

Introduction to structured programming with Fortran

<https://forge.uclouvain.be/barriat/learning-fortran>



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CISM/CÉCI Training Sessions

Fortran : shall we start ?

- You already know one computer language ?
- You understand the very basic programming concepts :
 - What is a variable, an assignment, function call, etc. ?
 - Why do I have to compile my code ?
 - What is an executable ?
- You (may) already know some Fortran ?
- How to proceed from old Fortran, to much more modern languages like Fortran 90/2003 ?

Why to learn Fortran ?

- Because of the execution speed of a program
- Well suited for numerical computations :
more than 45% of scientific applications are in Fortran
- Fast code : compilers can optimize well
- Optimized numerical libraries available
- Fortran is a simple language and it is (kind-of) easy to learn

Fortran is simple

- **We want to get our science done! Not learn languages!**
- How easy/difficult is it really to learn Fortran ?
- The concept is easy:
variables, operators, controls, loops, subroutines/functions
- **Invest some time now, gain big later!**

History

FORMula TRANslation

invented 1954-8 by John Backus and his team at IBM

- FORTRAN 66 (ISO Standard 1972)
- FORTRAN 77 (1978)
- Fortran 90 (1991)
- Fortran 95 (1997)
- Fortran 2003 (2004) → "standard" version
- Fortran 2008 (2010)
- Fortran 2018 (11/2018)

Starting with Fortran 77

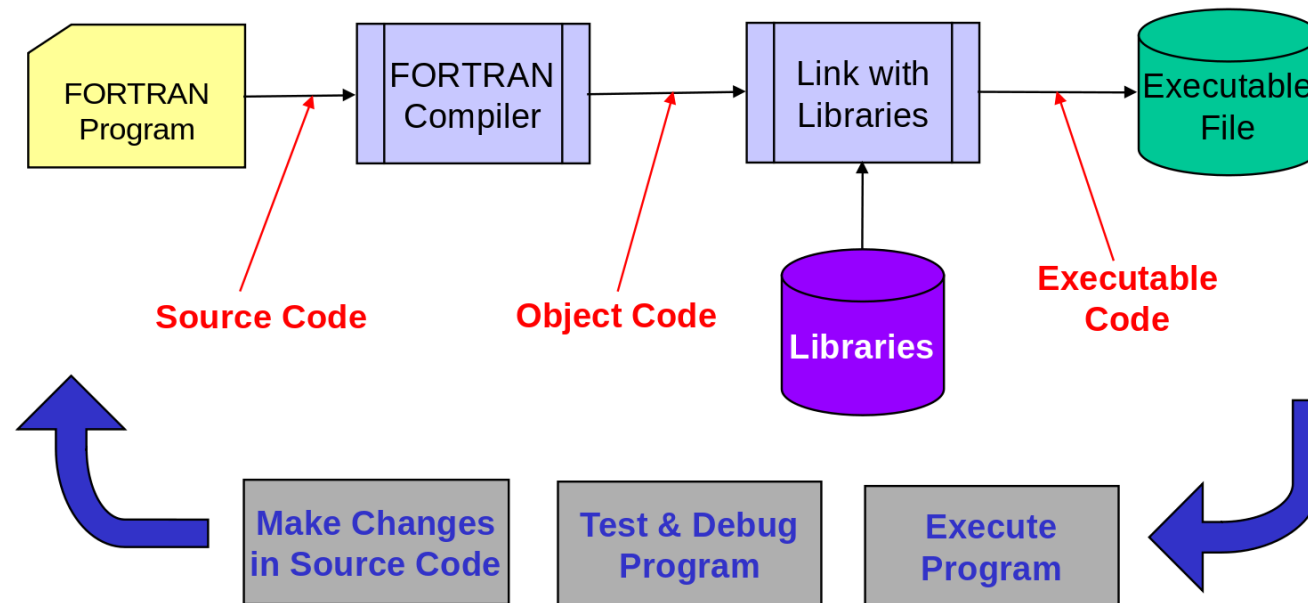
- Old Fortran provides only the absolute minimum !
- Basic features
 - data containers (integer, float, ...), arrays, basic operators, loops, I/O, subroutines and functions
- But this version has flaws
 - no dynamic memory allocation, old & obsolete constructs, "spaghetti" code, etc.
- Is that enough to write code ?

Fortran 77 → Fortran >90

- If Fortran 77 is so simple, why is it then so difficult to write good code ?
- Is simple really better ?
 - ⇒ Using a language allows us to express our thoughts (on a computer)
- A more sophisticated language allows for more complex thoughts
- More language elements to get organized
 - ⇒ Fortran 90/95/2003 (recursive, OOP, etc)

How to Build a FORTRAN Program

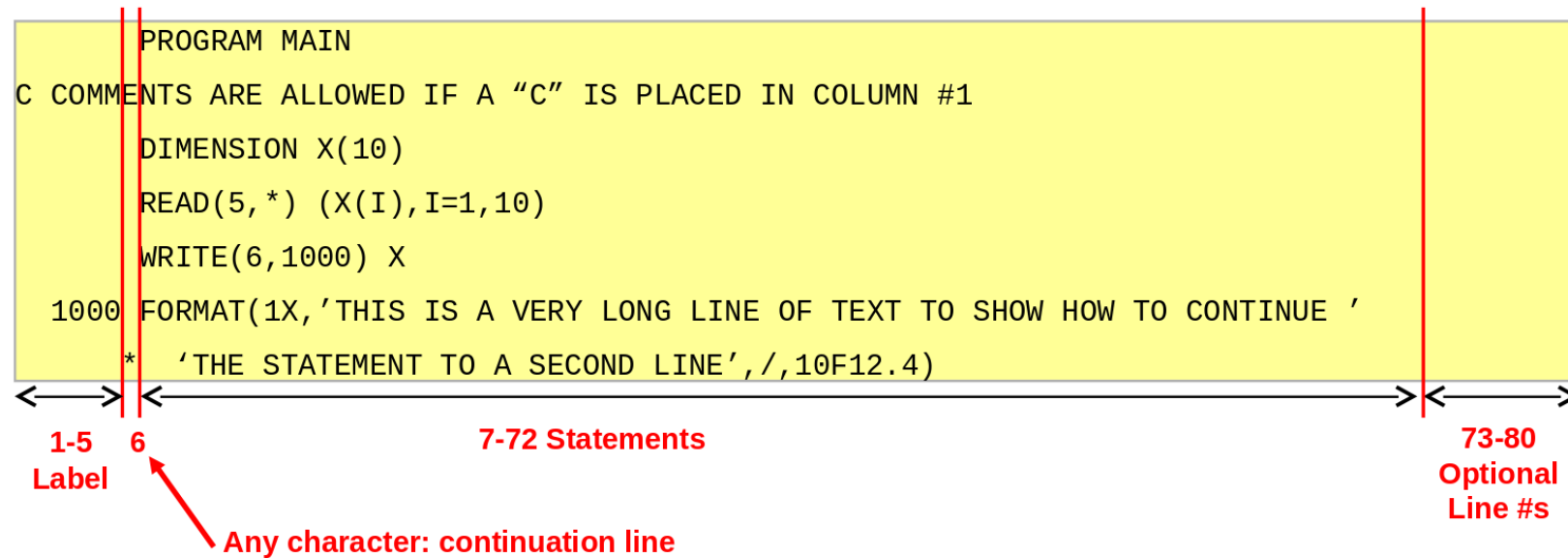
FORTRAN is a compiled language (like C) so the source code (what you write) must be converted into machine code before it can be executed (e.g. Make command)



Fortran 77 source code [hello_world.f](#)

FORTRAN 77 Format

This version requires a fixed format for programs



- max length variable names is 6 characters
- alphanumeric only, must start with a letter
- character strings are case sensitive

FORTRAN >90 Format

Versions >90 relaxe these requirements:

- comments following statements (`!` delimiter)
- long variable names (31 characters)
- containing only letters, digits or underscore
- max row length is 132 characters
- can be max 39 continuation lines
- if a line is ended with ampersand (`&`), the line continues onto the next line
- semicolon (`;`) as a separator between statements on a single line

Program Organization

Most `FORTRAN` programs consist of a main program and one or more subprograms

There is a fixed order:

```
Heading  
Declarations  
Variable initializations  
Program code  
Format statements  
  
Subprogram definitions  
(functions & subroutines)
```

Data Type Declarations

Basic data types are :

- `INTEGER` : integer numbers (+/-)
- `REAL` : floating point numbers
- `DOUBLE PRECISION` : extended precision floating point
- `CHARACTER*n` : string with up to **n** characters
- `LOGICAL` : takes on values `.TRUE.` or `.FALSE.`

Data Type Declarations

`INTEGER` and `REAL` can specify number of bytes to use

- Default is: `INTEGER*4` and `REAL*4`
- `DOUBLE PRECISION` is same as `REAL*8`

Arrays of any type must be declared:

- `DIMENSION A(3,5)` - declares a 3 x 5 array
- `CHARACTER*30 NAME(50)` - directly declares a `character` array with 30 `character` strings in each element

Implicit vs Explicit Declarations

By default, an implicit type is assumed depending on the first letter of the variable name:

- A-H, O-Z define REAL variables
- I-N define INTEGER variables

Can use the IMPLICIT statement:

```
IMPLICIT REAL (A-Z)
```

makes all variables REAL if not declared

Implicit vs Explicit Declarations

IMPLICIT CHARACTER*2 (W)

makes variables starting with W be 2-character strings

IMPLICIT DOUBLE PRECISION (D)

makes variables starting with D be double precision

Good habit: force explicit type declarations

IMPLICIT NONE

user must explicitly declare all variable types

Assignment Statements

Old assignment statement: `<label> <variable> = <expression>`

- `<label>` : statement label number (1 to 99999)
- `<variable>` : FORTRAN variable
(max 6 characters, alphanumeric only for standard FORTRAN 77)

Expression:

- Numeric expressions: `VAR = 3.5*COS(THETA)`
- Character expressions: `DAY(1:3) = 'TUE'`
- Relational expressions: `FLAG = ANS .GT. 0`
- Logical expressions: `FLAG = F1 .OR. F2`

Numeric Expressions

Arithmetic operators: precedence: `**` (*high*) → `-` (*low*)

| Operator | Function |
|-----------------|----------------|
| <code>**</code> | exponentiation |
| <code>*</code> | multiplication |
| <code>/</code> | division |
| <code>+</code> | addition |
| <code>-</code> | subtraction |

Numeric Expressions

Numeric expressions are up-cast to the highest data type in the expression according to the precedence:

(low) logical → integer → real → complex *(high)*

and smaller byte size *(low)* to larger byte size *(high)*

Examples:

Fortran 77 source code [01_arith.f](#)

Fortran 77 source code [02_sphere.f](#)

Character Expressions

Only built-in operator is **Concatenation** defined by `//`

```
'ILL'//'- '//'ADVISED'
```

`character` arrays are most commonly encountered

- treated like any array (indexed using `:` notation)
- fixed length (usually padded with blanks)

Character Expressions

Example:

```
CHARACTER FAMILY*16  
FAMILY = 'GEORGE P. BURDELL'  
  
PRINT*, FAMILY(:6)  
PRINT*, FAMILY(8:9)  
PRINT*, FAMILY(11:)  
PRINT*, FAMILY(:6)//FAMILY(10:)
```

```
GEORGE  
P.  
BURDELL  
GEORGE BURDELL
```

Relational Expressions

Two expressions whose values are compared to determine whether the relation is true or false

- may be numeric (common) or non-numeric

character strings can be compared

- done character by character
- shorter string is padded with blanks for comparison

Relational Expressions

| Operator | Relationship |
|---|--------------------------|
| <code>.LT.</code> or <code><</code> | less than |
| <code>.LE.</code> or <code><=</code> | less than or equal to |
| <code>.EQ.</code> or <code>==</code> | equal to |
| <code>.NE.</code> or <code>/=</code> | not equal to |
| <code>.GT.</code> or <code>></code> | greater than |
| <code>.GE.</code> or <code>>=</code> | greater than or equal to |

Logical Expressions

Consists of one or more logical operators and logical, numeric or relational operands

- values are `.TRUE.` or `.FALSE.`
- need to consider overall operator precedence

can combine logical and integer data with logical operators but this is tricky
(avoid!)

Logical Expressions

| F77 Operator | >F90 Operator | Example | Meaning |
|---------------------|-------------------------|-------------------------|--|
| <code>.AND.</code> | <code>&&</code> | <code>A .AND. B</code> | logical <code>AND</code> |
| <code>.OR.</code> | <code> </code> | <code>A .OR. B</code> | logical <code>OR</code> |
| <code>.EQV.</code> | <code>==</code> | <code>A .EQV. B</code> | logical equivalence |
| <code>.NEQV.</code> | <code>/=</code> | <code>A .NEQV. B</code> | logical inequivalence |
| <code>.XOR.</code> | <code>/=</code> | <code>A .XOR. B</code> | exclusive <code>OR</code> (same as <code>.NEQV.</code>) |
| <code>.NOT.</code> | | <code>.NOT. A</code> | logical negation |

Arrays in FORTRAN

Arrays can be multi-dimensional (up to 7 in F77) and are indexed using `()`:

- `TEST(3)` or `FORCE(4,2)`

Indices are by default defined as `1...N`

We can specify index range in declaration

- `INTEGER K(0:11)` : `K` is dimensioned from `0-11` (12 elements)

Arrays are stored in column order (1st column, 2nd column, etc) so accessing by **incrementing row index first** usually is **fastest** (see later)

Whole array reference (only in >F90): `K(:)=-8` assigns -8 to all elements in `K`

Avoid `K=-8` assignement

Unconditional `GO TO` in F77

This is the only GOTO in FORTRAN 77

- Syntax: `GO TO label`
- Unconditional transfer to labeled statement

```
10  -code-  
    GO TO 30  
    -code that is bypassed-  
30  -code that is target of GOTO-  
    -more code-  
    GO TO 10
```

- **Problem** : leads to confusing "*spaghetti code*" 🌟

IF ELSE IF Statement

Basic version:

```
IF (KSTAT.EQ.1) THEN  
  CLASS='FRESHMAN'  
ELSE IF (KSTAT.EQ.2) THEN  
  CLASS='SOPHOMORE'  
ELSE IF (KSTAT.EQ.3) THEN  
  CLASS='JUNIOR'  
ELSE IF (KSTAT.EQ.4) THEN  
  CLASS='SENIOR'  
ELSE  
  CLASS='UNKNOWN'  
ENDIF
```

Spaghetti Code in F77 (and before)

Use of `GO TO` and arithmetic `IF`'s leads to bad code that is very hard to maintain

Here is the equivalent of an `IF-THEN-ELSE` statement:

```
10  IF (KEY.LT.0) GO TO 20
    TEST=TEST-1
    THETA=ATAN(X,Y)
    GO TO 30
20  TEST=TEST+1
    THETA=ATAN(-X,Y)
30  CONTINUE
```

Now try to figure out what a complex `IF ELSE IF` statement would look like coded with this kind of simple `IF ...`

Loop Statements (old versions)

do loop: structure that executes a specified number of times

Spaghetti Code Version

```
      K=2
10    PRINT*,A(K)
      K=K+2
      IF (K.LE.11) GO TO 10
20    CONTINUE
```

F77 Version

```
      DO 100 K=2,10,2
      PRINT*,A(K)
100    CONTINUE
```

Loop Statements (>F90)

```
DO K=2, 10, 2  
  WRITE(*,*) A(K)  
END DO
```

- `loop_control` can include variables and a third parameter to specify increments, including negative values
- loop always executes ONCE before testing for end condition

```
READ(*,*) R  
DO WHILE (R.GE.0)  
  VOL=2*PI*R**2*CLLEN  
  READ(*,*) R  
END DO
```

- Loop will not execute at all if `logical_expr` is not true at start

Comments on Loop Statements

To exit a loop

- in old versions: use a `GO TO` statement
- in new versions: use an `EXIT` statement

you cannot transfer out of multiple nested loops with a single `EXIT`
use named loops if needed : `myloop : do i=1,n` and then `EXIT myloop`

To skip to next loop cycle

- in new versions **only** : use a `CYCLE` statement

File-Directed Input and Output

Much of early FORTRAN was devoted to reading input data from "cards" and writing to a line printer

Today, most I/O is to and from a file: it requires more extensive I/O capabilities standardized until FORTRAN 77

I/O = communication between a program and the outside world

- opening and closing a file with `OPEN` & `CLOSE`
- data reading & writing with `READ` & `WRITE`
- can use **unformatted** `READ` & `WRITE` if no human readable data are involved (much faster access, smaller files)

READ Statement

Syntax: `READ(dev_no, format_label) variable_list`

```
      READ(105,1000) A,B,C  
1000  FORMAT(3F12.4)
```

device numbers 1-7 are defined as standard I/O devices

- each `READ` reads one line of data

any remaining data in a line is dropped if not translated in
`variable_list`

- `variable_list` can include implied `DO` such as :

```
      READ(105,1000)(A(I),I=1,10)
```

READ Statement - cont'd

- input items can be integer, real or character
- characters must be enclosed in ' ' (or " ")
- input items are separated by commas
- input items must agree in type with variables in `variable_list`
- each `READ` processes a new record (line)

```
INTEGER K
REAL(8) A,B
! reads one line and look for floating point values for A & B and an integer for K
OPEN(105, FILE='path_to_existing_file')
READ(105, *) A,B,K
```

WRITE Statement

Syntax: `WRITE(dev_no, format_label) variable_list`

```
WRITE(*,1000) A,B,KEY
1000 FORMAT(F12.4,E14.5,I6)
```

```
|-----+-----0-----+-----0-----+-----+-----|
      1234.5678   -0.12345E+02      12
```

- device number `*` is by default the screen (or *standard output* - also 6)
- each `WRITE` produces one or more output lines as needed to write out `variable_list` using `format` statement
- `variable_list` can include implied `DO`

FORMAT Statement

| data type | format descriptors | example |
|-----------------------------|--------------------|---|
| integer | iw | <code>write(*,'(i5)') int</code> |
| real (<i>decimal</i>) | fw.d | <code>write(*,'(f7.4)') x</code> |
| real (<i>exponential</i>) | ew.d | <code>write(*,'(e12.3)') y</code> |
| character | a, aw | <code>write(*,'(a)') string</code> |
| logical | lw | <code>write(*,'(l2)') test</code> |
| spaces & tabs | wx & tw | <code>write (*,'(i3,2x,f6.3)') i, x</code> |
| linebreak | / | <code>write (*,'(f6.3,/,f6.3)') x, y</code> |

OPEN & CLOSE example (>F90)

Once opened, file is referred to by an assigned device number (a unique id)

```
character(len=*) :: x_name
integer          :: ierr, iSize, guess_unit
logical          :: itsopen, itexists
!
inquire(file=trim(x_name), size=iSize, number=guess_unit, opened=itsopen, exist=itexists)
if ( itsopen ) close(guess_unit, status='delete')
!
open(902,file=trim(x_name),status='new',iostat=ierr)
!
if (iSize <= 0 .OR. .NOT.itexists) then
  open(902,file=trim(x_name),status='new',iostat=ierr)
  if (ierr /= 0) then
    ...
    close(902)
  endif
  ...
endif
```

Examples

Fortran 77 source code [03_histogram.f](#)

Fortran 90 source code [03_histogram.f90](#)

Fortran 90 source code [04_plot.f90](#)

NAMelist

It is possible to pre-define the structure of input and output data using `NAMelist` in order to make it easier to process with `READ` and `WRITE` statements

- Use `NAMelist` to define the data structure
- Use `READ` or `WRITE` with reference to `NAMelist` to handle the data in the specified format

This is not part of standard F77 but it is included in >F90

NAMelist - cont'd

On input, the `NAMelist` data must be structured as follows:

```
&INPUT  
  THICK=0.245,  
  LENGTH=12.34,  
  WIDTH=2.34,  
  DENSITY=0.0034  
/
```

Fortran 90 source code [05_namelist.f90](#)

Namelist file [05_namelist.def](#)

Internal **WRITE** Statement

Internal **WRITE** does same as **ENCODE** in F77 : **a cast to string**

```
INTEGER*4 J,K  
CHARACTER*50 CHAR50  
DATA J,K/1,2/  
...  
WRITE(CHAR50,*) J,K
```

Results:

```
CHAR50= '    1    2'
```

Internal **READ** Statement

Internal **READ** does same as **DECODE** in F77 : **a cast from string**

```
INTEGER K  
REAL A, B  
CHARACTER*80 REC80  
DATA REC80/'1.2, 2.3, -5'/  
...  
READ(REC80, *) A, B, K
```

Results:

```
A=1.2, B=2.3, K=-5
```

Structured programming

Structured programming is based on subprograms (functions and subroutines) and control statements (like `IF` statements or loops) :

- structure the control-flow of your programs (e.g. give up the `GO TO`)
- improved readability
- lower level aspect of coding in a smart way

It is a **programming paradigm** aimed at improving the quality, clarity, and access time of a computer program

Functions and Subroutines

Subprograms allow **structured coding**

FUNCTION : returns single explicit function value for given function arguments

it's also a variable → so must be declared !

SUBROUTINE : any values returned must be returned through the arguments

no explicit subroutine value is returned !

- Subprograms are not recursive in F77
- Subprograms use a separate namespace (variables are local)
- Variables stored in **COMMON** may be shared between namespaces

Functions and Subroutines - cont'd

Subprograms must (should) include at least one `RETURN`

`FUNCTION` example:

```
REAL FUNCTION AVG3(A, B, C)
AVG3=(A+B+C)/3
RETURN
END
```

Use:

```
AV = WEIGHT*AVG3(A1, F2, B2)
```

`FUNCTION` type is implicitly defined as REAL

Functions and Subroutines - cont'd

Subroutine is invoked using the `CALL` statement

```
SUBROUTINE AVG3S(A, B, C, AVERAGE)
AVERAGE=(A+B+C)/3
RETURN
END
```

Use:

```
CALL AVG3S(A1, F2, B2, AVR)
RESULT = WEIGHT*AVR
```

Any returned values must be returned through argument list

Arguments

Arguments in subprogram are **dummy** arguments

arguments used in invocation are called "actual" or "real"

- passed by **reference** (memory address) if given as *symbolic*
 - the subprogram can then alter the actual argument value since it can access it by reference
- passed by **value** if given as *literal* (so cannot be modified)

```
CALL AVG3S(A1, 3.4, C1, QAV)
```

2nd argument is passed by value and others by reference

Arguments - cont'd

Arguments used in invocation (by calling program) may be *variables, array names, literals, expressions* or *function names*

Using symbolic arguments (variables or array names) is the **only way** to return a value (result) from a `SUBROUTINE`

It is considered **BAD coding practice**, but functions can return values by changing the value of arguments

this type of use should be strictly **avoided** !

Arguments - cont'd

The `INTENT` keyword (>F90) increases readability and enables better compile-time error checking

```
SUBROUTINE AVG3S(A, B, C, AVERAGE)
  IMPLICIT NONE
  REAL, INTENT(IN)      :: A, B
  REAL, INTENT(INOUT)   :: C      ! default
  REAL, INTENT(OUT)     :: AVERAGE

  A = 10                  ! Compilation error
  C = 10                  ! Correct
  AVERAGE=(A+B+C)/3      ! Correct
END
```

compiler uses `INTENT` for error checking and optimization

FUNCTION versus Array

REMAINDER(4,3) could be a 2D array or it could be a reference to a function

If the name, including arguments, **matches an array declaration**, then it is taken to be an array, **otherwise**, it is assumed to be a FUNCTION

Be careful about implicit versus explicit type declarations with FUNCTION

```
PROGRAM MAIN
  INTEGER REMAINDER
  ...
  KR = REMAINDER(4,3)
  ...
END

INTEGER FUNCTION REMAINDER(INUM, IDEN)
  ...
END
```

Arrays with Subprograms

Arrays must be passed by reference to subprogram

How do you tell subprogram how large the array is ?

| answer varies with FORTRAN version and vendor (dialect)...

- when an array element, e.g. `A(1)` , is used in a subprogram invocation , it is passed as a reference (address), just like a simple variable
- when an array is used by name in a subprogram invocation, it is passed as a reference to the entire array.

| the array must be appropriately dimensioned (and this can be tricky...)

Data layout in multi-dimensional arrays

- always increment the left-most index of multi-dimensional arrays in the innermost loop (i.e. fastest)
- **column major** ordering in Fortran vs. **row major** ordering in C
- a compiler (with sufficient optimization flags) may re-order loops automatically

```
do j=1,M
  do i=1,N ! innermost loop
    y(i) = y(i)+ a(i,j)*x(j) ! left-most index is i
  end do
end do
```

Arrays - dynamic allocation

Using `ALLOCATABLE` on declaration, and using `ALLOCATE` and `DEALLOCATE` later

```
integer :: m, n
integer, allocatable :: idx(:)
real, allocatable :: mat(:, :)
m = 100 ; n = 200
allocate( idx(0:m-1))
allocate( mat(m, n))
...
deallocate(idx , mat)
```

It exists many array intrinsic functions

SIZE, SHAPE, SUM, ANY, MINVAL, MAXLOC, RESHAPE, DOT_PRODUCT,
TRANSPOSE, WHERE, FORALL, etc

COMMON & MODULE Statement

A variable declared in a `Main` program can be made accessible to subprograms

- `COMMON` statement allows variables to have a more extensive scope
 - | can group into **labeled** `COMMON`
- with > F90, it's better to use a `MODULE` subprogram
 - | this can be selective (don't have to share all everywhere) with `ONLY`

Fortran 77 source code [06_common.f](#)

Fortran 90 source code [06_module.f90](#)

Hands-on

Fortran 90 source code [07_plot_newton.f90](#)

Fortran 90 source code [07_newton.f90](#)

Text file [08_ChristmasTree.txt](#)

Modular programming (>F90)

Modular programming is about separating parts of programs into independent and interchangeable modules :

- improve testability
- improve maintainability
- re-use of code
- higher level aspect of coding in a smart way
- *separation of concerns*

The principle is that making significant parts of the code independent, replaceable and independently testable makes your programs **more maintainable**

Data Type Declarations

FORTRAN >90 allows user derived types

```
TYPE my_variable
  character(30)      :: name
  integer           :: id
  real(8)           :: value
  integer, dimension(3,3) :: dimIndex
END TYPE variable

type(my_variable) var
var%name = "salinity"
var%id   = 1
```

Subprograms type

`MODULE` are subprograms that allow modular coding and data encapsulation

The interface of a subprogram type is **explicit** or **implicit**

Several types of subprograms:

- `intrinsic` : explicit - defined by Fortran itself (trigonometric functions, etc)
- `module` : explicit - defined with `MODULE` statement and used with `USE`
- `internal` : explicit - defined with `CONTAINS` statement inside (sub)programs
- `external` : implicit (but can be manually (re)defined explicit) - e.g. **libraries**

Differ with the **scope**: what data and other subprograms a subprogram can access

MODULE type



```
MODULE example
  IMPLICIT NONE
  INTEGER, PARAMETER :: index = 10
  REAL(8), SAVE      :: latitude
CONTAINS
  FUNCTION check(x) RESULT(z)
    INTEGER :: x, z
    ...
  END FUNCTION check
END MODULE example
```

```
PROGRAM myprog
  USE example, ONLY: check, latitude
  IMPLICIT NONE
  ...
  test = check(a)
  ...
END PROGRAM myprog
```

internal subprograms

```
program main
  implicit none
  integer N
  real X(20)
  ...
  write(*,*), 'Processing x...', process()
  ...
contains
  logical function process()
    ! in this function N and X can be accessed directly (scope of main)
    ! Please note that this method is not recommended:
    ! it would be better to pass X as an argument of process
    implicit none
    if (sum(x) > 5.) then
      process = .FALSE.
    else
      process = .TRUE.
    endif
  end function process
end program
```

external subprograms

- `external` subprograms are defined in a separate program unit
- to use them in another program unit, refer with the `EXTERNAL` statement
- compiled separately and linked

!!! DO NOT USE THEM: modules are much easier and more robust !

They are only needed when subprograms are written with different programming language or when using external libraries (such as BLAS)

It's **highly** recommended to construct `INTERFACE` blocks for any external subprograms used

interface statement

```
SUBROUTINE nag_rand(table)
  INTERFACE
    SUBROUTINE g05faf(a,b,n,x)
      REAL, INTENT(IN)      :: a, b
      INTEGER, INTENT(IN)   :: n
      REAL, INTENT(OUT)     :: x(n)
    END SUBROUTINE g05faf
  END INTERFACE
  !
  REAL, DIMENSION(:), INTENT(OUT) :: table
  !
  call g05faf(-1.0,-1.0, SIZE(table), table)
END SUBROUTINE nag_rand
```

Fortran Compiler and libraries

Examples:

```
module load netCDF-Fortran/4.5.3-gompi-2021b
gfortran -ffree-line-length-none \
-o OceanGrideChange.exe 07_OceanGrideChange.f90 \
-I${EBROOTNETCDFMINFORTRAN}/include -L${EBROOTNETCDFMINFORTRAN}/lib -lnetcdff
```

```
module load netCDF-Fortran/4.5.3-impi-2021b
ifort -O3 \
-o OceanGrideChange.exe 07_OceanGrideChange.f90 \
-I${EBROOTNETCDFMINFORTRAN}/include -L${EBROOTNETCDFMINFORTRAN}/lib -lnetcdff
```

Fortran 90 source code [09_OceanGrideChange.f90](#) with the input file [09_input.nc](#)

Conclusions

- Fortran in all its standard versions and vendor-specific dialects is a rich but confusing language
- Fortran is a modern language that continues to evolve
- Fortran is still ideally suited for numerical computations in engineering and science
 - most new language features have been added since F95
 - "High Performance Fortran" includes capabilities designed for parallel processing