

PH 566- Advanced Simulation Methods in Physics

- We will be using the language **Fortran** in this course. This section contains the syntax for the language.

* Basic Syntax -

```
program <name>
  real :: a, b, c
  integer :: a1, b1, ...
  ...
  write(*,*) "Enter value"
  read(*,*) a
  write(*,*) "Value: ", a
  ...
end program <name>
```

Begin program scope, like main

Declare variables. MUST be done at start

Use Vars in program

End program

* If-then-Else

```
if (<condition>) then
  ...
else if (<condition>) then
  ...
else
  ...
end
```

* Logical Operators

> - .gt.	< - .lt.
≥ - .ge.	≤ - .le.
= - .eq.	≠ - .ne.

* Do Loops

```
do i = 1, n
  ...
end do
```

integer i
takes 1 to n

```
do while (condition)
  ...
end do
```

repeat
until
false

* Reading from and Writing to files

open (<Id>, file = "<name>", status = "old")
 ↳ #, used for reference.
 ↳ means file is already present.
 "New" would create a blank file

write (<Id>, *) " Hey "

Read (<Id>, *) a

- Write to that file
- Read from the file and store in a.
- At end of last line, you must add a new line. Otherwise, Fortran encounters end of file before /n and gives an error.

* Formatting

- Write statements can be formatted in 3 ways.

1) Ix - Integer with x columns

2) Fw.d - Fraction with total w columns, d decimal reserved.

3) Ew.d - Scientific with total w, d for decimal

- Examples: 8.3 in F5.2 — 8.30

8.3×10^5 in E8.2 — 8.30E+5

- Used as 3 format(I7)
write(*,3) a

* Function

```
<return-type> function f(<arguments>)
    real :: ... — declare arguments here
    ...
    f = result — Equate f to return value
    return
end
```

* Subroutine

— Used when multiple return values are needed.

In main program

```
call function (i1, i2, o1, o2)
      name
```

Syntax

```
Subroutine function (i1, i2, o1, o2)
      name
    real :: ... — declare arguments
    declare i1, i2 — say i1, i2 are
                   inputs
    ...
    return
end
```

* Finding Approximate Root for function

1) Newton-Raphson method

A fairly simple way to find roots. We draw a tangent at any guess of the root, then switch over to the x-intercept of the tangent.

$$x_{n+1} = x_n - f(x_n) / f'(x_n)$$

This usually works very well. The req. are:-

1) $f(x)$ is continuous \rightarrow graph is smooth

2) $f'(x) \neq 0$

2) Secant Method

Instead of tangent, we use a secant for estimation.

$$x_{n+1} = x_n - f(x_n) / Q(x_n, x_{n-1})$$

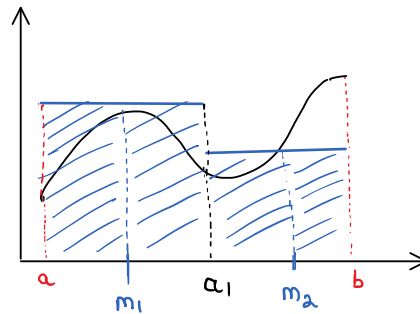
$$Q(x_n, x_{n-1}) = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Statistically takes 45% more steps, but each step is cheaper.

* Integration

1) Midpoint Rule.

- We need to compute $\int_a^b f(x) dx$. Divide the interval into n parts.

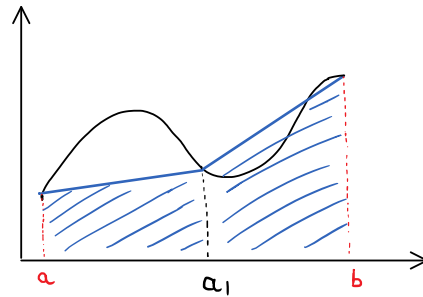


$$\Delta x = \frac{b-a}{n}$$

$$\Rightarrow I = \Delta x \sum f(m_i)$$

2) Trapezoidal rule

Instead of taking f at midpoints, we consider a trapezoid.



$$I_1 = \frac{1}{2} \Delta x (f(x_0) + f(x_1))$$

$$I_2 = \frac{1}{2} \Delta x (f(x_1) + f(x_2)) \rightarrow I = \sum I_i$$

⋮

3) Simpson's 1/3rd Rule

$$I_1 = \frac{\Delta x}{3} (f(x_0) + 4f(x_1) + f(x_2))$$

$$I_2 = \frac{\Delta x}{3} (f(x_2) + 4f(x_3) + f(x_4))$$

⋮

$$I_{\text{net}} = \sum I_i$$

Solving Differential Equations

We shall initially look at first order differential equations, and the techniques used to solve them. But before that, let's set a notation so that rest of the text is easy to follow.

$$\frac{dy}{dx} = f(x, y)$$

We have also been provided with the values of $\left. \frac{dy}{dx} \right|_{x=a}$ and $y(a)$; we wish to find the value of $y(b)$.

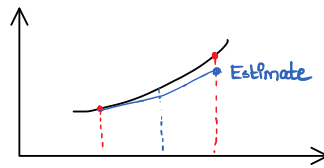
1) Euler's method

Take a step size h . Smaller step size gives better accuracy.

Let $(x_0, y_0) = (a, y(a))$. Perform the following recursion.

$$x_{n+1} \leftarrow x_n + h$$

$$y_{n+1} \leftarrow y_n + h \cdot f(x_n, y_n)$$



Stop when $x_{n+1} > b$. The value of y_n is the estimated value of $y(b)$.

2) 2nd Order Runge Kutta

$$k_1 = h f(x_n, y_n)$$

$$k_2 = h f(x_n + h/2, y_n + k_1 h/2)$$

$$y_{n+1} \leftarrow y_n + k_2$$

$$x_{n+1} \leftarrow x_n + h$$

3) 4th Order Runge-Kutta

$$K_1 = hf(x_n, y_n)$$

$$K_2 = hf(x_n + h/2, y_n + K_1/2)$$

$$K_3 = hf(x_n + h/2, y_n + K_2/2)$$

$$K_4 = hf(x_n + h, y_n + K_3)$$

$$\begin{aligned} y_{n+1} &\leftarrow y_n + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \\ x_{n+1} &\leftarrow x_n + h \end{aligned}$$

* Second Order differential equations

The above methods can be quite easily applied to second order DE as well, after some clever manipulation has been done.

$$\frac{d^2y}{dx^2} = f(x, y, \frac{dy}{dx}) \rightarrow \text{Let } \frac{dy}{dx} = v$$

$$\begin{aligned} \Rightarrow \frac{dv}{dx} &= f(x, y, v) \\ \frac{dy}{dx} &= v \end{aligned} \quad \left. \vphantom{\begin{aligned} \Rightarrow \frac{dv}{dx} &= f(x, y, v) \\ \frac{dy}{dx} &= v \end{aligned}} \right\} \begin{array}{l} \text{Simultaneously solve both 1st order} \\ \text{DE} \end{array}$$

We are provided with the values of y , $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x=a$. We wish to find value of $y(b)$.

1) Euler's Method

$$x_{n+1} \leftarrow x_n + h$$

$$y_{n+1} \leftarrow y_n + hv_n$$

$$v_{n+1} \leftarrow v_n + hf(x_n, y_n, v_n)$$

2) 4th Order Runge Kutta's Method

$$K_1 = U_n, \quad l_1 = f(x_n, y_n, U_n)$$

$$K_2 = U_n + hU/2, \quad l_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{hK_1}{2}, K_2\right)$$

$$K_3 = U_n + hU/2, \quad l_3 = f\left(x_n + \frac{h}{2}, y_n + \frac{hK_2}{2}, K_3\right)$$

$$K_4 = U_n + hU, \quad l_4 = f(x_n + h, y_n + hK_3, K_4)$$

→

$$y_{n+1} \leftarrow y_n + \frac{h}{6} (K_1 + 2K_2 + 2K_3 + K_4)$$

$$U_{n+1} \leftarrow U_n + \frac{h}{6} (l_1 + 2l_2 + 2l_3 + l_4)$$

$$x_{n+1} \leftarrow x_n + h$$