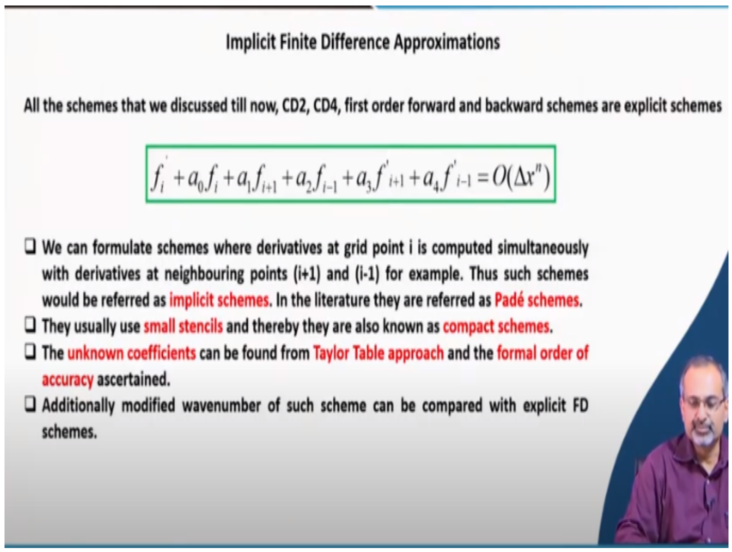
Introduction to CFD
Prof. Arnab Roy
Department of Aerospace Engineering
Indian Institute of Technology-Kharagpur

Lecture - 16
Taylor Table Approach for Constructing Finite Difference Schemes (Contd.)

In this lecture we will continue our discussion on the Taylor table approach.

(Refer Slide Time: 00:31)

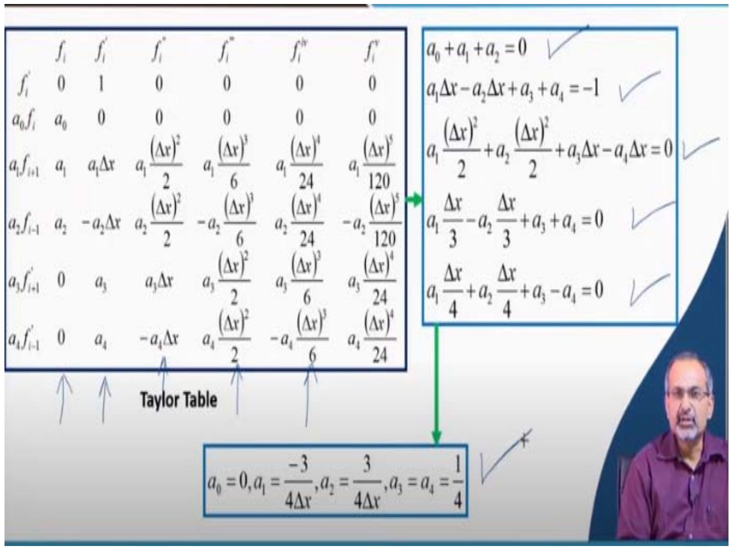


In the previous lecture, we had started discussing about implicit finite difference approximations and application of Taylor table in such approximations. So we recall that there could be finite difference approximations possible where you could have number of derivatives as unknowns in a given finite difference approximation.

And this would mean that you would not be able to compute the finite difference approximation for each grid point using a single equation. So we would call these as implicit schemes. And in the literature they are also referred as Pade schemes and they use small stencils to achieve comparable formal accuracies compared to explicit schemes. And therefore, they are often referred to as compact schemes as well in the literature.

We would take up an example and try to see how the formulation works out.

(Refer Slide Time: 01:48)

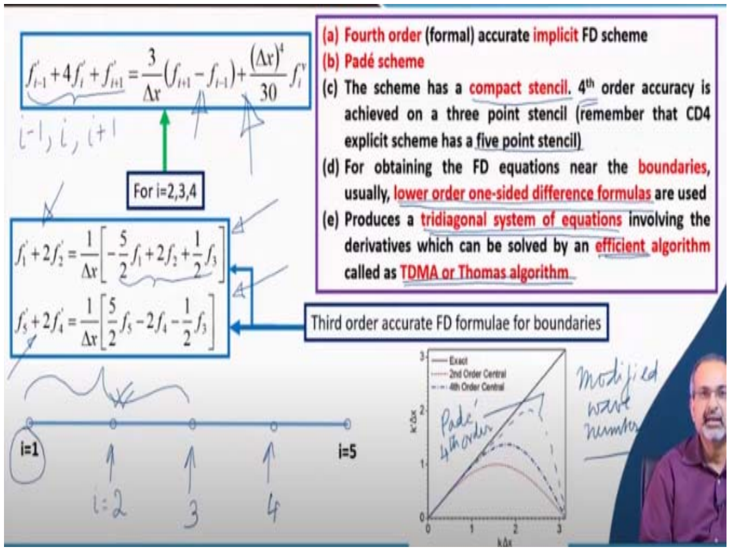


We are looking at the formulation which was shown in the previous slide and we have now constructed the Taylor table for it and you can now see the Taylor table populated with all the relevant terms. By now we have become familiar with the Taylor table approach. So it should be a straightforward exercise. And if we look at the number of unknowns in this formulation, we have 5 unknowns to be solved, starting from a_0 to a_4.

And therefore, we would need 5 linear algebraic equations to be defined in order to solve for these unknowns. We start the procedure by looking at the column for f_i and that column produces this equation. Then we move on to f_i', we get the second equation f_i'', the third equation; f_i''' the fourth and the fourth derivative and we get the fifth equation.

Now we simultaneously solve these linear equations, linear algebraic equations, and we come up with the values of the coefficients. If we just plug in these values of coefficients into the initial equation that we defined earlier, we should be able to get the scheme.

(Refer Slide Time: 03:25)



If we do that, we have the scheme defined over here for us. And we can show that this gives us a fourth order formally accurate implicit finite difference scheme. Because we cannot obtain the value of the first derivative, say at the grid point i, which is the reference grid point from this equation alone, we have to solve a system of simultaneous linear equations in order to obtain the values of the derivatives not only at that point, but all the remaining points in the domain simultaneously. Additionally we can show that it has fourth order accuracy.

As we mentioned earlier that in the literature these schemes are often called as the Pade schemes and they have a compact stencil. If you remember, to obtain fourth order accuracy with the CD4 scheme we needed 5 point stencil while this scheme uses a 3 point stencil because you are using the grid points i – 1, i, and i + 1 to define the derivatives on the left hand side of the finite difference equation.

Functional values are being used from points of that stencil namely i + 1 and i - 1 respectively. Now when you try to apply this scheme to the inner points of the domain, points like i equal to 2, 3, 4 provided that you call the first grid point as i = 1, then you can happily use this scheme. Because if you notice that if you are applying the scheme here at the point 2, then your stencil is this.

At the point 4 the stencil would comprise of 3, 4, 5 and so on. But when you move on to the boundary points, this scheme would not work. Because there will be a point at which the functional value and one of the derivatives will be required to be put into that equation where those values are not available to you. Therefore, you need to have a different way of defining the derivatives at the boundaries.

Usually, we go ahead with lower order one side finite difference schemes for the boundaries. In this case, we have used a third order accurate approximation which are given by these two equations.

$$f_1^{'} + 2f_2^{'} = \frac{1}{\Delta x}\left[-\frac{5}{2}f_1 + 2f_2 + \frac{1}{2}f_3\right]$$

$$f_5^{'} + 2f_4^{'} = \frac{1}{\Delta x}\left[\frac{5}{2}f_5 - 2f_4 - \frac{1}{2}f_3\right]$$

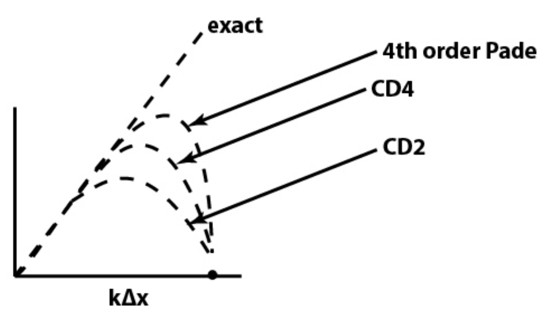
These two equations are again of implicit kind because on the left hand side of both the equations you can see that there are two derivatives, rather derivatives of two grid points which are shown simultaneously on the left hand side.

So at the left boundary, you have the derivative at points 1 and 2, the finite differences at points 1 and 2. And again at points 4 and 5 for the right boundary which are showing up on the left hand side of the equations which means that the equations remain implicit even at the boundaries. And on the right hand side, you can see that the functional values are invoked from three points near to the boundary including the boundary point.

So the stencil width as such does not change as far as the functional values are concerned on the right hand side. However, the stencil width has changed in as far as the derivatives are concerned because on the left hand side you no longer have three derivatives as unknowns, but rather two. This has an influence on the matrix representation of this system of equations.

This kind of a structure would lead to what is called as a tridiagonal system of equations when you try to write down these equations in matrix form. And this type of tridiagonal system is rather efficiently solved with an algorithm which is called as the tridiagonal matrix algorithm abbreviated as TDMA or Thomas algorithm. We will talk more about this algorithm in a later lecture.

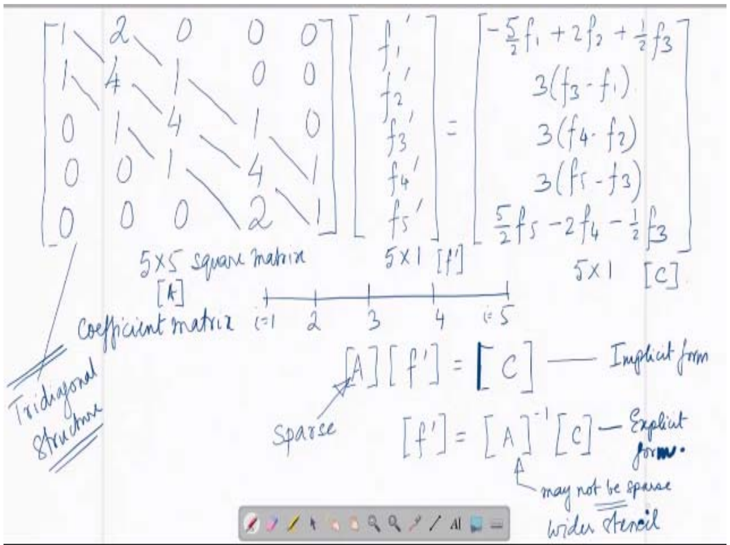
We also need to discuss about one point that what is the kind of accuracy this scheme is going to exhibit when we look at it from the modified wave number perspective. So we recall that this was the plot we made to study the modified wave number approach and it can be shown that this scheme would do more superiorly than the CD4 scheme that we discussed before.



So we call this as Pade fourth order scheme which displays more superior characteristics than the CD4 which comes from the explicit formulation. So this is a very interesting point of implicit schemes that with the same formal accuracy, it is exhibiting a superior accuracy from the modified wave number perspective. However, we are not going about obtaining the expression for the modified wave number for the scheme.

This can be attempted as a homework problem. We will just spend a little time discussing about the matrix structure of this problem.

(Refer Slide Time: 09:36)



The kind of discretization equations that we wrote in the previous slide for both the boundary stencils and the inner stencils can be written down in matrix form like this keeping in mind that we are considering 5 grid points. You recall that our grid looks like this starting from i equal to 1, 2, 3, 4 and 5. Points i equal to 2-4 are the inner grid points or internal grid points.

The grid points 1 and 5 are the boundary grid points. And then let us try to write it down in matrix form. If you write down the individual equations for each grid point, you will be able to generate this coefficient matrix and what you put on the right hand side are the functional values. They are all known to you. So this is a 5 by 5 square matrix. Let us call it as matrix A.

This is often called as the coefficient matrix. This is essentially a column vector which contains the unknown derivatives at the 5 points. Let us call it as a vector f'. And then this is again a column vector 5×1 which comprises of the known terms, let us call it as [C]. So this matrix equation can in principle be written like this

$$[A][f'] = [C]$$

And you could get a solution for f' in principle, if you can find out the inverse of the coefficient matrix and multiply it by the right hand side column vector. So this is essentially the system of equations in implicit form while this is the system in explicit form.

$$\left[f'\right]=\left[A\right]^{-1}\left[C\right]$$

So if you look back at the coefficient matrix a little carefully, then you can identify three nonzero diagonals in that matrix.

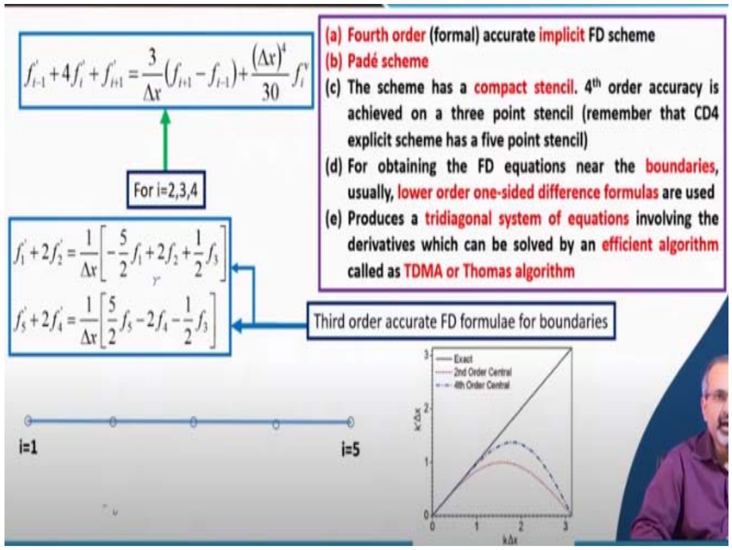
It is a very interesting structure. So only these three diagonals contain nonzero terms. The rest of the terms in that matrix happen to be 0. This structure was referred to as the tridiagonal structure. And whenever you have this structure in the coefficient matrix, it is very efficiently solved through the TDMA or Thomas algorithm.

We have to remember that though the matrix [A] has a rather sparse nature, that means only few number of the elements are nonzero, the inverse of that matrix may not be sparse. In fact, in the explicit form of this scheme, you have larger contributions coming from the A inverse matrix in computing the finite differences.

Larger influence in the sense that if you have more number of nonzero entries in $[A]^{-1}$ matrix that means effectively it has a wider stencil than is visible in the implicit form. And we have seen that in explicit schemes when you have wider stencil that usually helps us achieve greater accuracy.

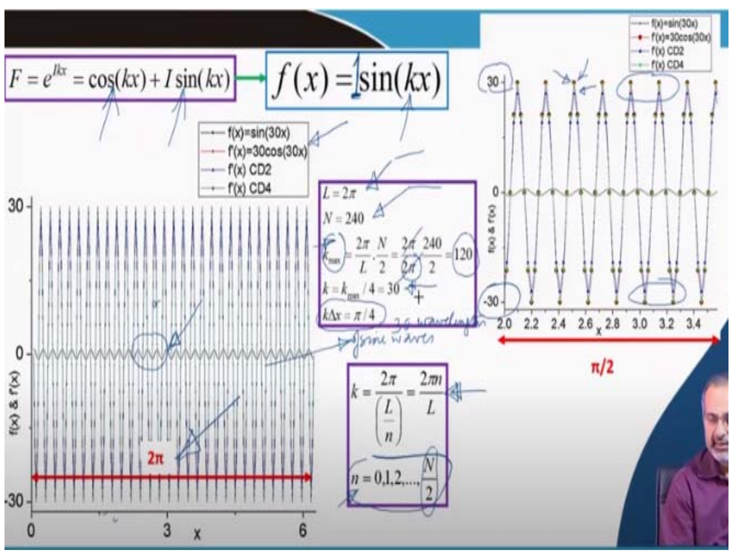
Now all this indicates towards one fact that in the implicit form, though the scheme is having a rather narrow stencil because of which we are calling it as a compact scheme, its explicit counterpart could be showing a much wider footprint, a much wider stencil. And therefore, that could be the reason behind its superior performance in the modified wave number sense.

(Refer Slide Time: 15:58)



Before we close our lecture on Taylor table approach, we would like to look at one example where we revisit the CD2 and CD4 schemes that we have discussed in earlier lectures and try to do a small example problem using these two schemes and see how they perform with a particular eye on the modified wave number approach implication.

(Refer Slide Time: 16:26)



We take up a problem over here by defining a function f(x)=sin(kx). Now you may recall that when we were talking about the Fourier representation of the function f (x) we had used a complex representation. So this was the real and this was the imaginary parts. And we said that this is a convenient way of accounting for both the sine and the cosine terms.

And then we had discussed how accurate the different finite difference schemes are in handling sine or cosine kind of terms. And that was the basis of the modified wave number approach. We are revisiting the problem now by doing an example.

And we have just taken up a sine term but with the wave number embedded here with x so that we have a control over choosing the wave number and therefore, we can look at waves whose wave lengths could be varied conveniently and thereby we can see how the finite difference schemes CD2 and CD4 are doing in calculating the first derivative of this function for different values of k.

For doing this we have made a few choices in terms of the parameters. We are going to choose a domain length L is equal to 2π. And we are going to use 240 grid intervals to be spanning this length 2π.

And then if you do that, you remember from the definition of the maximum wave number that you can entertain in that kind of a discretization going by the basic definition that wave number is nothing but $2\pi/\lambda$ where λ is the wavelength of the wave that you are accommodating, that wavelength can be changed based on the values of n that you are choosing.

So we remember that n is equal to 0 would give us a constant value and then n is equal to N/2 will give us a highly oscillatory nature of the function. And we remember that when we choose the value as capital N/2 that is the highest wave number that we can end up accommodating over such a discretization. The discretization being given by the length and the number of intervals that you have accommodated over that length.

So based on this, we can state that for this discretization the maximum wave number that you can accommodate k_{max} will be given by $(2\pi\times N/2)/N$ and we have chosen the L conveniently as 2π so that these two terms cancel out altogether. And we are then left with 240 by 2 which means, this length 2π can accommodate 120 wave number as the maximum wave number.

Now what we are going to do is we are going to choose different values of k subject to this maximum wave number that we can accommodate over this domain. So when we choose k of $k_{max}/4$ that gives us a k value of 30, which basically means that you will have 30 sine waves; 30 wavelengths of sine waves accommodated within the 2π domain, which is shown in this figure on the left.

So this functional value is actually showing as the ripple that you can see over here. So these ripples are nothing but the sine waves. And the amplitude essentially happens to be 1. Here we are trying to see that how the finite difference scheme CD2 and CD4 are doing in finding out the derivative f'. So we know that the exact derivative in this case will be given by $30\times\cos(30x)$.

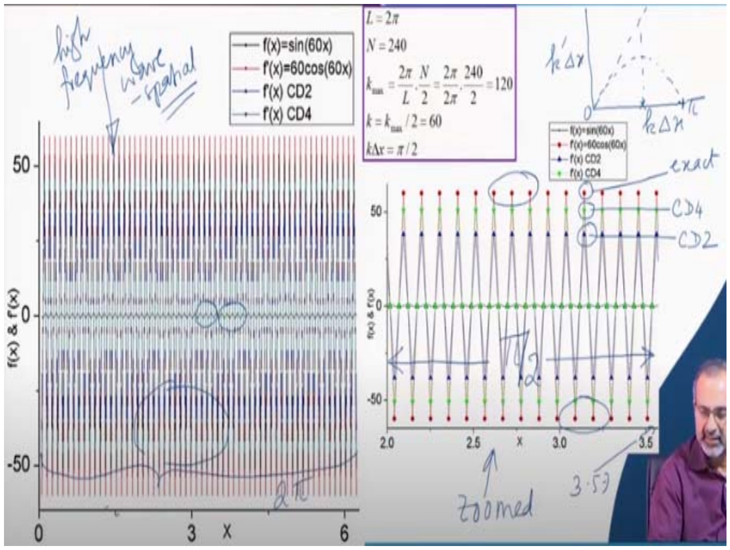
And then we need to see how well that is approximated by the CD2 and CD4 schemes. Remember that the k that we have chosen corresponds to $\pi/4$. And you may recall that $\pi/4$ is a rather small value compared to the full scale value of π in the modified wave number plot. So we are having an anticipation that the schemes will do reasonably well in capturing the derivative for this value of $k\Delta x$.

So when you look at their performance, you can see that the red spots are showing the exact values, the blue spots are showing the CD2 values, and the green spots are showing the CD4 values. You can make out that the green spots are going fairly close to the red spots and the blue spots are not far from the red spots when it goes to capturing the peak values.

We are more interested in seeing how well the schemes are doing in capturing the peaks. They could be crests or troughs. So going on the positive as well as on the negative sides as you can see, the peak positive value is 30 and the negative value -30. They are swinging between that. And for this value of $k\Delta x$ both the schemes are not doing badly, they are in fact doing fairly well.

So you would be interested to stretch the limit and go further and see that for higher wave numbers, how the performance would be. And of course, we know through our previous experience that there would be a degradation in the performance, but we are interested to know that how much the performance may be degrading.

(Refer Slide Time: 23:15)



So for that, we go to the case of kΔx equal to π/2, which is exactly at the half midpoint of the interval on the x axis of the modified wave number plot. And by then if you remember the plot, the response of both the schemes would have drooped off from the exact value.

So just to recall what we are talking about, you remember we made a plot like this and the exact plot used to go like this, while any of the approximations used to droop down like this, and this range was from 0 to π. So when we are at π/2, we are exactly midway of the x axis range. And by then you can imagine that the wave that you are trying to model over here has become a more high frequency wave in a spatial sense of course.

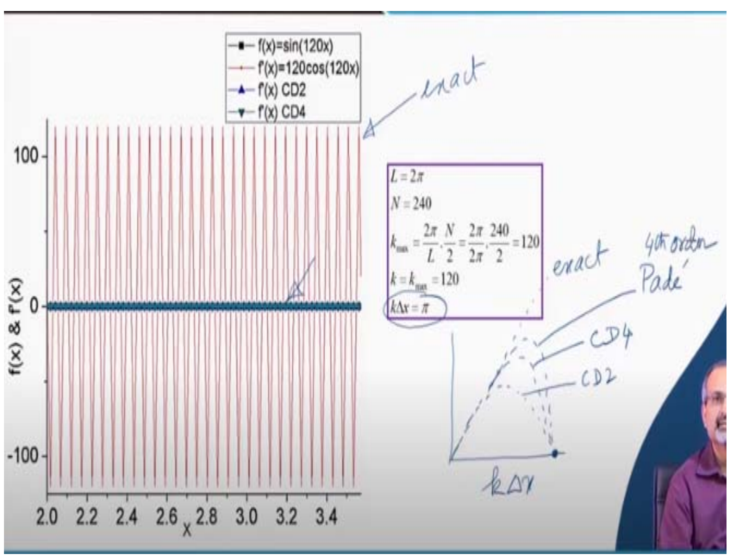
So this frequency essentially means that you have a shorter wave length to capture. You can notice that these waves are having half the wavelength as what they were in the previous plot. If you try to compare them one is to one that is how it will appear. Also remember that this continues to be the 2π interval while this is showing you a zoomed view of only one fourth that interval so that you can look at the features better.

For that we have just chosen one fourth of the total domain width and therefore, we have chosen it as π/2. So that is the span between 2 and say 3.57. That is the range which we have chosen for plotting the wave. It is like somewhere here. So it would be somewhere in this range that you have expanded it and you have shown it here. You can make out that more number of wavelengths have now got accommodated in this π/2 width.

And the more important thing to notice that the schemes, both CD4 and CD2 are now deviating off from the exact values. So the red is the exact value while the discrete schemes are now wavering off from the exact values. So you can clearly see that the green dots are closer to the peak values than the blue dots which is expected.

Which means CD4 is still doing more superior than CD2, though it is increasingly falling off from the exact value. It happens on both the crests and the troughs as we mentioned earlier. Now the ultimate test for them of course would be to stretch the wave number further and take it to the maximum point that is the k_{max} value. And we recall that of course, all schemes see a very massive degradation in the performance as you move towards the highest wave numbers.

(Refer Slide Time: 26:39)



And this is not a surprising outcome, because we have looked at it earlier. And you now see that the red plot happens to be the exact one while all the discretizations have fallen off and become very close to 0, which means they have failed in capturing the behavior of first derivative at the highest wave numbers.

So you are at the highest wave number where $k\Delta x$ equal to π has been reached, which is essentially the endpoint of that plot that we were talking about. So you remember that the behavior actually droops off here. And therefore, you are far away from the exact and that was irrespective of the kind of scheme. So we finally saw the behavior of three schemes. CD2, and CD4 were directly shown over here through these previous plots.

It would be a good exercise to try out for the Pade scheme, which we discussed about today on your own as a homework exercise. Thank you.