

Topic: Fortran Programming

Objectives

- Basics of Fortran programming

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```
program test
  implicit none

  real    :: s1, s2, s3, total

  s1 = 27.2
  s2 = 23.9
  s3 = 22.5

  total = s1 + s2 + s3

  write(*,*) ' Sum ', total

end program test
```

Output

Sum 73.5999985

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```
program test
  implicit none

  real    :: s(3), total

  s(1) = 27.2
  s(2) = 23.9
  s(3) = 22.5

  total = s(1) + s(2) + s(3)

  write(*,*) ' Sum ', total
end program test
```

Output

Sum 73.5999985

Introducing the arrays

Syntax: array_name(length_array) (one-dimensional)

array_name(array_length, array_length) (two-dimensional)

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How do you read this? 1D or 2D array?

Cartesian coordinates of 9 atoms (particles)

```
1.2361419  1.0137761 -0.0612424
0.5104418  0.8944555  0.5514190
1.9926927  1.1973129  0.4956931
-0.9957202  0.0160415  1.2422556
-1.4542703 -0.5669741  1.8472817
-0.9377950 -0.4817912  0.4267562
-0.2432343 -1.0198566 -1.1953808
0.4367536 -0.3759433 -0.9973297
-0.5031835 -0.8251492 -2.0957959
```

- Array operations:

- $a = a + 2.0$
- $a = a * 2.0$
- $a = a + a$
- $a = a * a$
- $a(1,:) = a(1,:) * 2$ or $a(1,:) = a(1,:) + 2$

$a(27)$ or $a(9)$



$a(9,3)$

(1,1)	(1,2)	(1,3)
(2,1)	(2,2)	(2,3)
(3,1)	(3,2)	(3,3)
(4,1)	(4,2)	(4,3)
(5,1)	(5,2)	(5,3)
(6,1)	(6,2)	(6,3)
(7,1)	(7,2)	(7,3)
(8,1)	(8,2)	(8,3)
(9,1)	(9,2)	(9,3)

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DO Loops

DO LOOP is used to repeat a block of statements.

Syntax

```
DO index_variable = start, end, step  
  ---  
  ---  
END DO
```

- Index_variable must be 'integer' type
- 'step' is optional

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Example of DO Loops

```
program num
  implicit none

  integer :: i

  do i=1,10

    write(*,*) "num", i

  enddo

end program num
```

```
do x = 1, 10
  ! block 1
enddo
```

```
m=1
n=10
do x = m, n
  ! block 1
enddo
```

```
m=1
n=10
do x = m, n, 1
  ! block 1
enddo
```

```
m=1
n=10
x=1
do x= m, n*x
  ! block 1
enddo
```

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CYCLE and EXIT Statements

- EXIT statement helps in transferring the control outside the DO loop
- CYCLE statement takes the control to the beginning of the next iteration in the DO loop

Syntax

```
DO index_variable = start, end, step
  ! block 1 statements
  exit
  ---
  ! block 2 statements
END DO
```

block 2 statements will not
be executed

Usually both CYCLE and EXIT statements are used along with IF condition

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DO WHILE Loops

Syntax

```
DO WHILE (logical argument)
```

```
    ! block statements
```

```
END DO
```


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Example of DO WHILE Loops

```
program num
  implicit none

  integer :: i

  i=0
  do while (i<10)

    i=i+1
    write(*,*) "num", i

  enddo
end program num
```

```
i=0
n=10
do while ( i < n)
  ! block 1
enddo
```

```
n=10
i=20
do while (.not. i < n)
  ! block 1
enddo
```

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Infinite DO Loops

Syntax

```
DO
    ! block statements

    If (logical expression) then
        exit
    endif

    ! block statements

END DO
```

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nested DO loops

Syntax

```
DO index_variable = start1, end1  
  ! block 1 statements
```

```
DO index_variable = start2, end2  
  ! block 2 statements
```

```
DO index_variable = start3, end3  
  ! block 3 statements
```

```
END DO  
! block 4 statements
```

```
END DO  
! block 5 statements
```

```
END DO
```

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```
program test
  implicit none

  integer :: i
  real    :: s(100), total

! initialize the variable s

  do i = 1, 100
    s(i) = i
  enddo

! main part of the program

  total=0.0
  do i = 1, 100
    total = total + s(i)
  enddo

  write(*,*) ' Sum ', total

end program test
```

Output

Sum 5050.00000

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```
program test
  implicit none

  integer :: i
  real    :: s(100), total

! initialize the variable s

  do i = 1, 100
    s(i) = i
  enddo

! main part of the program

  total=0.0
  do i = 1, 100
    total = total + s(i)
  enddo

! condition
  if(i>50) then
    total = total + 1
  endif

enddo

  write(*,*) ' Sum ', total

end program test
```

Output

Sum 5100.00000

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- Write a FORTRAN program that computes the average and standard deviation of N real numbers. Use arrays and DO loops in the program.

Standard deviation $\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \mu)^2}.$

Where

x_i is an individual value

μ is the mean/expected value

N is the total number of values

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Tips

- Don't worry about declaring variables initially. Identify the main part of the program and start writing
- All real numbers should be in double precision (add d0 in the end), eg. 10.0d0
- Always use indentation, leave black spaces to improve readability
- Always use 'parameter' in case when assigning the values to integer datatype
- Use internal functions to convert datatypes, eg. real(x)
- Read compiler error messages more carefully
- For debugging, use 'write' statement at several places in the program and check for the output
-

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FORTRAN – Reading material

- Please go through this FORTRAN program for a quick overview,
 - <https://learnxinyminutes.com/docs/fortran95/>
- Please go through this document for quick overview of FORTRAN
 - <https://www.ideo.columbia.edu/~mspieg/mmm/Fortran.pdf>
- For a video on FORTRAN programming, look at
https://www.youtube.com/watch?v=__2UgFNYgf8
- Book: Computer Programming in Fortran 90 and 95, V. Rajaraman