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

* Basic Syntax -

```
program <name>
```
Begin program scope, like main

```
  real :: a, b, c ..
  integer :: a1, b1, ..
```
Declare variables. MUST be done at start

```
    :
  write(*,*) " Enter value"
  read(*,*) a
  write(*,*) " Value:  ", a
```
Use Vars in program

```
    :
end program <name>
```
End program

* If - then - Else

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

* Logical Operators

$>$ - .gt.	$<$ - .lt.
$\geq$ - .ge.	$\leq$ - .le.
$=$ - .eq.	$\neq$ - .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")

<Id> → #, used for reference.

"old" → 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 . 3 0

  8.3×10^5 in E8.2 – _ 8 . 3 0 E + 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 → graph is smooth

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

2) Secant Method

Instead of tangent, we use a secant for estimation.

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

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

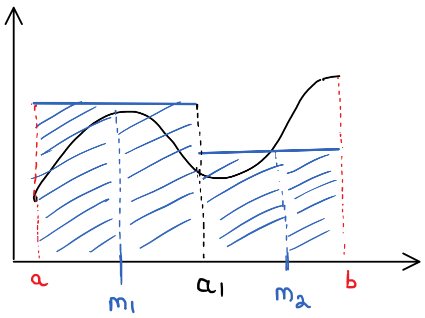
Statistically takes 45% more steps, but each step is cheaper.

* Integration

1) Midpoint Rule.

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

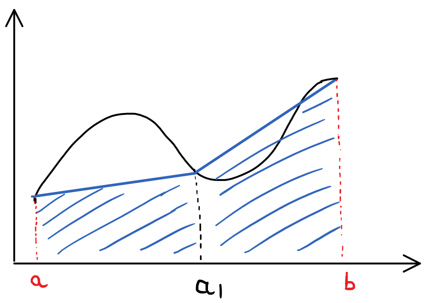
$\Delta x = \frac{b-a}{n}$



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

2) Trapezoidal rule

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



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

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

$$\vdots$$

3) Simpson's $1/3^{rd}$ Rule

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

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

$$\vdots$$

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

Solving Differential Equations

We shall initially look at first order differential equations, and the techniques used to solve them. But before that, lets 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 $y(b)$.

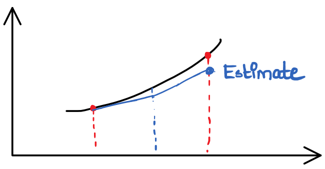
1) Euler's method

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) 2^{nd} Order Runge Kutta

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

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

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

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

3) 4th Order Runge-Kutta

$$K_1 = hf(x_n, y_n)$$
$$K_2 = hf(x_n + h/2, y_n + K_1/2)$$
$$K_3 = hf(x_n + h/2, y_n + K_2/2)$$
$$K_4 = hf(x_n + h, y_n + K_3)$$

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

* 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.

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

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

Simultaneously solve both 1st order DE

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

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

$$K_2 = v_n + hl_1/2, \quad l_2 = f\left(x_n + \tfrac{h}{2}, y_n + \tfrac{hK_1}{2}, K_2\right)$$

$$K_3 = v_n + hl_2/2, \quad l_3 = f\left(x_n + \tfrac{h}{2}, y_n + \tfrac{hK_2}{2}, K_3\right)$$

$$K_4 = v_n + hl_3, \quad l_4 = f\left(x_n + h, y_n + hK_3, K_4\right)$$

$\rightarrow$

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

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

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

* Solving Linear Equations

Assume that you need to solve the following system of linear equations.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ & & \vdots & & \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$A \cdot X = B$$

Method 1 The Jacobi Method

Let E_i represent the i'th row in the system of Linear Equations shown above. That is,

$$E_i \equiv a_{i1}x_1 + \ldots + a_{ii}x_i + \ldots + a_{in}x_n = b_n$$

Assume that $\forall i \in \{1, \ldots, n\}$ $a_{ii} > 0$ Then, let x_i^0 be x_i at 0^{th} iteration. We iterate as follows:-

$$x_i^{t+1} = \frac{1}{a_{ii}}\Big(b_i - \underbrace{a_{i1}x_1^t - \ldots - a_{i(i-1)}x_{i-1}^t}_{\text{" before" } x_i} - \overbrace{a_{i(i+1)}x_{i+1}^t - \ldots - a_{in}x_n^t}^{\text{" after" } x_i}\Big)$$

Rearrange E_i

Method 2 Gauss - Seidel Method

This is very similar to the Jacobi method with a small change in the recursion. Instead of waiting for the $(t+1)^{th}$ iteration for using the value of x^t_i, we use it directly after calculating it.

$$x_i^{t+1} = \frac{1}{a_{ii}}\Big(b_i \underbrace{- a_{i1}x_1^{t+1} - \dots - a_{i(i-1)}x_{i-1}^{t+1}}_{\text{" before " } x_i} \overbrace{- a_{i(i+1)}x_{i+1}^{t} - \dots - a_{in}x_n^{t}}^{\text{" after " } x_i}\Big)$$

Rearrange E_i

* These both methods are not guaranteed to be convergent. A good heuristic is to order the equations such that 'A' matrix is Strictly diagonally dominant.

<u>Definition of Strictly Diagonally Dominant Matrix</u>

An nxn matrix A is strictly diagonally dominant if the absolute value of each entry on the main diagonal is greater than the sum of the absolute values of the other entries in the same row. That is,

$$|a_{11}| > |a_{11}| + |a_{12}| + \dots\dots\dots\dots + |a_{1n}|$$
$$|a_{22}| > |a_{21}| + |a_{23}| + \dots\dots\dots\dots + |a_{2n}|$$
$$\vdots$$
$$|a_{nn}| > |a_{n1}| + |a_{n2}| + \dots\dots\dots\dots + |a_{n,n-1}|$$

Now, rearrange the above set of equations to the following

$$7x_1 - x_2 = 6$$
$$x_1 - 5x_2 = -4$$

If you now use the initial approximation (x1,x2)=(0,0), you will see that both Jacobi and Gauss-Seidel method will converge.

P.S. Please note that, strict diagonal dominance is not a necessary condition for convergence of Jacobi or Gauss-Seidel methods.