Scientific Computing using Matlab

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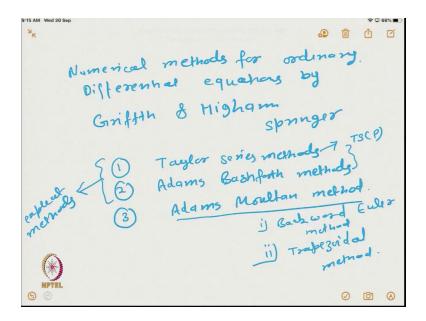
Indian Institute of Technology, Delhi

Lecture 62

Linear Multistep Method (LMM) For Ordinary Difference Equations

Welcome to all of you in the second class from my side in this course. So, first of all I would like to mention what is the book which we are following.

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Let me write that book, numerical methods for ordinary differential equations by, authors are Griffith and Higham and the book is published by Springer. So, this is the book which we will be following for this part of the course.

Now, let me recall what we have done in the last lecture, in the last lecture initially we have seen Taylor series methods. Then we saw Adams Bashforth methods and after that we looked at Adams Moulton method.

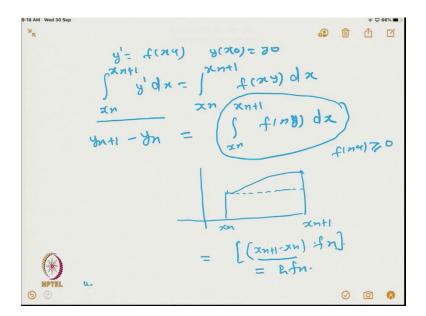
So, Taylor series methods and Adam Bashforth methods were the category of explicit methods and both can be of different order as we have seen that it is called TS(P) and when P is one, means it is first order that create method in that case it is called forward Euler method.

Similarly, Adam Bashforth method of order one is also called forward Euler methods. So, the first category of method in both the cases are the same which is the forward Euler method. While in the case of Adams Moulton method the first order method was called backward Euler method and second was called Trapezoidal method.

Trapezoidal method in some literature is also called modified Euler method and we have already seen that Adams Moulton methods is a way to develop general implicit methods and both of them are implicit, backward Euler method is also implicit and trapezoidal method is also implicit and that is what we have already seen in the last lecture.

But if you look at the derivation of these methods that we discussed in the last lecture, they were through the Taylor series by some manipulations of high order derivative terms, etc. Now, in this lecture, we can also see the alternate way of driving these methods, what is that through numerical integration, that is what I am going to show now.

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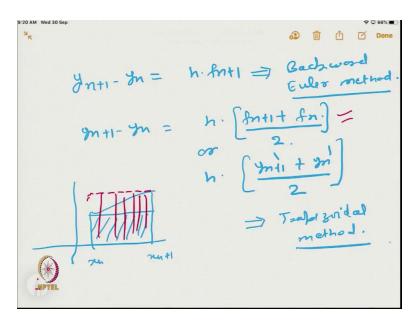


So, suppose this is my problem, y' = f(x, y), $y(x_0) = y_0$ let me integrate both the sides from x_n to x_{n+1} . So, now left hand side will become $y_{n+1} - y_n$, while on the right hand side we have to of course, if we are integrating as such then it corresponds to

analytical method but our role is to drive the numerical method for which we do not know the, how to integrate these terms.

So, in that case like that is the role of numerical Quadrature formulas also which you have seen in the previous part of this course. So, basically I wanted to integrate, suppose this is my function f(x,y) from x_n to x_{n+1} . So, if, just for simplicity I am considering, let us say this is positive. So, if I choose the sample point at the left hand like this then the approximation of this integration will be this $(x_{n+1} - x_n)f_n$, so which is basically hf_n so it means it is a forward Euler method and if I choose a sample point here at the right hand which you.

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Let me show you, in that case $y_{n+1} - y_n = h\left(\frac{f_{n+1} + f_n}{2}\right)$, so it corresponds to the backward Euler method. Why am I saying sample point? Because that is the way how you approximate numerical integral by Riemann sum, by choosing the sample point and if I choose the sample point at the average of both in that case this will become this or this which is basically a Trapezoidal method.

So, we have seen, like if this is a function we are integrating from x_n to x_{n+1} sometimes we are approximating the area under this curve with the help of this rectangle and sometimes we are approximating this with the area of this rectangle. So, we are overshooting the real area, in the previous case we are underestimating the real area, sometime we are choosing

with the help of Trapezoidal because this is the area of also trapezoid that is why it is called Trapezoidal method.

So, that is how you can also see how these methods can be derived otherwise with the help of numerical Quadrature method. So, though we have seen only a few special cases like forward Euler, backward Euler, Trapezoidal method, let me see one more case of implicit method which is the second order Adams Moulton method because we have already seen the difference equation of that method in the last lecture.

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$$\frac{y = f(xu)}{xnt^{2}} \quad y(x_{0}) = y_{0}$$

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$$\frac{xnt^{2}}{xnt^{2}} \quad y(x_{0}) = y_{0}$$

$$\frac{xnt^{2}}{xnt^{2}} \quad xnt^{2}$$

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$$\frac{x^{2}}{x^{2}} = u$$

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$$\frac{x^{2}}$$

So, again I am writing differential equation y' = f(x, y), $y(x_0) = y_0$ let me integrate it, this time I am integrating from x_{n+1} to x_{n+2} So basically, if we do this and we approximate this function with Newton's interpolating polynomial which you remember from the previous part of this course, then you must have derived the interpolating polynomials.

So, this will be $f_n + \left(\frac{x - x_n}{h}\right) \Delta f_n$, so the left hand side will become this and the right hand side will be this.

So, let me substitute $\frac{x - x_n}{h} = u$ So in that case the limit of u will become this and this

will become hdu, so this will become $f_n + \frac{3}{2}(f_{n+1} - f_n)$

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$$y_{n+2} - y_{n+1} = h \left[f_n + \frac{3}{2} \left(f_{n+1} - f_n \right) \right]$$
$$= \frac{3h}{2} f_{n+1} - \frac{h}{2} f_n.$$

So, the scheme will be this

the scheme we observed in the second order Adam Bashforth method because just this starts

from n+2 so this is recursive I can write $y_{n+1} - y_n = \frac{h}{2} \left[3f_n - f_{n-1} \right]$. In the last lecture, you must have seen in the following form that it does not matter because n can be here. I am replacing n with n-1 so we can get the following terms.

So, I have also shown you how to derive these difference schemes with the help of numerical Quadrature which you have already seen in the previous part of this course. So, basically we have derived forward Euler, backward Euler, Trapezoidal method as well as we have also developed the difference scheme for a second order Adam Bashforth formulae which was not specified by this special name but the differences scheme was the following.

And it was explicit anyway Adam Bashforth methods are explicit moreover, the specific point about this scheme was that it is a two step method because there are terms involving n-1, n and n+1 that is why it was called two step method.

Similarly, as I was saying that, we can develop trapezoidal method also in the following way but in that case I have to integrate if you, because last time what I have done I have chosen the sample point at the average of 2 so that was through the, if you look at the definition of

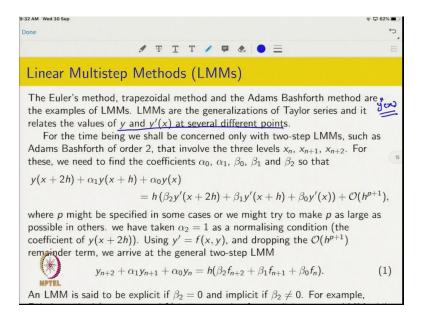
the Riemann sum as an approximation of a numerical integration but more formally if you do the following way and then you interpolate this function with fn this, you will get the same difference equation which we got in Trapezoidal method.

But now one specific thing about this and the previous case was that in previous case I was integrating from x_{n+1} to x_{n+2} and inside this interpolating polynomial I was keeping the term which was involving only points at $x = x_n$ but in this case I am integrating from x_n into x_{n+1} but still inside this I am keeping the same terms. So, why?

Because we know accordingly we will get, Trapezoidal method is just a single step method, they involve terms with n and n+1, while in case of a this two step method terms were involved n+1 and n+2 from here, n-1, n and n+1 here so that is why we have not started integration from x_{n+1} to x_{n+2} . So, it all depends how you want to manipulate and what are the terms you want to keep in your difference equation accordingly you will get to a difference equation.

So, this is the alternative way of driving the formulas for numerical solutions to ODE. Similarly, you can also go for higher order. You can take one third Simpson rule to approximate numerical integration 3/8 Simpson's rule so there are a lot of rules for that, so accordingly you will get different types of formulas or difference equations. Now, just let me open the slides, yes.

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So, let me mention you Linear Multistep methods, Linear Multistep methods because so far we have seen single step method or two step method. In fact, we have seen only one variant of a two step method which was the second order Adam Bashforth method, the Euler method, Trapezoidal method and the Adam Bashforth methods are example of Linear Multistep method, single step, two step all the, both category comes under multistep.

So, Linear Multistep methods are the generalisation of Taylor series. Why is it a generalisation of a Taylor series? Because you will see that when we were looking at the Taylor series methods the term involving second order derivatives and higher order derivatives were kept as such. While in other cases, which we have seen so far the terms involving were having only y and the value of its derivative so that is what I am saying here also and it relates the value of y and y' at several points.

So, basically it relates the value of y and y' At several points, that is the difference in Linear Multistep method and Taylor series methods. In Taylor series methods terms also involve y'', value of y'', while in Taylor series methods we are relating only the value of y and y' at several different points so I will be explaining this in detail also.

For the time being we shall be concerned only with two step Linear Multistep methods. Of course, what I am explaining here can be generalised to more than two step but right now our concern is just to drive two step Linear Multistep method in general like Adam Bashforth method of order 2 which we have already seen that involves the three level X_n , X_{n+1} , X_{n+2} for this we need to find the coefficients α_0 , α_1 , β_0 , β_1 , β_2 so that we are writing

 $y(x + 2h) + \alpha_1 y(x + h) + \alpha_0 y(x) = h(\beta_2 y'(x + 2h) + \beta_1 y'(x + h) + \beta_0 y'(x)) + O(h^{p+1})$ So, where p might be specified in some cases means I wanted to, if I wanted to drive a first order method, I have to specify p and or sometimes depending on the template, we wanted to choose p means what are the points we wanted to keep in the difference equation accordingly we have to choose p.

So, sometimes we want, we might to try to make p as large as possible so in this case we have taken alpha two which are suppose to become here, as a normalising condition, we have chosen $\alpha_2 = 0$ the coefficient of y(x+2h) that is what you can observe from here.

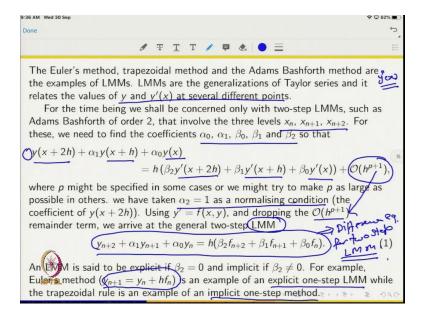
And using y' = f(x, y) and dropping the term $O(h^{p+1})$ that term so once we started dropping this term, this is some equation but once we start dropping the truncation error it will be a difference equations we arrive at general two step linear multi step method

 $y_{n+2} + \alpha_1 y_{n+1} + \alpha_0 y_n = h(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n)$. and LMM is the abbreviation for Linear Multistep method which we will be seeing now onwards.

So, now, this is your difference equation for the two step Linear Multistep method. So, if you observe this difference equation carefully, if I say $\beta_2 = 0$ in that case this will be called explicit method, the method corresponds to this difference equation will be called explicit method if I choose $\beta_2 = 0$ but if I choose because then there is no term which will be involving y_{n+2} in the right hand side so that is the definition which we have already seen in the last lecture corresponds to explicit and implicit methods. I do not need to repeat that definition again.

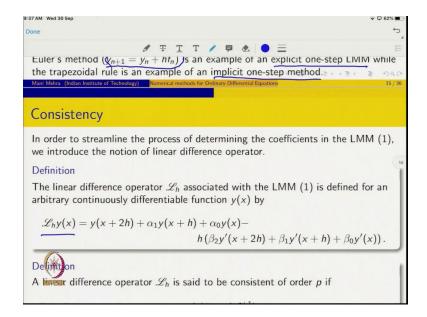
While if I say $\beta_2 = 0$ it is explicit, if $\beta_2 \neq 0$ it is implicit Linear Multistep methods. So, for example, in case of Euler methods when we got this difference equation earlier so basically it is an example of a explicit 1 step Linear Multistep method while the Trapezoidal rule is a example of a implicit 1 step methods, you know some people call it as a method, some people call it as a rule, some people call it as a formula these are just synonyms of the same thing.

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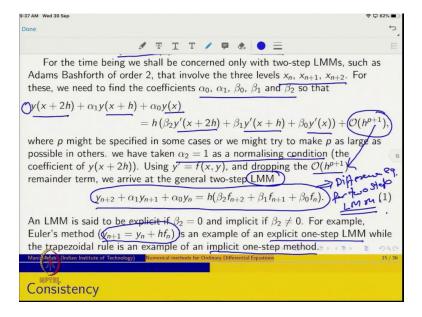
Now, in order to streamline the process of determining the coefficient of this Linear Multistep method, we introduce the notion of a linear difference operator because difference equation is here it is clear to you but how to choose this coefficient of course, we cannot randomly say that α_1 is 0 α_0 is 0, β_2 is something else and β_1 is something else, we have to choose according to some process so what is that process that I am going to explain to you.

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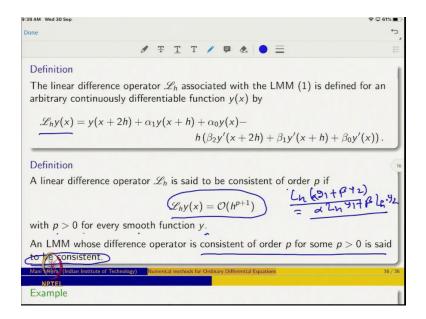
The linear difference operator L_h associated with the LMM is defined for an arbitrary continuously differentiable function y(x) by the following definition so here this is the definition of a linear difference operator which we are introducing right now, $L_h y(x)$ So, what are we doing?

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We are taking the difference of the left hand side and right hand side term if you observe this carefully.

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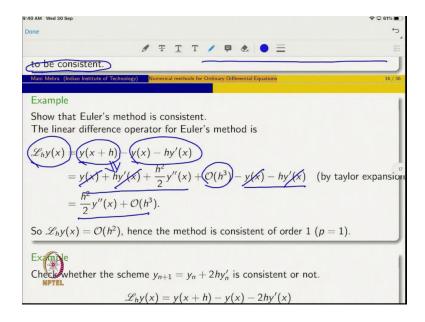
So, what is, what should be our expectation from any difference equation? Our expectation of any difference equation should be that a linear difference operator should be of $O(h^{p+1})$ where p > 0 for every smooth function p because if p > 0 only then I can say that truncation error will tends to 0 as $h \to 0$ because only in that case difference equation will approximate that differential equation if truncation error is not tending to 0 it will not converge that is what we have seen in the last lecture also.

So, to define this truncation error concept in an alternative way, what we are writing, a linear difference operator L_h is said to be consistent of order p, if $L_h y(x) = O(h^{p+1})$ with p > 0 for every smooth function y. So, you can observe that consistency is necessary for the convergence.

If you look at this more carefully of course consistency is necessary condition for the convergence because basically this is a truncation error which should tends to 0 because when I proved the theorem in the last lecture corresponds to forward Euler method also then also I was able to prove the convergence because truncation error was tending to 0 as $h \to 0$ and of course every time why we are calling as a linear difference operator because this is a linear operator which you can check.

Because what is the definition of linear operator $L_h(\alpha y_1 + \beta y_2) = \alpha L_h y_1 + \beta L_h y_2$ so you can check that is why we are calling it as a linear difference operator so an LMM whose difference operator is consistent of order p for some p > 0 is said to be consistent that is what I have already said.

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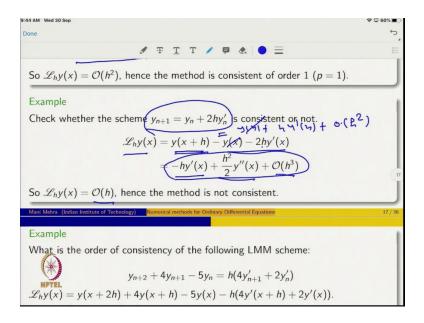
So, now though we already know that Euler method is consistent because in fact we have gone one step ahead for that method, we have proved the convergence also of that method but still by this way also we can start proving the same thing the linear difference operator of Euler method will be this.

So, again this y(x+h) and that is how we can define it, so now, I will be writing a Taylor series corresponds to this up to this term and this is the truncation error and then, this I am retaining as such so this can be cancelled out with this and this is here so basically $L_h y(x)$ is $O(h^2)$.

So, this is just the same way to look at truncation error in alternate way because this way helps you if some difference equation is also given to you, you can prove whether it is consistent or it is not consistent that is one thing, another thing is you can drive the method according to fixing the template, template means, what points you wanted to keep in the method x, x+h, x+2h, while in Taylor series that is not very easy task because you have to approximate y''(x), y'''(x) the order is also fixed, you can keep it.

So, hence the method is consistent of order p so that is the advantage of looking this way, if difference equation is given to you, you can prove whether it is consistent or not consistent similarly, sometimes you want, you are very particular that only I am wanted to construct a two step implicit method so I should fix the points at x, x+h and x+2h only so in those cases it helps.

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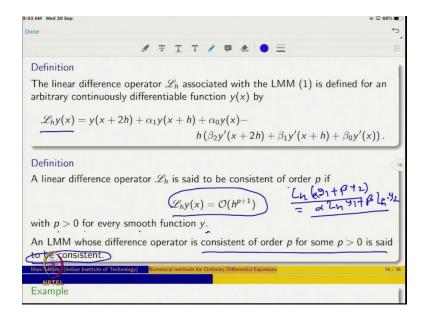
Now, let me give you one example because most of the time if you drive a difference equation through Taylor series, we end up with a consistent difference equation because we leave the truncation error which is always $O(h^2)$ but if suppose some difference equation is given to you like this example.

Now, our job is to prove whether it is consistent or not so for this let me define linear difference operator again which will be $L_h y(x) = y(x+h) - y(x) - 2hy'(x)$ This is the definition of a linear difference operator which we have seen earlier, so again if I write the Taylor series of this points then $y(x+h) = y(x) + hy'(x) + O(h^2)$.

So, this is the term I will be getting after rearranging term because this will be get cancelled

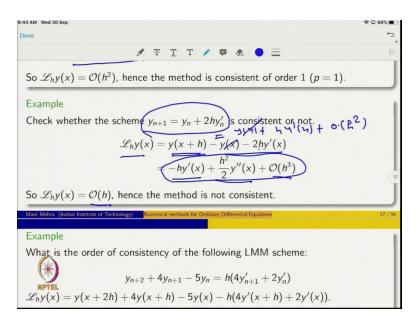
$$L_h y(x) = -hy'(x) + \frac{h^2}{2}y''(x) + O(h^3)$$
 so hence the method is not consistent because basically p is here, p is not greater than 0.

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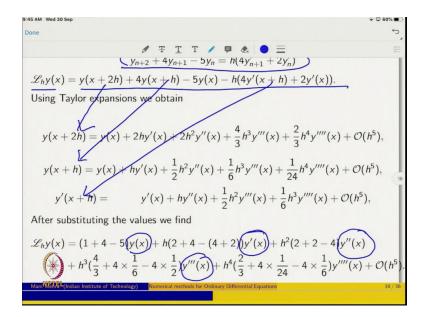
Because we have said in the definition that p should be greater than 0.

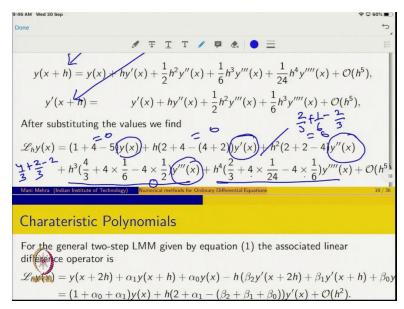
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So, this is the example of an inconsistent difference equation, which is very rare to see once we drive the difference equation with the help of a Taylor series because most of the time we end up with the consistent difference scheme. So, now in these two examples, we have seen how we can prove that our method is consistent or not consistent.

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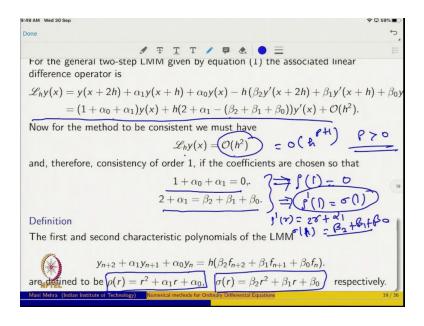
Now, in the next example, our aim is to find out what is the order of consistency of the following Linear Multistep method or difference scheme so the scheme is given to us this so now if I wanted to determine the order again I have to follow the same procedure.

Let me define linear difference operator, which is this using Taylor series expansion for this function and for this function as well as for these functions and after rearranging some terms, you can see this is the term corresponds to y(x), this is the term corresponds to y''(x), this is the term corresponding to y'''(x), y''''(x) we will keep adding that term till we get non-zero.

So, because this is also if you look at 2/3 this what is the calculation here $\frac{2}{3}+1/6$ -2/3 and here also so what, if this is $O(h^5)$, if this term is non-zero this will be $O(h^4)$ if this term is non-zero this will be $O(h^3)$, because this is 0, let us do it this is also 0, this is also 0, so and here we have to see so this is 4/3+2/3-2 so this will again be 0, this we have to see so this will be 2/3+1/6-2/3 so this is the non-zero term so this will be $O(h^4)$.

So, the order of difference scheme will be 3 in that case, if $L_h y(x) = O(h^4)$ the order of consistency will be 3 that is what we have already seen, so this way you can also determine the order of any difference scheme which is given to you, if it is consistency, consistent difference scheme you can determine the order, in fact you can also prove whether it is consistent at all or not that is what we have seen in the previous example.

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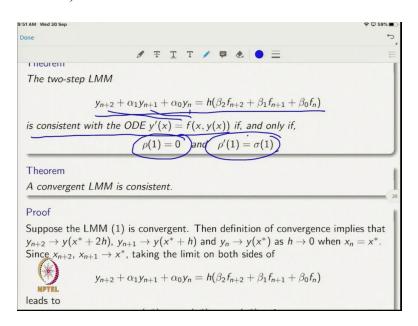
So, now generally as we have already seen that consistency is necessary for the convergence so let us formalise those concepts of consistency in a more formal way with the help of characteristic polynomials that is what we are going to do right now. For the general two step Linear Multistep method given by the equation 1 which we have seen earlier, the associated linear difference operator is this. So, now the method to be consistent, we must have $L_h y(x) = O(h^2)$ that is what we have already seen that it should be h^{p+1} where p should be greater than 0.

So, for any difference scheme to be consistent, we have to put that this and this is 0 if that is not the case you will not end up with the consistent difference scheme so $1 + \alpha_0 + \alpha_1 = 0, 2 + \alpha_1 = \beta_2 + \beta_1 + \beta_0$ so we are formalising these two necessary conditions for the consistency or you can say for the convergence in the form of a characteristic polynomial.

The first and second characteristic polynomial of the Linear Multistep method is given by the following formula: this is called first characteristic polynomial and this is called second characteristic polynomial. Why are we calling it as a first characteristic polynomial and second characteristic polynomial? Because we want it to redefine this condition in terms of characteristic polynomials which are easy to remember and doing some analysis.

So, the first condition corresponds to this becomes $\rho(1) = 0$ and second condition will become $\rho'(1) = \sigma(1)$ because $\rho'(r) = 2r + \alpha_1$ and $\sigma(1) = \beta_2 + \beta_1 + \beta_0$ so that is how we could get the second condition in the form of characteristic polynomials.

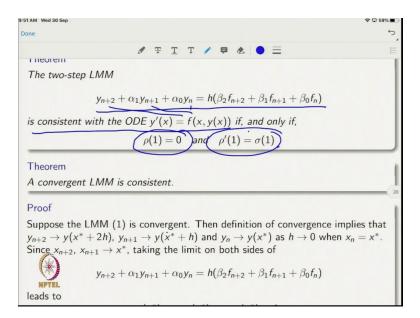
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So, basically what we have already said we are writing in the form of a theorem, the two step Linear Multistep method which is given by this is consistent with the ODE which we are going to solve with the help of this Linear Multistep method two step because the term is n, n+1, n+2 if and only if following conditions will be satisfied that is what we have already derived here.

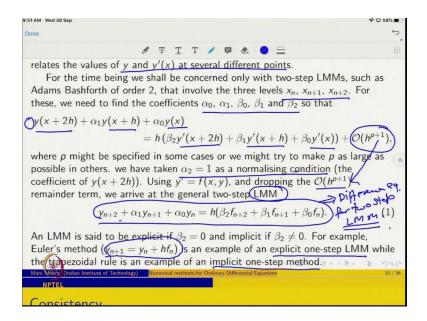
So, the two step Linear Multistep method is said to be consistent with the ODE if and only if these two conditions are satisfied so basically you write either in the form of a characteristic polynomial or you write in the following way both are equivalent ways of saying the same thing.

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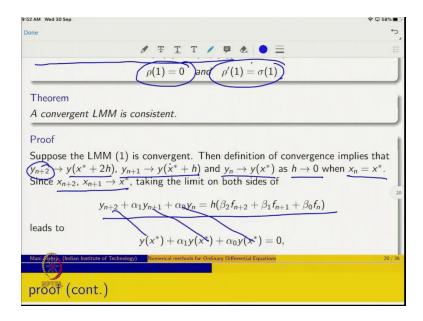
And now, let me prove one theorem which says that a convergence Linear Multistep method is consistent so it means consistency is a necessary condition for the convergence. Suppose that the Linear Multistep method is convergent and the Linear Multistep method corresponds to one which we have already seen earlier.

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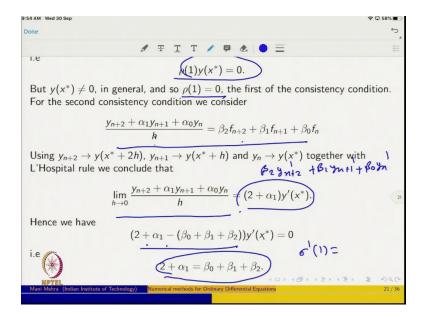
This is this.

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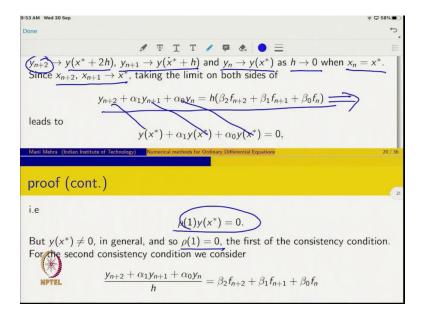
The definition of convergence implies that y_{n+2} will, which is a solution of a difference equation at x_{n+2} will converge to this so here basically x^* is x_n Similarly, using the definition of convergence we can say this also similarly, we can say this also as $h \to 0$ this is the definition of a convergence we have seen earlier also. Since, these points will also converge to x_n as $h \to 0$ taking the limit on both the sides so we are taking the limit of means, if this tends to x_n it means x_n it means x

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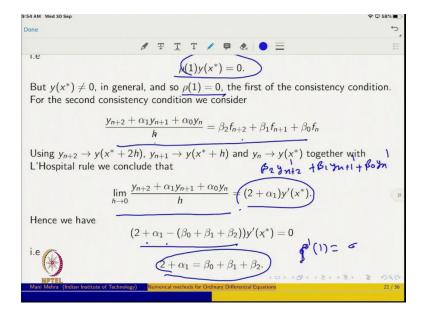
And then, if we write in the form of a first characteristics polynomial this will become this in general this cannot be 0, in general non trivial solution so $\rho(1) = 0$ the first of the consistency conditions so this is the first consistency condition which we always get with the help of convergent Linear Multistep method or a difference equation which is convergent.

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For that second consistency condition we are rewriting the same difference equation in an alternative way.

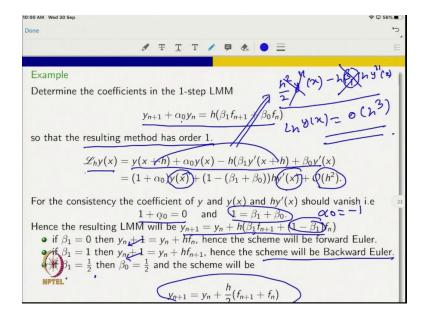
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We are dividing with h so this becomes this now, if we apply the limits, left hand side becomes this and right hand side is basically this so right hand side is basically $\beta_2 y'_{n+2} + \beta_1 y'_{n+1} + \beta_0 y'_n$

So, if left hand side will become this $2 + \alpha_1$ so all the things will if you use the definition of a convergence we can rearrange the terms in the following way and we end up with this which is again the second consistency condition because $2 + \alpha_1$ is basically $\rho'(1)$ so $\rho'(1) = \sigma(1)$ which is this second consistency condition. So, we have proved that convergent Linear Multistep method is consistent because both the condition should be satisfied which is this or this, one is that first consistency condition, this is called second consistency condition.

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So, now we have seen the proof of the theorem now let us take one example again: determine the coefficient in one step Linear Multistep methods. So, if you remember so far most of the time whatever examples we have done to prove the consistency there coefficients were given to us and we were proving whether it is consistent or not or in one case in fact we have determined the order of the consistency but this is the first example, where we are trying to find out the coefficient of the difference equation.

Determine the coefficient in the one step Linear Multistep method and we are fixing the order that resulted as order 1. So, with the help of this example, you will also learn how to determine the coefficient of course, this time just for simplicity I have kept only 1 step method so we define the linear difference operator according to the definition which we have seen in the just now this way and then, we will collect the terms of y(x), we will collect the terms of y'(x) after expanding the Taylor series for this and this. So, here I have skipped a few steps which you can do very easily just by writing a Taylor series and recollecting the terms.

So, for the consistency, the coefficient of y'_n should vanish that is what we have already seen because if it is consistent at least $O(h^2)$ should be there and in fact, in this case, we have set resulting method as order 1 so like truncation error determines the order of the method similarly, consistency determines the, because consistency is just the alternate way of looking in the truncation error $1 + \alpha_0 = 0$ and this is the second condition we are getting.

Hence, the resulting Linear Multistep method will be this because from this equation, you can get $\alpha_0 = -1$ so this is 0 so $\alpha_0 = -1$ which you can keep here and then we get this $\beta_0 + \beta_1 = 1$ which I am keeping here.

So, if you want that resulting method as order 1 it has given us some flexibility to choose β_1 , so if I am choosing $\beta_1 = 0$ So in that case we ended up with an explicit method and which is the same as the difference equation which we got in case of a forward Euler method if $\beta_1 = 1$ in that case of course, this should be, this 1 should be here, this is just a little typo.

So, $y_{n+1} = y_n + hf_{n+1}$ hence, the scheme will be same as backward Euler which we got and if I choose $\beta_1 = \frac{1}{2}$ the scheme will be this which is Trapezoidal method and fortunately, you will see if you expand this series and collect the terms of y'(x), one term

will come from here so this will be $\frac{h^2}{2}y''(x)$ and one term will come from here $h\beta_1 hy''(x)$

So, if you substitute $\beta_1 = \frac{1}{2}$ both the terms can be obtained, both the terms will be cancelled. So, that is why the resulting method will be of second order accurate which we already know in case of a Trapezoidal method so fortunately our aim was to resulting method

as order 1 but when we choose $\beta_1 = \frac{1}{2}$ it corresponds to the trapezoidal method and which we already know that it is a second order accurate method so the order, so $L_h y(x)$ in that case will be $O(h^3)$. So, clear to everyone?

So, this is the first example, where we have learned how to find out a coefficient of a difference equation by keeping the template fixed. What do you mean by template? Template means I wanted to retain only the points which use n and n+1 similarly, and it is not my aim that whether I end up with the explicit method or implicit method anything is fine that is why we have kept the term f_{n+1} as well as f_n , if our aim is to drive explicit methods then, we

would have kept this term with $\beta_1 = 0$ or basically it means that we would have not kept this term at all. So, with this I am closing now, thank you very much for your attention and I hope everything is clear to you. Thank you.