

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

**Lecture - 12**  
**Taylor Table Approach for Constructing Finite Difference Schemes**

In this lecture, we are going to talk about the Taylor table approach for constructing finite difference schemes.

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We are looking for a general technique to construct finite difference schemes

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

*Truncation error*

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

*leading error terms*

- We recall that these formulae were derived from Taylor series
- They are 2<sup>nd</sup> order accurate finite difference schemes for first and second order derivatives respectively


- Any finite difference formula is characterized by the points at which the functional values are used and its **order of accuracy**
- A set of points to be used in a formula is called a **stencil**. It is desirable to construct the formula with the **highest order accuracy** that involves those points.

*backward forward difference 3 point stencil*

$x-h$   
○  
← (-1)

$x$   
○  
← (0)

$x+h$   
○  
← (1)



Let us try to understand what we intend to discuss here to begin the discussion. So we are aiming to find a general technique to construct finite difference schemes. Now what is the necessity for such a general technique? We need to understand the relevance of that to begin with. Before we do all that, we first try to recall some of the things we did when we discussed finite difference method in some previous lectures.

You can see two formulae on the slide, one for the first derivative of a function  $f(x)$  and the other for the second derivative. And these formula as you may recall, were derived from Taylor series.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \left(-\frac{h^2}{6} f'''(x) \dots\right)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \left(-\frac{h^2}{12} f^{iv}(x) \dots\right)$$

So we expanded the function  $f(x)$  about the point  $x$  and we evolved these expressions for the derivatives. Of course, they are approximations, they are finite difference approximations of the first and second derivative.

And incidentally, both of them are second order accurate finite difference schemes representing the first and second derivatives that comes out from the order of these terms, which you have in the truncation error. You may recall that these terms are the leading error terms. If you look a little deeper into these equations, you find that these finite difference formula are dependent on functional values at different points.

So these are different points  $x+h$ ,  $x$ ,  $x-h$  and you are essentially invoking the functional values. That means the value of  $f$  at those different points, they are essentially the grid points. So if you have  $x$  here and  $x+h$  here,  $x-h$  here and so on we assign grid numbering to all these points in a finite difference grid. And therefore, whether in physical space or grid space, they are different points at which the functional values are being invoked.

So we use functional values at different points. And we also look at the order of accuracy of the discretization. So these are the two important things that we look at. Now depending on what points we have chosen, we come up with the so called stencil. That means, if I have these 3 grid points  $i$ ,  $i+1$  and  $i-1$  then I have a stencil which includes these three points. It is a 3 points stencil.

But just specifying 3 points is not enough, because 3 points could comprise of other possibilities also. You may have  $i$ ,  $i-1$  and  $i-2$ , which also is 3 points. But then it is not centered around  $i$ . So you may have centered stencils and non-centered stencils or skewed stencils. Also when we discussed about finite difference last time, we talked about backward and forward differences.

So we said that if you are looking at lower (smaller) indices, then you are talking about backward differencing. If you are looking at forward (larger) indices, you are talking about forward differencing. That means, you may have a forward difference expression looking like this, where you take a difference in functional values between these two points. Whereas, a backward difference expression may actually involve something like this, a difference in functional values between points  $i$  and  $i - 1$ .

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Use of Taylor series to generate a FD scheme of desired accuracy in a given stencil (which could be central or biased, i.e., forward/ backward scheme) **could be tedious, especially for schemes with higher stencil size/ higher accuracy.** Therefore a more convenient framework is desirable.

Therefore we are revisiting the finite difference method to explore a **general technique** to construct finite difference formulae using a given stencil.

The technique should ensure that the highest possible accuracy is achieved with the given stencil.

$f_i + \sum_{k=m}^n a_k f_{i+k} = O(1,2,3..?)$

Handwritten notes: *function terms* (pointing to the summation), *first derivative* (pointing to the O term), *i+k* (pointing to the index k).

What is the highest formal order of accuracy possible on a given stencil of grid points?

The stencil depends on the range of values of the index  $k$ .

Now using Taylor series to generate a finite difference scheme with desired accuracy and in a given stencil, which could be central or biased like what we discussed, sometimes could be quite tedious especially if you have a large stencil. That means, if you have large number of points. Let us say you have a 5 point stencil then you will see that to manipulate the Taylor series in a way that you can finally come to an expression for the derivative becomes increasingly more complex.

However, higher stencil sizes are usually associated with higher accuracy. And therefore, when you look for higher accuracy in approximating the derivatives very often you have to use them. Therefore, you need to have a more convenient and generalized framework where irrespective of stencil size and irrespective of the order of derivative that you want to calculate or approximate you should have a very robust and convenient scheme to work it out.

Now we are actually proposing such a general technique to construct finite difference formula on given stencils. And that is what we try to do when we talk about the

Taylor table. Now before we actually form the Taylor table, we essentially write down the discrete form or rather the semi discrete form if you call it that way of the derivative in this form where you are actually talking about a first derivative approximation.

So this term is the first derivative at the point  $i$  and what you have over here is the summation of terms where the functional values have been invoked from its neighbors. How do you create the numbers? As you can see the index here, it gives you  $i + k$ , where  $k$  varies from  $m$  to  $n$ , which means you can take neighbors. You can account for neighbors in the functional values.

Because these numbers  $m$  to  $n$  will define your neighbors. And then there are coefficients associated with the functional values at those neighbors. And then you sum them up which is visible through the sigma and then you equate it to very small terms which should actually approximate to 0. What are the ones you will see on the right hand side? They are essentially going to be some truncation terms.

And the leading term in that series would of course, give you the order of accuracy of the scheme. So you need to understand that all possible approximations of the first derivative can actually be expressed in a generalized form of this kind. Now the question to ask is that how wide is my stencil here? So that will be answered by those numbers  $m$  and  $n$ .

The second question to ask is that given that stencil, on that stencil what would be the highest order of accuracy that I can achieve? When we talk about order of accuracy in the Taylor series sense, we often use a word formal accuracy. So we are interested in maximizing the formal order of accuracy of the approximation for the given stencil. That is essentially our target.

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**Example problem**

|               |       |         |                        |                        |
|---------------|-------|---------|------------------------|------------------------|
|               | $f_i$ | $f'_i$  | $f''_i$                | $f'''_i$               |
| $f'_i$        | 0     | 1       | 0                      | 0                      |
| $a_0 f_i$     | $a_0$ | 0       | 0                      | 0                      |
| $a_1 f_{i+1}$ | $a_1$ | $a_1 h$ | $a_1 \frac{h^2}{2}$    | $a_1 \frac{h^3}{6}$    |
| $a_2 f_{i+2}$ | $a_2$ | $2ha_2$ | $a_2 \frac{(2h)^2}{2}$ | $a_2 \frac{(2h)^3}{6}$ |

Taylor Table

$f'$

uniform grid

- We would like to construct the **most accurate finite difference scheme** that involves the functional values at points  $i$ ,  $(i+1)$ , and  $(i+2)$ .
- There is a **restriction that has been imposed on the choice of points**. Given these points, we ask for the highest order of accuracy that can be achieved.

Let us take an example problem where we have a stencil comprising of 3 points  $i$ ,  $i+1$  and  $i+2$ . It goes without saying that you are using constant interval between the grid points. That means it is a uniform grid. Obviously, this is not a centered stencil. It is a skewed stencil. And the stencil has been given to us. There is no choice, we have to actually evolve an expression for  $f'$ , that means the first derivative on this given stencil, but we have to ensure that we come up with the highest possible accuracy in the approximation.

Now how do we go about it? For doing that, we of course have to do a few things in terms of the Taylor series expansions. So let us try doing that. We can write down the statement of the problem in this manner.

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$$\underline{f'_i} + a_0 \underline{f_i} + a_1 \underline{f_{i+1}} + a_2 \underline{f_{i+2}} = \underline{O(?)}$$

maximize  
order or  
accuracy

$$f_{i+1} = f_i + hf'_i + \frac{h^2}{2!} f''_i + \frac{h^3}{3!} f'''_i + \dots$$

$$f_{i+2} = f_i + \underline{(2h)} f'_i + \frac{(2h)^2}{2} f''_i + \frac{(2h)^3}{6} f'''_i + \dots$$

That we want to evaluate the problem in this manner.

$$f'_i + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = O(?)$$

That means, we are going to evaluate the first order derivative based on the functional values available at  $i$ ,  $i + 1$  and  $i + 2$ . And we do not know exactly what these weightages are, we have to work them out. And at this point we cannot answer what order of accuracy we will be able to achieve. But the aim is to maximize it.

As we do that, we need to write down the Taylor series expansions. So  $f_{i+1}$  for example would be written as this;  $f_{i+2}$  remember that you have a  $2h$  interval separating the point  $i$  and  $i + 2$ .

$$f_{i+1} = f_i + h f'_i + \frac{h^2}{2!} f''_i + \frac{h^3}{3!} f'''_i + \dots$$

$$f_{i+2} = f_i + (2h) f'_i + \frac{(2h)^2}{2} f''_i + \frac{(2h)^3}{6} f'''_i + \dots$$

And therefore the interval comes up as  $2h$  here.  $2h$  gets squared here.  $2h$  gets cubed here and so on. So this is the way you have Taylor series expansions for  $f_{i+1}$  and  $f_{i+2}$ . Now coming to how we form the Taylor table.

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|               | $f_i$ | $f_i'$     | $f_i''$                | $f_i'''$               |
|---------------|-------|------------|------------------------|------------------------|
| $f_i$         | 0     | 1          | 0                      | 0                      |
| $a_0 f_i$     | $a_0$ | 0          | 0                      | 0                      |
| $a_1 f_{i+1}$ | $a_1$ | $a_1 h$    | $a_1 \frac{h^2}{2}$    | $a_1 \frac{h^3}{6}$    |
| $a_2 f_{i+2}$ | $a_2$ | $a_2 (2h)$ | $a_2 \frac{(2h)^2}{2}$ | $a_2 \frac{(2h)^3}{6}$ |

$a_1 f_{i+1} = a_1 f_i + a_1 h f_i' + a_1 \frac{h^2}{2} f_i'' + a_1 \frac{h^3}{6} f_i'''$

$a_2 f_{i+2} = a_2 f_i + a_2 (2h) f_i' + a_2 \frac{(2h)^2}{2} f_i'' + a_2 \frac{(2h)^3}{6} f_i'''$

1st 2nd 3rd 4th  
 $a_2 f_{i+2} = (a_2) f_i + (a_2 (2h)) f_i' + (a_2 \frac{(2h)^2}{2}) f_i'' + (a_2 \frac{(2h)^3}{6}) f_i'''$

Let us see, how we draw the table. Remember that the table will contain no different information other than what the Taylor series have generated for you. Only thing is we will lay this information in such a manner that it conveniently suits our objective. So let us see what are the things we put in the table. We put the function and its different derivatives in increasing order in the first row, leaving this corner blank.

Here, we put the different terms that we saw on the left hand side of the discrete equations. Sorry, there should be no dash here. It is just the functional value. So let us erase that off to prevent any confusion. So we have  $a_0 f_i$ . And then you have  $a_1 f_{i+1}$ . And you have  $a_2 f_{i+2}$ . Let us see how we fill these boxes. This is  $a_1 h^3/6$ . So let us try to understand what we did.

For that it would be a good idea to write down the expression for  $a_1 f_{i+1}$  for example. So we will quickly write down the Taylor series once again over here. Now a little quicker because we can then map the terms coming from this Taylor series in the table. So let us go row by row.  $f_i'$  has an entry equal to 1 in the column of  $f_i'$  here. And it has 0 entries in other columns.

$a_0 f_i$  has an entry in the column of  $f_i$  and it has 0 entries in the others. Which means that in the expression whatever terms are coming are essentially coming from these numbers multiplied with the column titles, alright. So  $f_i'$  comes from a  $f_i'$  here

multiplied by 1 here.  $a_0 f_i$  comes from  $a_0$  here multiplied by  $f_i$  here and so on. So that should give you a clue as to how these entries have come.

Because now you actually can see that the first term here maps with this one because this term has to be essentially multiplied with the column head to give you this term. Similarly, this term  $a_1 h$  has to be multiplied with a  $f_i'$  and that is the second term in the Taylor series and so on. So likewise you can compare this term and this term which figure here and here respectively.

That means, all the terms that you have through  $a_1 f_{i+1}$  are actually coming in these four boxes provided that you multiply them with the column heads. Let us try to again repeat it for the last row here. So for that, we recall that  $a_2 f_{i+2}$  will be, this is triple dash and so on. Now you can easily map this  $a_2$  is here, and that needs to be multiplied with  $f_i$ . This  $a_2$  into  $2h$  is here.

This term is here and the last one is here. So we could map all of them. Now we will actually sum up the respective columns. This is the first column, this is the second column, third and fourth. If we sum all the columns, we would essentially have accounted for all the terms that we had generated through the Taylor series expansions.

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Example problem

|               |       |         |                        |                        |
|---------------|-------|---------|------------------------|------------------------|
|               | $f_i$ | $f_i'$  | $f_i''$                | $f_i'''$               |
| $f_i$         | 0     | 1       | 0                      | 0                      |
| $a_0 f_i$     | $a_0$ | 0       | 0                      | 0                      |
| $a_1 f_{i+1}$ | $a_1$ | $a_1 h$ | $a_1 \frac{h^2}{2}$    | $a_1 \frac{h^3}{6}$    |
| $a_2 f_{i+2}$ | $a_2$ | $2ha_2$ | $a_2 \frac{(2h)^2}{2}$ | $a_2 \frac{(2h)^3}{6}$ |

Taylor Table

1   2   3   4

- We would like to construct the **most accurate finite difference scheme** that involves the functional values at points  $i$ ,  $(i+1)$ , and  $(i+2)$ .
- There is a **restriction that has been imposed on the choice of points**. Given these points, we ask for the highest order of accuracy that can be achieved.



So if we put it that way, we can now see that through this Taylor table that we have formed if we sum up all these entries in the four columns, we can actually write down an equation which looks like this.

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = (a_0 + a_1 + a_2) f_i + (1 + a_1 h + 2h a_2) f_i'' + \left( a_1 \frac{h^2}{2} + a_2 \frac{(2h)^2}{2} \right) f_i''' + \left( a_1 \frac{h^3}{6} + a_2 \frac{(2h)^3}{6} \right) f_i^{(4)} + \dots$$

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The slide displays a Taylor table with the following structure:

|               | $f$   | $f'$     | $f''$                  | $f'''$                 |
|---------------|-------|----------|------------------------|------------------------|
| $f$           | 0     | 1        | 0                      | 0                      |
| $a_0 f$       | $a_0$ | 0        | 0                      | 0                      |
| $a_1 f_{i+1}$ | $a_1$ | $a_1 h$  | $a_1 \frac{h^2}{2}$    | $a_1 \frac{h^3}{6}$    |
| $a_2 f_{i+2}$ | $a_2$ | $2h a_2$ | $a_2 \frac{(2h)^2}{2}$ | $a_2 \frac{(2h)^3}{6}$ |

Below the table, the summation equation is shown with arrows indicating the source of each term:

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = (a_0 + a_1 + a_2) f_i + (1 + a_1 h + 2h a_2) f_i'' + \left( a_1 \frac{h^2}{2} + a_2 \frac{(2h)^2}{2} \right) f_i''' + \left( a_1 \frac{h^3}{6} + a_2 \frac{(2h)^3}{6} \right) f_i^{(4)} + \dots$$

Text on the slide:

- The left-hand side of the above equation is the sum of the elements in the first column of the Taylor Table.
- The right-hand side of the equation will comprise of the sum of the respective columns of the Taylor table from the second to the fourth columns.
- In this manner we ensure inclusion of all the terms of the Taylor series arranged in the form of a summation where each term comprises of a coefficient and a derivative. First term would involve zeroth order derivative, which is the function itself.

More terms from Taylor series to include higher derivatives of  $f$ . However, that would lead to more number of unknown constants.

So these are the summation of the columns essentially. How do you do? See that, just go back to the Taylor table, it is here. And you can see that all these terms have been summed  $a_0 + a_1$  into  $a_1 + a_2$  and multiplied with the column head here, that is  $f_i$  and then summed up with all the entries in this column multiplied by a  $f_i'$ , which gives you this. This should be a single derivative.

Then comes the terms in the third column, which figure over here multiplied by  $f_i''$ , which figures at the column head. And then the last column here, which gives you these terms multiplied by and you could have more and more of them. So more terms from the Taylor series to include the higher order derivatives could be put in here. But that would mean that there will be more number of unknown constants to solve.

And you need to check whether you can have enough number of equations to do that. Now the point is that you would like as many terms as possible on the right hand side of this equation to go to 0. What is the motivation behind it? The motivation behind it is that if you watch carefully, then the first bracket term contains h terms with zeroeth order because you do not have any h terms at all over there.

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$$f_i' + \sum_{k=0}^2 a_k f_{i+k} = O(?)$$

- The left-hand side of the above equation is the sum of the elements in the first column of the Taylor Table.
- The right-hand side of the equation will comprise of the sum of the respective columns of the Taylor table from the second to the fourth columns.
- In this manner we ensure inclusion of all the terms of the Taylor series arranged in the form of a summation where each term comprises of a coefficient and a derivative. First term would involve zeroth order derivative, which is the function itself.

$$f_i' + a_0 f_i + a_1 f_{i+1} + a_2 f_{i+2} = (a_0 + a_1 + a_2) f_i + (1 + a_1 h + 2h a_2) f_i' + \left( a_1 \frac{h^2}{2} + a_2 \frac{(2h)^2}{2} \right) f_i'' + \left( a_1 \frac{h^3}{6} + a_2 \frac{(2h)^3}{6} \right) f_i''' + \dots$$

More terms from Taylor series to include higher derivatives of  $f$ . However, that would lead to more number of unknown constants.

The second set of terms are h to the power of 1 terms. The third bracket terms are h squared terms. Fourth bracket ones are h cube terms and so on. So this is the kind of thing you saw in the Taylor series truncation error term. So you were looking at leading error term and you were trying to figure out what is the order of accuracy of the scheme. That is how we did last time.

This time the aim would be to have as many of those bracketed terms set to 0 as possible so that we can maximize the order of accuracy of the scheme. Now how many of them can we actually set to 0? That will be answered by the question that how many unknowns do we have on the left hand side of the equation. So we have three unknowns, three unknown coefficients;  $a_0$ ,  $a_1$  and  $a_2$ .

So we can have precisely three set of bracketed terms set to 0 on the right hand side of the equation, which would hopefully yield three independent linear algebraic equations, which can then be simultaneously solved to obtain the values of  $a_0$ ,  $a_1$  and  $a_2$ , which will set all three bracketed terms to 0 and also give you the highest possible

order of accuracy for this stencil. So let us go ahead and do that problem of setting these bracketed terms to zero.

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$a_0 + a_1 + a_2 = 0$   
 $a_1 h + 2h a_2 = -1$   
 $a_1 \frac{h^2}{2} + 2a_2 h^2 = 0$

To get the highest accuracy, we must set as many of the low-order terms to zero as possible. We have three free coefficients. Hence we can set the coefficients of the first three terms to zero.

$a_0 = \frac{3}{2h}, a_1 = -\frac{2}{h}, a_2 = \frac{1}{2h}$

Solution of the simultaneous linear equations

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

Second order accurate FD scheme

If you look at the equations carefully, they are going to yield these three conditions, alright? So we have essentially set the first three bracketed terms to 0 by doing that. And they have yielded three linear algebraic equations in the three unknowns  $a_0$ ,  $a_1$  and  $a_2$ . If you solve them simultaneously these will be the values for  $a_0$ ,  $a_1$  and  $a_2$ .

$$a_0 = \frac{3}{2h}, a_1 = -\frac{2}{h}, a_2 = \frac{1}{2h}$$

And therefore, you will now have a finite difference formula for the first order derivative for the given stencil of points  $i$ ,  $i + 1$  and  $i + 2$ , ensuring that you have achieved the highest formal order of accuracy in the process. That equation happens to be this.

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

So interestingly, because it is a skewed stencil, you can see that these coefficients do not have symmetry. So you have a - 3 here, you have a - 1 here and 4 at the center.

If it was a centered stencil, you would have seen symmetry in these coefficients. We will do more of these exercises later. So this was the first example we solved using

the Taylor table approach. In the subsequent lectures, we will solve more of such problems. And we will try to understand how the Taylor table approach may be extended to higher order derivatives and both to centered as well as non-centered stencils. Thank you.