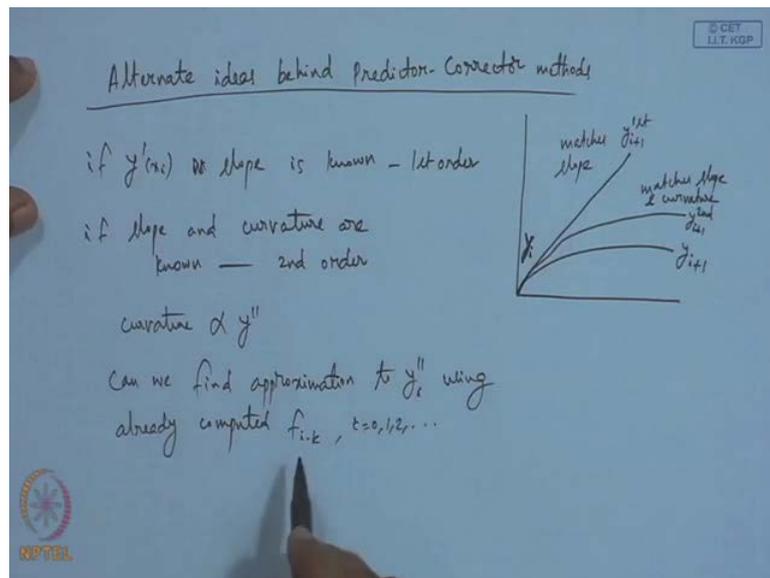


Numerical Solutions of Ordinary and Partial Differential Equations
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Lecture - 15
Some Comments on Multi-Step Methods

Hello. In the last few lectures, we have been discussing about multistep methods. So, we started with explicit methods then implicit, then we discussed some stability aspects, and then how a combination of explicit implicit methods can be used as predictor corrector methods to improve upon the solution. So, well we have given some motivation for the multistep methods, but however I would like to mention here a different motivation and then some comments on multistep methods. So, it is a kind of alternative approach, but it is a intuitive.

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So, let us start with that. So, alternate ideas behind corrector, suppose this is our y_{i+1} and this is the approximation, let us denote some other notation. So, this is matches slope for this. So, this can be thought of us first approximation suppose this matches slope and curvature. So, then this can be thought as second order approximation. So, if y' at x_i is slope is known, then it is a first order approximation. If slope and curvature are known second order approximation, but the fact is curvature is proportional to y''

double prime. So, hence the question is can we find approximation to y_{i+1} using already computed values.

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Handwritten mathematical derivation on a blue background:

$$y_i'' = \frac{y_i' - y_{i-1}'}{h} + O(h) = \frac{f_i - f_{i-1}}{h} + O(h)$$

$$y_{i+1} = y(x_i+h) = y_i + h y_i' + \frac{h^2}{2} y_i'' + O(h^3)$$

$$= y_i + h f_i + \frac{h^2}{2} \left(\frac{f_i - f_{i-1}}{h} + O(h) \right) + O(h^3)$$

$$= y_i + h \left(\frac{3}{2} f_i - \frac{1}{2} f_{i-1} \right) + O(h^3) \quad \text{--- (*)}$$

Remark (*) becomes exact rather than approximate if $y^{(2)} = P_2(x) = ax^2 + bx + c$
 $y_i' = 2ax + b$; $y_i'' = 2a = \frac{y_i' - y_{i-1}'}{h}$

Logos: NPTEL (bottom left), © IIT KGP (top right)

So, this is the motivation can we approximate this person. So, usual approximations y_{i+1} double minus by h , usual difference approximation then y_{i+1} is Taylor series. So, y_{i+1} double prime can we approximate this using past points. So, here is the answer, we substitute. So, this we got a kind of a multistep method. So, what did we do just this is the Taylor series expansion, but then the second derivations have been approximated by the corresponding finite differences which involve past points, but star becomes exact rather than approximate if y of x is polynomial degree 2 because y_i' is $2ax + b$ then y_i'' is $2a$ by h . So, this star becomes exact rather than approximation if because the coefficients are determined.

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⊗ is second order
 However, if one needs 3rd order?

$$y_i''' = \frac{y_i' - 2y_{i-1}' + y_{i-2}'}{h^2} + O(h)$$
 then
$$y_{i+1} = y_i + h y_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i''' + O(h^4) \quad \otimes$$
 In order to use $y_i'' = \frac{f_i - f_{i-1}}{h} + O(h)$ in \otimes , we need an expression for the $h O(h)$ term with accuracy $O(h^2)$.

So star is second order, however if one needs third order what would we do, let us consider this. So, then finite difference approximation then we get . So, this is our new star, but the question see in the earlier case we have a substituted in the earlier case we have substituted for y i double only of after order h, but now we would like to go for a higher. So, in order to use y i double which is after order of h in star we need an expression for this because we have to increase right an expression see this is h square. So, you need third order, you need an expression for this. So, that h square times this you get third order. So, an expression for the order h term with accuracy h square.

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$$\frac{y_i' - y_{i-1}'}{h} = \frac{y(x_i) - y(x_{i-1}))}{h}$$

$$= \frac{y_i' - (y_i' - h y_i'' + \frac{h^2}{2} y_i''' + O(h^3))}{h}$$

$$= y_i'' - \frac{h}{2} y_i''' + O(h^2)$$

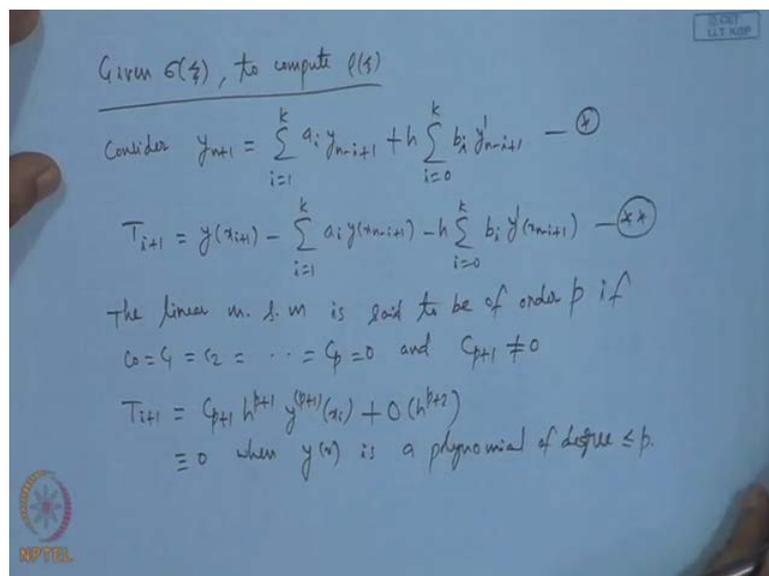
$$\therefore y_i'' = \frac{y_i' - y_{i-1}'}{h} + \frac{h}{2} y_i''' + O(h^2)$$

$$\otimes \Rightarrow y_{i+1} = y_i + \frac{h}{12} (23f_i - 16f_{i-1} + 5f_{i-2}) + O(h^4)$$
 Adams-Bashforth 3rd order

So, how do we do it y_i prime minus for the second derivative we want to increase the order. So, therefore, now if we substitute this star would lead to which is Adams Bashforth third order method. So, this is a kind of a alternative thought i mean this is a little unusual, but this is a kind of a alternative thought. So, this gives the multistep method. So, one can derive other methods.

Now, if you recall in one of the earlier lectures. So, given see a general linear multistep method can be expressed in terms of a 2 characteristic polynomials that is a first characteristic the second. Now, one of the question that was posed was given the first one can we determine the second characteristic polynomial, so that they corresponding multistep method is determined, that was a bit unfinished.

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So let us try to recall this and then try to compute for a particular case. So, given to compute, we consider a multistep method i would like to make a remark. So, this can be written in different notations. So, I do not want you to remember, we should be able to write within any general notation. Sometimes, like this sometimes with a n plus j combination. So, this is our multistep method then the corresponding error, now linear multistep method said to be of order p equal to 0 and C_{p+1} non 0. So, accordingly t_{i+1} plus 1, we get this that is identically 0, when $y(x)$ is a polynomial of degree less than equal to p $y(x)$.

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Observe that c_i and p are independent of $y(x)$!

Choose $y(x) = e^{\lambda x}$, $y_j = e^{\lambda x_j}$

then $(**)$ \Rightarrow

$$T_{i+1} = e^{\lambda x_{i+1}} - a_1 e^{\lambda x_i} - a_2 e^{\lambda x_{i-1}} - \dots - a_k e^{\lambda x_{i-k+1}}$$

$$- h [b_0 e^{\lambda x_{i+1}} + b_1 e^{\lambda x_i} + \dots + b_k e^{\lambda x_{i-k+1}}]$$

$$= \left[e^{\lambda kh} - a_1 e^{\lambda (k-1)h} - a_2 e^{\lambda (k-2)h} - \dots - a_k \right]$$

$$- h [b_0 e^{\lambda kh} + b_1 e^{\lambda (k-1)h} + \dots + b_k] e^{\lambda x_{i-k+1}}$$

Now, observe that c_i and p , order of the method are independent of y of x k . So, choose y this y of x is e power x . Accordingly this then your double star which is the error this. So, this is e power if I take e power x_i minus k plus 1 common e power $k h$ e power h minus x this.

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$\therefore T_{i+1} = (p(e^h) - h\sigma(e^h)) e^{\lambda x_{i+1}}$

$$= \left(\sum_{k=1}^k c_k h^{k-1} + O(h^{k+2}) \right)$$

\Rightarrow $p(e^h) - h\sigma(e^h) = \sum_{k=1}^k c_k h^{k-1} + O(h^{k+2})$

Let $e^h = \xi$, $h = \log \xi$

as $h \rightarrow 0$, $\xi \rightarrow 1$

$$\log \xi = \log [(\xi-1)+1] = (\xi-1) - \frac{1}{2}(\xi-1)^2 + \dots$$

$$h^{k+1} = (\log \xi)^{k+1} = (\xi-1)^{k+1} + O((\xi-1)^{k+2})$$

So, using this notation this can be written as $\rho(h, \sigma)$ because this is the characteristic first characteristic and second. So, but then this must be equals to, from these 2 we can. So, by some terms of this will be left that is e power 1 minus k . So, that e

power k minus 1. So, this is h times 1 minus k . So, that is given to this coefficient. So, with adjustment it can be written like this, now this becomes the basis for finding given this how to find the second characteristics polynomial. How do we do it, let us proceed set this as h goes to 0 1 then $\log z$ we write it as z minus 1 plus 1 and we write it an expansion further h power p plus 1 is $\log z$.

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$$\therefore \rho(\zeta) - h\sigma(\zeta) = \sum_{p=1}^k \binom{k}{p} (\zeta-1)^{p+1} + O((\zeta-1)^{k+2}) \quad \text{--- } \oplus$$

if $\sigma(\zeta)$ is given, the above \oplus can be used to find $\rho(\zeta)$

- expand $\log \zeta$, $\sigma(\zeta)$ in $(\zeta-1)$, retain terms of required order.
- implicit $\rho(\zeta)$ & $\sigma(\zeta)$ are of same order
- explicit $\rho(\zeta)$ is one higher

Now, these two we use it here therefore, if is given the above can be used to find ρ , how do we do it expand in then retain terms of required order. So, another remark is implicit are of same order or the degree explicit ρ is 1 higher.

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example Given $\rho(z) = z(z-1)$, find $\sigma(z)$
 degree $\rho(z) = 2 \Rightarrow$ degree $\sigma(z) = 1$
 $\rho(z) = z(z-1) = (z-1)^2 + z-1$
 $\rho(z) = \frac{(z-1)^2 + z-1}{\log(1+(z-1))} = \frac{(z-1)^2 + z-1}{z-1 - \frac{1}{2}(z-1)^2 + \dots}$
 $= (1+(z-1)) \left[1 - \frac{1}{2}(z-1) - \dots \right]^{-1}$
 $= (1+(z-1)) \cdot \left[1 + \frac{1}{2}(z-1) + \dots \right]$
 $= 1 + \frac{3}{2}(z-1) + 0(z-1)^2$

So, let us work it out with an example, given find this, so looking at this. So, this implies. So, degree of 1 for of course, for a explicit method. So, this can be further simplified as, what we have taken we have cancelled out z minus 1. So, we expanded therefore, this equals to because of a, the second degree, we have expanded up to that.

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$\therefore \sigma(z) = 1 + \frac{3}{2}(z-1) = \frac{3}{2}z - \frac{1}{2}$
 \therefore method
 $\rho(E)y_{n+1} - h\sigma(E)y'_n = 0$
 $\Rightarrow (E^2 - E)y_{n+1} - \frac{h}{2}(3E-1)y'_n = 0$
 $\Rightarrow y_{n+1} = y_n + \frac{h}{2}(3y'_n - y'_{n-1})$

We have got sigma, therefore the method is explicit which is of second order. So, what did we do given this we have expanded. So, this is h , h is a log zeta. So, I have divided, this rho by h rho by log zeta we have expanded. So, rho by log zeta we expanded, so then

up to second order. So, that should be of order sigma neglecting of second order that should be sigma and hence the method is given by this. So, this gives a sense of computing first characteristic polynomial second characteristic polynomial vice versa.

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Stiff systems

$$\dot{\bar{x}} = A\bar{x}, \quad A = \begin{pmatrix} 998 & 1998 \\ -999 & -1999 \end{pmatrix}$$

$$\bar{x} = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}, \quad x_1(0) = x_2(0) = 1.$$

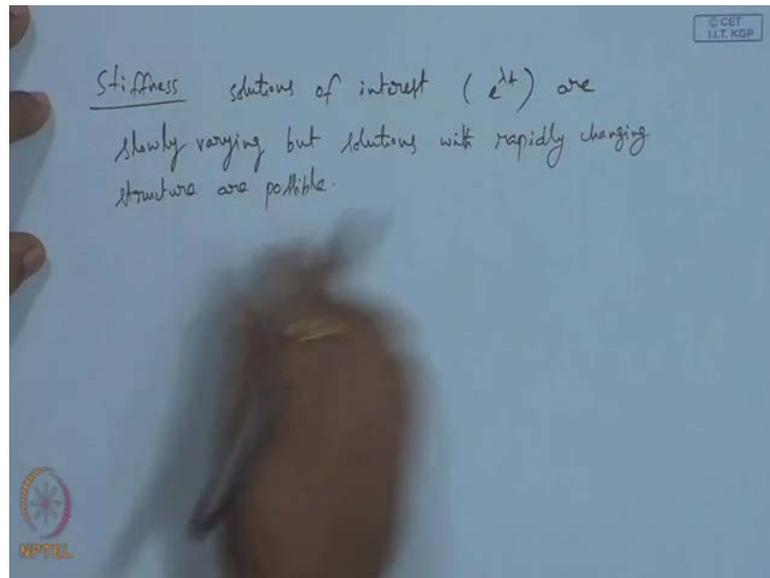
$$\Rightarrow x_1(t) = 4e^{-t} - 3e^{-1000t} \Rightarrow x_1 \sim 4e^{-t}$$

$$x_2(t) = -2e^{-t} + 3e^{-1000t} \Rightarrow x_2 \sim -2e^{-t}$$

as $t \rightarrow \infty$
time

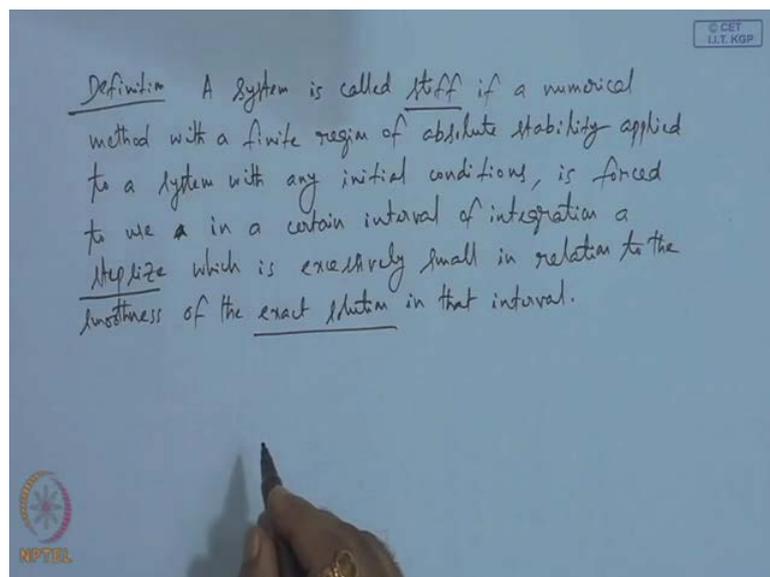
So, there is another aspect related to multistep methods which I would like to mention stiff systems. So, stiff systems has to do with the system of equations, but however while solving using multistep methods, it is a important study stiff systems in the context of multistep methods. So, we have a system, example say A is with conditions where x bar is say x 1 of t and x 1 of 0. So, this implies x 1 of t is, we have an equation like this system the coefficient matrix is like this with this initial conditions we get the solution. So, this becomes this is after a short time the reason is you have a big coefficient multiplying t. So, after short time this decays faster than this. So, after short time we have this solution.

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So, what is great about this system it is a very fuggy kind of a term, stiffness, solution of interest what are they, we expect solutions of interest means they are of the form $e^{\lambda t}$ kind of solutions right are slowly varying, but solutions with rapidly changing structure are possible. So, look at this, these are the solutions of interest, but however you have solutions that are rapidly changing.

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So, let us define more precisely, a system is called stiff if a numerical method with a finite region of absolute stability applied to a system with any initial conditions, is forced

to use in a certain interval of integration a step size, which is excessively small in relation to the smoothness of the exact solution in that interval.

So, what it says a system is called stiff if a numerical method with a finite region of absolute stability, applied to a system with any initial conditions is forced to use in a certain interval of integration, a step size which is excessively small, that means your exact solution is really smooth up to some order, but however the step size that the method is demanding is not in correlation. So, we can analyze this a little more carefully. So, let us analyze with respect to system

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Consider a system

$$\begin{cases} \bar{y}' = \bar{f}(x, \bar{y}) \\ \bar{y}(a) = \bar{y}_0 \end{cases} \quad \text{--- (1)}$$

where $\bar{y} = (y_1, y_2, \dots, y_m)^T$

eg. $y_1' = x + y_1 - y_2, \quad y_1(0) = 1$ $\bar{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$ $\bar{f} = \begin{pmatrix} x + y_1 - y_2 \\ x^2 - y_1 \end{pmatrix}$
 $y_2' = x^2 - y_1, \quad y_2(0) = -1$

A linear k-step method for the numerical solution of (1) has the form

$$\sum_{j=0}^k a_j \bar{y}_{n+j} = h \sum_{j=0}^k b_j \bar{f}_{n+j}$$

Consider system that means a system of IVPs, so where these are the unknowns. So, example here our y was and this is an example. Now, we have learnt how to solve an IVP for a single component, but then suppose if we extend similar method to this we must arrive at a multistep method. So, a linear k step method for the numerical solution of one solution of one we expect to have the following form.

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Let us assume that $\bar{f}(\bar{y}, \bar{y}) = A\bar{y} + \bar{b}$

$$\bar{f} = \begin{pmatrix} x + y_1 - y_2 \\ x^2 - y_1 \end{pmatrix} = A \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \bar{b} = \begin{pmatrix} 1 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} x \\ x^2 \end{pmatrix}$$

$A_{m \times m}$ - constant matrix
 $\bar{b}_{m \times 1}$ - column.

(M) $\Rightarrow \sum_{j=0}^k (a_j I - h b_j A) \bar{y}_{n+j} = h \sigma(1) \bar{b}$
 where $\sigma(1) = \sum_{j=0}^k b_j \neq 0$

So, now let us assume that this f vector is of this form. So, for example, f bar is x plus y_1 minus y_2 . So, this we need to express, this is possible. So, we need to get y_1 minus y_2 and 0 plus. So, this is our A , this is suppose we are assuming like this. So, constant matrix and b bar column, this is the column matrix then your multistep method gets reduced to where. So, this is a simple exercise with reference to this split up, if you put it in your multistep method we can check the multistep method reduces to this.

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Let the eigenvalues of the matrix A are distinct $\lambda_i, i=1, \dots, m$.

Then \exists a non-singular matrix $H \Rightarrow$

$$H A H^{-1} = \Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & \lambda_m \end{pmatrix}$$

define $\bar{z} = H\bar{y}$ and $\bar{c} = h\sigma(1)H\bar{b}$ then (M*) \Rightarrow

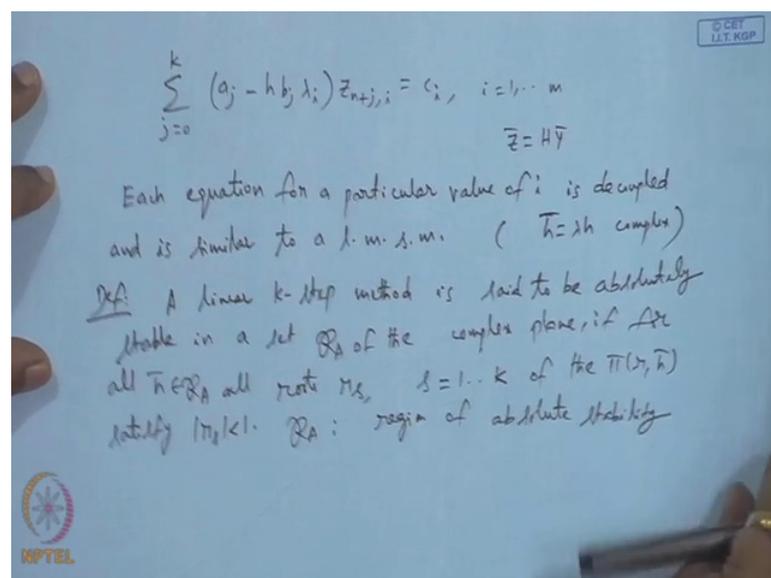
$$\sum_{j=0}^k (a_j H^{-1}H - h b_j H^{-1}\Lambda H) \bar{y}_{n+j} = h\sigma(1)\bar{b}$$

$$\Rightarrow \sum_{j=0}^k (a_j I - h b_j \Lambda) \bar{z}_{n+j} = \bar{c}$$

Let the Eigen values of matrix a are distinct the λ_i , then there exists a non singular matrix h such that can you guess what would be the matrix yes of course, the Eigen values entries. The diagonal matrix with Eigen values. Then define what for we are doing, see look at this we know how to solve a single multistep method for a single component. So, you have initial value problem, let us say this is single component we have multistep method then we know how to compute the solution and how to analyze whether the method is stable or not, but then for a system it is coupled you can see.

So, unless you arrive at a corresponding multistep method which is decoupled we can we are not in a position to comment on the stability and overall behavior of the system. So, we are trying to do that. So, define this and c is, then we get. So, then this is m star, then m star becomes a j . So, your m star contain identity matrix. So, this one can write h inverse h . So, I would like to write minus $h b j$ and a so it can be written like this.

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The same thing can be written as this is a component i th component of the vector. So, this is you can see this is a corresponding Eigen value. This is the corresponding component of a the vector z and what was our definition. So, what did we achieve, each equation for a particular value of i is decoupled and is similar to a linear multistep method, but only one remark h bar equals λh can be complex.

Now, one can discuss the stability because now each equation is like a multistep method, but only thing is this is complex. So, within the context of this complex, let us discuss

the absolute stability region. So, a linear k step method is said to be absolutely stable in a set $R \subset \mathbb{C}$ of the complex plane, if for all h this all roots r_1 to r_k of the stability polynomial satisfy this, then the set $R \subset \mathbb{C}$ is called region of absolute stability.

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Example $2y_{n+2} = y_{n+1} - \frac{h}{3}(2f_{n+1} - f_n)$.

$$\rho(z) = 2z^2 - z, \quad \sigma(z) = -\frac{1}{3}(2z-1)$$

$$\pi = 2z^2 - z + \frac{h}{3}(2z-1) = 0$$

$$\Rightarrow z = \frac{3-2h \pm \sqrt{9+4h^2-12h+24h}}{12}$$

$$= \frac{1}{2}, \frac{-h}{3}$$

$$|r_1| < 1 \Rightarrow |h| < 3.$$

So, let us see for a single component case. So, for example, we have this and we have. So, π is this equals to 0 this implies z equals to. So, we need a the region, this implies the region.

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Euler method $y_{n+1} = y_n + h f_n$.

$$\pi = z - 1 - h$$

$$\Rightarrow z = 1 + h$$

$$RA : \{ h \in \mathbb{C} \mid |1+h| < 1 \}$$

open circle centred at -1.

Suppose, consider Euler method then ρ is given by, implies r is $1 + h\lambda$ and the region R will be $h\lambda$ belongs to the complex plane such that. So, what is this, this is an open circle centered at -1 . So, this is the stability region, for a system also one can discuss and one can observe that for the system, if the stability region is dictating some range, however the solution is demanding very smaller h due to the extraneous terms. So, then really the system is stiff in that context. So, this gives a some idea on the stiff system. So, you can refer the notes by Julie for a better understanding with respect to examples. So, more or less this gives some idea of multistep methods, predictor corrector methods.

Thank you bye.