Introduction to CFD
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Lecture - 14
Taylor Table Approach for Constructing Finite Difference Schemes (Contd.)

In this lecture, we begin by looking at the CD4 formula that we derived last time, and we continue our discussion. Today we will additionally discuss about the wave number approach.

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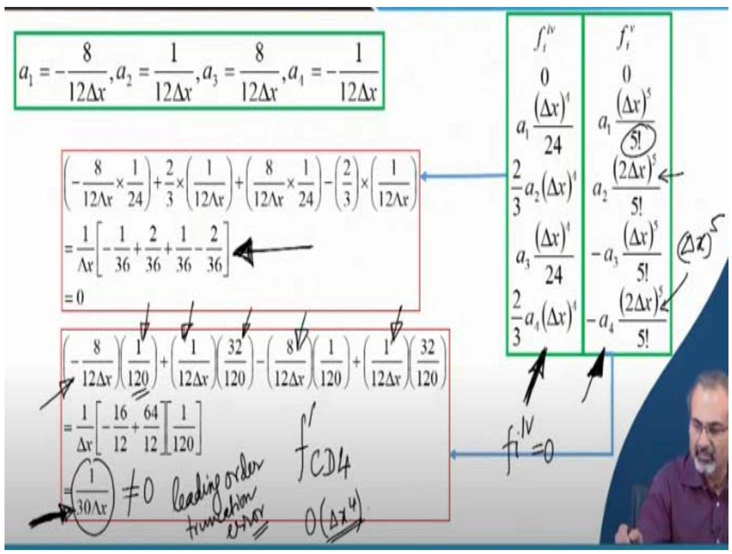

Last time, we had looked at the derivation of the CD4 scheme for first derivative. So just to recapitulate, towards the end of the last lecture we had even formally shown that why we have been able to achieve the fourth order accuracy formally through this approach through the Taylor table based calculations that we showed.

And we remember that this particular column which comes from the f_i^{iv} had yielded a 0 because all the terms summed up to zero when we substituted the values of the coefficients a_1, a_2, a_3 and a_4 in the associated expressions in the f_i^{iv} column. While the f_i^{v} column elements when they were summed up with the values of the coefficient substituted, which you can see here, so this is a_1, a_2, a_3 and a_4 respectively.

And the other coefficients are essentially coming from these numbers which you have. So you have 1 by factorial 5, which is 120. You have 2 to the power of 5 by factorial 5, which is 32 by 120, and so on. And then you find that this does not sum to 0. So this is a nonzero number what you produce over here. And therefore this column, these column entries would lead to the leading order truncation errors.

And that we showed it to be of the order of $(\Delta x)^4$. Because we said that we have $(\Delta x)^5$ terms in the denominator and 1 by delta x coming from the coefficients and therefore, ultimately you will be left with fourth order accuracy. So we have been successful in obtaining a fourth order accurate central difference formula using a 5 point stencil, which we had set out to achieve.

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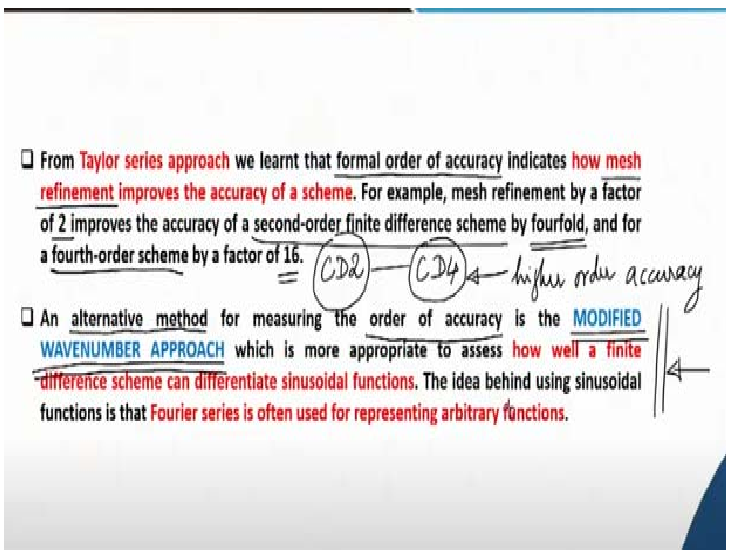

Just to recapitulate, from the Taylor series approach, what we learned was that, this is a method by which we can quantify the formal order of accuracy of a scheme through the truncation error based approach. And we also learned that the accuracy is essentially linked with mesh refinement. So if we are defining the mesh of the grid that we are using for calculations by a factor of 2, it can improve the accuracy of a second order finite difference scheme fourfold.

While if we are using a fourth order accurate scheme a twice fine mesh would improve the accuracy 16 times and that is the reason why one would actually like to explore higher and higher order accuracies in a formal sense and try to apply them in grids of different refinements and trying to look at how the errors reduce and accuracy gets enhanced.

So even on a relatively coarse mesh, the CD4 scheme is expected to do comparatively better or quite significantly better than the CD2 scheme. So that is primarily the motivation behind looking for higher order accuracy. Well, that is one possible way by which we can assess accuracy of finite difference scheme. But that is not the only one.

There could be an alternative method, which often turns out to be more effective than the formal order of accuracy, which we do by the Taylor series approach. And that approach is known as the modified wave number approach. And what we try to assess over here is that how well is a finite difference scheme doing in differentiating sinusoidal functions which could include both sine as well as cosine terms.

Now the motivation behind doing such an exercise would be that we are all aware that Fourier series is a very powerful tool in representing arbitrary functions, and we often come across very complex functional forms where the Fourier series approach is very robust and sometimes the most effective way of representing such complex functional forms.

And then if we have a finite difference scheme doing a good job in differentiating sine or cosine terms that occur in Fourier series, then we can be rest assured that they would be appropriate in application of finite differencing of complex functional forms.

And that basically gives the motivation of pursuing the modified wave number approach where we try to look at the suitability of a finite difference scheme in differentiating sinusoidal functions. So with that motivation in mind, we try to look at this alternative approach for assessing accuracy of a finite difference scheme, which we are naming as the wave number approach.

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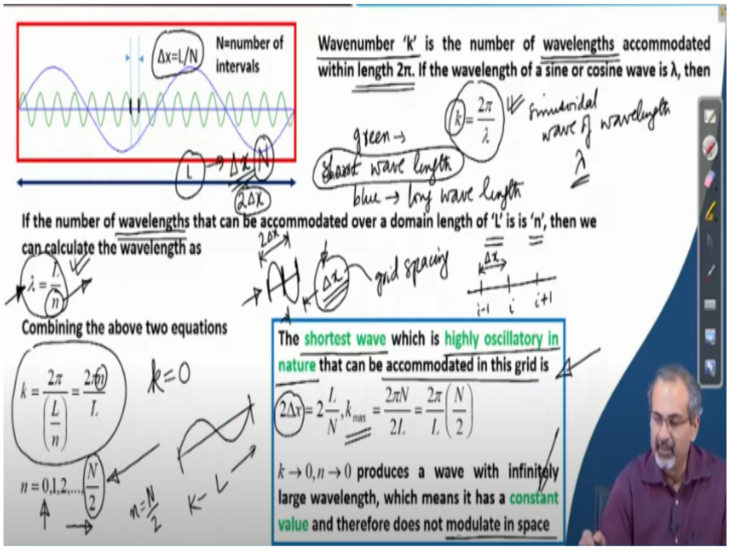

Before we do more detailed discussions on what the wave number approach actually means, let us look at some typical waveforms and briefly relook at some of the facts that we know about such waveforms so that we can formally address the issue of the wave number approach. Here in the diagram we have a certain domain length L that we have specified along which we can see waves disposed.

The blue colored wave completes two full wavelengths over that domain while the green colored wave ends up having many more wavelengths. Incidentally, both the waveforms are having integer number of wavelengths accommodated within the same length that is L. Now the green wave has a very short wavelength while the blue wave has a comparatively long wavelength.

So what it means is that if you have a minimum length scale defined here based on which you can accommodate the shortest possible wave, then you are essentially defining a bound. That means, you cannot express a wave which has a shorter wavelength than the one that we have represented over here provided that this interval is defined.

So here what we are trying to say is that if you have a domain length L which you are representing in the form of the small interval Δx times the number of intervals that you have then that way you are also defining how short the wavelength can get. Because you cannot have a wave, which has a wavelength more than 2Δx on such a discretized domain. Now we have a wave number associated with these waves.

The blue and the green wave would have very different wave numbers associated with them. So by definition, we say that the number of wavelengths that can be accommodated within a length of 2π would give you the wave number. So by definition if you have a wave, a sinusoidal wave of wavelength λ then the wave number of such a wave will be given by $2\pi/\lambda$.

Now when the interval is not 2π in length, but rather some other length like we are calling as L over here and we are seeing that small n number of wavelengths can be accommodated within such a length, then obviously, the λ corresponding to such a wave will become L/n. And this n is a general quantity. It can be applicable for a long wavelength wave or a medium wavelength wave.

Or could be a very short wavelength wave as well. So n is a kind of a variable. That will essentially mean that you end up producing waves of different wavelengths by tuning the value of n. If you combine these two equations, the equation for λ here and the equation of wave number that we already defined earlier, then we end up getting an expression for wave number of this kind, which gives you k is equal to $2\pi n/L$.

And now we have to decide what is the range of values of n that we can accommodate so that the necessary condition is that whichever wave we accommodate in the process within this domain L, the wave should end up completing integer number of wavelengths within the domain length L. It cannot be a portion of the wave left at the end of the domain which is not completed.

So if you look back at the picture on top, you can very clearly see that both the blue as well as the green colored waves have ended up satisfying that condition. You could have more number of waves of intermediate wavelengths which could be coming in between based on how the value of small n changes. Now coming to the range of values that we have for small n, if small n is equal to 0 that yields the condition that k will become equal to 0.

Now if k is equal to 0, that means the function is not showing any wavy nature whatsoever, it is just a constant. Whereas, if n is equal to 1, then you will end up just filling up the entire length L through one wavelength. That means, if this is your L, then you will see a sinusoidal wave going like this and filling up the domain which is a fairly large wavelength wave.

Now gradually as you keep increasing n and bring it to a large value, if the capital N value is a large value than N/2 is also quite large. In that case, you will have waves with much higher wave numbers, which will look closer to the green one that you have. In fact, the green one satisfies the condition that n is equal to capital N/2, because the green one is the limiting case where one wavelength is accommodated within $2\Delta x$ length.

That means, half of the wave gets accommodated within the smallest length scale that is available in the discrete space, which we are offered referring as the grid spacing, like the way we did it on a finite difference mesh, for example. So this was the grid spacing that we were talking about when we did the finite difference calculations. So it is a very similar sense that we are trying to convey over here.

So if this length L was discretized using a set of grid points, then Δx is the grid spacing that we have. And you can accommodate the shortest possible wave which has a wavelength of $2\Delta x$ on such a grid. So we are just reemphasizing this point here in the box right up here that the shortest wave has a very highly oscillatory nature. And this is the shortest way we can accommodate within the given grid with this wavelength, $2\Delta x$ wavelength.

And that gives you the highest value of the wave number k_{max}. Similarly, we said that for n is equal to 0, we have no functional variation. There is no modulation that we see in the functional value in space. So these are the two N's of the spectrum. Now this concept will be very useful when we develop the modified wave number approach for assessing the accuracy of a finite difference scheme.

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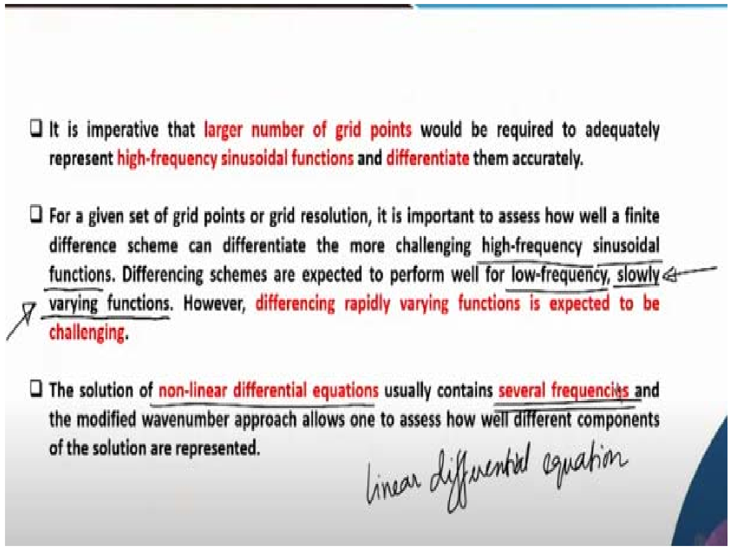

We will just try to look at a few points before we go over to the wave number approach. We have understood that a large number of grid points will be required when we try to capture high frequency sinusoidal function within a discrete space, where you have a certain length discretized using large number of grid points.

And then if you are trying to differentiate such a wave function, then you also of course need very accurate differencing methods. When you have a given set of grid points or grid resolution, you need to assess that whether the finite difference scheme that you are using is capable of capturing the high frequency part of the sinusoidal function effectively.

Because it is expected that the low frequency portion will be captured with more efficiency because they are associated with slowly varying functions while the high frequency part is associated with rapidly varying functions and capturing them through the difference operations may be very challenging.

And therefore, the accuracy of the scheme from the wave number approach would be to focus on this that how effective is a numerical scheme in capturing high frequency oscillatory behavior of functions. And we need to remember that we have in the earlier part of this course discussed more on linear differential equations. But very often in fluid mechanics we have to handle nonlinear differential equations.

Very often they are also going to be of partial differential nature. And it would be found that such differential equations contain a large number of frequencies. They could be several frequencies at least. And therefore, the finite difference scheme should have enough capability to resolve the different frequencies which would be there in the solution with sufficient efficacy, without which the solutions will not be satisfactory.

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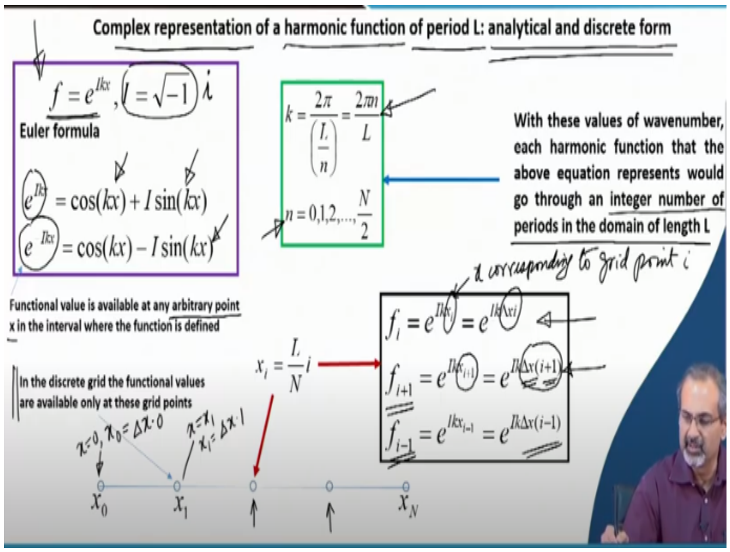

Going to a more formal way of setting up the stage for doing the wave number approach, we first introduce a harmonic function of period L. And we introduce it in a complex form, a complex representation because very often it is more convenient to represent a harmonic function that way because you can accommodate the sine and cosine terms more compactly through a complex representation.

And we are going to show both the analytical as well as the discrete form of such a function here. So first looking at the analytical form, we are defining the function $f = e^{Ikx}$. Here we are using capital I as under root minus 1. Usually, we use the small i for doing that, but because we have exhausted the small i for meaning grid index here we are going to call the under root minus 1 as capital I ($I = \sqrt{-1}$).

And this is essentially going to cater to a large number of waves, possible waves having different wave numbers. So in Fourier series representations for example, we could be having some coefficient terms also coming on over here, but we are not including them, but we will be looking at behavior of such coefficients later on in a future lecture, where we deal more on stability analysis.

So as far as the modified wave number approach is concerned, we will not be needing the coefficient term and therefore, we are not including it here. We recall the Euler formula where we can have representation of this e^{Ikx} in terms of the cosine and the sine terms. And we may often come across even with e^{-Ikx}.

Now we need to remember that this is an analytical form which would give us the value of this function at arbitrary points x within an interval where the function is valid or defined. But when we do discrete grid based calculations, the function will be available only at the respective grid points. And therefore, we have to have an equivalent representation of this function in the discrete space.

Before we go on to that, we just recall from the previous slides that we had defined wave number like what we have done over here. And we also recall that there will be an integer number of periods in the domain of length L irrespective of the wave number that we accommodate, and that the wave number varies with this index small n. So as we said that, on a discrete grid, we have specific points at which the functional values will be available.

So if we have the function defined at a grid point i we call it f_i. And then what we do essentially is that in the index we convert x to x_i, where x_i stands for the x coordinate corresponding to the grid point i. Now we can very easily see from this nomenclature that at x = 0, we have the x_0 expressed as $\Delta x \times 0$, at $x = x_1$ we have $x_1 = \Delta x \times 1$ and so on.

So that way we can say that at x_i the coordinate will be represented by multiplying Δx by i, the grid index. So likewise, f_{i+1} can be represented this way, where you have x_{i+1} here in the index and x_{i+1} is nothing but $\Delta x \times (i + 1)$. So again the grid spacing times the index of that grid point. Similarly, f_{i-1} will be given by an expression like this.

So we need to keep these nomenclatures in mind, because when we do the wave number approach calculations, all these things that we discussed over the last few minutes will come in very handy. Now let us do a few calculations.

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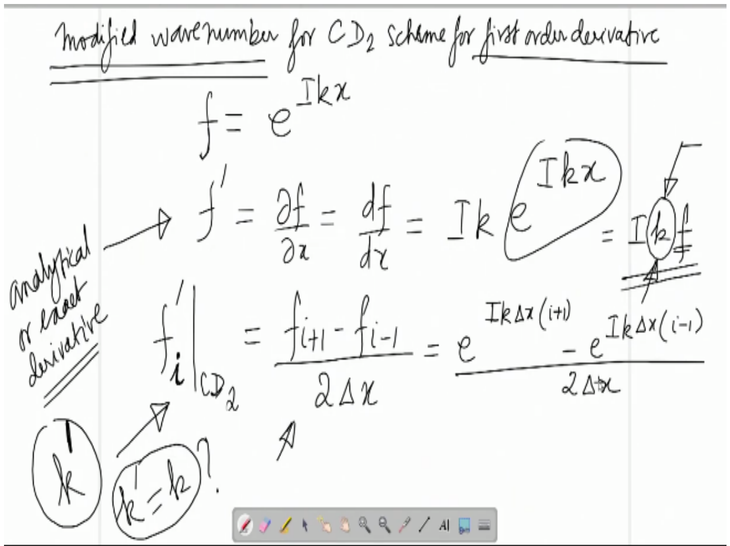

We will start off with a calculation where we try to understand what would be the modified wave number for CD2 scheme for first order derivative. Of course, we still do not know precisely what we are meaning by modified wave number, but as we do this example, we will understand better that what is the meaning of this whole process.

We remember that the analytical function that we had defined was $f = e^{Ikx}$. And we are talking about first order derivative. So if we take the analytical derivative f' that essentially means, here it will essentially mean df/dx and that will be equal to Ike^{Ikx}. We can represent it as *Ikf*.

So this is the analytical derivative or exact derivative. And now you can perhaps guess that we will also find an approximate expression for the derivative through our finite difference scheme. So when we do that, we can call it as f'_{CD2}. Then compare f'_{CD2} with *Ikf* that you have from the analytical part. That is the whole idea.

In the analytical part, we have the wave number figuring here in the expression of f'. We have to figure out that in the f' expression that we work out for CD2 scheme, the

k that comes up, is it exactly equal to the k that we have from the analytical approach or it is some other value. The one that will come up in the CD2 expression we will mark it as k' and the idea would be to find out whether k' is equal to k or not.

So that is the question we are raising at this point. Now if we manage to find that both the wave numbers are matching we would be most happy because then what it means is that CD2 is doing as good a job as the exact derivative. Now how do we go about finding the f' for CD2 scheme? Let us try to put the approximation that we have for the CD2 scheme and then try to work our way ahead from that point.

So this is the approximation we have for f' for CD2 scheme and remember that this f' is being calculated at the grid point i. So now it is a matter of just substituting those expressions which we already wrote previously.

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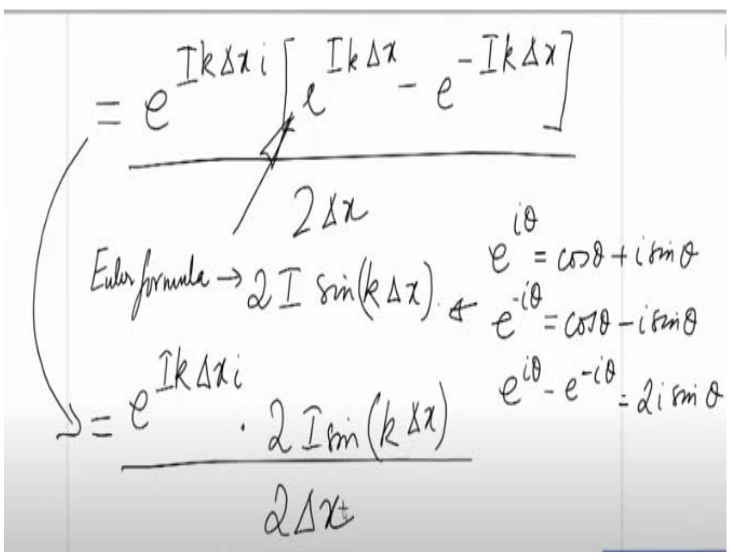

We take out a common factor. Again from Euler formula you can show that the bracketed term in the numerator can be seen simplified as this. Why is it because

$$e^{i\theta} = \cos\theta + i\sin\theta$$

while

$$e^{-i\theta} = \cos\theta - i\sin\theta$$

and therefore, if you take a difference you are left with $2i\sin\theta$.

$$e^{i\theta} - e^{-i\theta} = 2i\sin\theta$$

So based on that we can show this to be coming up in the numerator. So what do we have finally from this step?

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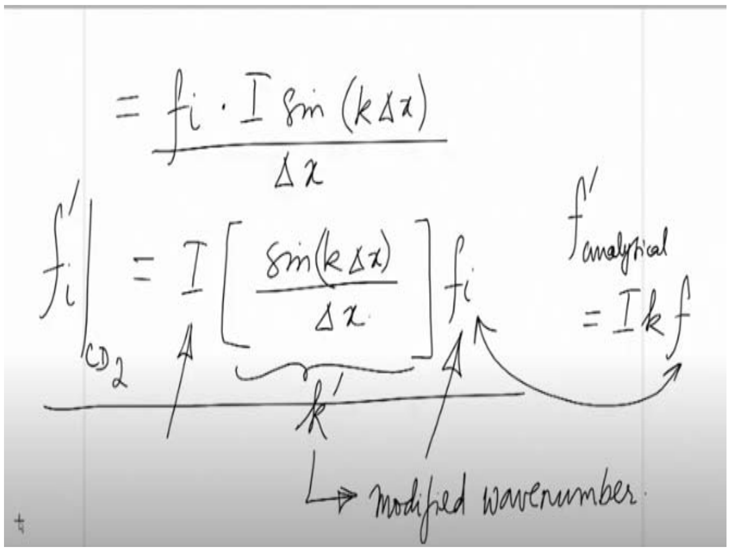

We have, this may be written as f_i. Now we will just rewrite this whole thing in a format which becomes very easy for us to compare with the analytical expression. So we now recall that the f' analytical was equal to *Ikf*. And through the discrete scheme that we have used over here, we have the *i* the f_i which is nothing but a counterpart of *f*.

And an expression in between, which is not the same as *k* unfortunately, and that is the one which we will call as the modified wave number. So since *k* and k' are not the same, it is as though through a numerical means *k* has been translated to a different expression which involves $\sin(k\Delta x)/\Delta x$.

$$f_i'\Big|_{CD_2} = I\left[\frac{\sin(k\Delta x)}{\Delta x}\right] f_i$$

OR

$$f_i'\Big|_{CD_2} = I\underbrace{\left[\frac{\sin\left(k\Delta x\right)}{\Delta x}\right]}_{k'} f_i$$

$$f'_{\text{analytical}} = Ikf$$

So that means a wave with a certain wave number or frequency is now having a different frequency associated with it, when it is being captured in the discrete calculations using the CD2 finite difference scheme. We will discuss more on this in the next lecture. Thank you.