorial * i
  end do
  write(*, '(i4,a,i15)') n, '!= ', factorial
end program factorial1
```
If a condition is to be tested at the top of a loop, a do ... while loop can be used

**DO WHILE** construct

```plaintext
[do name:] do while ( expression )
    executable statements
end do [do name]
```

The loop only executes if the logical expression is `.TRUE.`.
DO WHILE example

finite: do while ( i <= 100 )
    i = i + 1
    inner: if ( i < 10 ) then
        print *, i
    end if inner
end do finite
Exercise

We know that the summation of the first $n$ positive integers is given by the arithmetic sequence formula

$$1 + 2 + 3 + \ldots + n = \sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$

Write a Fortran program that uses a do loop to compute the sum of the first $n$ integers. You may assume a value of $n$, or read in as input. After computing the sum, use an if clause to compare the computed sum with the expected value (RHS), and print an affirmation to the output.
15 minute break
Section 4

Program Sub-units
Typical Fortran program structure

```fortran
PROGRAM program-name
  IMPLICIT NONE
  [specification part]
  [execution part]
  [subprogram part]
END PROGRAM program-name
```

The `PROGRAM` statement (optional) gives a name to the program. The first character of the name must be a letter. Use the `IMPLICIT NONE` statement to avoid implicit typing rules. The `END` statement terminates the program and returns control to the computer’s operating system.
A Fortran program can consist of one or more program sub-units, **SUBROUTINE, FUNCTION, MODULE**. Why?

- Break down a complex program into smaller, coherent units
- To avoid repeating code blocks
- Allow "Unit" testing and debugging
- Enhance code readability
Temperature Conversion between Fahrenheit and Celsius

```plaintext
program temp
    implicit none
    real :: tempC, tempF
    ! Convert 10C to fahrenheit
    tempF = 9.0 / 5.0 * 10.0 + 32.0
    ! Convert 40F to celsius
    tempC = 5.0 / 9.0 * (40.0 - 32.0)
    call display(tempc, tempF)
end program temp
```

Typical Fortran subroutine structure

```fortran
SUBROUTINE subroutine-name (dummy arguments)
  IMPLICIT NONE
  [specification part]
  [execution part]
  [subprogram part]
END SUBROUTINE subroutine-name
```
CALL Statement:
- The CALL statement evaluates its arguments and transfers control to the subroutine.
- Upon return, the next statement is executed.

SUBROUTINE Statement:
- The SUBROUTINE statement declares the procedure and its arguments.
- These are also known as dummy arguments.

The subroutine’s interface is defined by
- The subroutine statement itself
- The declarations of its dummy arguments
- Anything else that the subroutine uses
A Subroutine Example

Calculate the sum of input variables

SUBROUTINE calc(a,b,c)
    IMPLICIT NONE
    real :: a,b,c
    c = a + b
    return
END SUBROUTINE calc
Fortran functions operate on the same principle as subroutines. The only difference is that function returns a value and does not involve the call statement.

**Calculate the sum of the input variables**

```
FUNCTION calc(a,b)
    IMPLICIT NONE
    real :: a,b,calc
    calc = a + b
END FUNCTION calc
```
Subroutine definition

SUBROUTINE calc(a,b,c)
  IMPLICIT NONE
  real :: a,b,c
  c = a + b
END SUBROUTINE calc

Function definition

FUNCTION calc(a,b)
  IMPLICIT NONE
  real :: a,b,calc
  calc = a + b
END FUNCTION calc

Subroutine call

CALL calc(x,y,z)

Function call

z = calc(x,y)
A module is a program unit whose functionality can be exploited by other programs which attaches to it via the \textbf{USE} statement.

\begin{verbatim}
MODULE mymod
IMPLICIT NONE
integer, parameter :: dp = 8
CONTAINS

  FUNCTION calc(a,b)
    IMPLICIT NONE
    real :: a, b, calc
    calc = a + b
  END FUNCTION calc

END MODULE mymod
\end{verbatim}

\begin{verbatim}
PROGRAM test
  USE mymod
  IMPLICIT NONE
  REAL(KIND=dp) :: x, y, z
  z = calc(x, y)
END PROGRAM test
\end{verbatim}
Exercise

We already computed the roots of a quadratic equation as:

\[ q = \frac{1}{2a}(-b \pm \sqrt{b^2 - 4ac}) \]

Convert your previous Fortran program to use subroutines. The main program should read in (or assume) the coefficients \(a\), \(b\) and \(c\), and then call the subroutine as:

```fortran
CALL quad_roots(a,b,c, q1, q2, is_complex)
```

where \(q1\) and \(q2\) are the output roots of type REAL, and \texttt{is\_complex} is an output boolean variable that specifies if roots are real or complex.
Section 5

Array Handling
Arrays (or matrices) hold a collection of different values at the same time. Individual elements are accessed by subscripting the array. Fortran arrays are defined with the keyword `DIMENSION(lower bound: upper bound)`

**Arrays**

```
INTEGER, DIMENSION(1:106) :: atomic_number
REAL, DIMENSION(3, 0:5, -10:10) :: values
CHARACTER(LEN=3), DIMENSION(12) :: months
```

In Fortran, arrays can have up to seven dimensions. Fortran arrays are column major.
Array Handling

Row Major vs Column Major

Row-major order

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

Column-major order

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

In Fortran

\[
\begin{bmatrix}
1 \\
2 \\
3 \\
4 \\
5 \\
6 \\
7 \\
8 \\
9
\end{bmatrix} =
\begin{bmatrix}
a_{11} \\
a_{21} \\
a_{31} \\
a_{12} \\
a_{22} \\
a_{32} \\
a_{13} \\
a_{23} \\
a_{33}
\end{bmatrix}
\]

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Arrays in use

\[ y = Ax = \sum_{j=1}^{N} a_j x_j \]

\[
\begin{bmatrix}
  y_1 \\
  y_2 \\
  y_3
\end{bmatrix} =
\begin{bmatrix}
  a_{11} & a_{12} & a_{13} & a_{14} \\
  a_{21} & a_{22} & a_{23} & a_{24} \\
  a_{31} & a_{32} & a_{33} & a_{34}
\end{bmatrix}
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3 \\
  x_4
\end{bmatrix}
\]

INTEGER :: m = 3, n = 4, i, j
REAL :: A(m,n), x(n), y(m)

y = 0.0
do j = 1, n
  y(:) = y(:) + A(: ,j)*x(j)
end do
Section 6

Input and Output in Fortran
Simple I/O

Any program needs to be able to read input and write output to be useful and portable.

**Simple output with PRINT**

```fortran
print *, <var1> [, <var2> [, ... ]]
```

**Simple input with READ**

```fortran
read *, <var1> [, <var2> [, ... ]]
```

The * indicates that the data is unformatted.
Interactive hello world via I/O

PROGRAM hello
   IMPLICIT NONE
   character(len=100) :: your_name
   print *, 'Your Name Please'
   read *, your_name
   print *, 'Hello ', your_name
END PROGRAM hello
Files are identified by some form of file handle, in Fortran called the unit number.

- The default unit number 5 is associated with the standard input,
- Unit number 6 is assigned to standard output.

**Read and write through unit number**

```fortran
read(unit,*)
write(unit,*)
```
Fortran provides functions to open, read, write, inquire, and close files. A file may be opened with the statement

\begin{verbatim}
OPEN([UNIT=]un, FILE=fname [, , options])
READ(un, options)varlist
WRITE(un, options)varlist
INQUIRE([UNIT=]un, options)
CLOSE([UNIT=]un [, , options])
\end{verbatim}
If data is read/written from/to standard input/output, then
- the unit number can also be replaced with *.
- use alternate form for reading and writing i.e. the READ *, and PRINT start mentioned earlier.
- If data is unformatted i.e. plain ASCII characters, the option to WRITE and READ command is *.
A formatted data description must adhere to the generic form: 
\[ nCw.d \]

- \( n \) is an integer constant that specifies the number of repetitions (default 1 can be omitted),
- \( C \) is a letter indicating the type of the data variable to be written or read,
- \( w \) is the total number of spaces allocated to this variable, and,
- \( d \) is the number of spaces allocated to the fractional part of the variable. Integers are padded with zeros for a total width of \( w \) provided \( d \leq w \).
- The decimal (.) and \( d \) designator are not used for integers, characters or logical data types.
In the simplest form, the format is enclosed in single quotes and parentheses as argument to the keyword.

```fortran
print '(I5,5F12.6)', i, a, b, c, z ! complex z
write(6, '(2E15.8)') arr1, arr2
read(5, '(2a)') firstname, lastname
```

If the same format is to be used repeatedly or it is complicated, the FORMAT statement can be used. The `FORMAT` statement must be labeled and the label is used in the input/output statement to reference it.

```fortran
label FORMAT(formlist)
PRINT label, varlist
WRITE(un, label) varlist
READ(un, label) varlist
```
The **FORMAT** statements can occur anywhere in the same program unit. Most programmers list all **FORMAT** statements immediately after the type declarations before any executable statements.

**Format statement examples**

10  **FORMAT**(I5,5F12.6)
20  **FORMAT**(2E15.8)
100 **FORMAT**(2a)

`print 10, i, a, b, c, z ! complex z`

`write(6,20) arr1, arr2`

`read(5,100) firstname, lastname`
Section 7

Online Resources for Fortran
Numerical Recipes - http://numerical.recipes/

Lahey Fortran Resources -
http://www.lahey.com/other.htm