

Computational Science in Engineering
Prof. Ashokee De
Department of Aerospace Engineering
Indian Institute of Engineering – Kanpur

Lecture – 37
Numerical Analysis

So, let us continue the discussion on the integration that has last towards the end of that we have looked at the composite integration method.

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Numerical Analysis

Composite Integrative Methods
 $[a, b]$ or $[-1, 1]$

Composite Trapezoidal

$h = \frac{b-a}{N}$

$\int_a^b f(x) dx = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \dots + \int_{x_{N-1}}^{x_N} f(x) dx$

$= \frac{h}{2} [f_0 + 2f_1 + 2f_2 + \dots + 2f_{N-1} + f_N]$

$[a, b] \leftarrow N$

$(x_{i-1}, x_i) \rightarrow (z_i, \dots, N)$

$x_0 = a, x_N = b, x_i = x_0 + ih$

$(i=1, \dots, N-1)$

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Just like where we stopped here with the composite trapezoidal rule. And this is what we looked at.

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Numerical Analysis

error : $-\frac{h^3}{12} [f''(x_1) + f''(x_2) + \dots + f''(x_n)]$

$x_1 < \dots < x_n$

Comp. Simpson's Rule
 $(a, b) \rightarrow 2N$ sub-int. $h = \frac{b-a}{2N}$
 $x_0 = a, x_{2N} = b, x_i = x_0 + ih$
 $i = 1, \dots, 2N-1$

$\int_a^b f(x) dx = \int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots + \int_{x_{2N-2}}^{x_{2N}} f(x) dx$

$= \frac{h}{3} [f_0 + 4(f_1 + f_3 + \dots + f_{2N-1}) + 2(f_2 + f_4 + \dots + f_{2N-2}) + f_{2N}]$

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And the one which we wanted to talk about the composite Simpson's rule, this case also you have this domain (a, b) which is divided into $2N$ sub interval where the length $h = \frac{b-a}{2N}$ and so, we get $(2N + 1)$ abscesses where $x_0 = a, x_{2N} = b$, and $x_i = x_0 + ih$, where i goes from 1 to $(2N - 1)$. So, what do we write here that

$$\int_a^b f(x) dx = \int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots + \int_{x_{2N-2}}^{x_{2N}} f(x) dx$$

So, now, in the right hand side each of these interval we can evaluate the integral by Simpson's rule and what then finally, the total integration that we will get as an composite rule which is

$$= \frac{h}{3} [f_0 + 4(f_1 + f_3 + \dots + f_{2N-1}) + 2(f_2 + f_4 + \dots + f_{2N-2}) + f_{2N}]$$

So, this is what you get.

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Numerical Analysis

$$\text{Error} = -\frac{h^5}{90} [f^{(iv)}(\xi_1) + f^{(iv)}(\xi_2) + \dots + f^{(iv)}(\xi_N)]$$

$x_{2i-2} < \xi_i < x_{2i}$

$$f^{(iv)}(\eta) = \max_{a \leq x \leq b} |f^{(iv)}(x)|, \quad a < \eta < b$$

$$|R_2| \leq \frac{Nh^5}{90} f^{(iv)}(\eta) = \frac{(b-a)^5}{2880N^4} f^{(iv)}(\eta)$$

$$= \frac{(b-a)}{180} h^4 f^{(iv)}(\eta)$$

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And here in this composite Simpson's rule the error which would be associated with that is

$$\text{Error} = -\frac{h^5}{90} [f^{(iv)}(\xi_1) + f^{(iv)}(\xi_2) + \dots + f^{(iv)}(\xi_N)]$$

where $x_{2i-2} < \xi < x_{2i}$. So, this is for the error which is associated with that. So, let us say

$$f^{(iv)}(\eta) = \max_{a \leq x \leq b} |f^{(iv)}(x)|$$

where $a < \eta < b$ then the error which should be bounded by

$$|R_2| \leq \frac{Nh^5}{90} f^{(iv)}(\eta) = \frac{(b-a)^5}{2880N^4} f^{(iv)}(\eta) = \frac{(b-a)}{180} h^4 f^{(iv)}(\eta)$$

So, this is what you get.

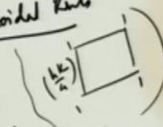
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Numerical Analysis

Double Integration

$$I = \int_a^b \int_c^d f(x,y) \, dx \, dy$$

Trapezoidal Rule



$$I_T = \frac{d-c}{2} \int_a^b [f(x,c) + f(x,d)] \, dx$$

$$= \frac{(b-a)(d-c)}{4} [f(a,c) + f(b,c) + f(a,d) + f(b,d)]$$

$$= \frac{hk}{4} \left[\begin{aligned} & \{ f_{10} + f_{1M} + 2(f_{21} + f_{22} + \dots + f_{2,M-1}) \} \\ & + 2 \sum_{i=1}^{M-1} \{ f_{i0} + f_{iM} + 2(f_{i1} + f_{i2} + \dots + f_{i,M-1}) \} \\ & + \{ f_{M0} + f_{MM} + 2(f_{M1} + f_{M2} + \dots + f_{M,M-1}) \} \end{aligned} \right]$$

$h = \frac{(b-a)}{N}$
 $k = \frac{(d-c)}{M}$
 x_0, x_1, \dots, x_N
 y_0, y_1, \dots, y_M
 $x_{i-1}, x_i, \dots, x_{i+1}$
 $y_{j-1}, y_j, \dots, y_{j+1}$

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Now, the last one which we can look at is that the double integration. So, this double integration so, this is where you want to evaluate that

$$\int_a^b \int_c^d f(x, y) dx dy$$

So, this can be evaluated numerically, for example, we can use a trapezoidal rule to do that, let us say we like this integral

$$I_T = \frac{d - c}{2} \int_a^b [f(x, c) + f(x, d)] dx$$

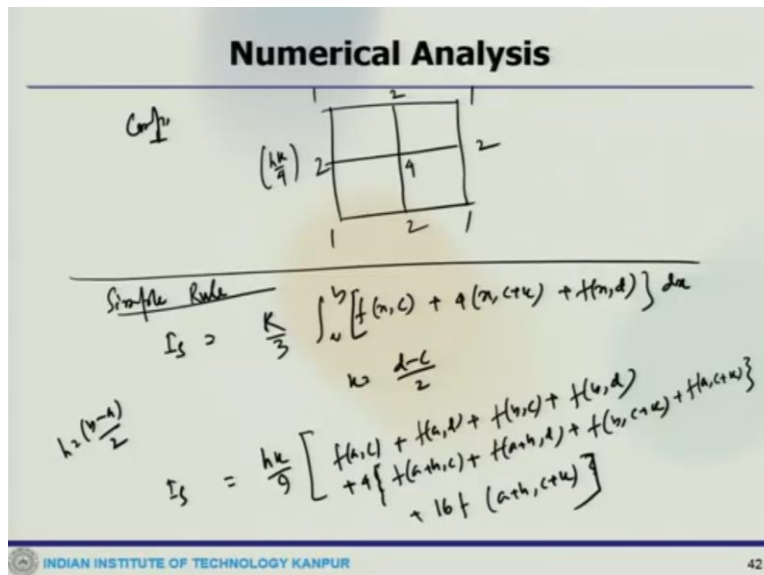
So, this is what we can do. Now, what one can write here that

$$= \frac{(b - a)(d - c)}{4} [f(a, c) + f(b, c) + f(a, d) + f(b, d)]$$

Now the composite trapezoidal rule for evaluating this which will get us that, So, this is what we get when evaluate this. So, what is h and K, $h = \frac{b-a}{N}$ and $K = \frac{d-c}{M}$. So, $x_i = x_0 + ih$, $y_j = y_0 + jK$ for i goes from 1 to (N - 1), j goes from 1 to (M - 1) and $x_0 = a$, $x_n = b$, $y_0 = c$, $y_m = d$.

So, these are the constant that you get where now, this is how the thing would look like in that trapezoidal rule.

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And now, when I go to composite trapezoidal rule, the picture is subdivided into sub interval. So, this is $\left(\frac{hk}{4}\right)$ and this is 1, 2, 1, 1, 1, 2, 4, 2, 2. So, this is how it looked like. And so, this is how one

can get it. Similarly, for the Simpson's rule, you can get the double integration or using the Simpson's rule. So, the double integration using Simpson's rule will get like

$$I_s = \frac{k}{3} \int_a^b [f(x, c) + 4f(x, c + k) + f(x, d)] dx$$

here $k = \frac{d-c}{2}$.

So, this is what you get the complete where $h = \frac{b-a}{2}$. Now, obviously, you can also use the composite Simpson's rule which would be bit kind of involved.

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Numerical Analysis

Composite Simpson's

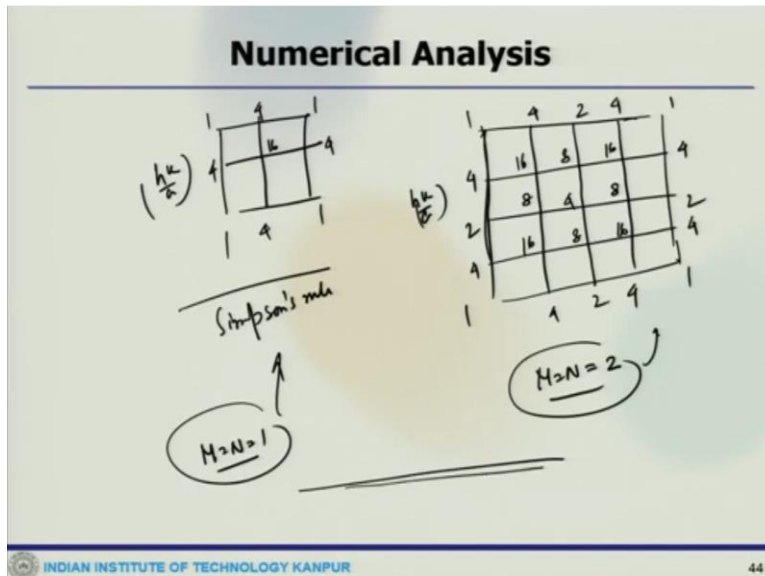
$$I_s = \frac{hk}{9} \left[\left\{ f_{0,0} + 4 \sum_{i=1}^N f_{i,0} + 2 \sum_{i=1}^{N-1} f_{i,0} + f_{2N,0} \right\} + 4 \sum_{j=1}^M \left\{ f_{0,y_{j-1}} + 4 \sum_{i=1}^N f_{i,y_{j-1}} + 2 \sum_{i=1}^{N-1} f_{i,y_{j-1}} + f_{2N,y_{j-1}} \right\} + 2 \sum_{j=1}^{M-1} \left\{ f_{0,y_j} + 4 \sum_{i=1}^N f_{i,y_j} + 2 \sum_{i=1}^{N-1} f_{i,y_j} + f_{2N,y_j} \right\} + \left\{ f_{0,y_M} + 4 \sum_{i=1}^N f_{i,y_M} + 2 \sum_{i=1}^{N-1} f_{i,y_M} + f_{2N,y_M} \right\} \right]$$

$h = \frac{b-a}{2M}, \quad k = \frac{d-c}{2N}$
 $x_i = 2n + ih, \quad i=1, 2N-1$
 $y_j = y_0 + jk, \quad j=1, 2M-1$
 $x_0 = a, \quad x_{2N} = b$
 $y_0 = c, \quad y_{2M} = d$

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So, if you do that the composite Simpson's, then what you write I_s would be as shown on the screen

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So, these are the things, so I mean one can see how it looks like. So, this is what $\left(\frac{hk}{9}\right)$, this is 1, 4, 1, 4, 1, 1, 4, 16. So, this is what you get in simple Simpson's rule, or when you have the composite, then you sub divided into 1, 2, 3, 1, 2, 3, 4. So, this is 1, 1, 1, 1 $\left(\frac{hk}{9}\right)$. So, this is 4, 2, 4, 4, 2, 4, 4, 2, 4, 4, 2, 4 16, 8, 16, 8, 4, 8, 16, 8, 16. So, this is how the whole domain would look like in computational domain usually module what you take $M = N = 1$ which is this is for Simpson's rule.

And when you take $M = N = 2$ this is for the composite Simpson's rule. So, this is how you can get this numerical integration done for the given integration and all these things. So, now we can move to the looking at the solution to the differential equation.

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Numerical Analysis

ODE - Solution

IVP

mth order

vector form

$y' = f(x, y)$

$y(a) = \eta$

$y = [y_1 \dots y_m]^T$

$\eta = [\eta_1 \dots \eta_m]^T$

1st BVP

mth order

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

$y(a) = \eta$

$L y = r(x)$

$U_\mu y = \gamma_\mu, \mu = 1, \dots, m$

L = mth order differential operator.

$r(x)$ = given function of x

U_μ = mth order B.C.

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So, we will start with the solution of the ordinary differential equation. Now, this is what would be interesting because we have looked at differential equation and now, there are one thing which is important is that we have all these initial value problems. So, the initial value problem, what we have is, if we have a system of equations, where let us say, we can define as

$$y' = f(x, y)$$

and for any given value which is given as $y(a) = \eta$ then essentially y is nothing but

$$y = [y_1 \ y_m]^T$$

$$\eta = [\eta_1 \ \eta_m]^T$$

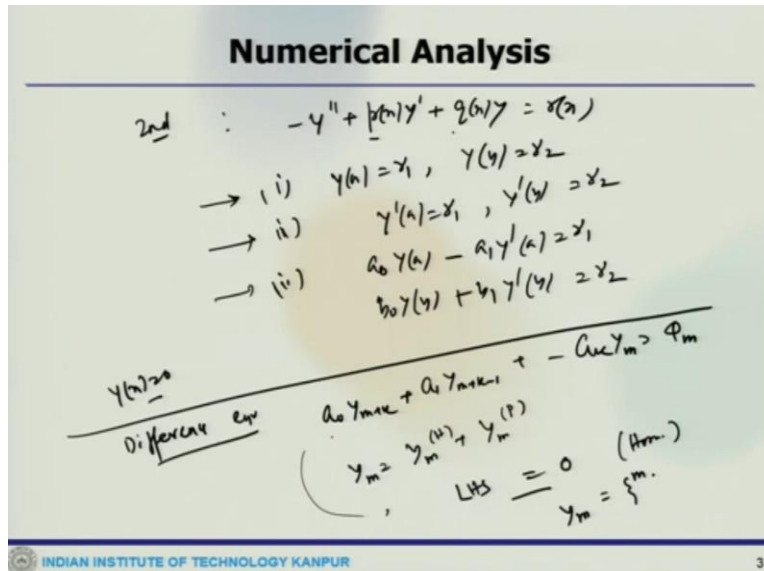
So, this is what you write in sort of in vector form that if you have that kind of a system, now, if we will look at the first order system, then it would simplify to $\frac{dy}{dx}$ the first order system would be

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

and you need 1 initial value at $y(a) = \eta$. So, that we can solve and that is how you are going to solve this initial value problem of a different order.

Now, you can have a similarly you can have the boundary value problem and let us say you have n th order boundary value problem. So, n th order boundary value problem which can be represented like $Ly = r(x)$ and where $U_\mu y = \gamma_\mu$, where μ is 1 to m , L here is the m th order differential operator and $r(x)$ is given function of x , U_μ at boundary condition.

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So, the simplest boundary value problem which can be given by the second order differential equation looks like

$$-y'' + p(x)y' + q(x)y = r(x)$$

now, $p(x), q(x), r(x)$ are a continuous function of x or constant with the 3 boundary conditions what you require one is that $y(a) = \gamma_1$ and $y(b) = \gamma_2$ that is first kind, the second kind would be $y'(a) = \gamma_1, y'(b) = \gamma_2$ and the third kind would be

$$a_0y(a) - a_1y'(a) = \gamma_1$$

Or

$$b_0y(b) - b_1y'(b) = \gamma_2$$

So, the boundary conditions which are given here are the kind of, this is the first kind boundary condition that is, this is second kind and this is the third kind. So, the homogeneous boundary value problem, we will only have a trivial solution for $y(x) = 0$. So, we therefore, considered those boundary value problems in which a parameter lambda occurs either in the differential equation or in the boundary conditions and will determine the value of lambda.

And that is called the Eigen values for which the boundary value problem has non-trivial solution and such a solution is called the Eigen function and the entire problem is called the Eigen value or a characteristic value problem. So, that is one thing, then one can also write these things in like difference equations like for example, we can write that difference equations like it is a Kth order linear non-homogeneous difference equation.

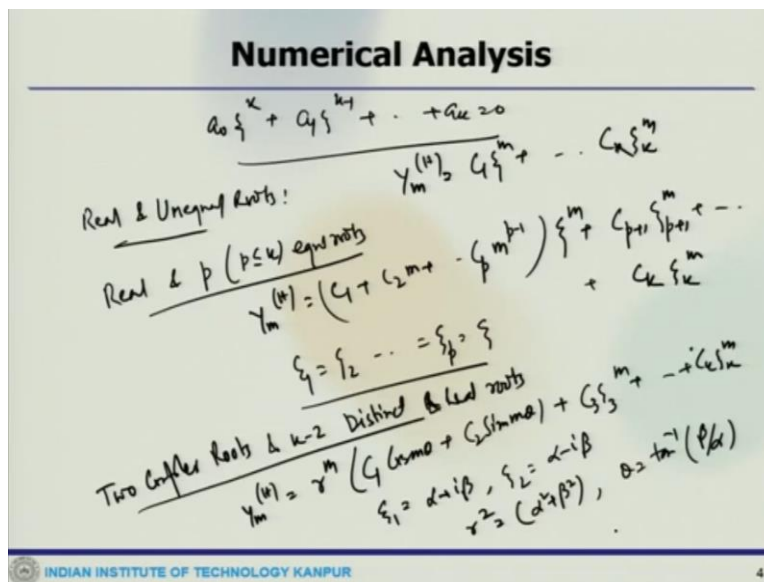
So, the general solution of this equation would be

$$y_m = y_m^{(H)} + y_m^{(P)}$$

Now, for the homogeneous equation to consider this left hand side would be there and the right hand side would be 0, for this is for homogeneous system. Let us say we find on homogeneous solution would be

$$y_m = \xi^m$$

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So, this equation would give us a polynomial equation like

$$a_0 \xi^k + a_1 \xi^{k-1} + \dots + a_k = 0$$

So, this is the polynomial equations and this is called the characteristics equations of the homogeneous equation system. Now, here we can have real and distinct root and unequal roots, then our homogeneous solution would be like

$$y_m^{(H)} = C_1 \xi^m + \dots + C_k \xi_K^m$$

C_i 's are all arbitrary constants, which goes from 1 to 1. Other case would be real and p which is p less than equals to K equal roots.

Then the solution would take the form the homogeneous solution is

$$y_m^{(H)} = (C_1 + C_2 m + \dots + C_p m^{p-1}) \xi^m + C_{p+1} \xi_{p+1}^m + \dots + C_K \xi_K^m$$

where $\xi_1 = \xi_2 = \dots = \xi_p = \xi$. So, they are equal. Now, you can have 2 complex roots and $(K - 2)$ distinct and real roots. So, the solution would be

$$y_m^{(H)} = (C_1 \cos m\theta + C_2 \sin m\theta)\xi^m + C_3 \xi_3^m + \dots + C_K \xi_K^m$$

here

$$\xi_1 = \alpha + i\beta$$

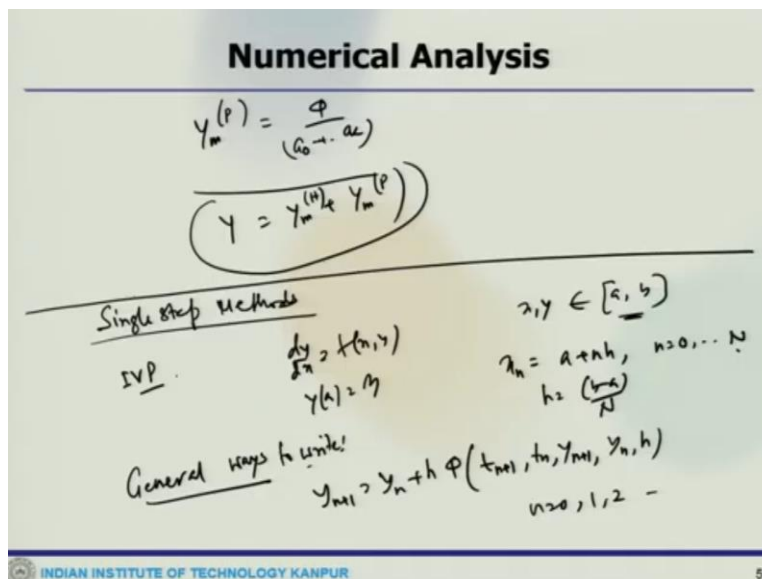
$$\xi_2 = \alpha - i\beta$$

and

$$r^2 = (\alpha^2 + \beta^2)$$

$$\theta = \tan^{-1}(\beta/\alpha)$$

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And so, particular solution could be

$$y_m^{(P)} = \frac{\phi}{(a_0 + \dots + a_K)}$$

So, now, then the general solution we can get like y would be

$$y_m = y_m^{(H)} + y_m^{(P)}$$

this would be the general solution of that. Now, obviously, we have already seen the stability criteria when you have this complex rule and all these things that the real part has to be a negative.

So, that already we have seen that when you have the stable system.

Now moved to that when you have this system like this will go to state with single step methods, how we can solve this ordinary differential equations. Let us say we consider an initial value problem, which is $\frac{dy}{dx} = f(x, y)$ where x, y lies between a and b and $y(a) = \eta$. So, that divide a and b this interval into in equally spaced sub intervals, so, that we get $x_n = a + nh$ where $h = \frac{b-a}{N}$ and n goes from 0 to N .

So, the parameter h is called the step size or mesh size, a single step method is related to first order difference equation. So, I mean kind of a general ways to write is that

$$y_{n+1} = y_n + h\phi(t_{n+1}, t_n, y_{n+1}, b_n, h)$$

like this n goes from $0, 1, 2$ and so, on. and the function is called the increment function.

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Numerical Analysis

Q, increment f_n

Explicit: $y_{n+1} = y_n + h\phi(t_n, y_n, h)$

Truncation error: $T_{n+1} = y(t_{n+1}) - y(t_n) - h\phi(t_n, t_n, y(t_n), y(t_n), h)$

$|h^{-1} T_{n+1}| = O(h^p)$

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So, this ϕ is called increment function and now, y_n and can be then simply by evaluating the right hand side of this equation, but now there are ways one can do either explicit method or implicit method. Now, if it is explicit method that is explicitly, we are finding that out then one can write that

$$y_{n+1} = y_n + h\phi(t_n, y_n, h)$$

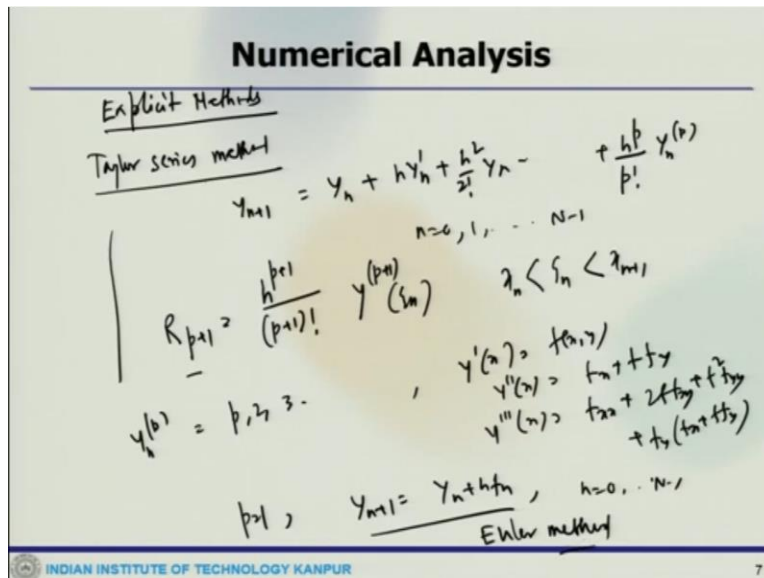
So, that means, this right hand side you can see depends on, so, this is what you write in the implicit method.

Now in the right hand side of this guy, which contents and that if you take into consideration then this goes into the implicit method. And the local truncation error which would come out to be like that, and the largest integer piece is that

$$|h^{-1}T_{n+1}| = O(h^p)$$

So, this is the order of single step method.

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There are a few single step methods that we will look how we can find solution for example; we look at a like explicit some of the explicit methods and where we write is that Taylor series method.

So, where you expand this function like

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2!} y''_n + \dots + \frac{h^p}{p!} y_n^{(p)}$$

where n goes from 0, 1 to (N - 1) and the remainder would be

$$R_{p+1} = \frac{h^{p+1}}{(p+1)!} y^{(p+1)}(\xi_n)$$

So, this called the Taylor series method of order p.

So, the p chosen such that the remainder is less than some p assigned accuracy or epsilon. So, then that it lies. Now derivative that $y_n^{(p)}$ where p could be 2, 3 and this can be successively determining the differential equation and then evaluating at $x = n$. So, we can say that

$$y'(x) = f(x, y)$$

$$y''(x) = f_x + f f_y$$

$$y'''(x) = f_{xx} + 2f f_{xy} + f^2 f_{yy} + f_y(f_x + f f_y)$$

such that. So, if we take $p = 1$ then we get

$$y_{n+1} = y_n + h f_n$$

n goes to 0 to $(N - 1)$. Euler method, which is one of the simplest one that one can evaluate the method the function like that.

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Numerical Analysis

Runge Kutta method

General $y_{n+1} = y_n + \sum_{i=1}^v w_i k_i, \quad n=0, \dots, N-1$

$k_i = hf(x_n + C_i h, y_n + \sum_{m=1}^{i-1} a_{im} k_m)$

with $C_1 = 0$

For $w_1=1, w_2=1 \rightarrow$ Euler's method with $p=1$

p	2	3	4	5	6	-
v	2	3	4	6	8	...

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Now slightly better method that we can have been the Runge Kutta method like the general RK methods, which is can be written as y_{n+1} this is in general how you can write so, that

$$y_{n+1} = y_n + \sum_{i=1}^v w_i k_i$$

where $n = 0$ to $(N - 1)$ and

$$k_i = hf(x_n + C_i h, y_n + \sum_{m=1}^{i-1} a_{im} k_m)$$

with $C_1 = 0$. So, for $v = 1, w_1 = 1$, the equation becomes now eulerian method.

So, this becomes eulerian method. So, this goes to Euler's method with $p = 1$. So, this is the lowest order RK method that one can get. So, for higher order methods, like there will be different values of p and v , like 2, 3, 4, 5, 6 so on, v would be 2, 3, 4, 6, 8 and so on. So, we will stop here. And

so, we have looked at the expression for the general RK method and we will look at some of those higher order RK method second order or third order and move to the next session.