Computational Fluid Dynamics
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Lecture - 12
Finite Difference Approximation of Second Order Derivatives

Welcome back to module 3 on finite difference method. We already finished our description of basic methodology for finite differences and in the last lecture we covered finite difference approximation of first order derivative. Today, we would focus on the finite difference approximation of second order derivatives.

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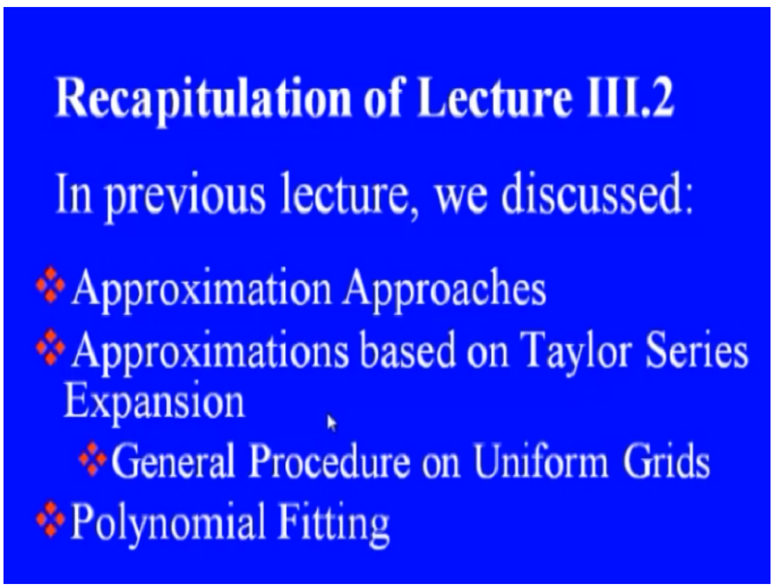

Now let us have a recapitulation of what we did in previous lecture. We discussed different approximation approaches for finite differences, then we obtained finite difference approximations for first order derivative based on Taylor series expansion and we also discussed a simplified general procedure on uniform grids based on Taylor series expansion and then we discussed a method based on polynomial fitting.

Now these methods were used to obtain finite difference approximation of first order derivatives. In today's lecture, which is third lecture in the series on finite differences. We will discuss finite difference approximation of second order derivatives. So let us have a look at outline of today's lecture.

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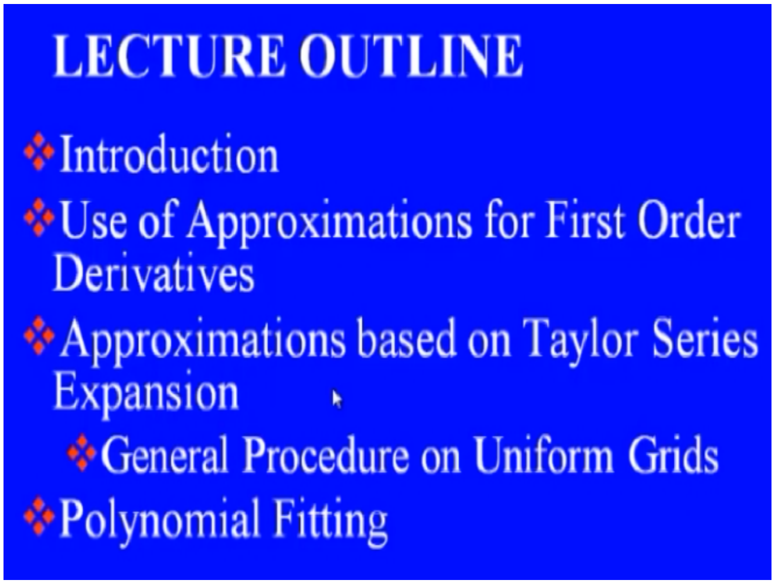

We will have brief introduction about the second order derivatives, do we need to have an approximation for them and then we will have a look at different approaches to obtain the approximation of second order derivatives. For instance, use of approximations, which we derived for first order derivatives. We can obtain ab initio approximation for second order derivatives based on Taylor series expansion.

So we will see similar procedure, which we have adopted in the case of first order derivatives, including a general procedure on uniform grids. We will take plentiful examples to explain the derivation process, so that you can independently obtain similar derivatives of other orders as well. Then, we will also have a look at the polynomial fitting approach in context of second order derivatives. Now let us come back to second order derivatives.

Why do we need an approximation for second order derivatives. The preamble were derivations of the governing equations whether we had dealt with energy equation or scalar transferred equation.

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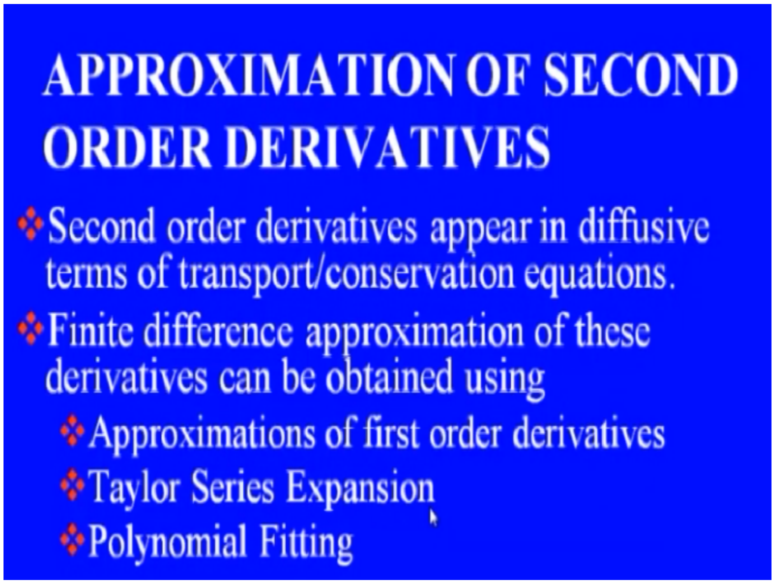

We had second order derivatives, which appear in diffusive terms. So that is why if you want to solve our fluid flow problems using finite differences, we must obtain approximations for second order derivatives and we can obtain finite difference approximation of the second order derivatives using approximations, which we have derived earlier for first order derivatives. We can use Taylor series expansion or polynomial fitting.

We can also use Pade approximants and explain fittings and so on, but we are going to focus today on all of these three that its use of approximation of first order derivatives, Taylor series expansion based approach and polynomial fitting approach. So now let us see what allows us to use approximation of first order derivative. So for that, let us have a brief look at the definition of second order derivative, how do you define it.

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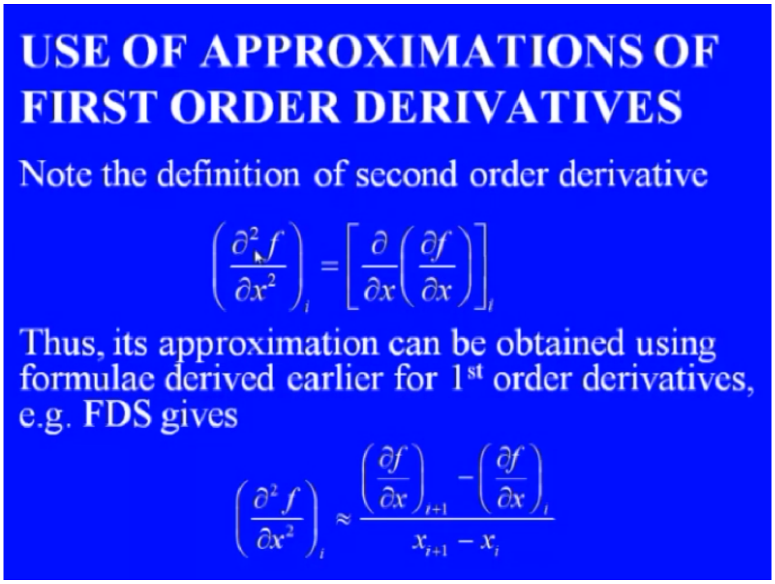

Del 2 f/del x square at i is a second order derivative of function of f with respect to x. This is basically derivative with respect to x that is del/del x of the first order derivative that is del f/del x. So we have already got the formula of how do we approximate this del/del x is first order derivative using finite differences. So our new function becomes the right hand side can be sort of del/del x of gx, where g is del f/del x.

And now we can use the first order derivative expressions, which we derived in the previous lecture to obtain a finite difference approximation of this del g/del x. This one simple example has like say we want to find out finite difference approximation of del 2f/del x square I, we can use simple forward difference scheme. So del f/del x at i+1. Now you can think of del f/del x at gx. So g at i+1 - g at i/xi+1 – xi. We have got plenty of choices.

We had forward difference scheme. We had backward difference scheme. We had central difference scheme. Any of those schemes can be used on this right hand side and similarly for these 2 derivatives, which appear in numerator, we can choose separate approximations. This could be back differences or central difference approximations.

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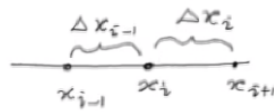
Approximations of 2nd Order Derivatives using formulae derived for FD approximation of 1st Order Derivative

FDS

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \left[\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)\right]_i$$

$$\approx \left[\frac{\left(\frac{\partial f}{\partial x}\right)_{i+1} - \left(\frac{\partial f}{\partial x}\right)_i}{x_{i+1}-x_i}\right]$$



Use Backward Difference scheme for 1st order derivative:

$$\left(\frac{\partial f}{\partial x}\right)_{i+1} \approx \frac{f_{i+1}-f_i}{x_{i+1}-x_i} = \frac{f_{i+1}-f_i}{\Delta x_i}$$

So we would deal with or we derive these approximations of second order derivatives using formulae derived for FD approximation of first order derivative. Let us continue with example, which we cited in our slide that is to say we have used a forward difference approximation. So let us allocate our grid. This is our grid point xi, xi+1, xi-1. Now this is equal to del/del x of del f/del x at i. Now for this term, now let us see what is our FD is.

So this becomes del f/del x at the forward point that is xi+1-del f/del x at i/xi+1-xi. Now we need to expand the first order derivative, which appear on the right hand side that is del f/del x at i+1 and del f/del x at i. So now let us use backward difference approximation for first order derivative on RHS. So use backward difference scheme for first order derivatives. So what do these become or del f/del x at i+1.

This can be approximated in terms of the function value at i+1- function value at the grid point i/xi+1-xi. Let us write it in a more compact form using del x notation of the grid spacing. We have used the convention. We are going to denote by del xi and the spacing between the node xi-1 and xi, we will call this as delta xi-1. So using this notation, we can write our right hand side as f of i+1 – fi divided by delta xi.

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Use Backward Difference scheme for 1st order derivative:

$$\left(\frac{\partial f}{\partial x}\right)_{i+1} \overset{BDS}{\approx} \frac{f_{i+1}-f_i}{x_{i+1}-x_i} = \frac{f_{i+1}-f_i}{\Delta x_i}$$

$$\left(\frac{\partial f}{\partial x}\right)_{i} \overset{BDS}{\approx} \frac{f_i-f_{i-1}}{\Delta x_{i-1}}$$

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_{i} = \frac{(f_{i+1}-f_i)/\Delta x_i - (f_i - f_{i-1})/\Delta x_{i-1}}{\Delta x_i}$$

$$\Rightarrow \boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_{i} \approx \frac{f_{i+1}\Delta x_{i-1} + f_{i-1}\Delta x_i - (\Delta x_i + \Delta x_{i-1}) f_i}{\Delta x_i^2 \Delta x_{i-1}}}$$

Similarly the second derivative, first order derivative we had. So del f/del x at i. Once again let us use BDS approximation. Make sure what we are saying, let us just start the scheme name, what is the symbol, this is fi – f of i-1/del xi-1. Now we can substitute these 2 expressions in our previous expression and simplify it further. So that will give us the finite difference approximation for second order derivative.

First f of i+1-fi/delta xi-second term in terms of del f/del x at i, we would write an fi-ffi-1/delta xi-1 and this whole thing divided by delta xi. We will write simplification straight forward. So del 2f/del x square at i, this is approximated by f of i+1 * delta xi-1+f of i-1 delta xi-delta xi+delta xi-1* f of i and our denominator becomes delta i square delta xi-1. So this is only one such approximation because we have got a variety of choices, which we can use first in obtaining this outer derivative and then for approximating these in our first order derivatives.

So we can get a family of such a finite difference approximations for first order derivative. Now I would like to leave it as an exercise for you.

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Ex. Find out truncation error for the above approximation.

- For uniform grid, $\Delta x_i = \Delta x_{i-1} \equiv \Delta x$

$$\boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i \simeq \frac{f_{i+1} + f_{i-1} - 2f_i}{\Delta x^2}}$$

Ex. Find out if TE for uniform grid approximation is $O(\Delta x^2)$ or $O(\Delta x)$

That verify or find out truncation error for the above approximation. This formula or this approximation can be simplified for uniform grids. So let us see what would happen for uniform grid. So let us start this special case. For uniform grid, that is our delta xi = delta xi-1 and this we can write as simple symbol delta x. So if you substitute it in the previous expression, we get the simplified form for this approximation del 2f/del x square at i. This is f of i+1+f of i-1 – 2fi/delta x square.

Now once again, I would leave it as an exercise. Find out if TE for uniform grid approximation is O delta x square or O delta x. That you should say, if you expand the terms on the right hand side in Taylor series expansion and see which other terms, which we have neglected in finding out this derivative, that will give you the expression for the truncation error and so if the results on uniform grid or any different grid from what you will get for non-uniform grid that you say if it is of the first order or it is of second order.

This particular approximation, which we have derived that here we have used only forward and backward difference approximations and both of these schemes we have seen earlier that they are first order accurate. Now can we expect to get somewhat weighter approximations to use central difference scheme. See if you use the central difference scheme, we have already seen that we get much more accurate approximations using CDS.

Now let us try and derive one approximation using central difference scheme.

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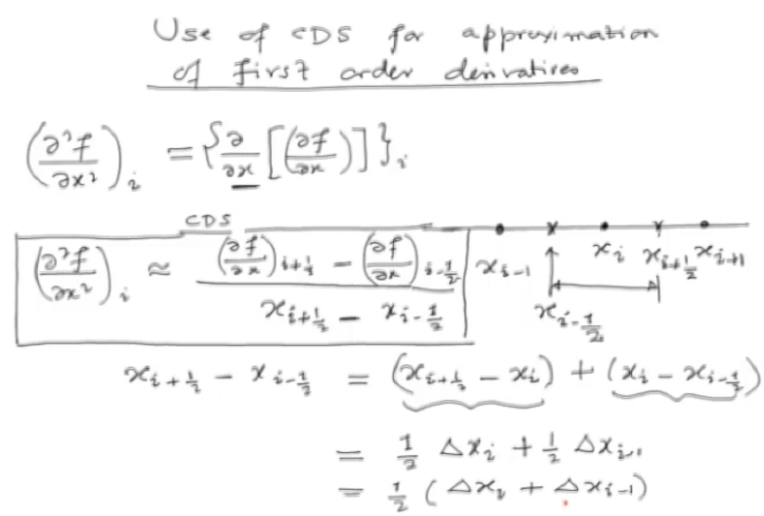

Use of CDS for approximation of first order derivatives. Once again, let us have a look at our grid center point xi that is where we would like to have our approximation for the second order derivative. The grid point of the right of it xi+1, grid point to the left of it xi-1. For CDS or central difference approximation, we need to choose the grid points, which are just mid point of these grid spacings. So one towards right, let us call it as xi+1/2 and the one at right we will give it as an index xi-1/2.

So now our del 2f/del x square at point i = del f/del x of del f/del x. Now let us use the CDS that if we are going to use the function values at grid locations i+1/2 and i-1/2, which is situated on both the sides of grid point xi. So we put the CDS, we can write their approximation as del f/del x at I+1/2-del f/del x at i-1/2/the spacing between these altered locations or the mid point locations. So we can write xi+1/2-xi-1/2. So this is the expression, which we have derived by applying central difference approximation to the outer derivative.

Now let us simplify this thing a bit further. Let us have a look at the denominator on the right hand side, xi+1/2-xi-1/2. This we can rewrite as xi+1/2-x of i-1/2. As xi+1/2 is mid point of xi and xi+1 similarly xi-1/2 is the mid point of this grid segment xi and xi-1/2. The first one would be half of the grid spacing between xi and xi+1/2, so we can write this term as 1/2 of delta xi.

Similarly our second term that will also, this distance is basically half of the spacing between grid points xi-1 and xi.

So half of delta xi-1. This takes factor 1/2 outside, so we can get a simplified form delta xi+delta x i-1. Next we would like to find out expressions for this first order derivatives. Once again, let us use CDS.

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$$= \frac{1}{2}\left(\Delta x_i + \Delta x_{i-1}\right)$$

$$\left(\frac{\partial f}{\partial x}\right)_{i+\frac{1}{2}} \overset{CDS}{\simeq} \frac{f_{i+1} - f_i}{x_{i+1} - x_i} = \frac{f_{i+1} - f_i}{\Delta x_i} \quad (3)$$

$$\left(\frac{\partial f}{\partial x}\right)_{i-\frac{1}{2}} \overset{CDS}{\simeq} \frac{f_i - f_{i-1}}{x_i - x_{i-1}} = \frac{f_i - f_{i-1}}{\Delta x_{i-1}} \quad (4)$$

Substitute Eqn. (2) – (4) into Eq. (1):

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i \simeq \frac{(f_{i+1} - f_i)/\Delta x_i - (f_i - f_{i-1})/\Delta x_{i-1}}{\frac{1}{2}\left(\Delta x + \Delta x_{i-1}\right)}$$

$$\Rightarrow \boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i \overset{CDS}{\simeq} \frac{f_{i+1}\Delta x_{i-1} + f_{i-1}\Delta x_i - f_i(\Delta x_i + \Delta x_{i-1})}{\frac{1}{2}\left(\Delta x + \Delta x_{i-1}\right)\Delta x\, \Delta x_{i-1}}}$$

So del f/del x at i+1/2 using central difference scheme, let us focus on the grid point i+1/2. The nodes to both of its sides are xi and xi+1. So we have to use the function values at these 2 adjoining nodes whose width point is i+1/2. We would use function values at fi+1-fi/spacing between these nodes that is xi+1-xi or using a delta x notation. This is f of i+1-f of i/delta xi. Similarly for the next derivative, which is involved on the right hand side del f/del x, which is to be obtained at the mid point of grid segment xi-1 to xi.

So once again this derivative can be approximated using central difference scheme using the function values at grid point xi and xi-1. So that this is = fi-f of i-1/xi-x of i-1 that is f of i-f of i-1/delta xi-1. Now we have to expand it for all the terms, which we need in our previous CDS representation of outer derivative. So let us substitute these expressions. Let us call the previous expression as 1, this is 2, 3, and 4.

So substitute equations 2 to 4 into equation 1and the resulting expression would be del 2f/del x square at i. This is approximately = f of i+1-fi/del xi-fi-f of i-1/delta xi-1 and denominator we have got 1/2 of delta x+delta xi-1. Simplify to obtain the final expression del 2f/del x square at i. This whole thing is based on CDS or central difference approximation for the first order derivatives, f of i+1 delta xi-1 +f of i-1 delta xi-fi *delta xi+delta xi-1/1/2 delta x+delta xi-1 * delta x/delta xi-1.

So this is the final form of CDS based or central difference approximation based approach for second order derivative. This expression, if you look at, the numerator is fairly similar to the one which we have obtained using first order scheme, but there is small difference in denominator here, see 1/2 delta x+delta xi-1. What difference will it make to the accuracy of this scheme, that you can explore yourself by using Taylor series expansions.

Let us have a look at simplified form for this expression for uniform grid. Delta xi+delta xi-1, which we will call as delta x.

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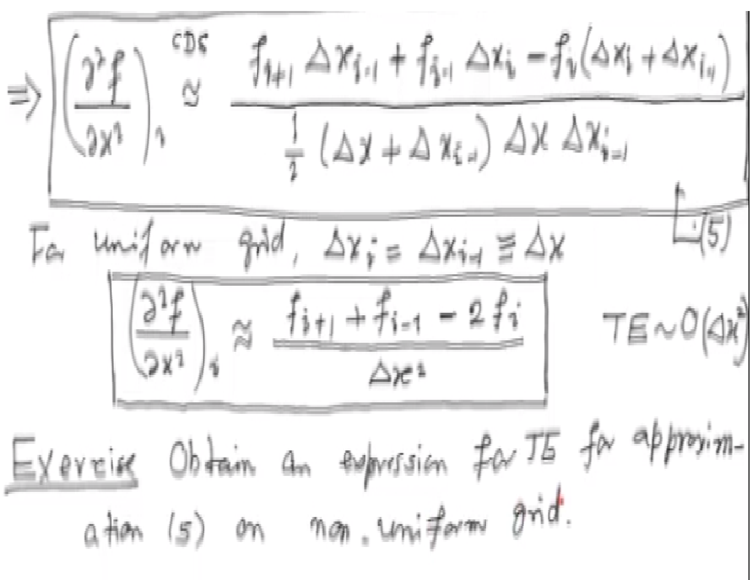

So we get del 2f/del x square i fi+1+f of i-1-twice of fi/delta x square. This is expression for uniform grid is identical to what we had obtained earlier. I just give you a hint, the truncation error for this approximation is of order delta x square, that is the second central difference based approximation on uniform grid for second order derivative is second order accurate. Now a simple exercise for you.

Once again obtain an expression for TE for the approximation, which we have derived on non-uniform grid or approximation on non-uniform grid. As I mentioned earlier, that we have just discussed 2 possibilities. The various other possibilities, which you can use to obtain the expression for the second order derivative based on the expression for the first order derivative. So the remainder type approximations you can explore yourself. Now let us proceed further to next approach.

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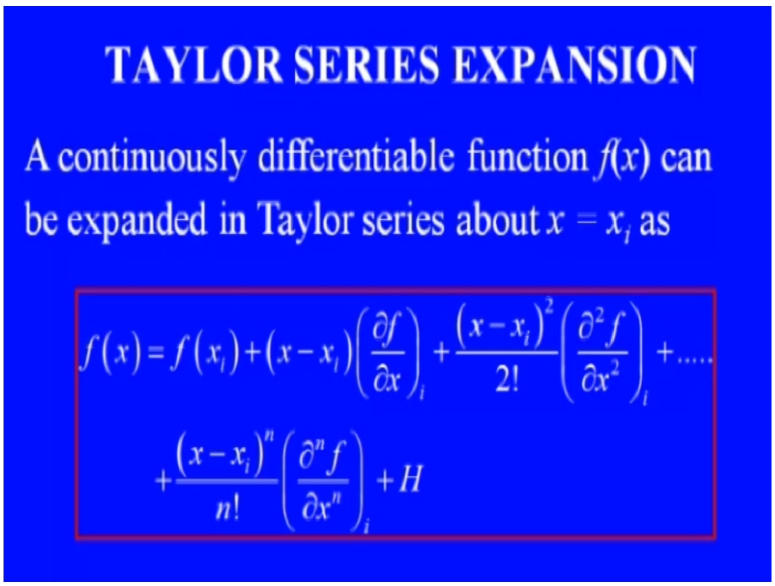

That is let us use our Taylor series expansion as an issue. This is once again a recap of what is Taylor series expansion, which we have seen earlier for any continuously differentiable function f(x). We had f(x) expanded around x=xi. So at point x in the neighborhood of point xi, the function values given is f(x)=f of xi+x-xi del f/del xi+x-xi square factorial to del 2f/del x square i+ so on. So can we use this expansion per se and perform certain algebraic manipulations to obtain an approximation for the second order derivative del 2f/del x square at i.

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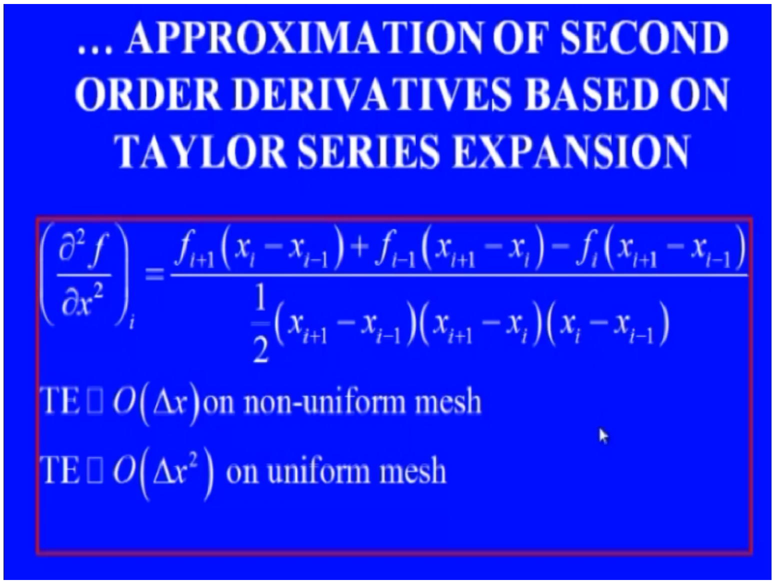

So now let us try obtaining an expression for the second order derivative based on Taylor series expansion. So let us get back to writing board.

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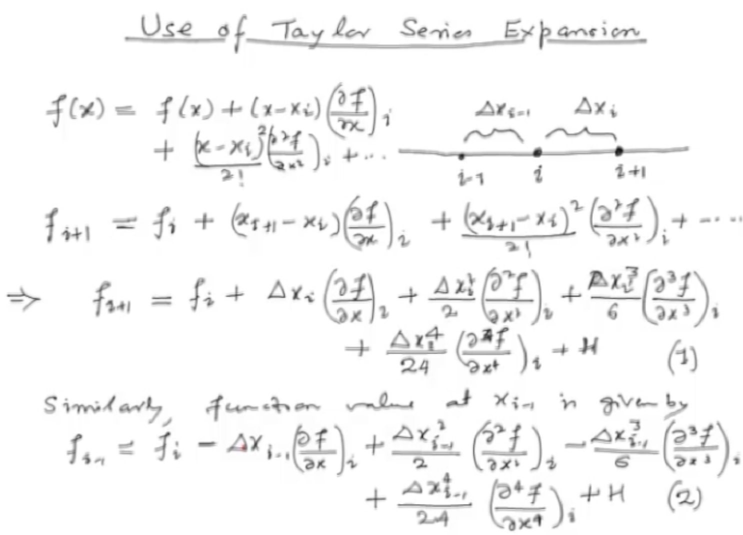

Use of Taylor series expansion. Let us first try to obtain an expression or an approximation of the second order derivatives in terms of the nodal values at grid point i, i+1, and i-1 grid spacing as usual xi between these points and delta xi-1. What will be the grid spacing between grid nodes xi and xi-1. So for a recap, let us write our Taylor series expansion once again. So f(x)= f(xi)+x-xi del f/del x at i+x-xi del 2f/del x square at i square of this/2 factorial+so on.

Now let us write down the function values as we did earlier. We obtained the function values at grid node i+1 in terms of this Taylor series expansion at point xi. So fi+1 thus becomes fi+x(i+1-xi) del f/del x at i+x(i+1-xi) square/2 factorial del 2f/del x square at i and so on. Let us use our delta notation to write it in more compact form, f(i+1)=fi+delta xi del f/del x at i+delta x square/2 del 2f/del x square at i+delta xi cube/6 del cube f/del x cube at i+delta x to the power of 4/24, del 4f/del x 4 at point i+ so on.

Let us call this as our high order terms. So let us term this equation as 1. Similarly function value at xi-1 is given by let us write straight away in terms of delta notation, so f(i-1)=fi-delta xi-1 del f/del xi+delta xi-1 square/2 del 2f/del x square at point i-delta xi-1 cube/6 del cube f/del x cube at point i+ delta xi-1 to the power of 4/24 del 4f/del x4 at i+remaining high order terms. Let us call this equation or number it as 2.

Now our task is of what we are looking for is to obtain an expression in terms of the function values at grid nodes and this grid spacing for second order derivative del 2f/del x square. That we can obtain, if you can eliminate the first order derivative from these 2 equations. So if you look at the coefficient of del f/del xi in the first equation is delta x and second one it is delta xi-1. So all that we need to do is multiply the first equation by delta xi-1 and the second one by delta xi and add that 2, thereby we would be able to eliminate the first order derivative.

Rearrange the resulting equation and we should be able to obtain an expression for the second order derivative. So let us do that.

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Multiply Eq. (1) by Δx_{i-1} and Eq. (2) by Δx_i and add:

$$\Delta x_{i-1} f_{i+1} + \Delta x_i f_{i-1} = f_i (\Delta x_i + \Delta x_{i-1}) + \frac{1}{2}(\Delta x_i^2 \Delta x_{i-1} + \Delta x_{i-1}^2 \Delta x_i)\left(\frac{\partial^2 f}{\partial x^2}\right)_i + \left[\frac{\Delta x_{i-1} \Delta x_i^3}{6} - \frac{\Delta x_i \Delta x_{i-1}^3}{6}\right]\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \left[\frac{(\Delta x_{i-1} \Delta x_i^4 + \Delta x_i \Delta x_{i-1}^4)}{24}\right]\left(\frac{\partial^4 f}{\partial x^4}\right) + H$$

$$\Rightarrow \frac{1}{2} \Delta x_i \Delta x_{i-1} (\Delta x_i + \Delta x_{i-1})\left(\frac{\partial^2 f}{\partial x^2}\right)_i = [\Delta x_{i-1} f_{i+1} + \Delta x_i f_{i-1} - f_i (\Delta x_i + \Delta x_{i-1})] + \frac{\Delta x_i \Delta x_{i-1}}{6}\{\Delta x_{i-1}^2 - \Delta x_i^2\}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \frac{\Delta x_i \Delta x_{i-1}}{24}(\Delta x_i^3 + \Delta x_{i-1}^3)\left(\frac{\partial^4 f}{\partial x^4}\right)_i + \cdots$$

So multiply equation 1 by delta xi-1and equation 2 by delta xi and add. So what do we get. On the left hand side, we will get delta xi-1 f of i+1 delta xi * f of i-1. On the right hand side, we will get fi*delta xi+delta xi-1. The terms this first order derivative terms, they get canceled. They cancel out each other. So next contribution will come from the second order terms, that is 1/2 delta xi square delta xi-1+delta xi-1 square*delta xi*del 2f/del x square at i.

The first equation will get a positive term. So this delta xi-1 delta xi cube/6-delta xi*delta xi-1 cube/6 and this whole thing * del cube f/del x cube at i+the expressions coming from the fourth order derivative, their coefficients. There will be delta xi-1 into delta xi to the power of 4+delta xi into delta xi-1 to the power of 4/24 *del 4f/del x4 at i+ remaining higher order terms. Now let us rearrange this equation and simplify because our task is to obtain and expression for this del 2f/del x square.

Put this on left hand side, transfer everything else on the right hand side and thereby obtain the expression for this del 2f/del x square, 1/2 delta xi*delta xi-1 delta xi+delta xi-1*del 2f/del x square at i. So this is the term, which we keep or retain in one side. The remaining go on the RHS. So let us at one go have the terms involving the functional values. So we get delta xi-1 f(i+1)+delta xi f(i-1) – fi*delta xi+delta xi-1.

Now the terms containing the higher order derivatives, we will get delta xi delta xi-1/6 (delta xi-1 square – delta i square del cube f/del x cube at i+ the terms coming from the fourth order derivative. We can again write it as delta xi delta xi-1/24*delta xi to the power 3+delta xi-1 to the power of 3 del 4f/del x4 at i+ higher order terms. So now we are ready to get the final form of the expression. So this would be given by.

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Therefore,

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_i = \underbrace{\left[\frac{[\Delta x_{i-1} f_{i+1} + \Delta x_i f_{i-1} - f_i(\Delta x_i + \Delta x_{i-1})]}{\frac{1}{2}\Delta x_i \Delta x_{i-1}(\Delta x_i + \Delta x_{i-1})}\right]} + \frac{1}{6}(\Delta x_{i-1} - \Delta x_i)\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H$$

Thus, approximation for second order derivative

$$\boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{\Delta x_{i-1} f_{i+1} + \Delta x_i f_{i-1} - f_i(\Delta x_i + \Delta x_{i-1})}{\frac{1}{2}\Delta x_i \Delta x_{i-1}(\Delta x_i + \Delta x_{i-1})}}$$

Therefore, what we get del 2f/del x square i=the function values, let us write them in numerator. So delta xi-1 f(i+1)+delta xi f(i-1)-fi delta xi+delta xi-1. So this completes our numerator part in terms of the function values/1/2 delta xi delta xi-1*delta xi+delta x (i-1). So this is basically the approximation, which we are looking for. Let us put in a big bracket. The remainder terms they are in the form of the multiple of higher order derivatives.

If you look at carefully, this is what we had obtained earlier by using central difference approximation of the first order derivatives previously. Let us also complete the higher order terms and terms containing the higher order derivatives, which will form the part of a truncation error. So it will be 1/6 of delta xi-1-delta xi*del cube f/del x cube+ higher order terms. So we can clearly say that if we use this approximation.

Thus this approximation for the second order derivative del 2f/del x square of i = delta xi-1 f(i+1)+delta xi f(i-1)-fi delta xi+delta xi-1/1/2 delta xi delta xi-1*delta xi+delta xi-1. So this is the approximation which we have obtained for the second order derivative on a non-uniform grid using Taylor series expansion. How about its truncation error. Truncation error is the terms, which we have neglected.

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$$TE \sim O(\Delta x)$$

$$TE = \frac{1}{6}\underbrace{(\Delta x_{i-1} - \Delta x_i)}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + H$$

On uniform grid, $\Delta x_i = \Delta x_{i-1}$

$$\boxed{\left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{f_{i+1} + f_{i-1} - 2f_i}{\Delta x^2}}$$

$$TE \sim O(\Delta x^2)$$

Very widely used in CFD

So first term which we will see that is the one which is multiplying our third order derivative and formally we will say this is of the order of the grid spacing delta x, but at the same time say this TE=1/6 delta xi-1-delta xi del cube f/del x cube i+the higher order terms. Since here we have got a difference of the grid spacing. It is actually more than first order accurate in fact is closer to the second order of the TE is more likely to be of second order when the grid spacing is nearly uniform.

Because this difference will be fairly small. Then the next term is the one, which will come into play that will dominate over this term. The next term, which multiplies is del 4f/del x cube that term in truncation error would dominate and that is clearly of the order delta x to the power of 4. You can just try and see if we assume our grid to be uniform, so on uniform grid that is delta xi=delta xi-1, we get back our familiar expression, which we have derived previously.

So this del 2f/del x square at i, this is f of i+1+fi-1-twice of fi/delta x square and you can easily verify from the first term or the s term which I just left as such. This truncation error in this case is of the order delta x square. Now this simple three-point scheme for the second order derivative, this has got a number of advantages and this expression is very widely used in CFD.

If you want, you can use the Taylor series expansion to derive the approximations of much higher order, which will involve many more points, but as you can see from the simple three-point case. We have to do considerable amount of algebra, so if you use more number of points, the algebra would become more involved. However, in the case of uniform grid, we have put a simple general formula, which can simplify our task.

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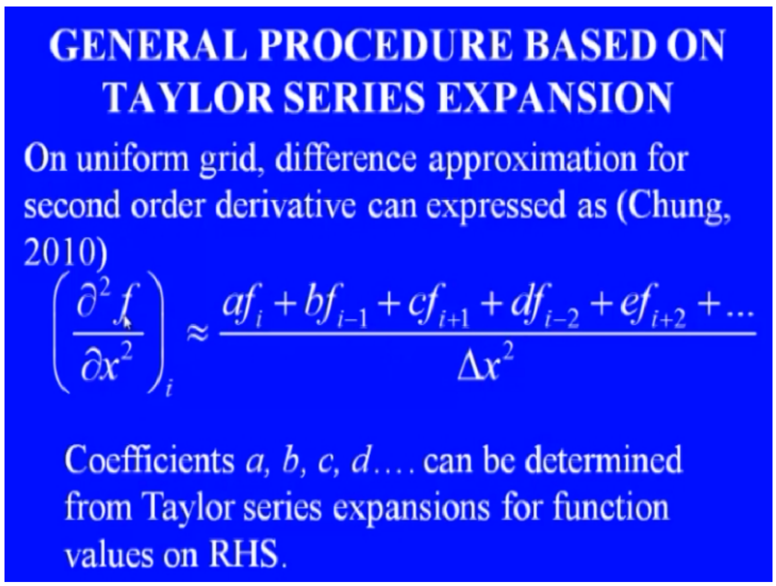

Like instead of guessing that which equation to multiply by what factor and what sort of eliminations we need to perform. Chung suggested that look on uniform grid we can write the difference approximation for a derivative and so we can write the difference approximation for second order derivative on a uniform grid as del 2f/del x square at point i in terms of the function values at grid point i and neighbouring nodes by multiplying by some factors.

Afi+bfi-1+cfi+1+d times fi-2+e times f of i+2+ so on/delta x square. Now these coefficients a, b, c, d they can be determined from Taylor series expansions for the functional values this fi-1, fi+1, fi-2 and so on and compare the terms on both the sides of this equation. We will get a set of equations, which can be solved to obtain the values of these numerical constants a, b, c, d. For instance the three-point central difference formula, which we have derived previously.

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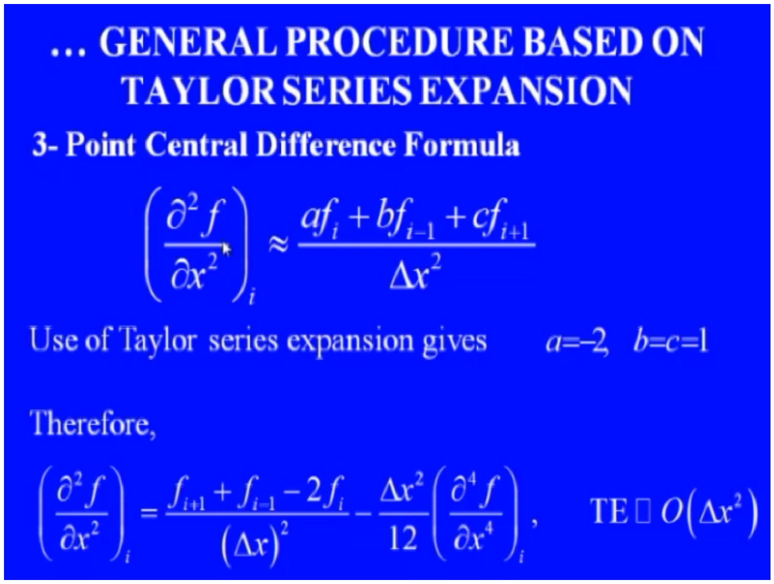

Let us try this general scheme for that and let us verify if we can get the same approximation. So we will derive these three-point formula using our general procedure based on Taylor series expansion in the next class. So thank you, let us wait for the next class and we would derive three-point central difference backward difference and a five-point formula and we will continue with polynomial fitting and future derivations for second order derivatives.