Introduction to CFD
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Lecture - 15
Taylor Table Approach for Constructing Finite Difference Schemes (Contd.)

In this lecture, we continue our discussion on the modified wave number approach.

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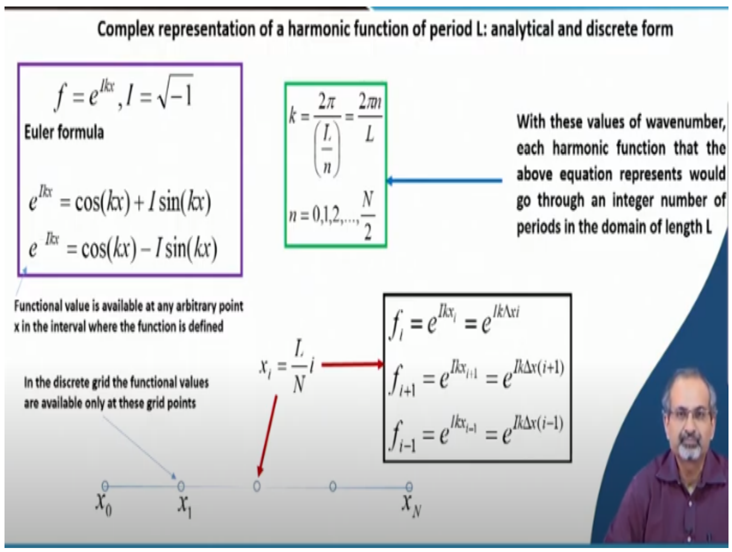

Last time, we had introduced the complex representation of a harmonic function and we looked at the analytical form of its derivative, and then we derived the discrete form of the derivative using the CD2 scheme. Then we showed that the wave number that we see coming from the analytical derivative does not exactly match with the wave number expression that we get from the finite difference approximation using the CD2 scheme.

We use the nomenclature k' for representing the so called modified wave number. So just to recall, we will write the expression for the modified wave number once more for the CD2 scheme.

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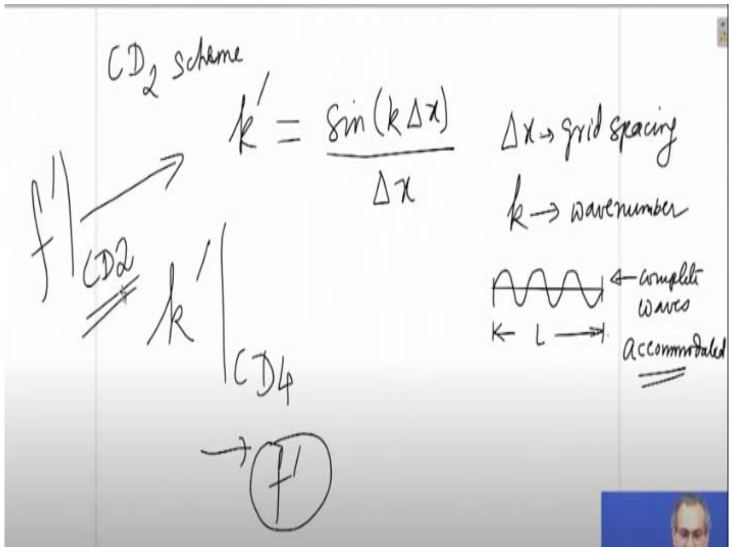

We found last time that for the CD2 scheme, k' is equal to $\sin(k\Delta x)/\Delta x$. So Δx is of course our grid spacing. And k is the wave number of a sinusoidal wave that you are accommodating within your domain which has a length of L. And we said that the waves could be coming in like this in integer form. That means, we have complete waves accommodated.

These are some of the things we already discussed in the last lecture. Today we work out another example. We have earlier derived the CD4 discretization for the first derivative using the Taylor table approach. Let us discuss about the wave number approach with respect to the CD4 scheme. The target is that we try to work out the k' for the CD4 scheme now, of course for the first derivative.

We have already achieved that for the CD2 scheme. That's how the k' looks for f' using central differencing of second order accuracy. So we use the same methodology, but this time by using the CD4 discretization.

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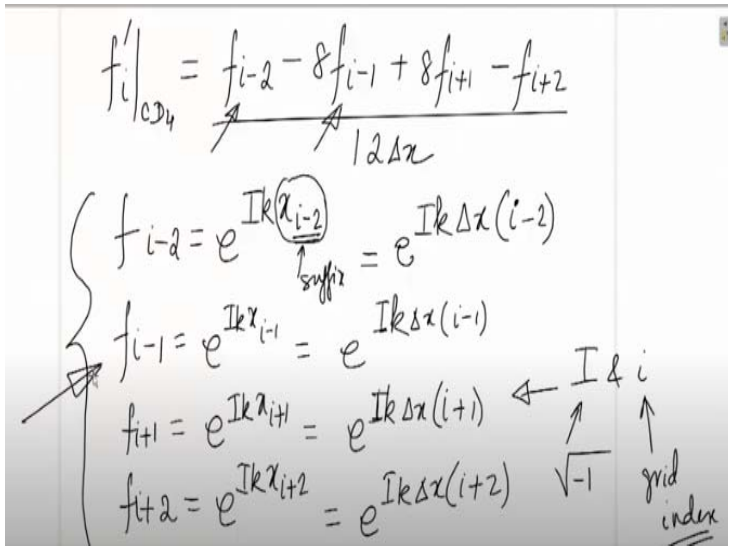

We recall that the f' expression for CD4 which we had already derived using the Taylor table approach is given by this expression. Now, like we discussed earlier, we need to have representations for all these functional values at the different grid points. Let us try to do that. We just recall this nomenclature, which we discussed earlier, that here, i – 2 is in the suffix.

You need to convert it to a length in terms of the grid spacing. And for that, what you do is multiply the grid spacing by the grid index corresponding to that point. In a similar manner, we define it for f_{i-1} and then we need an expression for f_{i+1} and f_{i+2}. You have to be a little careful with the use of *I* and *i*. So just to recall, *I* stands for under root – 1 and *i* is the grid index.

We need one more expression, that of f_{i+2}. Now we are ready with all the expressions for the functional values on the grid. We have a discrete domain. So we need the functional values at the discrete grid points and we have them all. Now we would just substitute them in the expression for f'.

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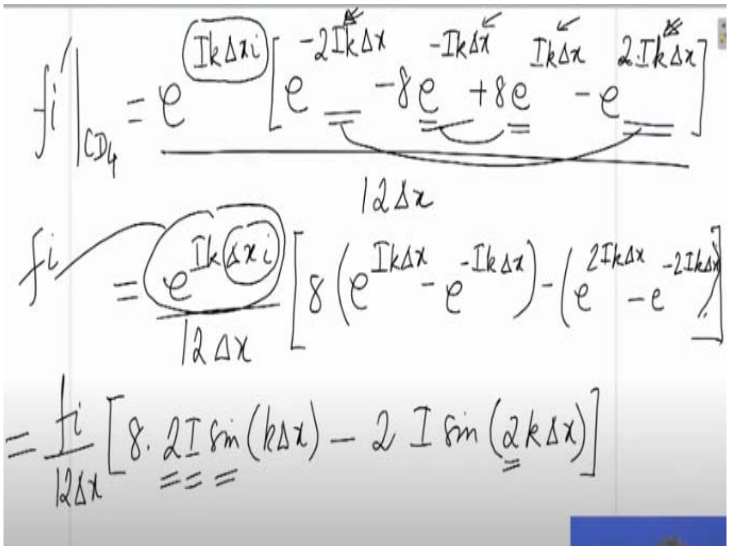

So what we have, we could write it this way, where you take out the common factor. So this $e^{Ik\Delta xi}$ is common to all of those functions and the rest of it could be put in the bracketed term. This would be plus 2IkΔx the whole divided by 12Δx. That will be the expression. So we need to now club the terms. These two terms will be clubbed together.

And again these two terms will be clubbed together. You can figure out why. Because you have similar looking indices here. And you have similar looking indices here for the starting and the end terms. Let us do that exercise. Remember that this is a product $\Delta x \times i$; i is not a suffix here. This expression can be called as f_i. So what we have here is $f_i/(12\Delta x)$.

And then we can write $8\times 2I \sin(k\Delta x)$. We have explained earlier why we get a two times sine with the capital I here. This comes from the Euler formula. Be careful to put in this 2 inside.

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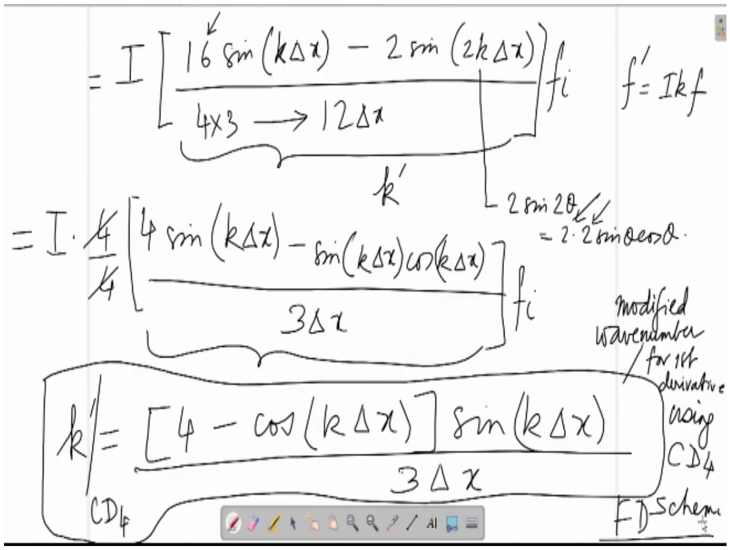

So this can be written as, as you can see, we are gradually getting it arranged into a form which can be easily compared with the analytical form. So you remember that f' was equal to Ikf. So you can very well imagine that whatever comes out from here will actually become the k' for the CD4 scheme. We continue in that direction. We can expand this term for example.

So this is like 2sin2θ. So that will give you 2×2sinθcosθ. So that means, once you do that, you can have a 4 coming out here and then you already have a 16. That means 4 will come out as a common factor from the numerator. You also have a 4 into 3 from the denominator. So the 4 and 4 cancel out, whatever you extract as common factors from numerator and denominator.

So you have 4sin(kΔx) left with the first term and you have sin(kΔx)cos(kΔx)/(3Δx) times f_i. So we have arrived at the expression for k'.

$$k'\Big|_{CD_4} = \frac{\left[4-\cos\left(k\Delta x\right)\right]\sin\left(k\Delta x\right)}{3\Delta x}$$

So what we have here is k' for CD4 scheme and of course for the first derivative. And the expression turns out to be 4 sin. So let us take sin common. We will put (4- cos(kΔx)sin(kΔx))/(3Δx).

So this is our expression for the modified wave number for first derivative using CD4 scheme. We achieved our goal of obtaining the modified wave number expression for CD4 scheme and now we still do not know how far these k' expressions are from the analytical k that we were talking about.

And we certainly need to plot and see how well the k' expressions for CD2 scheme and CD4 schemes are comparing with the analytical expressions for different values of k. We already realized that there is a provision for accommodating different values of k. That means, waves of different frequencies to span the domain L.

And as you try to apply these finite difference schemes to approximate the derivatives, when these derivatives are working on waves of different frequencies, how well are we doing using these approximations. So we need to find out more by doing a few calculations using these k' expressions. So let us try to do that.

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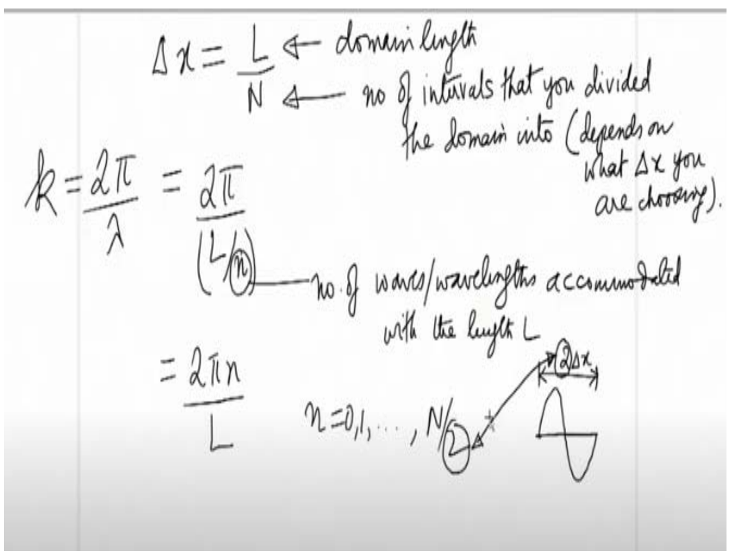

We will just go back to how we defined these parameters Δx and k. So Δx was defined as L/N. L is the domain length, N is the number of intervals that you divided that domain into. That of course depends on what Δx you are choosing. That means the smaller the Δx, the larger would be N and vice versa. And we remember that k by definition was 2π/λ.

And how did we obtain λ? We said λ is equal to the domain length divided by the number of wavelengths we are accommodating within that length. That means, the small n was the number of waves or wavelengths accommodated within the length L. And so this would become $2\pi n/L$. And we know that n varies from 0 to N/2.

Again, you must be remembering that the shortest wave would take up a distance of $2\Delta x$. And this factor 2 basically is connected with the fact that the shortest wave takes up two times the grid spacing.

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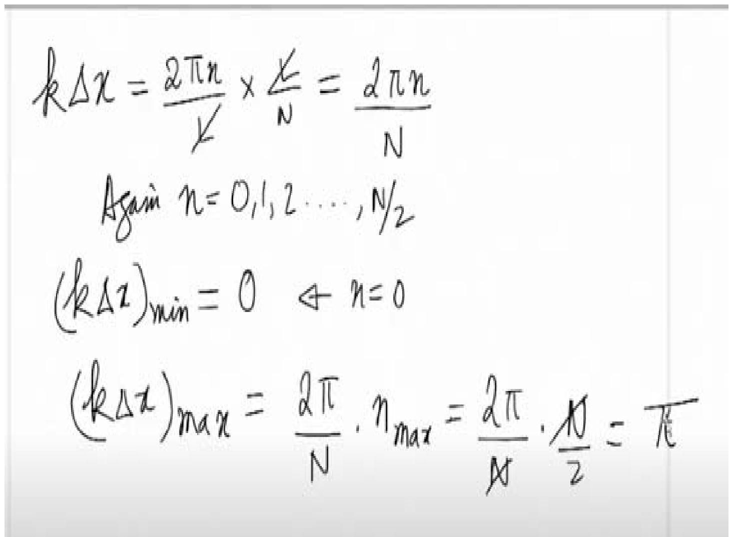

Now the important thing to look at is what is this $k\Delta x$ that we had seen in the modified wave number expressions both for the CD2 as well as the CD4 scheme. You may be noticing that in both the formulae we are seeing this $k\Delta x$ coming up. So what is this $k\Delta x$? Let us try to substitute those expressions and try to work out what this $k\Delta x$ is all about.

We find that it is nothing but $2\pi n/N$. And again n is anything, of course in terms of integers varying from 0 to N/2. That will give me the maximum and minimum values of $k\Delta x$, because that is basically the maximum and minimum values of small n. So the minimum of $k\Delta x$ is 0, which corresponds to $n = 0$.

And the maximum $k\Delta x$ is equal to $2\pi n_{max}/N$, which is $(2\pi\times N/2)/N$ and you get π. So the maximum value of $k\Delta x$ would be π. So we have to look at a range of $k\Delta x$ spanning between 0 to π as we look at these expressions of k' and then see that for those values of k, where these k' values are. So we can do a few simple hand calculations to do a quick check on this.

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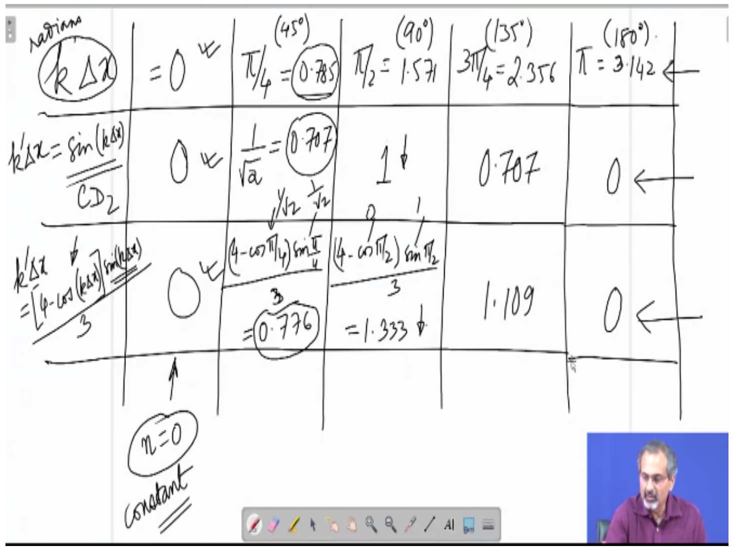

Let us try to do that. We form a kind of a table for our hand calculations. And let us take a few discrete values and try to check how the k' values are doing for the two schemes. We will choose values of this kind. Remember that this kΔx is in radians. So when we operate the sine or cosine operator on the angle, we know that we apply the expression in terms of radians.

I choose radian values of the angles say π/4, which means 45 degrees. So here the kΔx will have a value of 0.785. For π/2 it is 1.571. This is the degree value. And then 3π/4 would have a value of 2.356. Of course, they are approximate values correct to three places after decimal. And the last value will correspond to π. So this is 180 degrees.

And then we try to find out what $k'\Delta x$ is for the CD2 scheme. Sorry, the expression for $k'\Delta x$ is equal to sin(kΔx) for the CD2 scheme. And the $k'\Delta x$ for the CD4 scheme will be $(4-\cos(k\Delta x))\sin(k\Delta x)/3$. Now as you can understand that when kΔx is equal to 0, then this is going to yield a 0.

Now how about this? You will get a 4 - 1 because cos 0 is 1. But then it gets multiplied with sin(kΔx) which is 0. So finally, you will get a 0 here. That means, you actually can match exactly between the analytical and the approximate forms here when kΔx is 0. Again remember it corresponds to n = 0 which means you just have a constant value of the function.

So the derivative is 0. And the finite difference is turning out to be 0, which is consistent. When you go to π/4, this will give you a value of $1/\sqrt{2}$, which is approximately 0.707. Here you will get a value of (4 – cos(π/4))×sin(π/4), both of them being $1/\sqrt{2}$ whole divided by 3. And that will give you a value of 0.776.

So you can figure out that this value is already falling short of the analytical value which is 0.785. Whereas, this CD4 approximation is still fairly close till kΔx equal to π/4. Now let us look at π/2. So at π/2 this will give you a value of 1 which is already quite low compared to 1.57.

Now as far as CD4 is concerned, you will get a 0 here, you will get a 1 here and then the final value will be 1.33 approximately, which is falling short of 1.57, but still better than what CD2 is giving you. Then as you move on to the other angles, you can calculate the values like we did for the lower values of kΔx.

And then finally, you find that both the schemes are showing up with a value of zero when the actual value should have been 3.14. That means, in this range, both of them have deviated far from the exact expression.

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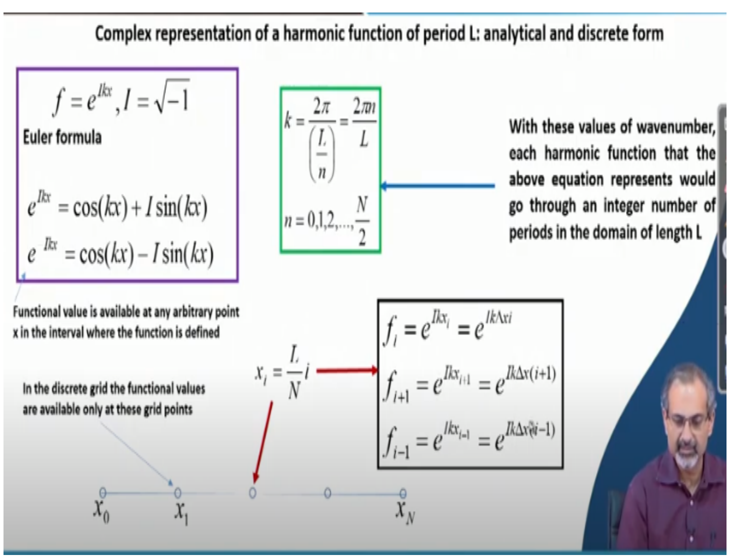

Now if we were to plot this exactly over the range of values of k, we would be able to see a graph which looks like this.

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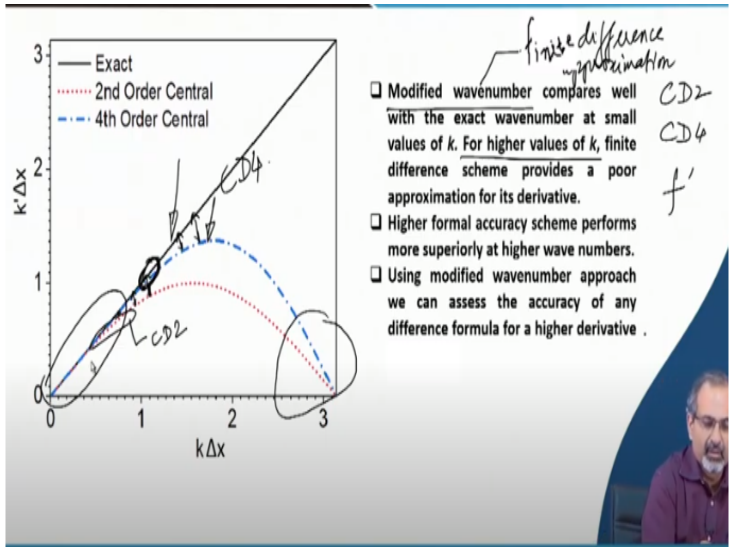

And you find that in the lower ranges of kΔx, you have a fairly good match, but then you can see that the red dotted line which stands for CD2 is deviating off from the exact plot earlier than the blue plot which stands for CD4. So essentially CD4 is close to the exact values up to these ranges and then the deviation is enlarging here. But, you can see deviation starting for CD2 earlier.

And of course, what we noticed was that at much higher values of kΔx, both of them have deviated significantly. Now what is the outcome of this analysis or what are the conclusions that we can draw from an analysis of this kind? So we can say that the modified wave number which comes from a finite difference approximation, of which we tested two schemes for first derivative, that compares well with the exact wave number at small values of k.

However, for higher values of k, the finite difference schemes are having poor approximation. The question is that even if you go for still higher orders of formal accuracy, you may not still be able to achieve very good performance at higher wave numbers.

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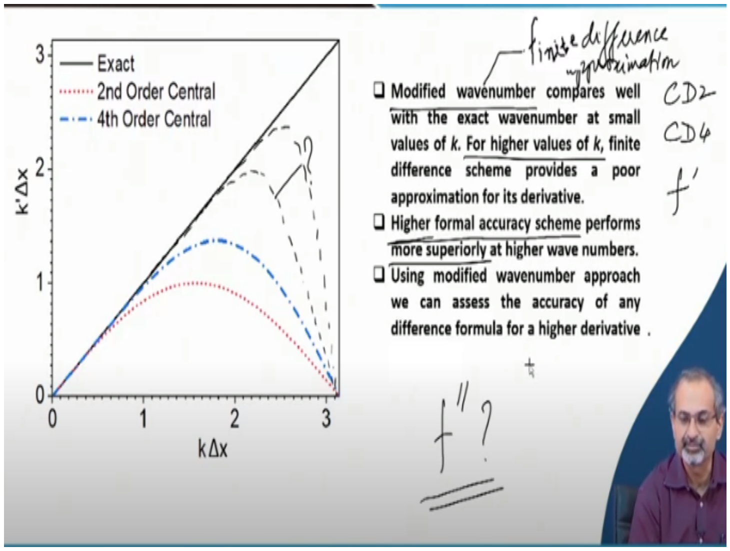

But the motivation would be to push higher and higher so that you get superior accuracy up to a fairly large value of kΔx before it droops down. So can we have schemes which are having superior performance of this kind? We have seen that the higher formal accuracy schemes have performed more superiorly because CD4 has excelled over CD2 in the modified wave number plot.

And like we did for the first derivative, we can also do a similar exercise for second derivatives because many of the fluid dynamics equations involve second order derivatives. We need to know how the schemes are doing on second order derivatives. So we learnt a more contemporary way of assessing accuracy of finite difference schemes. And in all these exercises that we did, we have shown that the expressions that have been derived are essentially explicit expressions.

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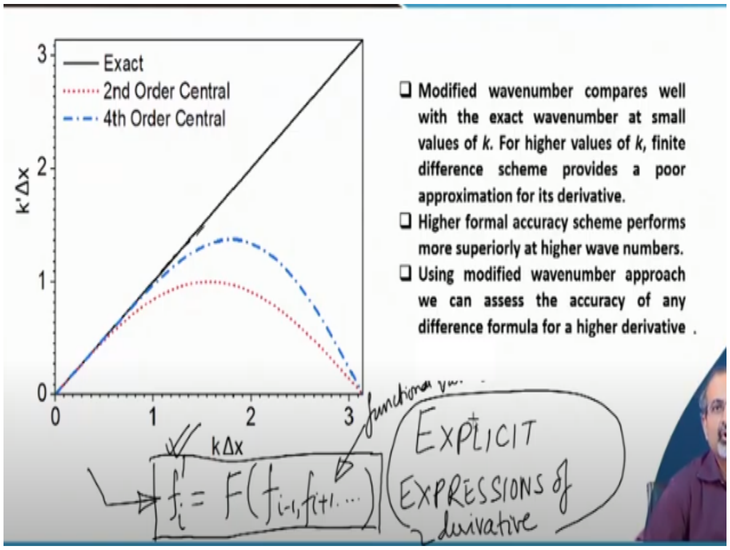

Explicit expressions of the derivative, which means that the finite difference approximation gives you a formula for calculating f' at a grid point i in terms of functional values in the neighborhood. So which may involve i – 1, i + 1 and other points.

That means, you can get the expression for f', the approximate expression for f' can give you the value at that grid point the moment you substitute for the functional values on the right hand side of the equation. So that kind of a calculation is called as an explicit calculation.

As long as you have the functional values which we normally have, we can substitute on the right hand side of this equation and immediately the difference expression helps us to calculate the f' approximately at the grid point i. Now there could be schemes where such explicit calculations are not done, calculations of the derivatives are done by so called implicit means. Let us have a quick look at the appearance of such schemes.

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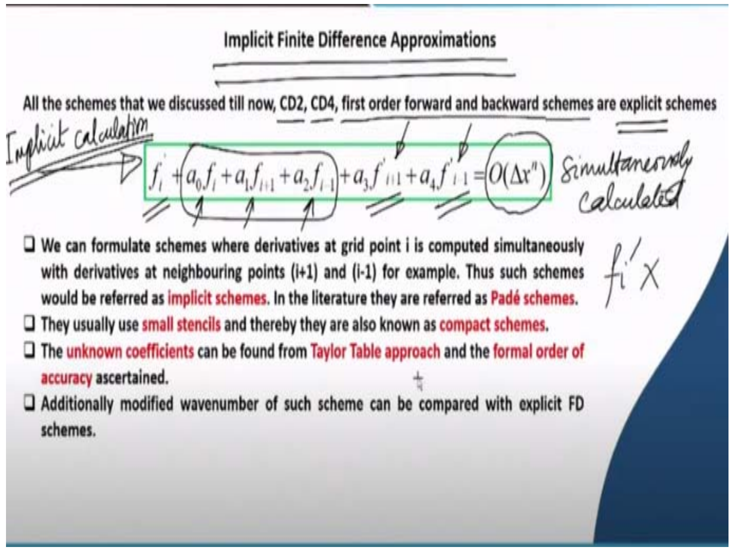

We could be having implicit finite difference approximations. So as we mentioned earlier that the schemes that we have discussed till date say CD2, CD4 or earlier we have discussed about first order accurate schemes involving forward and backward differences, all of them were explicit schemes, which we just discussed about what the explicit scheme essentially means.

But if you look at a scheme like this, where the derivative at the grid point i, the derivative at the grid point i + 1 and the derivative at the grid point i - 1 all first derivatives are being simultaneously calculated here. Now even if you substitute the functional values at these points, you cannot get a direct value of f_i' from this equation. This will not be possible because there are more derivatives involved here in this equation.

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i-1} + a_3 f_{i+1} + a_4 f_{i-1}' = O(\Delta x^n)$$

And of course, we do not know what is the formal accuracy of this approximation, but that is a question that we need to look at later. Right now we are just trying to figure out that, where this implicitness comes from. So what we understood was that an implicit expression would mean that the derivative cannot be calculated at a grid point just by substituting the functional values which are involved in the finite difference approximation directly.

But rather the derivatives have to be calculated at that grid point as well as the derivatives at some neighboring grid points in a simultaneous manner. And therefore, what you can understand is that there would be a system of linear algebraic equations which will come out in the process and then you need to solve the system of linear algebraic equations to obtain these derivatives at the different grid points simultaneously.

So once you solve for the system, all the derivatives will be worked out at a time, but they cannot be just worked out by substituting the functional values by using a single equation. So this kind of a calculation is an implicit calculation. We will talk more about this implicit formulation in the next lecture. Thank you.