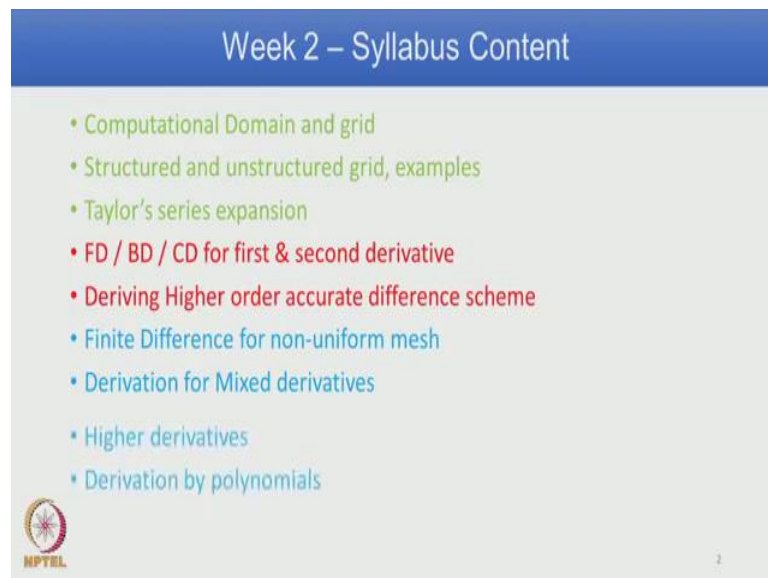


Foundation of Computational Fluid Dynamics
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Lecture - 08

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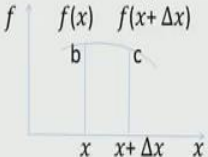


Welcome you all again to this course on CFD. We are now onto module three of week two. So far, we have done definition of computational domain, structured grid and unstructured grid, and how to obtain difference formula from Taylor's series expansion. In today's class, we will take this to the next level of obtaining finite difference scheme for first as well as second derivative, and then how to obtain higher order accurate scheme again by all three methods for the both first as well as second derivative. After that we will move to the remaining syllabus content in the subsequent modules.

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Finite Difference Formulations - FD & BD


- Slope of the function at 'b' using values at 'b' and 'c':



- First order forward difference of $O(\Delta x)$ is given by:

$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{f(i+1) - f(i)}{\Delta x} \quad \text{As } \Delta x \text{ is reduced, error is reduced}$$

- Similarly for backward difference we have,


$$\left. \frac{\partial f}{\partial x} \right|_i = \frac{f(i) - f(i-1)}{\Delta x}$$

So, towards end of last class, we have derived forward difference scheme from Taylor's series expansion and by using i notation form, we wrote expression for first derivative as $\frac{df}{dx} \Big|_i = \frac{f(i+1) - f(i)}{\Delta x}$. And graphically it is shown here; f on y -axis, x on x -axis, and $\frac{df}{dx}$ is evaluated at point b ; for the function that is represented here. And we also wrote down the final formula for the same first derivative by using backward difference scheme and that is shown here as $\frac{df}{dx} \Big|_i = \frac{f(i) - f(i-1)}{\Delta x}$. We also noticed that this is the order of Δx , which is a leading term that we have not consider. It also to be noted the derivative error associated with the derivative gets reduce as the Δx is reduced. Now, in today's class, we will see detail steps on how to obtain this backward difference scheme formula.

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Finite Difference Formulations


- Taylor series expansion of function $f(x)$ in backward direction:

$$f(x - \Delta x) = f(x) - \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) - \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots$$

or

$$= f(x) + \sum_{n=1}^{\infty} \frac{(-\Delta x)^n}{n!} \left(\frac{\partial^n f}{\partial x^n} \right)$$

First derivative by backward difference formula,

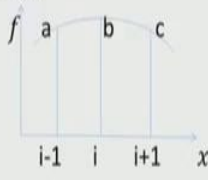

$$\frac{\partial f}{\partial x} \Big|_i = \frac{f(i) - f(i-1)}{\Delta x}$$


So, as we did for difference scheme, we write down Taylor series expansion for the function f of x in backward direction as f of x minus Δx equal to f of x minus Δx into $\frac{\partial f}{\partial x}$ plus all other higher order terms. And you have to notice that this is alternate sign with Δx first term, then third term and so on. As we did in the case of forward difference scheme, one can also write the entire expression in this format with summation sign going from n is equal to one to infinity and minus Δx to the power of n by n factorial and all other higher order terms. So, we are interested only in the first derivative, so we take only the term $\frac{\partial f}{\partial x}$ and remaining terms are not consider. And so this Δx is taken to the other side then we are able to write in i form $\frac{\partial f}{\partial x}$ evaluated at i has f of i minus f of i minus one by Δx , and this also of the order Δx .

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Finite Difference Formulations - CD

• Central difference:


$$f(x + \Delta x) = f(x) + \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 3$$
$$f(x - \Delta x) = f(x) - \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) - \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 4$$


So, in the next is we had forward differences scheme, backward differences scheme, there is also what is known as a central differences scheme. So, in forward differences scheme, we had expression for example, for $\frac{df}{dx}$ at b is related to values of the function at b and c . And in the case of backward differences scheme, it is related to value of the function at b and a . Now, in central difference scheme, it is related between a and c . Now, we will see the steps. So, we again write down expression for Taylor series expansion f of $x + \Delta x$ like this, and f of $x - \Delta x$ as shown here in equation four, and these two are familiar. Now, we have to do again a small arithmetic operation, and we observed here $\frac{df}{dx}$, another $\frac{df}{dx}$ from equation three and four respectively.

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Finite Difference Formulations - CD

$$f(x + \Delta x) = f(x) + \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 3$$


$$f(x - \Delta x) = f(x) - \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) - \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 4$$

Subtracting Eq.4 from Eq.3 we get,

$$f(x + \Delta x) - f(x - \Delta x) = 2\Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{2\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots$$

- Solving for $\left(\frac{\partial f}{\partial x} \right)$, we get :

$$\left(\frac{\partial f}{\partial x} \right) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + O(\Delta x)^2$$



$$\text{Or } \left(\frac{\partial f}{\partial x} \right) = \frac{f(i+1) - f(i-1)}{2\Delta x} + O(\Delta x)^2$$

So, if you subtract equation four from equation three, so this is equation four, which is the backward expansion formula. And this is expansion in the forward direction. So, if you subtract equation four from equation three, you can get f of x plus Δx minus f of x minus Δx , the first term get canceled, second term, it becomes positive, so two times Δx $\text{d}f$ by $\text{d}x$ plus all other higher order terms. Again we are only interested in the first derivative here, so we retain the first derivative and take remaining terms to the other side. So, if you write down $\text{d}f$ by $\text{d}x$ f of x plus Δx minus f of x minus Δx by two Δx , and here it is Δx to the power of three, and this Δx here when it is divided here, the power gets reduced by one, so it is of order Δx square. In i form, it is written here $\text{d}f$ by $\text{d}x$ equal to f of i plus one minus f of i minus one by two Δx and order of Δx square.

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Forward Difference for higher derivative

- Forward difference for second derivative:

$$f(x+2\Delta x) = f(x) + (2\Delta x) \left(\frac{\partial f}{\partial x}\right) + \frac{(2\Delta x)^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{(2\Delta x)^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad \dots 5$$

$$f(x+\Delta x) = f(x) + \Delta x \left(\frac{\partial f}{\partial x}\right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad \dots 6$$

Subtracting Eq. 5 from two times Eq. 6 we get,

$$f(x+2\Delta x) - 2f(x+\Delta x) = -f(x) + \frac{2\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{6\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots$$


Now, we will also see how to write down difference formula for higher derivative. We had seen so far f of x plus Δx ; now we can also do the expansion for any length of Δx . So, what is shown here is for two Δx , so f of x plus two Δx , the formula is almost same except that Δx is now replaced with two Δx . So, if you subtract equation five from equation six, because we are interested in the second derivative $\text{d}^2 f$ by $\text{d}^2 x$. And we need to have other terms cancelled. So, we do operation subtracting equation five from two times equation six, so we get f of x plus two Δx minus two times f of x plus Δx , then some of the term will get cancelled. Now, you see here only the second derivative term that is $\text{d}^2 f$ by $\text{d}^2 x$. We are again interested only in the second derivative, so we retain that on side and bring all other terms to the other side. Again, we have written here up to the next term only all other terms are not written here. So, if you bring Δx square from one side to the other side, this Δx cube will get reduced to only Δx .

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Forward / Backward Difference for higher derivative

- Solving for $\left(\frac{\partial^2 f}{\partial x^2}\right)$, we get :

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(x+2\Delta x) - 2f(x+\Delta x) + f(x)}{\Delta x^2} + O(\Delta x)$$

Or $\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(i+2) - 2f(i+1) + f(i)}{\Delta x^2} + O(\Delta x)$

- Similarly for Backward difference, we get:

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(i) - 2f(i-1) + f(i-2)}{\Delta x^2} + O(\Delta x)$$


If you do that way then we get f of x plus two delta x minus two f of x plus delta x plus f of x by del x square and of order delta x for the second derivative dou square f dou x square. And in i form, it is written here, f of i plus two minus two f of i plus one plus f of i by del x square and again of order delta x . Now, this is getting the second derivative in the forward direction that is i plus two and i plus one function values are these two locations are used. Just like we did for forward differencing, in the case of first derivative here also we have expression evaluated based on function values in i plus two on i plus one. Similarly, you can also get expression in backward difference form following the same procedure, and what is shown here is the final form which is f of i minus two f of i minus one plus f of i minus two by del x square for the same second derivative, again with the order delta x .

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Central Difference for higher derivative


$$f(x + \Delta x) = f(x) + \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 3$$

$$f(x - \Delta x) = f(x) - \Delta x \left(\frac{\partial f}{\partial x} \right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2} \right) - \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3} \right) + \dots \quad \dots 4$$

- For central difference, adding Eq. 3 and Eq. 4 we get:

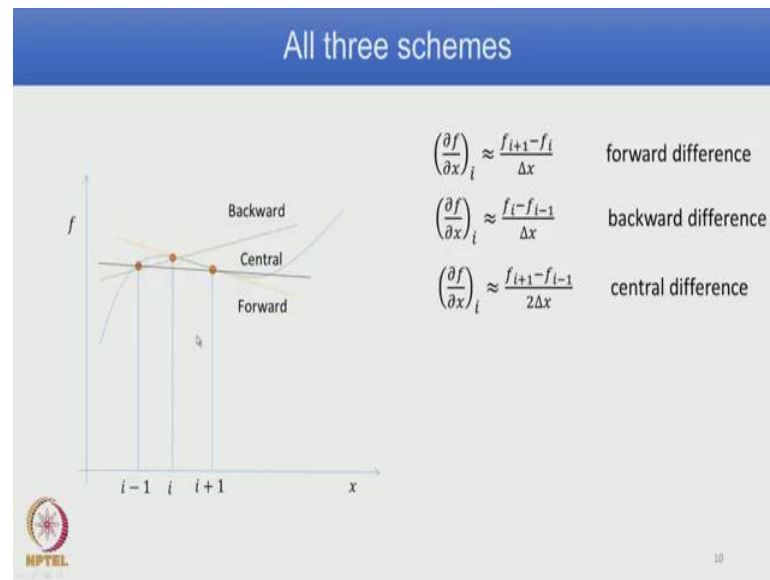
$$\left(\frac{\partial^2 f}{\partial x^2} \right) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + O(\Delta x)^2$$

Or

$$\left(\frac{\partial^2 f}{\partial x^2} \right) = \frac{f(i+1) - 2f(i) + f(i-1)}{\Delta x^2} + O(\Delta x)^2$$


You can also obtain central difference scheme for the same second derivative, so again we write down Taylor series expansion in forward direction as well as in backward direction, and we do the arithmetic operation at equation three and equation four. So, we get $f(x + \Delta x)$ and here $f(x)$ here two times, and we want only the second derivative, so after doing this operation then we get $\frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + O(\Delta x)^2$. So, you can observe the function value at that point of interest, and function value on either side, so which is $x + \Delta x$ on the forward direction and $x - \Delta x$ on the backward direction these values are used, so it is called central difference scheme and this evaluated for second derivative. And you can also write in i form that is what is given here as $\frac{f(i+1) - 2f(i) + f(i-1)}{\Delta x^2} + O(\Delta x)^2$ of order Δx square.

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So, if you put all the three terms together in graphical form to get an idea of how these are evaluated, so what is shown here is function on the y-axis that is f ; and on the x-axis, you have x mark; i is point of interest, i plus one and i minus one are immediate neighbor on the right side and left side. And you see a curve here that is actually the function and you are evaluating slope of the function, so when you say derivative, when you say first derivative, you are actually evaluating slope of the function, so $\frac{df}{dx}$ is evaluated at the point of interest at i . So, by following forward difference formula, which is written here again $f_{i+1} - f_i$ by Δx , it is evaluated the first derivative slope is evaluated by considering function values at i and i plus one. For backward differencing, it is evaluated using the functions values at i and i minus one; and for central difference scheme, it is evaluated using function values at i plus one and i minus one.

So, you see here the function curve actually is this way, and you are evaluating slope by three different methods, and for each method there is an error associated, it is not always perfect. And we can also observed as you decrease the Δx that is the distance between two subsequent grid points, in this case, it is i and i plus one or i and i minus one, one can get a slightly error reduced value for the same slope.

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Higher order FD

- By considering additional terms in the Taylor series expansion, accurate approximations can be made

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x+\Delta x) - f(x)}{\Delta x} - \frac{\Delta x}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) - \dots$$

- Substituting a forward difference approximation for $\left(\frac{\partial^2 f}{\partial x^2}\right)$, i.e.

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(x+2\Delta x) - 2f(x+\Delta x) + f(x)}{\Delta x^2} + O(\Delta x)$$

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Now, we also have higher order FD, in the sense we have seen first derivative evaluated by Taylor series formula with order of accuracy of Δx . We observed that you can reduce the error by reducing the grid spacing, but that is not always possible, we have a limitation in having number of grid points or other practical difficulties to have a finer grid. So, is there a way to get higher order without increasing the mesh size, it is possible by considering additional terms in the Taylor series expansion and that is what we are going to see that is known as getting higher order finite differences scheme again for any derivative, first derivative, second derivative or any other derivative. So, in this case, we write down here the first derivative formula $\frac{df}{dx}$ by forward difference method, so $f(x + \Delta x) - f(x)$ by Δx and remaining term.

And you can observe that $\frac{d^2 f}{dx^2}$ is an immediate term, previously we did not consider, now we know that we also got expression for the second derivative again by all the three schemes that is forward difference, backward difference and central differences scheme. So, if we can replace this second derivative appropriately, then follow some simplification, we will be able to get higher order finite differences scheme for the same first derivative and we are going to see that. So, in the case of first time when we did, we considered only the two terms, now to get the higher order we will consider one more term. So, you have substitute, because we are interested here forward difference, so you substitute for the second derivative in terms of forward difference and that we already obtained the previous steps that is given here once again, which is given

as $f(x + 2\Delta x) - 2f(x + \Delta x) + f(x)$ by Δx^2 of order Δx .


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Higher order FD

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x + \Delta x) - f(x)}{\Delta x} - \frac{\Delta x^1}{2!} \left[\frac{f(x + 2\Delta x) - 2f(x + \Delta x) + f(x)}{\Delta x^2} \right] - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) - \dots$$

- Forward difference approximation for $\left(\frac{\partial f}{\partial x}\right)$, i.e.

$$\left(\frac{\partial f}{\partial x}\right) = \frac{-f(x + 2\Delta x) + 4f(x + \Delta x) - 3f(x)}{2\Delta x} + O(\Delta x)^2$$

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x + \Delta x) - f(x)}{\Delta x} + O(\Delta x)$$


So, if you substitute this expression for the second derivative in this equation, and then simplify you just try to account for all the terms together reorganize then one can get forward difference approximation for the first derivative and that is shown here, $\frac{d}{dx} f$ by $\frac{d}{dx} x$ as $\frac{-f(x + 2\Delta x) + 4f(x + \Delta x) - 3f(x)}{2\Delta x}$. And here, the leading term that we have not considered is here. After dividing Δx , you find this is Δx square; the term that is not considered becomes order so order of Δx square. And if you compare what expression we got the first step that is considering only the first term so that we have $\frac{f(x + \Delta x) - f(x)}{\Delta x}$ and that is of order Δx for the same first derivative.

So, if you observe these two expressions very closely, here we consider immediate neighbor that is $x + \Delta x$ and the higher order expression we consider immediate neighbor $x + \Delta x$ and one more immediate neighbor, which is $x + 2\Delta x$. So, you can get idea that by considering more number of nodal points function values at more number of nodal points, you are able to increase the order of accuracy; and in this case, as you can observe of order Δx to of order Δx square. Once again, this is not a permanent solution or a solution for all situations that is you can get higher accuracy by considering more nodal points. There is always a limitation when it comes

to applying, for example, if you are in a computational domain, if you are on the right side of the boundary then you have a very very limited choice of considering more points beyond the boundary limit. To consider a forward difference scheme to get a derivative by forward differences scheme, so you are limited by number of grids points available beyond boundary location. So, either it is forward or backward, there is always a limitation.

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Higher order FD

- For backward difference

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x) - f(x - \Delta x)}{\Delta x} + \frac{\Delta x^1}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots$$
- Substituting a backward difference approximation for $\left(\frac{\partial^2 f}{\partial x^2}\right)$, i.e.

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(x - 2\Delta x) - 2f(x - \Delta x) + f(x)}{\Delta x^2} + O(\Delta x)$$
 in the above eq., we get:

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x) - f(x - \Delta x)}{\Delta x} + \frac{\Delta x^1}{2!} \left[\frac{f(x - 2\Delta x) - 2f(x - \Delta x) + f(x)}{\Delta x^2} \right] - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots$$



So, just like we obtain higher order finite differences scheme by forward difference procedure, we can also obtain higher order finite difference scheme by backward difference procedure. So, what is shown here is backward differencing formula for the first derivative, which was already obtained, and we follow the same procedure that is the second derivative that is the next term that we have to consider; replace that second derivative term by backward differencing formula that we also be obtained and that is shown here as f of x minus two delta x minus two f x minus delta x plus f of x by del x square and this of order by independently these are order delta x . Now, we replace the second derivative term by this backward differencing formula for that term. And again properly reorganize with the corresponding term and we end up getting backward differencing formula, higher order finite difference scheme for the first derivative $\text{dou } f$ by $\text{dou } x$, and you can again observe that this is rearranged.


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Higher order FD

Backward difference approximation we get,

$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x-2\Delta x) - 4f(x-\Delta x) + 3f(x)}{2\Delta x} + O(\Delta x)^2$$

- Compare BD formula obtained with lesser points


$$\left(\frac{\partial f}{\partial x}\right) = \frac{f(x) - f(x-\Delta x)}{\Delta x} + O(\Delta x)$$
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And we get finally, a formula like this, and as we observed in the case of forward difference scheme f of x minus Δx is an immediate neighbor point in the backward direction, and x minus two Δx is one more additional point in the backward direction. Now, if you compare this formula with lesser accuracy that is first order accurate then you get formula here, so only two points are considered, and we have an additional point considered and that results in a slightly next order that is order second order accuracy. So, as I mentioned in the forward difference scheme, it is not always possible to implement though it appears a solution to get a higher order accuracy. So, earlier we have seen by decreasing Δx , you can slightly get a higher accurate approximation, alternatively as shown here by considering more points, you can get a higher order approximation for the same first derivative.

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Higher order FD

- Similarly for $\left(\frac{\partial^2 f}{\partial x^2}\right)$ by central differencing

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{-f(x-2\Delta x) + 16f(x-\Delta x) - 30f(x) + 16f(x+\Delta x) - f(x+2\Delta x)}{12\Delta x^2} + O(\Delta x)^4$$
$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} + O(\Delta x)^2$$
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Now, the last few slides, we have seen how to obtain higher order finite difference scheme by both forward differencing as well as backward differencing for the first derivative. We will now extend this procedure to get higher order finite differences scheme for the second derivative, for example, by central differencing procedure. What is shown here is the final obtained formula; and as you can observe here this is of order four, and if you compare this with the original expression that we obtained by second order accurate scheme, you observe that second order accurate scheme has point of interest and one node on the left, and one node on the right. To get fourth order accurate scheme, we have in addition two more nodes; one more extra on the left, and one more extra on the right. So, by considering additional points, one is able to obtain higher order, it is also possible to do similar exercise for higher derivative schemes. Now, with this, we come to end of this class, we will take another interesting part in the next class.

Thank you.