

# Introduction to Scientific Programming

## Control Constructs and Arrays

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# Fortran Part 2

- Control constructs
  - `if, else if, else, endif`
  - `select case, case, end select`
  - `do, enddo, cycle, exit`
- Arrays
  - static arrays, dimension
- Subprograms
  - Functions and Subroutines
- Full story
  - Control constructs
  - Arrays
  - Structures
  - Subprograms: Functions and Subroutines

# IF

```
[label0:] if (logical expression) then
    {if-block}
[else if (logical expression) then
    {else-if-block} ]
[else
    {else block} ]
end if [label0]
```

- Use labels in complicated (and/or long) if or do constructs  
In case that an **endif** or **enddo** is missing, the compiler will be able to tell which one is missing
- Always indent code in **if** and **do** constructs

# IF

optional label

```
real      :: x
complex :: root

imag: if (x < 0.0) then
    root=cmplx(0.0,sqrt(-x))
else
    root=cmplx(sqrt(x),0.0)
end if imag
```

```
integer :: n, factorial

if (n < 0) then
    print "n should be
positive"
    exit
else if (n == 0) then
    factorial=1
else if (n >= 1) then
    ...
end if
```

# SELECT CASE

```
[label:] select case (expression)
  [case selector
    block]
  [case default
    block]
end select [label]
```

- **expression** may be integer or character (or logical)
- **selector** is list of non-overlapping values

# SELECT CASE

```
select case (n)
case (:-1)      ! Range from smallest integer to -1
    print*, "n should be positive"
    exit
case (0:)       ! Range from 0 to largest integer
    factorial=1
    <factorial code>
end select
```

# DO

```
[label:] do variable=expr1, expr2[, expr3]  
    block  
end do [label]
```

**variable** is a scalar integer variable

**expr1, expr2 & expr3** are integer expressions

# DO

```
factorial=1  
do i=2,n  
    factorial=factorial*i  
end do
```

- when  $n \leq 1$ , loop is not executed
- lower and upper limits could be any valid expression that evaluates to an integer

```
dotp = 0.0  
do i=1,n,3  
    dotp = dotp+a(i) * b(i)  
    dotp = dotp+a(i+1)* b(i+1)  
    dotp = dotp+a(i+2)* b(i+2)  
end do
```

stride of 3.  
stride=1, if not specified

- this is an example of loop unrolling
- assumes  $n$  is divisible by 3



# Arrays

```
program average  
  
real :: a, b, c, sum, average  
  
a = 3.4  
b = 4.5  
c = 5.6  
  
sum      = a + b + c  
average = sum / 3.  
  
print *, sum, average  
  
end program
```

This works to calculate the average of 3 variables (**a**, **b**, **c**), but ...

How would we deal with an example that has more than 3 variables, say 100?

Output:  
13.5000, 4.500000

# Arrays

```
program average

integer, parameter :: n = 3
real, dimension(n) :: a

a(1) = 3.4      ! Data from somewhere
a(2) = 4.5
a(3) = 5.6

sum = 0.        ! Initialize sum = 0

do i=1, n
    sum = sum + a(i)      ! Add up
enddo

average = sum / real(n)  ! Divide

print *, sum, average

end program
```

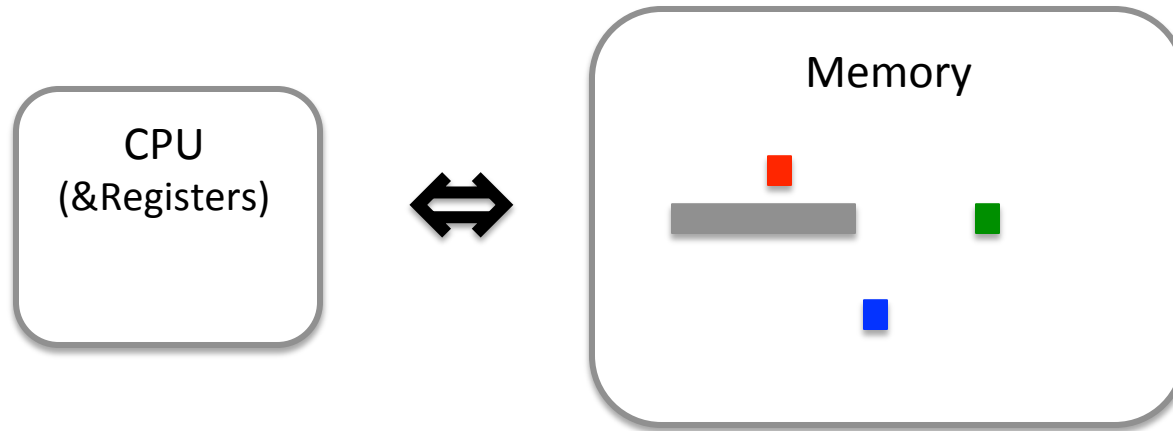
An array is a group of variables (or constants), all of the same type, that are referred to by single name. An individual value within the array is called an array element; it is identified by the name of the array together with a subscript.

`type, dimension(<constant>) :: var`

`a` is an array of type real  
`a(1)` is the first array element  
`a(3)` is the third array element

Output:  
13.5000, 4.500000

# Computer Architecture: Memory



Variables and arrays are stored somewhere:

a, b, c scalar variables

d array variable, contiguous in memory

# Arrays

What is the most important segment in this code?

```
program average_square

integer, parameter :: m = 30
real, dimension(m) :: squares

! Read from keyboard
print *, 'Enter the maximum number'
read *, n_squares
print *, 'Input is', n_squares

if (n_squares > m) then
    stop 'Error'
endif

! Calculate and store squares
do i=1, n_squares
    squares(i) = real(i)**2
enddo

! Calculate average
sum = 0.
do i=1, n_squares
    sum = sum + squares(i)
enddo
aver = sum / real(n_squares)
print *, 'average = ', aver
end program
```

# Multi-Dimensional Arrays

In this example, **a** is a 2D array with 3x7 elements, and **b** is a 3D array with 2x4x8 elements

```
program average

integer, parameter      :: n = 3
integer, parameter      :: m = 7

real, dimension(n,m)    :: a
real, dimension(2,4,8)  :: b

...

end program
```

# Arrays

```
integer, dimension(0:7,2) :: indArray
...
indArray(myTaskID,1) = myStart
indArray(myTaskID,2) = myEnd
```

- Ordered collection of elements
- Each element has an index
- Index may start at any integer number, not only 1
- Array element may be of intrinsic or derived type
- Array **size** refers to the number of elements
- The number of dimensions is the **rank**
- The size along a dimension is called an **extent**
- Array **shape** is the sequence of extents

indArray's size	16
indArray's rank	2
extent along 1st dimension	8
indArray's shape	(8,2)

# Derived Data Types and Structures

```
type person      ! Declaration of a
                  ! derived type
real              :: age
integer           :: year_of_birth
character(len=8)  :: name
end type person

! Declaration of a structure of
! the derived type
type(person)      :: you

! A structure can be an array
type(person), dimension(10) :: we

! Elements are references by %
you%age           = 29.2
you%year_of_birth = 1990
you%name          = 'John Doe'

print *, 'age = ', you%age
print *, 'you = ', you
```

A Derived Type is similar to an array. Like an array, a single derived type can have multiple components. Unlike an array, the components of a derived type may have different types. One component may be an integer (array), while the next component is a real (array), the next a character (array), and so forth.

Components are accessed with percent (%)  
**structure%component**

Output:

age =	29.20000	
you =	29.20000	1990 John Doe

# Derived Data Types and Structures

...

**! more examples of how to use structures**

**we(1)%age = 'John Doe'**

**we(1)%age = you%age**

**we(1)%year\_of\_birth = you%year\_of\_birth**

**we(1)%name = you%name**

**we(2) = you ! copies all components**

**we(3)%age = 1.5 \* we(3)%age**



# Derived Data Types - Structures

- Composed of one or more components
- Components may also be arrays or of a derived type

```
! Declaration of the type
type particle
    integer                :: partID
    real, dimension(3)     :: pos, vel, force
end type particle

! Declaration of variables of a type
type(particle) :: p1, p2

! Usage
p1%partID = 1
p1%pos    = 0.0; p1%vel = 0.0; p1%force = 0.0
p1%pos(1) = 1.5
p2 = p1; p2%partID = 2
```

# Derived Data Types and Structures

```
! structures can contain arrays  
! and other structures
```

```
type data  
    integer :: nx, ny, nz           ! Number of points in X, Y and Z  
    real, dimension(10,10,10) :: value ! 3D array  
end type data
```

```
type(data) :: set1, &  
             set2
```

```
type more_data  
    real, dimension(20,20) :: y  
    type(data) :: d  
end type more_data
```

```
type(more_data) :: more
```

```
set1%nx = 5; set2%value(1,1,1) = 7.3
```

```
more%y(1,1) = 5.
```

```
more%d%nx = 7
```

```
more%d%value(2,4,5) = 7.3
```

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