Topic: FORTRAN Programming

Objectives

- Basics of FORTRAN programming: Read, write

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Assigning values to input variables

```
program test
  implicit none

  integer :: s1, s2, s3, total

   s1 = 27

   s2 = 23

   s3 = 22

   total = s1 + s2 + s3

   write(*,*) ' Sum ',  total

end program test
```

How to read input variables while executing the program?

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Reading from standard input

```
program test
 implicit none

 integer :: s1, s2, s3, total

 write(*,*) 'Enter s1, s2, s3 values'
 read(*,*) s1, s2, s3

 total = s1 + s2 + s3

 write(*,*) ' Sum ', total

end program test
```

```
sandeep $ ./a.out
 Enter s1, s2, s3 values
27 23 22
  Sum           72
sandeep $ ./a.out
 Enter s1, s2, s3 values
27
23
22
  Sum           72
sandeep $
```

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Reading/writing from/to standard input/output

```
program test
 implicit none

 integer :: s1, s2, s3, total

 write(6,*) 'Enter s1, s2, s3 values'
 read(5,*) s1, s2, s3

 total = s1 + s2 + s3

 write(*,*) ' Sum ', total

end program test
```

read(*,*) == read(5,*)

write(*,*) == write(6,*)

Format status – either unformatted or formatted

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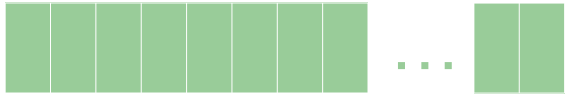
How do you read this? 1D or 2D array?

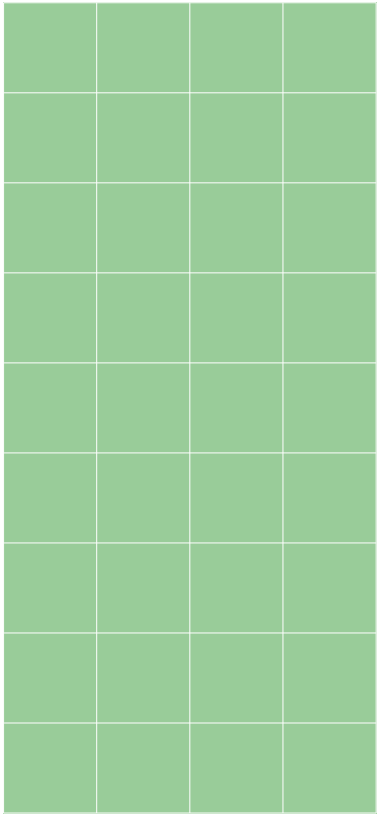
Cartesian coordinates of 9 atoms (particles)

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

a(27) or a(9)



a(9,3)



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Read statement

used to read input data from both terminal and text file

```
read(unit, fmt, ERR = err_label, iostat= val, end = end_label)
```

where **unit** is any integer

fmt is format specification mainly used for reading binary files

err_label is statement label where the control is transferred in case of error

end_label is statement label where the control is transferred after reaching the end of file

iostat = value is to check the status of execution of the statement

```
read(1, *)
read(10000, *)
read(10 + i, *)
read(1, *, err=100)
read(1,*, end=100)
read(1, *, iostat=value)
```

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Write statement

used to write output to both terminal and text file

```
write(unit, fmt, ERR = err_label, iostat= val)
```

where **unit** is any integer

fmt is format specification mainly used for reading binary files

err_label is statement label where the control is transferred in case of error

end_label is statement label where the control is transferred after reaching the end of file

iostat = value is to check the status of execution of the statement

```
write(1, *)
write(10000, *)
write(10 + i, *)
write(1, *, err=100)
write(1, *, iostat=value)
```

We discuss format identifiers in write statement in the next class

Opening files

```
open (unit = number, file = "name", action= action_string, status=status_string, iostat=val).
```

unit is any integer
file is filename (string) of any length
action possible values (string) read/write/readwrite -- default is readwrite
status possible values (string) old/new/scratch
iostat = value is to check the status of execution of the statement

```
open(unit=1, file='coord.xyz', action='read')

open(unit=1, file='coord.xyz', action='readwrite')

open(unit=1, file='coord.xyz')

filename = "coord.xyz"

open(unit=1,file=filename,action=write)

open(unit=1, file='coord.xyz', status=new, action='read', status='new', iostat=x)
```

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open statement - example

```
program test
 implicit none

 character(len=200) :: filename
 integer :: val,i

 i=1
 filename='coord.xyz'

 open(unit=i,file=filename,action='read')

end program test
```

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close statement - example

```
program test
 implicit none

 character(len=200) :: filename
 integer :: val,i

 i=1
 filename='coord.xyz'

 open(unit=i,file=filename,action='read')

 close(i)

end program test
```

- Files are automatically closed after the termination of the program
- The close statement flushes the output in the buffer to file and disconnects the unit with the filename
- Any file opened should be closed after writing the output

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Hands-on

1. Write a Fortran program to read the same data using 1D and 2D array.
   Input file='input1.xyz'.

2. Write a Fortran program to check if a file exists in the current directory

3. Write a program to read the data from a text file and write the same data to another file 'output3.xyz'. The program must use DO loops. Input file='input3.xyz'

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Writing the data to a file

```
program test
  implicit none

  integer, parameter           :: natoms=9

  integer           :: i, atom
  real(kind=8)      :: atm_coor(natoms,3)
  character(len=10) :: atm_name(natoms)

! unit = x where x can be any number except 5 and 6

  open(unit=100,file='coordinates.xyz',action='read')
  open(unit=101,file='output.xyz',action='write')

  do atom = 1, natoms

                    ??????????????????

  enddo

  do atom = 1, natoms

                    ??????????????????

  enddo

end program test
```

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.ldeo.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