

**Introduction to CFD**  
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**Lecture - 30**  
**Numerical Solution of Linear Wave Equation (Hyperbolic PDE) (continued)**

In this lecture, we will continue our discussion on the dissipation and dispersion error that we have been discussing in the last lecture.

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The image shows a handwritten derivation on a whiteboard. The title is "Relative phase error after one time step". The main equation is 
$$\frac{\phi_{\text{numerical}}}{\phi_{\text{exact}}} = \frac{\tan^{-1} \left[ \frac{-C \sin \theta}{1 - C + C \cos \theta} \right]}{-C \theta}$$
 To the right of the equation, there is a circled expression  $0 \leq C \leq 1$  with the text "CFL criteria" written below it. A small video inset of the professor is visible in the bottom right corner of the whiteboard frame.

So, this is where we ended in the last lecture by writing an expression for the dispersion error and we said that it is going to accrue over different time steps and in each time step, the difference between the phase angle for the exact  $\phi_{\text{exact}} - \phi_{\text{numerical}}$  will get added up N number of times, where N is the number of time steps of computation that you perform. And therefore, that would result in the total error that you commit in this portion.

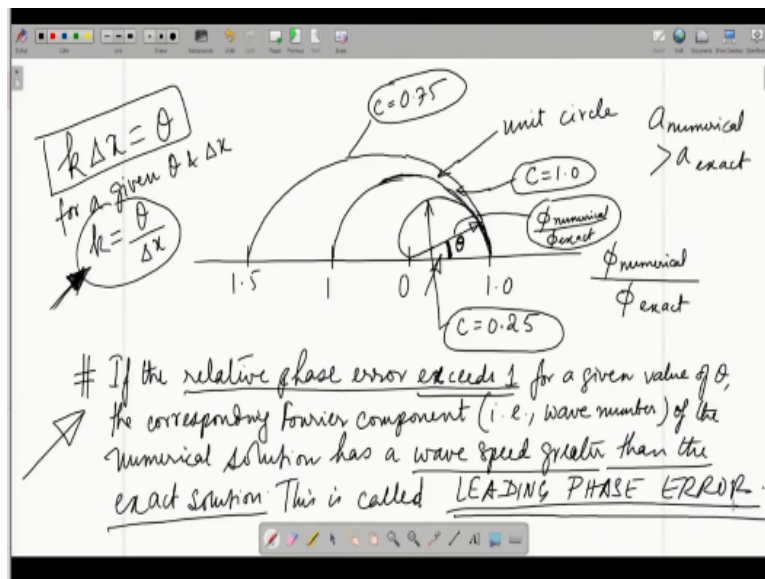
Earlier, we have discussed about the dissipation error. So, if we look at the first order upwind scheme for example, then it could be interesting to see what is the so called relative phase error after 1 time step. So, here what we are doing is we are taking a ratio between the face expression which comes from the numerical scheme. Here, in this case, it is first order upwind and the exact expression we had earlier derived.

So, that will be in the denominator. So, let us write down the expression for  $\phi$  for the first order upwind scheme. So, here we have  $-C \sin \theta$  divided by  $1 - C + C \cos \theta$ . So,  $\tan$

inverse of this by it was  $-C\theta$ , which is the  $\phi_{\text{exact}}$ . So, now, as you can understand that you would be varying  $\theta$  over the entire range of phase angles  $(0, 2\pi)$  space from 0 to  $2\pi$  and then you could also change  $C$ .

So,  $C$  is essentially a parameter which you can choose based on the constraint that  $C$  remains bounded by the CFL criteria which we discussed earlier. So, you could take different values of  $C$  based on this inequality and then check that how the relative phase error works out and remember that this is the phase error that you are committing in 1 time step as a ratio.

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So, we will make a simple plot to indicate how things can be compared in this manner. What we are plotting is essentially  $\phi_{\text{numerical}}$  by  $\phi_{\text{exact}}$  the first order upwind scheme. So, what we will do is we will first draw a unit circle and this is what comes when you use  $C$  is equal to 1. While this needs a bit of redrawing while if you are choosing a lower value of  $C$ , say  $C = 0.25$  then the plot looks like this, this curve.

And if you choose something like 0.75, then the plot looks like this. So, we try to jot down a few points. So, we have jotted down something to begin with. So, what we are saying is that if the relative phase error, which is nothing, but that ratio of files it exceeds the value of 1 for a given value of  $\theta$ , then the corresponding Fourier component of the wave number of the numerical solution has a wave speed greater than the exact solution and this is what is called as leading phase error.

Now, what does it mean? Let us go back to the definition of theta. So, in the wave number space, we have defined theta as the wave number times, the grid spacing, the spatial grid spacing  $k$  times  $\Delta x$ . So, for a given theta and also grid spacing you have a given wave number that means, as you vary theta, which we are showing in this diagram. You are essentially addressing different wave numbers.

So, as the wave numbers change, we are finding that the  $\phi$  numerical by  $\phi$  exact is taking up different values and the paths are different if the CFL number is also different that means for the chosen CFL number. It means that over the range of thetas, as you follow that (( )) **(08:33)**. There is no guarantee whether you will be following the unit circle. Where  $\phi$  numerical and  $\phi$  exact are in match with each other.

So, either it may exceed or it may be reduced on a comparative scale. So, then what happens when you have an excess. So, related phase error exceeds 1 that is what we have jotted down over here. That means, in that case, that particular wave number part will speed up with respect to the theoretical wave speed. So, the wave speed will be greater than the exact solution. Why? Because  $\phi$  numerical happens to be larger than  $\phi$  exact.

That is why the ratio is exceeding 1 and that means, the waves rather that wave number component of the wave is actually traveling faster than the analytical wave. That means, if I were to call a numerical then a numerical is greater than a exact at least for that wave number. And how is that wave number specified here? It is specified by the choice of theta you have already chosen  $\Delta x$  through your grid distribution.

And now you are varying theta, which means basically, that wave number  $k$  will get modified as you vary theta. You will go from lower wave numbers to higher wave numbers, that is how you cover the entire wave number range, which you can capture within your grid size. Right. And we already know that the highest wave number that you can capture depends on the grid spacing that we have discussed earlier.

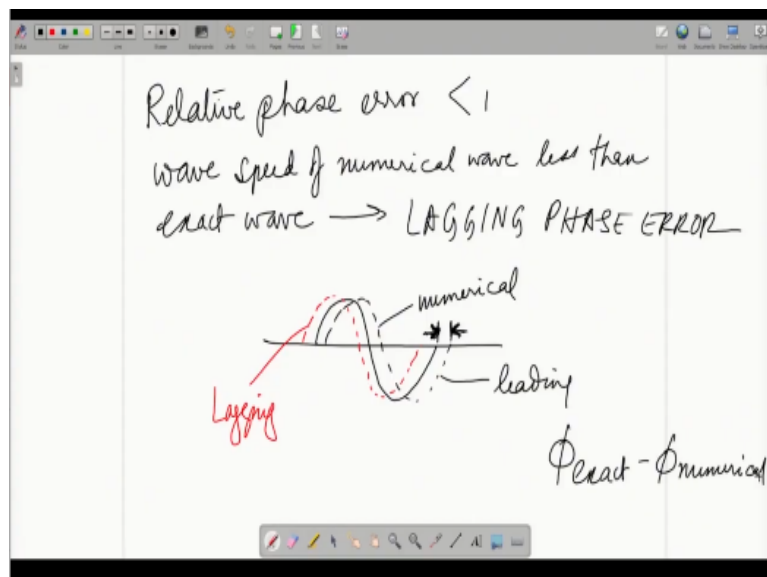
So, that way over the entire range of wave numbers that you can capture with your grid spacing, this is how the the ratio of  $\phi$  is how you can actually say that whether that wave number component of the mother wave will travel at a exact or greater than a exact or less

than a exact. So, we are just talking about a situation where the ratio exceeds 1. That means  $\phi_{\text{numerical}}$  is greater than  $\phi_{\text{exact}}$ .

In that case, that basically means that that wave number will travel faster than the theoretical wave. And this is what is called as leading phase error. If it is just the other way around that means a relative phase error is less than 1 then what will happen to the numerical wave, it will lag. It may not be this that the entire wave will lag. It is a certain wave number component of the mother wave which will lag.

So, for that particular  $k$  if the  $\phi_{\text{numerical}}$  by  $\phi_{\text{exact}}$  happens to be less than 1, then that wave number component of the mother wave will lag and that is what is going to be call as lagging phase error.

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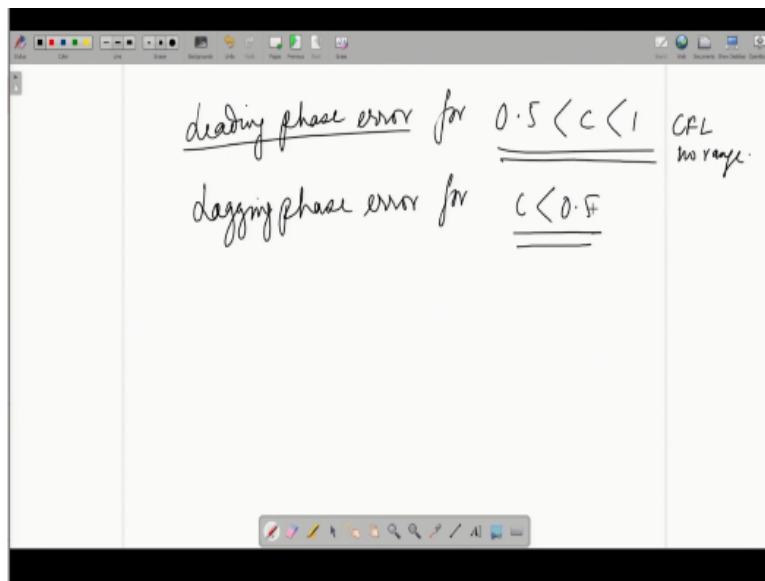
So, if relative phase error is less than 1 we have wave speed of numerical wave less than exact wave and that gives rise to what is called as lagging phase error. So, if we were to highlight on just one wave number, how would the situation look like? So, if this was location of the exact wave at a certain point of time, if you had a leading error, then this is how it would look like.

So, the numerical 1 would have speeded up. If you had a lagging error, then how would it look like? Let us try to put it on the same plot. So, in the case of a lagging error, it would be moving slower than their exact. So, this is a lagging case while the other one is a leading

case. And how do you quantify there, it is a gap between the two. Of course, this is an accrued gap over  $n$  time intervals of calculation.

But if this was the gap created in 1 time step, then this would be given by the relative phase error that is in a ratio form while this is in the actual form of values. That means, the difference between say  $\phi_{\text{exact}} - \phi_{\text{numerical}}$ , not the ratio. So, this is how phase error is quantified.

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Now, incidentally for the first order upwind scheme, we see leading phase error for this range of CFL number, this range of CFL number and the lagging phase error for a lower range. That is why in the previous plot we had seen if we go back and check in this figure that for lower values of  $C$  that is say 0.25 less than 0.5. What are we seeing the ratio happens to be less than 1 everywhere, wherever you are on that locus.

You are at a ratio less than 1 because the limiting ratio is the unit circle. If you are on the unit circle, there is no difference in phases. There, the numerical wave is exactly in phase with the exact 1 if you are having a  $C$  lying between say 0.5 and 1 slightly less than 1 like  $C$  is equal to 0.75, then you have a leading error. That means the numerical wave is going faster for a wide range of wave numbers only for very small wave numbers.

Is it close to the exact wave? But, the more we go to the higher wave numbers, it is having an increasing gap between the exact wave and the numerical wave. That is because this curve is going further away from the unit circle that is the indication and that is happening at higher

values of theta that means, higher wave numbers. So, usually complications are more as you go to the higher wave number range anyway.

So, we discussed quite a bit on the dissipation and the dispersion kind of errors for wave propagation problems. Now, we are going to discuss another aspect of the linear wave equation, which is often called as modified partial differential equation approach or equivalent partial differential equation approach.

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So, a little bit of recapitulation of what we have already discussed about. So, we have discussed about the upwind technique for doing finite differencing of the linear wave equation. And we understood that upwind technique is essentially a first order accurate technique with accounting the windward or upstream direction of the propagation of the waveform.

And we found that when a is greater than 0, it is equivalent to using the FTBS scheme the forward time backward space scheme. When a is less than 0, it is forward time forward space scheme and we understood that from Von Neumann stability analysis. This is the range of CFL numbers which need to be used. Now, we are going to discuss about a technique by means of which we use the Taylor series expansion for replacing the terms other than u<sub>i</sub><sup>n</sup> in the finite difference expression for the first order upwind scheme.

So, in the first order upwind scheme we have terms other than u<sub>i</sub><sup>n</sup>. So, now, we are going to substitute the Taylor series expansions for the other terms, which means u<sub>i</sub><sup>n+1</sup> and u<sub>i-1</sub><sup>n</sup>

n. And this we are doing to develop another new tool, which we will be discussing now. So, let us see how do we go about doing that. So, the Taylor series will be developed both in time as well as in space.

Because, as you can understand  $u_{i,n+1}$  is temporarily different from  $u_{i,n}$  in the sense that grid location wise spatial grid location wise, it is the same point  $i$  but time wise we are at a different time step. Therefore, when we do a Taylor series expansion, then we have to expand it in time. So, what we are doing is that you have, you are expanding it about  $u_{i,n}$  and you are expanding it in time.

Therefore, you are using time steps here to be multiplied with the time derivatives of  $u$ . So, these are the higher order time derivatives and these are the time steps. So, that is how we are having the Taylor series representation for  $u_{i,n+1}$  and of course, the representation for  $u_{i,n-1}$  is a very routine thing that is a Taylor series in space which we have dealt with adequately earlier also.

Only thing is that because it is  $i-1$ . So, it is in the negative direction and therefore, there will be flipping of sign of the different terms in the Taylor series. So, what we have got is a form of the original finite difference equation with Taylor series expansions incorporated in it.

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$$u_i + au_x = -\frac{\Delta t}{2} u_{it} + \frac{a\Delta x}{2} u_{ix} - \frac{(\Delta t)^2}{6} u_{itt} - \frac{a(\Delta x)^2}{6} u_{ixx} + \dots (1)$$

$$u_t + au_x = 0$$
  
*FOV → Approximate form*

Left hand side of the above equation (1) corresponds to the wave equation and the right hand side is the truncation error.

The significance of terms in the truncation error can be more easily interpreted if the temporal derivative terms are replaced by spatial derivatives.

In order to replace  $u_{it}$  by a spatial-derivative term, we take the partial derivative of above equation (1) with respect to time

$$u_{it} + au_{xt} = -\frac{\Delta t}{2} u_{itt} + \frac{a\Delta x}{2} u_{ixt} - \frac{(\Delta t)^2}{6} u_{ittt} - \frac{a(\Delta x)^2}{6} u_{ixxt} + \dots (2)$$

And take the partial derivative of equation (1) with respect to  $x$  and multiply by  $-a$

$$-au_{ix} - a^2 u_{xx} = \frac{a\Delta t}{2} u_{itx} - \frac{a^2 \Delta x}{2} u_{ixx} + \frac{a(\Delta t)^2}{6} u_{ittx} + \frac{a^2 (\Delta x)^2}{6} u_{ixxx} + \dots (3)$$

Now, if we arrange the terms, we will find that it can be represented this way. So, the original linear wave equation is this. And by means of the first order upwind scheme, we have

essentially approximated it. So, when we approximated we ended up generating error terms, which are truncation error terms and by means of the Taylor series approximations. We have essentially generated the total truncation error terms here on the right hand side of the equation.

So, the left hand side of (( )) (20:30) the equation it corresponds to the exact wave equation, while the right hand side is the total truncation error due to the particular numerical discretization that you have used. So, it is very specific to only the first order upwind approximation that we have used. For a different numerical scheme, the truncation error would look different as well.

Now, the significance of the truncation error term can be better interpreted if you can convert all the temporal derivatives that you see in the truncation error to spatial derivatives entirely. So, right now, as they stand you have a mix of spatial derivatives and temporal or time derivatives. So, we want the time derivatives to be converted to spatial derivatives as well. So, that is how we go ahead in restructuring the truncation errors.

So, what is the starting point, we want to replace  $u_{tt}$  that is the first term here on the right hand side by means of a spatial derivative term. So, in order to do that we take a partial derivative of the equation 1 with respect to time. So, when we do that that means, when we take a partial derivative of equation 1 with respect to time we come up with the equation 2. So, you can see that it is nothing but equation 1 with a partial derivative in time added to each one of the terms.

And then we do another operation we take a partial derivative of equation 1 with respect to  $x$  and multiply the resulting equation by  $-a$ . So, what do we do in this step we take a partial derivative with respect to  $x$  that means, the first term now has  $u_{tx}$  because you are taking a partial derivative with respect to  $x$ . So, originally it had  $u_t$  now, it has  $u_{tx}$  originally the second term had  $u_x$  and now it has  $u_{xx}$  and so on.

Additionally, each one of the terms has been multiplied by  $a - a$ . So, the first term now has  $a - a$  the second time has  $a - a$  square and so on. So, we have ended up generating 2 equations here the equations 2 and 3, which we will further use to replace the  $u_{tt}$  in equation 1. So, let us see how we go about doing it further.



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Adding equations (2) and (3) we get

$$u_{tt} = a^2 u_{xx} + \Delta t \left[ \frac{-u_{tt}}{2} + \frac{a}{2} u_{tx} + O(\Delta t) \right] + \Delta x \left[ \frac{a}{2} u_{xt} - \frac{a^2}{2} u_{xxx} + O(\Delta x) \right] \dots (4)$$

In a similar manner one can show

$$\begin{aligned} u_{tt} &= -a^3 u_{xxx} + O[\Delta t, \Delta x] \\ u_{tx} &= -a^2 u_{xxx} + O[\Delta t, \Delta x] \dots (5) \\ u_{xxx} &= -a u_{xxx} + O[\Delta t, \Delta x] \end{aligned}$$

In this process we are essentially **converting all mixed derivatives of space and time to derivatives IN SPACE ONLY.**

So, when we add the equations 2 and 3, we get an expression for  $u_{tt}$ . Now, what does this expression contain, it contains a leading term  $a^2 u_{xx}$  and then all the remaining terms that it has can be expressed like this. So, you have a  $\Delta t$  multiplied to a bracketed term which contains higher order derivatives either in time or in time and space mixed and you have still higher order terms which can be represented like this order of  $\Delta t$ .

Similarly, you would have terms which can be represented like this that they have a common factor  $\Delta x$  and then you have term sitting inside the bracket, which are derivatives of space or space and time combined, and then the remaining terms can be expressed in terms of order  $\Delta x$ . So, this can very well be done. So, you can do it at your own convenience and check for yourself. So, this is how we would end up replacing the  $u_{tt}$  term.

So, you remember that this we had to do because this  $u_{tt}$  was lying as the first term in the truncation error. So, we have to get that replaced by this expression now. Now, if you were to go through this exercise, you could similarly do this exercise or extend this exercise to generate expressions for higher order derivatives which figure in the truncation error and this truncation error is what we saw in equation 1.

So, likewise we can generate expressions for  $u_{ttt}$ ,  $u_{ttx}$ ,  $u_{ttxx}$  and so on. Now, interestingly you can see that  $u_{ttt}$  is a function of  $u_{xx}$  and has a coefficient  $-a^3$ .  $u_{ttx}$  is expressed as  $u_{xxx}$  and a coefficient of  $-a^2$ . So, the coefficient seems to be reducing here and each time, it is getting multiplied with the third order derivative in space.

That means, we are able to convert all the time derivatives to space derivatives or the mix of time and space derivatives to purely space derivative. That means, the ultimate objective is converting all mixed derivatives of space and time to derivatives in space alone or converting derivatives alone in time to alone in space. So, that way, we should be in a position to express the truncation error part entirely as a function of higher order space derivatives alone.

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Combining equations (1), (4) and (5) we get +  $u_t + a u_x = 0$

$$u_t + a u_x = \frac{a \Delta x}{2} (1-c) u_{xx} - \frac{a(\Delta x)^2}{6} (2c^2 - 3c + 1) u_{xxx} + O[(\Delta x)^3, (\Delta x)^2 \Delta t, \Delta x (\Delta t)^2, (\Delta t)^3] \dots (6)$$

**Modified Partial Differential Equation**

- The Modified PDE can be thought of as the PDE that is actually solved when a finite-difference method is applied to approximate a governing PDE (in the present case the Linear Wave Equation).
- Since it is an approximation, the governing PDE is never represented by the FD scheme.
- There is however a limitation in this approach. While solving the approximate form, suitable boundary & initial conditions are imposed keeping the governing PDE in mind. Sufficient boundary conditions for modified PDE would not be available as it has infinite number of derivatives.

So, combining these results, what we will be able to finally achieve is something like this that you now have the exact equation on the left hand side of of this equation 6 which has emerged. And now, the right hand side which is the truncation error contains all spatial derivatives like what we intended to do. And instead of writing still higher order derivatives.

We have bunch them up in terms of higher order terms, which would have delta x cube delta t cube or mix of delta x square delta t or delta x delta t square which are essentially third order terms. Now, you have now, a first order in delta x or a second order in delta x as the leading error or the next 2 leading error terms. And incidentally the leading error term now has second derivative of u and the coefficient associated with it.

So, the coefficient happens to be eight times delta x by 2 into 1 - c that is the coefficient associated with the second order derivative. Now, the form of the equation that we have achieved in the process is what is called as the modified partial differential equation. Now, what is the spirit behind this entire exercise? I mean what are we trying to really achieve for ourselves?

So, we look at the bullet points below and they would give us the clue. So, the modified partial differential equation, it can be thought of as the partial differential equation that we are actually solving. So, we intended to solve which equation we intended to solve this equation the linear wave equation, but we have used an approximation a finite difference scheme to approximate it that is the first order upwind scheme incidentally.

That is the one we are analyzing now. So, is the first order upwind approximation really solving the original exact equation? The answer is no, because errors are involved, because you are approximating and the errors are essentially modifying the nature of the partial differential equation you are solving. So, which equation do you end up solving at the end that is what is the modified partial differential equation.

It is the original equation along with the truncation error that the numerical discretization involves. That is what is called as the modified partial differential equation. And that is what we have in equation 6 for the first order upwind discretization of the linear wave equation. So, coming back to the bullet point, the modified partial differential equation can be thought of as the partial differential equation that we are actually solving.

And in the present case, it is not the linear wave equation but but a much more complicated equation. In fact, on the right hand side, we have innumerable terms, it is an infinite series. So, there is no end to this equation. So, as a numerical exercise, we cannot really go ahead with that. We can at best say that we look at the leading error term out of the truncation error.

And try to see what influence that has on the solution because the later terms would become smaller and smaller and smaller hopefully, because they involve higher powers of  $\Delta x$ . Of course, one can raise the critical question that are the higher derivatives small as well. Usually, for not too rapidly varying functions and not functions which have sharp jumps. That is true.

That means smooth looking functions generally have this behavior that the higher order derivatives when multiplied with higher powers of  $\Delta x$  would actually become very small terms. And that is the hope with which we are actually saying that the leading error term is going to essentially define the character of the modified partial differential equation. So we

can say that we will just retain 1 term on the right hand side and try to see how the new partial differential equation looks like.

However, we need to understand one thing that if you are going for a modified partial differential equation involving more higher order derivatives, that means ideally, you may need to change your boundary and initial conditions, because you are changing the order of the equation. But in principle, we do not do that. We impose suitable boundary and initial conditions keeping in mind the original partial differential equation.

That is the Spirit. And we often would run out of even possibilities of setting sufficient boundary conditions, if we were to consider the higher order derivatives of the modified partial differential equation. So keeping that in mind, we go about deciding the boundary and initial conditions as per the original non English. So we will discuss more about modified partial differential equations in the next lecture. Thank you.