Introduction to CFD
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Lecture - 13
Taylor Table Approach for Constructing Finite Difference Schemes (Contd.)

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

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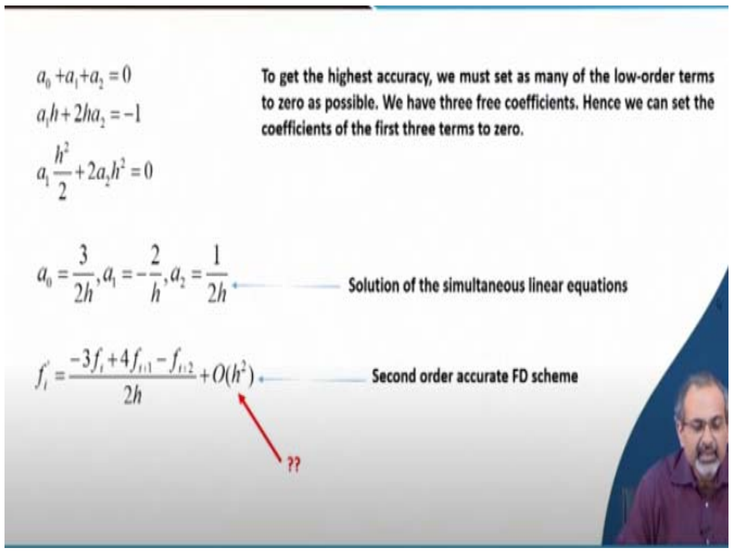

Last time, we had done a problem where three grid points were involved in the stencil, namely i, i + 1 and i + 2. With that stencil, we did the Taylor table calculations and we found that the scheme turns out to be a second order accurate scheme. But we did not do a very thorough discussion on how it comes up with a second order accuracy.

$$f_i^{'} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + O(h^2)$$

We just discussed that on the right hand side of the expression that we derived from the Taylor table approach, the bracketed terms would be set to 0 so that we are able to send as many of those terms as possible to 0 and thereby enhance the accuracy of the scheme in a formal sense. So by doing that, we could set three of those bracketed terms or expressions to 0 and thereby obtain the expressions for these unknown coefficients a_0, a_1 and a_2 which we set out to do.

And the remaining bracketed terms the higher order terms would still remain as the truncation error terms. So if you look at the truncation error terms and then you try to substitute these values of the coefficients that you have now obtained, then you can find out in a proper manner whether it really turns out to be a second order accurate scheme or not. So let us try to review that activity.

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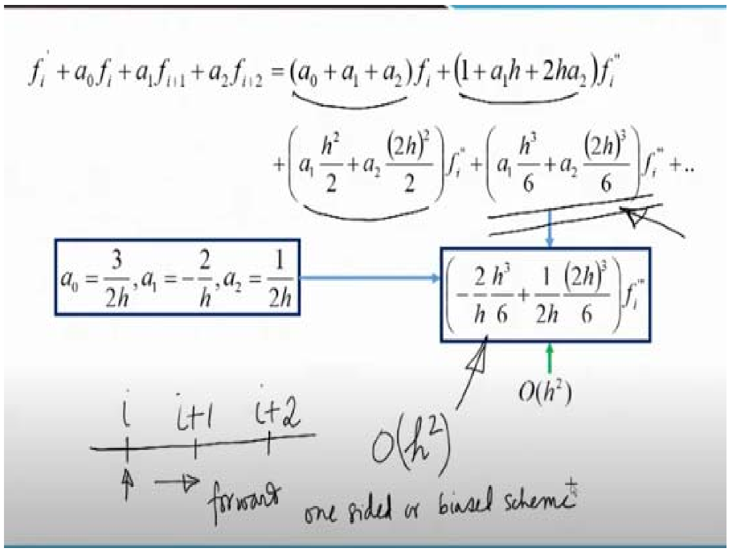

So here what we see is, we have these three bracketed expressions set to 0, which helped us calculate the values of those unknown coefficients a_0, a_1 and a_2. And then the leading order term in the truncation error was left here, the one that we just indicated.

So if you now substitute the values of a_1 and a_2 what you have worked out in that expression in the bracketed expression, then you find out that this actually produces h^2 terms. So that is what we need to show before we can justify that it actually produces a second order accurate scheme. So having said that, now let us try to do one more example problem, where we would have a symmetric stencil.

So you remember that he problem that we did had a kind of a biased stencil in the sense that it just had points disposed on one side of the reference grid point i that is to the right of the point i. That means, essentially the forward direction. So it gives you a kind of a one sided biased scheme. Whereas, now let us do an example, where we actually have a centered scheme. That means, the point i would lie at the center of the stencil.

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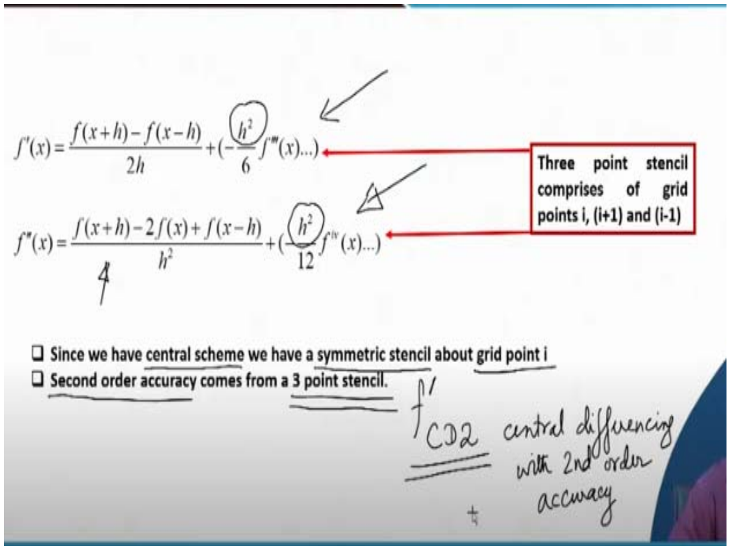

Before we do that, let us once again review the finite difference expressions that we have worked on till now. So when we worked on the first and second derivatives using a 3 point stencil, we have seen that the reference grid point was i and we had taken two points i +1 and i - 1 on two sides of that point. And that helped us to come up with these two expressions for the first and second order derivatives through the Taylor series approach.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + (-\frac{h^2}{6} f'''(x)...)$$
$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + (-\frac{h^2}{12} f^{iv}(x)...)$$

And both of them turned out to be second order accurate approximations of the first and second derivative. So we once again note that in central schemes, we find symmetric stencils being used about the grid point i. And the second order accuracy came from a 3 point stencil. We will for now focus only on the first derivative, when we do it for still higher order accuracy.

But we find that even for the second order derivative, the same 3 point stencil could be used. Now we found out the f' using central differencing of second order accuracy. This is often referred in the literature as CD2 scheme. That means central differencing with second order accuracy. So that is abbreviated as CD2.

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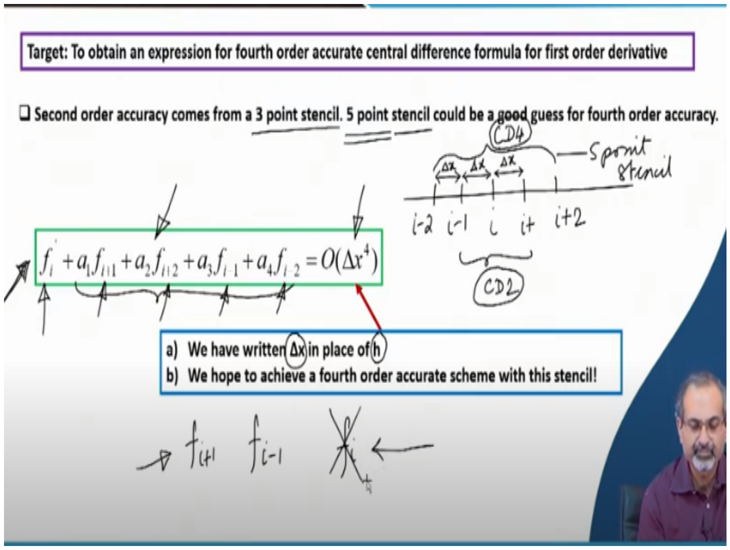

We might like to go ahead with an ambition to get a scheme with still higher order accuracy, let us say fourth order accuracy. And let us try to guess that what kind of stencil may help us achieve that. So we are setting out with the target to find an expression for fourth order accurate central difference formula for first order derivative.

What we mean to say is going by the previous nomenclature, we are interested to find out a finite difference scheme for f'_{CD4} because we continue with the central differencing but this time the target is to go to fourth order accuracy. Now we have to do a slightly intelligent guess at this point in choosing the stencil. We go ahead by saying that earlier it was a 3 point stencil. Let us see what happens when we use a 5 point stencil instead, which means, you have i here, i + 1 and i - 1 the stencil that gave you CD2 and then you are now guessing that you need to expand this stencil to another two points included which makes it i – 2 to i + 2 which means 5 point stencil and we are hoping that, that may just turn out to be adequate for a CD4 finite difference calculation.

So if that really works, we should be able to come up with a discretization of this form.

$$f_i' + a_1 f_{i+1} + a_2 f_{i+2} + a_3 f_{i-1} + a_4 f_{i-2} = O(\Delta x^4)$$

So here what do we have? We have now laid it out in the form we used earlier, which is more suitable for the Taylor table approach. So we have the derivative term here, f_i' and then comes all the functional values. And you notice that in your CD2 expression for example, you just had f_{i+1} and f_{i-1} in the formula.

But remember that f_i was missing. So going by the same trend, we have now chosen the functional values at i + 1, i – 1 like before and just added on i + 2 and i - 2, which means we continue to skip f_i. This is usually the trend for first order derivatives on central stencils. It works in general. And then we are hopeful that this kind of a stencil will help us achieve a fourth order accuracy.

Let us set out with this target and see how far we can achieve this. Note that we could have different kinds of nomenclature. Here we are using delta x for example, instead of h which we have been using for some time. You should be developing this habit of using alternative nomenclature because you might find these different nomenclatures being used in literature.

They all mean the same thing. Here, for example, if you want to indicate the spacing, and if you are following this nomenclature, each of these intervals would be indicated as Δx instead of h. There is nothing wrong in continuing with the h nomenclature, but just to keep things more flexible, we are using this different nomenclature here.

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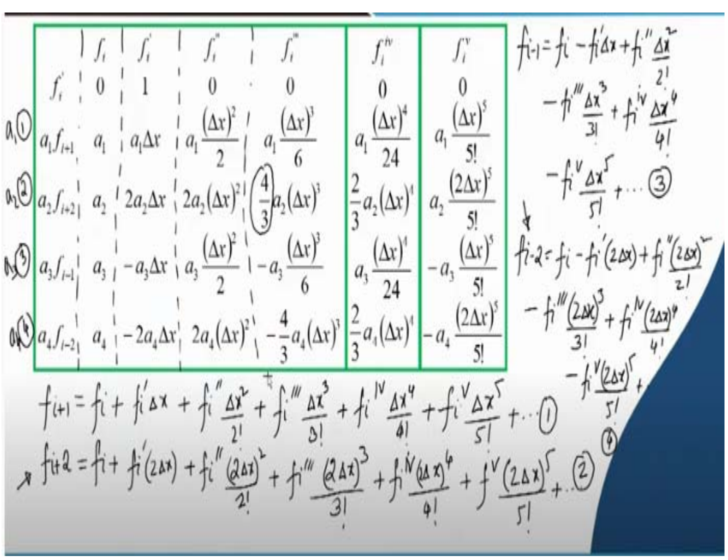

Let us look at the Taylor table that we have as a consequence. We are just trying to recall what we did last time. We would write down the Taylor series. What you can see is that we have written up to the fifth derivative. Let us go ahead and do that so that you can actually see the correspondence with the Taylor table here. We have the Taylor series for f_{i+1}. You could write it for f_{i+2}.

This should be 4. So these are the Taylor series expansions for f_{i+1} and f_{i+2}. Similarly, you can write it for f_{i-1} and then finally f_{i-2}. We have all the Taylor series for the grid points that we have written in the stencil. Now we are going to use all these equations that we wrote down. Let us number them 1, 2, 3, 4.

$$f_{i+1} = f_i + f_i' \, \Delta x + f_i'' \frac{\Delta x^2}{2!} + f_i''' \frac{\Delta x^3}{3!} + f_i^{iv} \frac{\Delta x^4}{4!} + f_i^{v} \frac{\Delta x^5}{5!} + \ldots (1)$$

$$f_{i+2} = f_i + f_i' \left(2\Delta x\right) + f_i'' \frac{\left(2\Delta x\right)^2}{2!} + f_i''' \frac{\left(2\Delta x\right)^3}{3!} + f_i^{iv} \frac{\left(2\Delta x\right)^4}{4!} + f_i^{v} \frac{\left(2\Delta x\right)^5}{5!} + \ldots (2)$$

$$f_{i-1} = f_i - f_i' \, \Delta x + f_i'' \frac{\Delta x^2}{2!} - f_i''' \frac{\Delta x^3}{3!} + f_i^{iv} \frac{\Delta x^4}{4!} - f_i^{v} \frac{\Delta x^5}{5!} + \ldots . (3)$$

$$f_{i-2} = f_i - f_i' \left(2\Delta x\right) + f_i'' \frac{\left(2\Delta x\right)^2}{2!} - f_i''' \frac{\left(2\Delta x\right)^3}{3!} + f_i^{iv} \frac{\left(2\Delta x\right)^4}{4!} - f_i^{v} \frac{\left(2\Delta x\right)^5}{5!} + \ldots . (4)$$

And what you need to do is you need to multiply 1 with a_1.

And then you have to multiply the equation 2 by a_2, the equation 3 by a_3 and equation 4 by a_4 in order to generate the rows in the Taylor table. And then these coefficients would have to be worked out based on the factorial expressions that you have and also for the f_{i+2} and f_{i-2} you have numerals in the numerator also because you have term 2 sitting inside the brackets raised to different powers.

So once you do those little calculations, you should be able to fill up the Taylor table in the manner we have shown here. Now we have purposely boxed the Taylor table in a manner that the larger part of the Taylor table box shows information which should be adequate for you to solve for the 4 unknown coefficients that you have. So we have 4 unknowns; a_1, a_2, a_3, a_4 which need to be solved.

And for doing that, you learned last time that we essentially identify these columns. And we try to sum up the contributions of all these columns. And those are the terms which come in the bracketed terms on the right hand side of the final expression. And then we use those bracketed terms to set them individually equal to 0, so that we are able to finally find out the values of these four unknown coefficients by solving 4 simultaneous algebraic equations.

So that was the procedure we followed last time. So let us try to look at that calculation once more in detail for this problem. It is little laborious, but we will do it nevertheless so that we can actually get a feel of the calculations which are involved. So the equations that we will have coming from those 4 columns of information, let us try to write them down one after the other.

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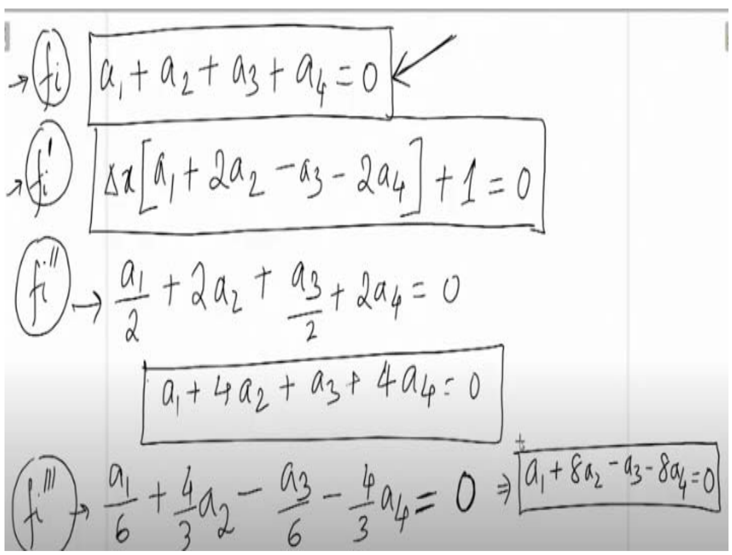

So if you look at the f_i' column, from there you will get an equation which looks like this. What it says essentially is that when you sum these coefficients the unknown coefficients, they should always go to 0. This is very easy to observe for central difference schemes. If you go back to your CD2 scheme for example, you will see that happening very simply.

And in the new scheme that we are trying to work out which hopefully will give us the CD4 scheme, even there you will see that the sum of these coefficients will come out to be 0 in the final formula also because you already have this constraint imposed through one of the equations. So that is essentially coming from the f_i' column. Now if you look at the f_i'' column, the equation that emerges from there looks like this.

This should be single dash, I am sorry. This should be a single dash. Let us write it down once more to avoid confusion and I made a mistake. This should have been from the f_i column not the f_i' column. Please take note of this. So the first equation comes from the f_i column.

$$a_1 + a_2 + a_3 + a_4 = 0$$

The second equation comes from the f_i' column.

$$\Delta x\left[a_1 + 2a_2 - a_3 - 2a_4\right] + 1 = 0$$

The third equation comes from the f_i'' column.

$$a_1 + 4a_2 + a_3 + 4a_4 = 0$$

And that looks like, so let us multiply this equation by 2 so that we can get rid of the fractions. So this becomes like this. Let us box the expressions. This is 1. This is the second one. This is the third one. And then we are looking for a fourth one so that we have 4 simultaneous equations to solve. So the fourth one, which comes from the f_i''' triple dash column looks like.

$$a_1 + 8a_2 - a_3 - 8a_4 = 0$$

Again, just to get rid of fractions, we would prefer to multiply it by 6, this should be equal to zero. So let us multiply this whole equation by 6 so that we can get rid of the fractions. And then you will see that the equation looks like this. So we now have 4 equations, which need to be solved simultaneously.

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$$(2) - (1)\Delta x \Rightarrow \left\{(2a_2 - a_2) + (-a_3 - a_3) + (-2a_4 - a_4)\right\}\Delta x + 1 = 0$$

$$\boxed{\Delta x (a_2 - 2a_3 - 3a_4) = -1} \quad - (5)$$

$$(3) - (1) \Rightarrow (4a_2 - a_2) + (a_3 - a_3) + (4a_4 - a_4) = 0$$

$$\Rightarrow 3a_2 + 3a_4 = 0 \Rightarrow \boxed{a_2 = -a_4} \quad (6)$$

$$(4) - (1) \Rightarrow (8a_2 - a_2) + (-a_3 - a_3) + (-8a_4 - a_4) = 0$$

$$\boxed{7a_2 - 2a_3 - 9a_4 = 0} \quad (7)$$

Now if you do a few simple calculations, you can generate equations in such a manner that you can gradually start eliminating the unknowns and therefore get closer to solving the system. Ideally when you will be doing this for larger stencils there could be larger number of equations to handle and it could be quite tedious to do it manually.

So in such situations it may be a better practice to involve some softwares which can do symbolic calculations for example MATLAB to ease the amount of effort required for generating these equations and solving them. So this equation you can obtain once you do the above calculation. Then if you do another calculation, you subtract equation 1 from equation 3. Then, so it finally gives you a_2 is equal to $-a_4$.

So you have generated one equation here involving a_2, a_3 and a_4. You have generated another condition that a_2 is equal to $-a_4$. And then if you do this calculation, you subtract equation 1 from 4. Then you generate another equation. So essentially what we have done now is we have got rid of one of the variables that is a_1 in these three equations.

So now we have three simultaneous equations in 3 variables a_2, a_3 and a_4. So if we name them, let us name them as say 5, 6 and 7.

$$\Delta x\left(a_2 - 2a_3 - 3a_4\right) = -1...(5)$$

$$a_2 = -a_4 ...(6)$$

$$7a_2 - 2a_3 - 9a_4 = 0...(7)$$

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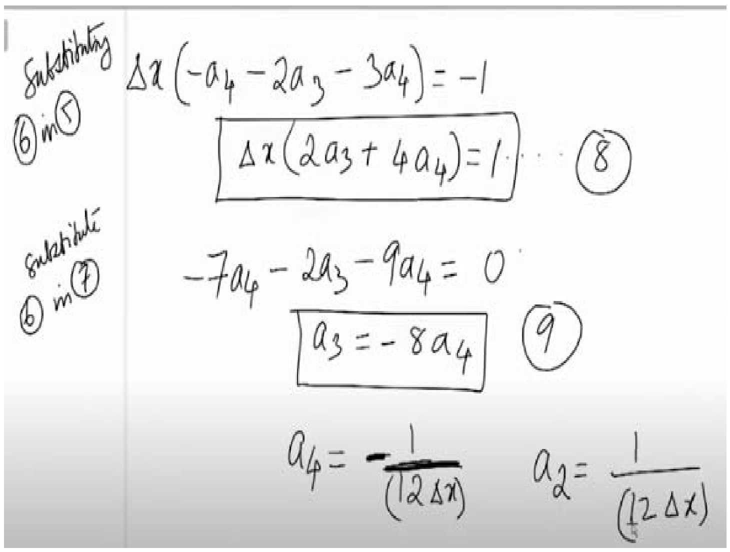

Now you substitute 6 in 5. Let us name this as 8. If you substitute 6 in 7, you have 9. And now you notice that you have reduced the problem to a two variable problem. So one more variable that is a_2 has gone out from the system. And now if you combine 9 and 8, you should be able to come up with a solution that a_4 is equal to – $1/(12\Delta x)$.

That means Δx is in the denominator. So $1/(12\Delta x)$ with a minus sign. And you remember that a_2 is equal to $-a_4$. So a_2 is $1/(12\Delta x)$. And let us try to work out a_3 and a_1.

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$$a_3 = \frac{8}{12\Delta x} = \frac{2}{(3\Delta x)}$$

$$a_1 = -\frac{8}{(12\Delta x)} = \frac{-2}{(3\Delta x)}$$

$$f_i' = \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{(12\Delta x)} + O(?)$$

So a3 can be obtained by substituting the value of a4 in equation 9. Then you will find that a_3 will come out to be $8/(12\Delta x)$ which is $2/(3\Delta x)$ and a_1 which can be obtained by substituting all these values a_2, a_3 and a_4 in equation 1. Then you will find that a_1 will come out to be $-8/(12\Delta x)$, which is $-2/(3\Delta x)$ in the denominator. Now you have solved for all the 4 unknown coefficients.

What do you have finally for the expression of the derivative? If you just substitute those values of the coefficients you will find that the scheme comes out to be like this. However, that does not answer that what is the order of accuracy that we have achieved here.

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	f_i	f_i'	f_i''	f_i'''	f_i^{iv}	f_i^{v}
f_i'	0	1	0	0	0	0
$a_1 f_{i+1}$	a_1	$a_1\Delta x$	$a_1\frac{(\Delta x)^2}{2}$	$a_1\frac{(\Delta x)^3}{6}$	$a_1\frac{(\Delta x)^4}{24}$	$a_1\frac{(\Delta x)^5}{5!}$
$a_2 f_{i+2}$	a_2	$2a_2\Delta x$	$2a_2(\Delta x)^2$	$\frac{4}{3}a_2(\Delta x)^3$	$\frac{2}{3}a_2(\Delta x)^4$	$a_2\frac{(2\Delta x)^5}{5!}$
$a_3 f_{i-1}$	a_3	$-a_3\Delta x$	$a_3\frac{(\Delta x)^2}{2}$	$-a_3\frac{(\Delta x)^3}{6}$	$a_3\frac{(\Delta x)^4}{24}$	$-a_3\frac{(\Delta x)^5}{5!}$
$a_4 f_{i-2}$	a_4	$-2a_4\Delta x$	$2a_4(\Delta x)^2$	$-\frac{4}{3}a_4(\Delta x)^3$	$\frac{2}{3}a_4(\Delta x)^4$	$-a_4\frac{(2\Delta x)^5}{5!}$

For doing that, we go back and try to see where we left our previous calculations in the Taylor table and try to figure out what these additional columns behind the larger box can do that for us so that we can actually work out the order of accuracy of the scheme confidently. We will take note of these two columns, and we will do some more calculations to come to the answer that what is the formal accuracy of this scheme.

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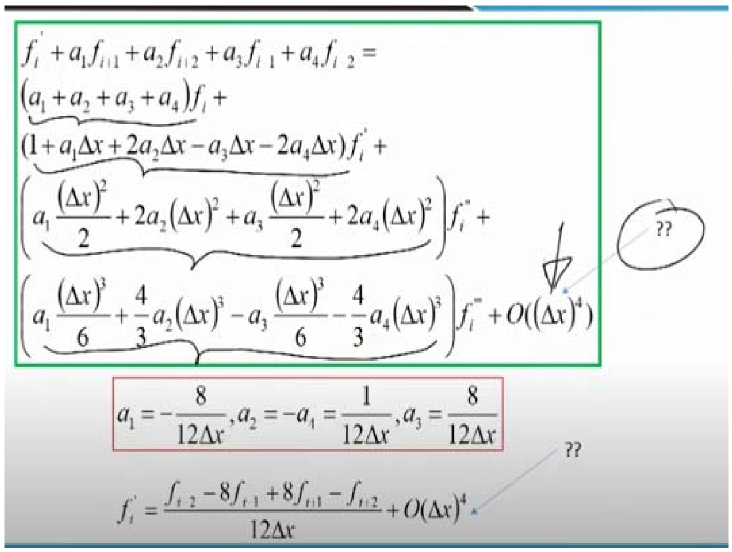

We have it all over here in the slide. You have already set these terms to 0. And you are still tentative whether you have got a fourth order accuracy or not.

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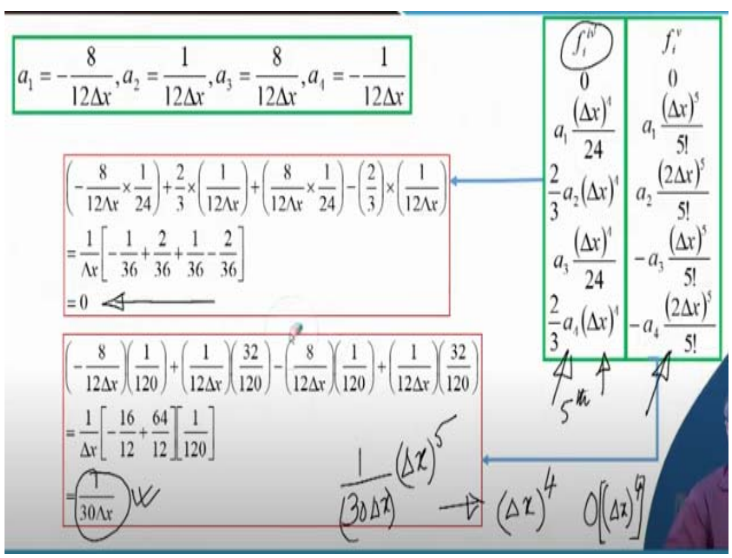

In order to answer that question you have to do some calculation out here. You take note of the 4 coefficients that you have solved for and you substitute it into the first column, which is actually the f_i^{iv} column and then you sum up all these terms in this column which is essentially the fifth column that we are looking at. Incidentally, when you substitute for all these terms, a_1, a_2, a_3, a_4 here, this comes out to be 0.

That means automatically that bracketed term goes to 0 even though you have not explicitly set it to zero. What that means is that the leading error in the truncation error terms is not this, but rather the contributions which comes from the next column, which is the f_i^{v} column. And that column incidentally gives you a nonzero summation.

When you substitute the values of a_1, a_2, a_3, a_4 into those respective expressions, this would give you a nonzero summation. And remember that you have $1/(30\Delta x)$ in the denominator and you have $(\Delta x)^5$ terms in the denominator in each one of those terms in the f_i^{v} column. So that is what is going to actually give you the $(\Delta x)^4$ terms, which means we have actually reached fourth order accuracy, like what we had set out to achieve. With this, we close this lecture. Thank you.