Computational Physics

⇒ Runge-Kutta Methods :-

→ In numerical analysis, there are several types of Runge-Kutta (RK) methods, to solve the initial value problems. And they are all based on one equation:

$\frac{dy}{dx} = f(x)$
$\Rightarrow dy = f(x)\,dx$
$\Rightarrow y + dy = y + f(x)\,dx$
$\Rightarrow y_{i+1} = y_i + f(x)\,h$

$$y_{i+1} = y_i + (\text{Slope} \times \text{interval size})$$
$$= y_i + mh$$

→ Where, m represents the slope, that is weighted average of the slopes at various points in the interval h. if we estimate 'm' using slopes at 'r' points in the interval (x_i, x_{i+1}), then

$$m = \omega_1 m_1 + \omega_2 m_2 + \dots + \omega_r m_r$$

→ Where, $\omega_1, \omega_2, \dots \omega_r$ are weights of the slopes at various points. The slopes $m_1, m_2, \dots, m_r$ are computed as follows:

$$m_1 = f(x_i, y_i)$$
$$m_2 = f(x_i + a_1 h,\ y_i + b_{11} m_1 h)$$
$$m_3 = f(x_i + a_2 h,\ y_i + b_{21} m_1 h + b_{22} m_2 h)$$
$$\vdots$$
$$m_r = f(x_i + a_{r-1} h,\ y_i + b_{r-1,1} m_1 h + \dots + b_{r-1,r-1} m_{r-1} h)$$

That is,

$$m_1 = f(x_i, y_i), \quad r = 1 \quad \text{—} ①$$

$$m_r = f\left(x_i + a_{r-1} h,\ y_i + h \sum_{j=1}^{r-1} b_{r-1,j}\, m_j\right), \quad \text{—} ② \quad r \geq 2$$

→ Note that, the computation of slope at any point involves the slopes at all previous points. Slopes can be computed recursively using eqn ②, starting from $m_1 = f(x_i, y_i)$.

→ Runge-Kutta (RK) methods are known by their order. For instance, an RK method is called the <u>r-order Runge-Kutta method</u>, when slopes at 'r' points are used to construct the weighted average slope m.

→ When, $r = 1$, we use only one slope at (x_i, y_i) to estimate y_{i+1}. This method is also known as the Euler method (1st order Runge-Kutta Method).

→ So, for Euler method, $y_{i+1} = y_i + mh$

where, m = slope at (x_i, y_i)

& h = step size (dx or Δx)

→ The Euler method can also be used to solve, the 2nd order differential equations. Suppose we have a 2nd order differential eq^n as:

$$\frac{d^2y}{dx^2} = f \quad \text{with,} \quad y(x_0) = y_0$$

(some function) & $y'(x_0) = y'_0$

→ Then, to get $y(x)$, we can solve two differential eq^{n}s successively given as,

$$\frac{dy}{dx} = y'(x) = u$$

So, $\boxed{y_{i+1} = y_i + h\,u_i(x_i, y_i)}$

and, $\frac{du}{dx} = f(x, y, u) = \frac{d^2y}{dx^2}$

So, $\boxed{u_{i+1} = u_i + h\,f(x_i, y_i, u_i)}$

→ So, by solving the above two differential eq^{n}s by Euler's method, we can get $y(x)$, provided the initial conditions.

→ Similarly, when, $n = 2$, we use two slopes as,

$$m_1 = f(x_i, y_i)$$

$$\& \quad m_2 = f\left(x_i + \tfrac{3}{4}h,\ y_i + \tfrac{3}{2}m_1 h\right)$$

as: $\boxed{y_{i+1} = y_i + \left(\frac{m_1 + 2m_2}{3}\right)h}$

This is known as <u>2nd order Runge Kutta Method or</u>

<u>Heun's method.</u>

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(*) Modified Euler's Method :-

$$y_{i+1} = y_i + Kh$$

where. $K = \frac{K_1 + K_2}{2}$

and, $K_1 = f(x_i, y_i)$

$K_2 = f(x_i + h, y_i + K_1 h)$

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⇒ So, from the above discussions, we get that, it is possible to construct RK Methods of different orders. However the commonly used ones are the fourth order methods. Although there are different versions of fourth order RK Methods, the most popular method is the classical fourth order Runge Kutta method given as:

$$y_{i+1} = y_i + \left(\frac{m_1 + 2m_2 + 2m_3 + m_4}{6}\right)h$$

where, $m_1 = f(x_i, y_i)$

$$m_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{m_1 h}{2}\right)$$

$$m_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{m_2 h}{2}\right)$$

$$m_4 = f\left(x_i + h, y_i + m_3 h\right)$$

→ Like, Euler Method, this can also be modified to solve 2nd order differential equations. Suppose we need to solve,

$$\frac{d^2y}{dx^2} = f(\,), \text{ with conditions, } y(x_0) = y_0$$

(Some function)

$$\& \; y'(x_0) = y'_0$$

Then, We need to solve two differential eq's by RK-4 method:

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

and, $y_{i+1} = y_i + \frac{h}{6}\left(K_1 + 2K_2 + 2K_3 + K_4\right)$

Again, $\frac{du}{dx} = f(x, y, u)$

and, $u_{i+1} = u_i + \frac{h}{6}\left(J_1 + 2J_2 + 2J_3 + J_4\right)$

→ where, $K_1 = u_i$, $J_1 = f(x_i, y_i, u_i)$

$K_2 = u_i + hJ_1/2$, $J_2 = f\left(x_i + \frac{h}{2}, y_i + \frac{hK_1}{2}, u_i + \frac{hJ_1}{2}\right)$

$$K_3 = u_i + \frac{hJ_2}{2}, \quad J_3 = f\left(x_i + \frac{h}{2}, y_i + \frac{hK_2}{2}, u_i + \frac{hJ_2}{2}\right)$$

$$K_4 = u_i + hJ_3, \quad J_4 = f\left(x_i + h, y_i + hK_3, u_i + hJ_3\right)$$

→ So, this is how we can solve the 2nd order DEs using RK-4 method.