Computational Fluid Dynamics
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Lecture - 13
Finite Difference Approximation of Second Order Derivatives-2

Welcome back to the next lecture in module 3 on finite difference method. We will continue from where we left in the first lecture on second order derivative. So we are going to focus on finite difference approximation of second order derivatives in this lecture. What we discussed in lecture 3, so previous lecture was we discussed approximation approaches.

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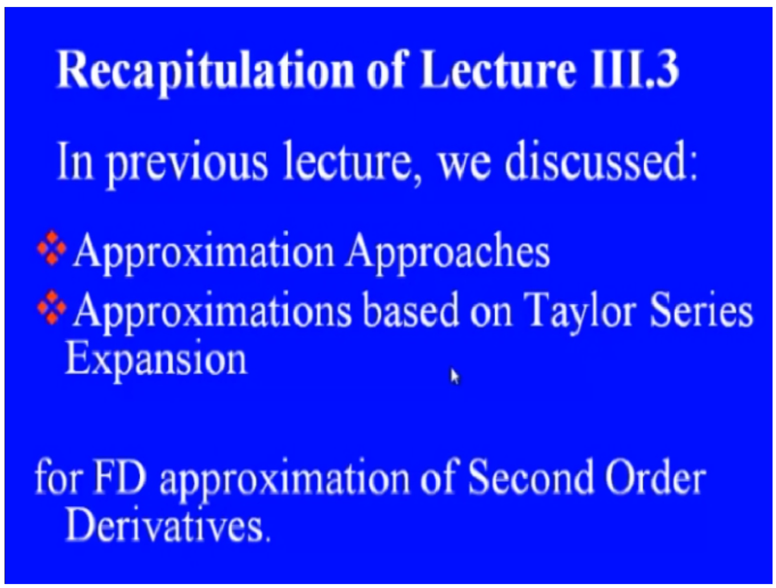

And we derived approximations based on Taylor series expansion for finite difference approximation of second order derivative. So we are going to continue the same part, that is we would derive finite difference approximation of second order derivatives.

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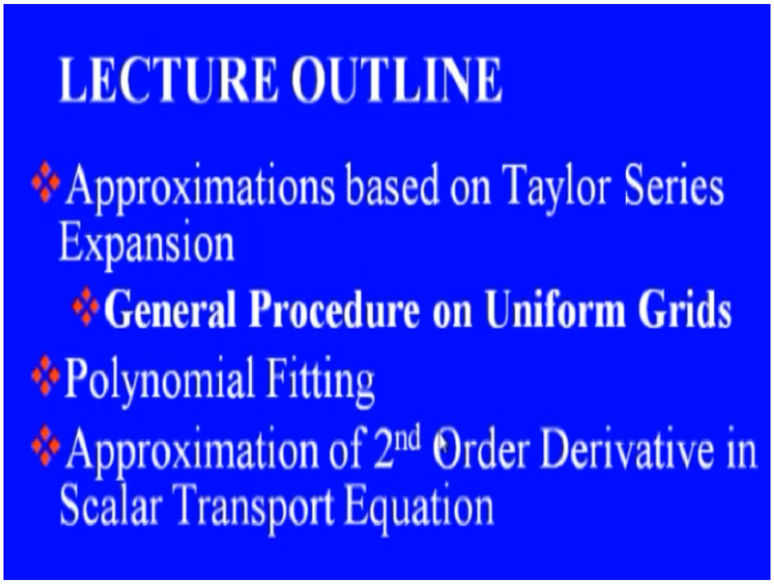

We will continue our approximations based on Taylor series expansion, particularly the one based on general procedure on uniform grids, then we will take up how do we obtain finite difference approximations based on polynomial fitting, and then we would try and obtain approximation of second order derivative in scalar transport equation. So now let us have a relook at a general procedure, which we outlined earlier.

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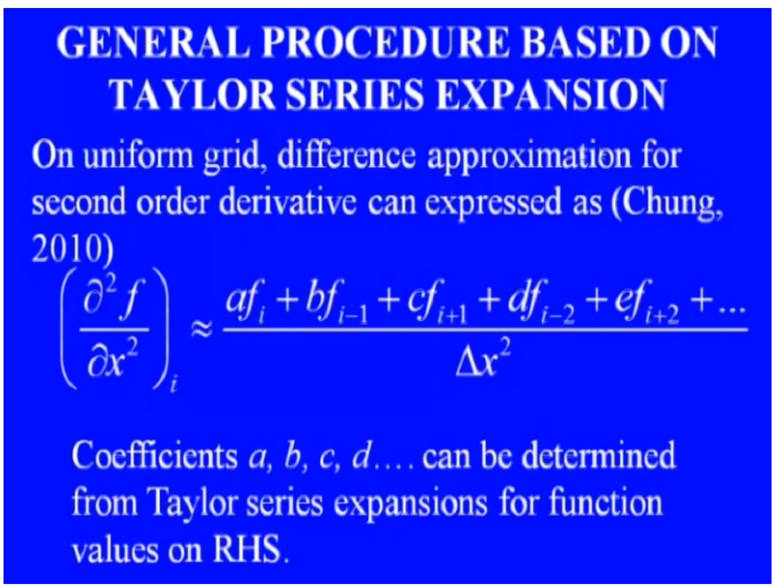

That on uniform grid, difference approximation for second order derivative can be expressed as del 2f/del x square i, this is approximately = a*fi+b*fi-1+c*fi+1+d*fi-2+e*fi+2 so on/delta x square and these coefficients a, b, c, d, can be determined from Taylor series expansions for function values fi, fi-1, fi+1 and so on. We will substitute them on the right hand side and try and equate the terms appearing on both the sides and thereafter you will get system equation.

From which we can determine a, b, c, d, etc. Let us take one or 2 examples of this approach, which is proposed by Chung in 2010. Now first thing we will take up is three-point central difference formula.

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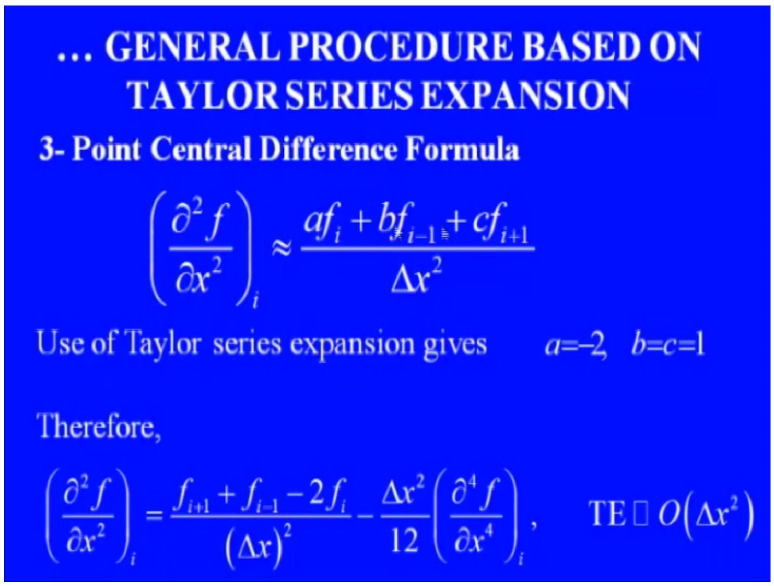

So this is our general formula del 2f/del x square i=afi+bfi-1+cfi+1/delta x square and using this formula, let us find out the values of a, b, and c involved in this approximation using Taylor series expansion.

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3-Point Central Difference Scheme for 2nd Order Derivative

(Uniform grid : Δx)

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

$i-1 \quad i \quad i+1$

$$a f_i + b f_{i-1} + c f_{i+1}$$
$$= a f_i + b\left\{ f_i - \Delta x \left(\frac{\partial f}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i - \frac{\Delta x^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \frac{\Delta x^4}{24}\left(\frac{\partial^4 f}{\partial x^4}\right)_i + H \right\}$$
$$+ c\left\{ f_i + \Delta x \left(\frac{\partial f}{\partial x}\right)_i + \frac{\Delta x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i + \frac{\Delta x^3}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \cdots \right\}$$
$$= (a+b+c) f_i + (-b+c)\Delta x \left(\frac{\partial f}{\partial x}\right)_i + \frac{\Delta x^2}{2}(b+c)\left(\frac{\partial^2 f}{\partial x^2}\right)_i$$
$$+ \frac{\Delta x^3}{6}(-b+c)\left(\frac{\partial^3 f}{\partial x^3}\right)_i + \frac{\Delta x^4}{24}(b+c)\left(\frac{\partial^4 f}{\partial x^4}\right)_i + H$$

So we want to find out a three-point central difference approximation or central difference scheme for second order derivative. The grid is supposed to be uniform and let us use symbol delta x to denote our grid size. So let us rewrite our formula or formula of Chung del 2f/del x square at the grid point i approximately = afi+bfi-1+cfi+1/delta x square. So basically what we have is, we have taken 2 points in the neighborhood of our grid point i.

So grid point i, we have taken the grid point i+1 to the right of it and grid point i-1 to the left of it. Now let us substitute on this formula the values of fi-1 and fi+1 using Taylor series expansion around point xi. So if you do that, let us have a look at the numerator, that is afi+bfi-1+cfi+1. The first term remains as such afi. Now for b*fi-1, now let us use Taylor series expansion. So it would be fi-delta x *del f/del x at i+delta x square/2 del 2f/del x square at i-delta x cube/6 del 3f/del x cube at i+delta x to the power 24 del 4f/del x4+other high order terms.

So this completes our expansion for value of fi-1 in terms of fi. Now c * the expansion for fi+1. This becomes fi+delta x *del f/del xi+delta x square/2 del 2f/del x square i+del x cube i6 del cube f/del x cube i and +other high order terms. Now let us collect the like terms like the ones which involve function values or first derivative, second derivative and so on. Let us collect them together.

So we have got three terms involving function values, afi, b* fi, and c*fi. So we will get a+b+c*fi. Now let us next collect the multipliers of the first derivative. So we get –b coming from the expansion of fi-1 and –b+c*delta x del f/del xi+delta x square/2 b+c del 2f/del x square at i+delta x cube/6 we will get (-b+c del cube f/del x cube at i+delta x to the power 4/24 b+c del 4f/del x4 at i+ higher order terms.

So now let us substitute this value which we have obtained for afi+bfi-1+cfi+1 into our generic formula, we have started off. We will call this equation 1, expansion of which we got as 2, so substitute 2 into equation 1.

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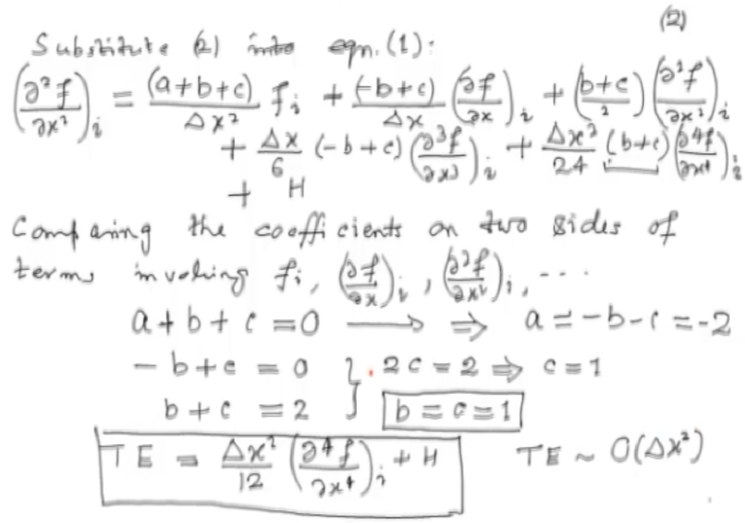

So what we will get, del 2f/del x square. This is what we get on the right hand side. This is =a+b+c/delta x square * f of i+(-b+c)/delta x del f/del xi+b+c/2 del 2f/del x square at i+delta x/6-b+c del cube f/del x cube of i+delta x square/24 b+c del 4f/del x4+higher order terms. So now let us compare the coefficients of the function values derivatives of different orders, which we have got in left hand side and right hand side.

So on the left hand side we do not have any term, which contains fi, we do not have any term containing first derivative or third derivative and so on. So if you compare the coefficients on 2 sides of terms involving fi del f/del x of i del 2f/del x square i and so on. What do we get. We get a+b+c=0. That is what we get. The coefficient of fi on the left hand side. There is no term on fi, so it coefficient is 0.

On the right hand side, we have got a+b+c/x square, so this should be set to 0, so we get this equation in terms of a, b, and c a+b+c=0. Similarly, this node term which contains the first derivative on the left hand side, but we have got one term-b+c/delta x del f/del xi in the right hand side, so its coefficient must vanish as well. So we get –b+c=0. We got three unknowns. We need one more equation. Now let us compare the coefficients of the second derivative.

The coefficient of second derivative del 2f/del x square i is the one on the left hand side. Its coefficient on the right hand side is b+c/2. So if we equate these 2, we get b+c=2. From these equations if you just add the last 2 equations, we get 2c=2, which implies c=1 and we can solve for b from second equation, b=c. We get b=c=1, substitute these values of b and c in the first equation, so this equation will give us the value of a, a=-b-c.

So thereby we get the value of -2. So let us summarize it on the slide. So by Taylor series expansion, we have got a=-2, b=c=1. So therefore we get pretty simple form for the second order derivative del 2f/del x square i=f of i+1+fi-1-twice of fi/delta x square. What happens to a truncation error. So truncation error, lets us see on the right hand side the terms, which involve the higher order derivatives.

The term containing the third derivatives –b+c, b and c are equal, so this term vanishes. So our truncation error is basically delta x square/12, we substitute for b and c here, so b+c we get 2, 2/24 that gives us 12. So delta x square/12 del 4f/del x4. So we can clearly say that this central difference approximation has got a truncation error of the order 2 of x square that is it is a second order accurate scheme.

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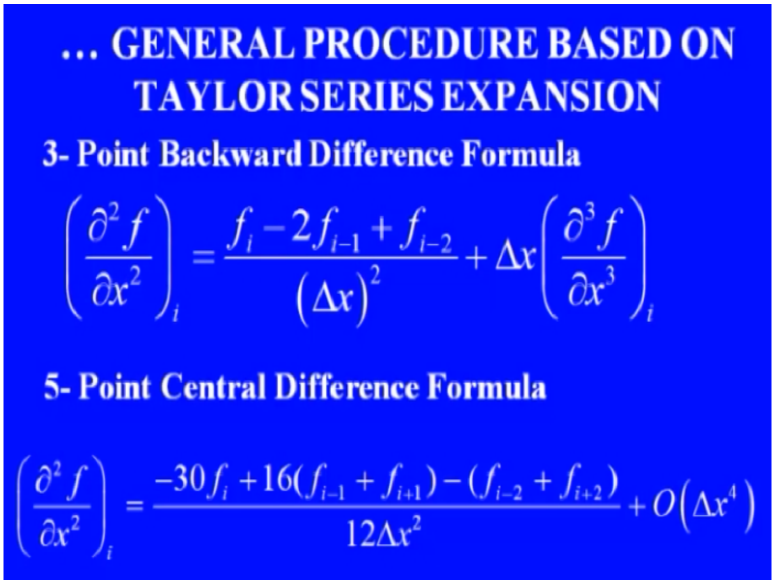

We can also find out a one side formula of 3-point backward difference formula by taking the values at point fi, fi-1 and fi-2 and in this case, our truncation error involves the terms of order delta x. So this 3-point one-sided difference formula, which we can get using this general procedure has got a first order accuracy. We can also obtain higher than second order formula using this Taylor series expansion. So let us take a 5-point central difference formula.

We will do part of the derivation and part will be left to you as an exercise.

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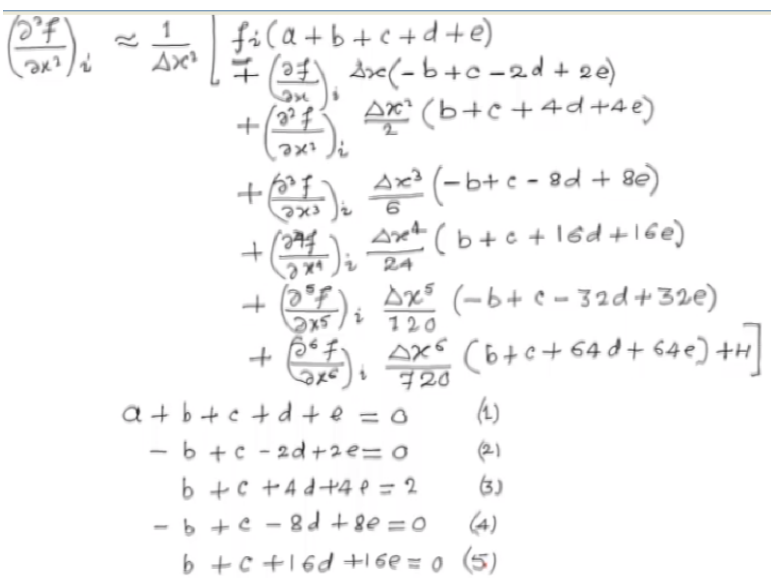

So we want to find out a 5-point central difference formula for second order derivative. This higher order formula is sometimes used in the finite difference course, which require extremely accurate finite difference approximations. So our first point would be our central point that is i-th grid point. We will take 2 points on each side. That is grid point i+1 and i+2 on the right hand side of point i and i-1 and i-2 to the left.

So difference scheme or difference formula, we can express as af of i+b*f of i-1+c*f of i+1+d*f of i-2+e*fi+2/delta x square. So we have got five unknown coefficients, which we must determine using Taylor series expansion and let us do that straight away by putting expanded forms for fi-1, fi+1, fi-2 and fi+2 on the right hand sides. We can write 1/delta x square, now let us try and collect similar terms, the terms which are going to multiply fi.

We will get a constant term fi in all these remaining 4 expansions, we will get fi would be multiplied by a+b+c+d+e. Now next we will have terms collecting coefficient of del f/del xi, so what do we get. The first term afi, that will remain as such. We will get this del f/del xi occurring in the expansions of fi-1, fi+1, fi-2, and fi+2. So let us take what do we get from expansion of fi-1. From here we will get simply a term containing delta x.

So here we will have, let us take delta x common. So from expansion of fi-1, we will get the contribution –b. From the expansion of fi+1 we have the coefficient delta x *c, delta x we have taken out, so we get +c, fi-2. Now here the difference is -2 delta x, so we get -2d and similarly the contribution coming from the expansion of fi+2/b 2e. So that completes our collection of the terms from expansion, which have del f/del xi.

Now let us collect the terms containing second order derivative del 2f/del x square at i. Let us take this delta x square/2 outside. So from expansion of fi-1, we will simply get +b, from fi+1 expansion, we get the contribution c, from fi-2 and fi+2, we have got 2 del x whole square. So we will get 4d+4e. Next, the third order derivative. Here let us take delta x cube/6 outside. So we get from expansion of fi-1, the contribution would be –bfi+1+c.

From fi-2, we will get 2 cube * d that is 8d fi+2 8e. Similarly del cube f/del x to the power 4i, let us take del x to the power of 4/4 factorial that is 24 outside. So we would be left with b+c+16d+16e. Next our fifth order derivative, del 5f/del x5 delta x to the power 5/120 is taken as common, so we get –b+c-32d+32e. Let us write one more term del 6f/del x 6 of i, common multiply del x to the power of 6/720 b+c+64d+64e and +remaining higher order terms.

Now to obtain the equations for a, b, c, d, now let us compare the terms on the LHS and RHS of this equation. Left hand side we have got only the second order derivative term. So coefficients of rest of the terms as a function value itself or first order derivative, third order derivative, forth order, fifth order, and so on. They can be all set to 0.

So we need five equations. First let us compare the coefficients of fi on both the sides. So this gives us a+b+c+d+e=0. Let us call this equation as 1. Second equation we can get by comparing the coefficient of del f/del xi in both LHS and RHS. In LHS, we have got value 0. So RHS we will get –b+c-2d+2e=0. Next compare the coefficients of del 2f/del x square. So this will give us b+c+4d+4e=2. Now I have got 3 equations. We need 2 more.

So let us next compare the coefficient of del cube f/del x cube i of both the sides. So we will get –b+c-8d+8e=0 and next equation we can get by comparing coefficient of del 4f/del x4. So that gives us b+c+16d+16e=0. Now we have got 5 equations and 5 unknowns a, b, c, d, e and you can solve these equations that I would leave as an exercise. I will just give you the summary of the results that if you solve these equations what do we get. We get the values of a, b, c, d, e.

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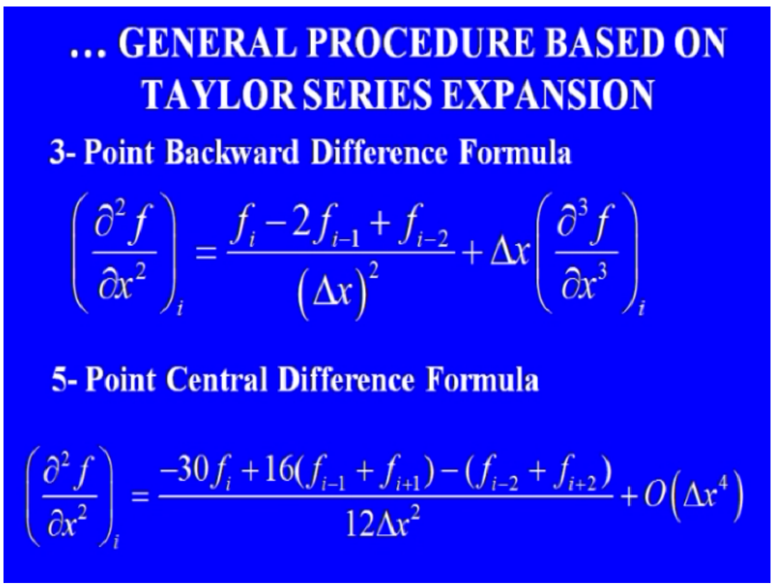

So we get on solving these equations, we get a=-5/2, b=c=, b and c they are both equal, that is 4/3. Similarly d and e are also equal d=e=-1/12. We can substitute these values and you can make few observations. By substituting the value, we get the final formula and the values of d and e are equal, so that will tell us that the coefficients, which multiplies del 5f/del x5 that becomes 0. So the leading coefficient and truncation error would be given by the multiply of del 6f/del x6.

So our truncation error for this scheme that is del 6f/del x6i b+c+64d+64e*delta x to the power of 4/720. Substitute the values of b, c, d, e and so on to get actual values of truncation error. You can clearly see this order of truncation error is delta x to the power of 4. So now let us have a look at the summary of this formula, which we derived. This 5-point difference formula, del 2f/del x square i=-30 fi+16*fi-1+fi+1-f of i-2+f of i+2/12 x square.

And the truncation error is of the order delta x to the power of 4. So this scheme is fourth order accurate. So now here we would put a stop to our approach or derivations based on Taylor series expansion. Let us have a look at the next scheme that is obtaining approximation of derivatives by polynomial fitting.

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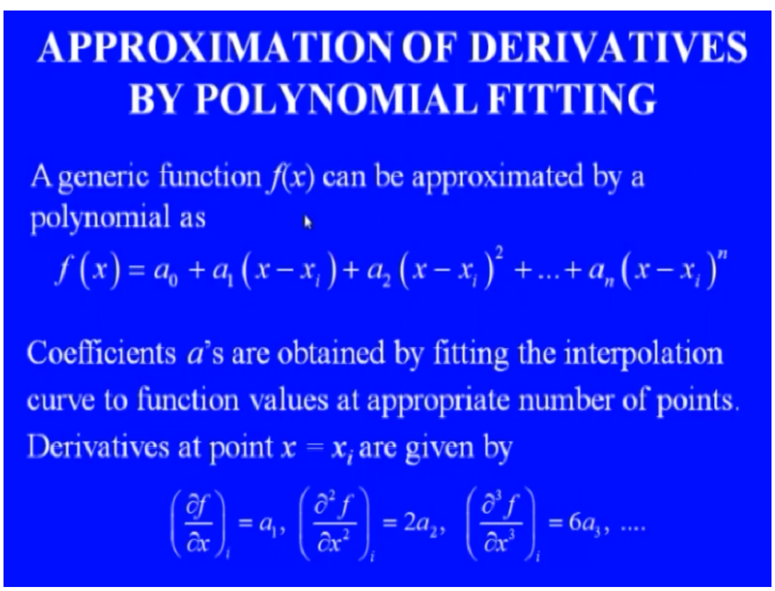

We have already seen this expansion earlier that a generic function fx can be approximated by a polynomial as f x=a0+a1*x-xi+a2*x-xi square+ so on an (-xi to the power n). We have taken in terms of x-xi so that we can easily obtain the expression for the derivative and x=xi and these coefficients a0, a1 and so on, we would obtain by fitting the interpolation curve. This is given by this polynomial to the function values at appropriate number of points.

And if you want to find derivatives, just simply differentiate this polynomial, so they get del f/del x this coefficient a1. The second order derivative xi is given by 2 *a2, third order derivative del cube f/del x cube is given by 6*a3 and so on. So we have already used this approach to derive few formulae for first order derivative. Now let us try and do one more and one derivation for our second order derivative.

In fact as part of the derivation, we can also obtain a formula or higher order formula for first order derivative as well.

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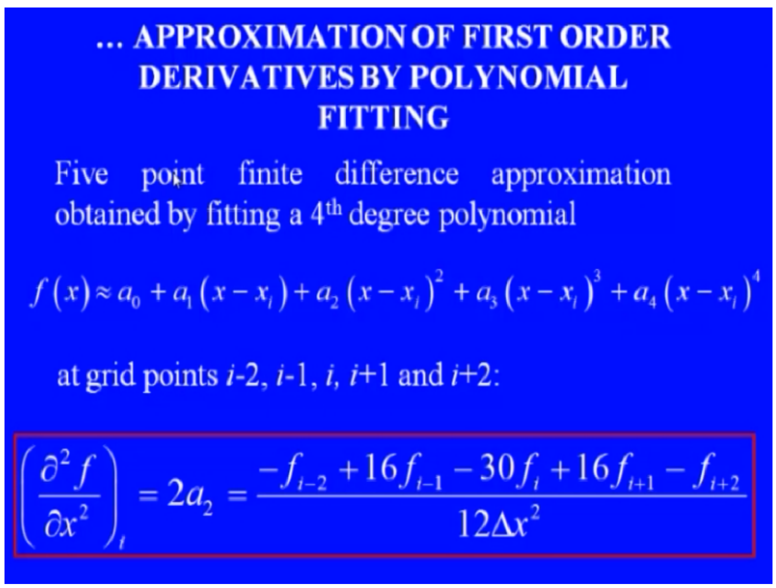

So what we would try to attempt is let us find out 5-point finite difference approximation by fitting a fourth degree polynomial. So fourth degree polynomial is given by fx is a0+a1*x-xi+a2*x-xi square+a3*x-xi cube+a4*x-xi to the power of 4. In this fourth order polynomial, we have got a0, a1, a2, a3, and a4, we have got a total of 5 unknown numerical coefficients, so that is why we need to equate this polynomial at 5 grid points to determine the values of a0, a1, a2 and so on.

For a central difference formula, let us take the grid points as i-2, i-1, i, i+1 and i+2. Let us get back to the board and try to derive our approximation based on fourth order polynomial fit.

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Add Eq. (5) and Eq. (6):

$$f_{i+2} + f_{i-2} = 2f_i + (8\Delta x^2)\, a_2 + (32\Delta x^4)\, a_4 \quad (7)$$

Add Eq. (3) and Eq. (4):

$$f_{i+1} + f_{i-1} = 2f_i + 2\Delta x^2 a_2 + 2\Delta x^4 a_4 \quad (8)$$

$$(8)\times 16 \Rightarrow \; 16(f_{i+1} + f_{i-1}) = 32 f_i + 32\Delta x^2 a_2 + 32\Delta x^4 a_4 \quad (9)$$

$$(9)-(7): \; 16(f_{i+1} + f_{i-1}) - (f_{i+2} + f_{i-2}) = 30 f_i + 24\Delta x^2 a_2$$

$$\Rightarrow \; 2a_2 = \frac{16(f_{i+1} + f_{i-1}) - (f_{i+2} + f_{i-2}) - 30 f_i}{12\Delta x^2}$$

$$\text{ie} \quad \left(\frac{\partial^2 f}{\partial x^2}\right)_i \approx \frac{-f_{i-2} + 16(f_{i-1} + f_{i+1}) - 30 f_i - f_{i+2}}{12\Delta x^2}$$

So polynomial fitting approach, first let us note down our grid points i, i+1, i+2, i-1, i-2. For the sake of simplicity of derivation, let us assume a uniform grid. So let us take an uniform grid and our grid spacing is delta x, so with reference to point i the spacing between i and i+1, this would be delta x. Similarly the difference between i and i+2 that would become 2 delta x and so on.

So if we choose our coordinate frame, centered at the grid location xi, we can obtain the values for the differences for these different points for substitution in our polynomial. Now let us write our fourth order polynomial fit, polynomial interpolation for function fx. So fx=a0+a1*x-xi+a2*x-xi square+a3*x-xi cube+a4*x-xi to the power 4. So if taken a fourth order polynomial, now let us equation this interpolation to the function values at points i, i+1, i-1, i+2, and i-2.

So let us do it 1 by 1. First by equating the function values at point xi, fxi is given by fi and that gives us a0. So straightly we have got the value for a0, which we can substitute in further expressions. Now f of i+1 that will give us fi+1 fi+1=fi+a1*delta x+a2*delta x square because difference between xi+1 and xi is simply delta x +a3*delta x cube+a4*delta x4. Interpolation equation 1, 2, let us call this equation as 3. Function value at fi-1=fi.

Now x is xi-1, so xi-1-x square that will give us –delta x, so we get a1*-delta x, this – sign comes here +a2*-delta x square, which simply gives us +delta x square-a3*delta x cube+a4*delta x4. Let us call this equation as 4. Next equate the values at point i+2. So f(i+2)=fi+2 delta x*a1. I have got 2 delta x as x-xi, so this square term would give us 4 delta x square*a2+8 delta x cube*a3+16 delta x4*a4. Let us call this equation as 5, f(i-2).

Now x-xi in this case would become -2 delta x, so fi-2 delta x*a1+4 delta x square*a2-8 delta x cube*a3+64 delta x4*a4. Let us call this equation as 6. Now we have got the required number of equations. The equation 2 gives us the value of coefficient a0. We are interested in finding out the values of coefficients a1 and a2, a2 will give us the second derivative and a1 will give us the approximation for first order derivative.

Now let us have a look at equations 5 and 6, let us add them together. So what we get f (i+2) +fi-2=2fi, see this a1 and a3, these 2 terms would vanish so we get 4 and 4 8 delta x square*a2+32 delta x to the power 4*a4. Similarly if we add equations 3 and 4, the ones in terms of fi+1 and fi-1, this is equation 7. So add equations 3 and 4. So this addition will again eliminate a1 and a3 terms, so we get yet another equation in terms of a2 and a4.

So we will get f of i+1+f of i-1=twice of fi+2 delta x square*a2+2 delta x to the power of 4*a4. So now this 7 and 8, these 2 equations involve only coefficients a2 and a4. So we can eliminate a4, thereby obtain a value for a2. So to eliminate a4, let us multiply equation 8 by 16. So equation 8*16 that will give us 16*f of i+1+f of i-1=32 fi+32 delta x square a2+32 delta x to the power of 4 a4. Now let us subtract equation 7 from equation 9, 9-7.

If you do that we would be able to eliminate a4, 16 of fi+1+f of i-1=30fi+24 delta x square a2 and on the left hand side we will have 8 and the term –fi+2+fi-2. So now let us rearrange and thus write down the value of 2a2, so 2a2 will become 16 of fi+1+fi-1-fi+2+fi-2-30fi/12 delta x square and this is what we are looking for because twice of a2 gives us the second derivative, so that is del 2f/del x square at i. Now we have got an approximation for it.

Now let us write the terms in index order –fi-2+16fi-1+fi+1-30fi-fi-2/12 delta x square. Now let us summarize this result on our slide. That is what we get del 2f/del x square i=twice of a2, which is –fi-2+16 of fi-1-30 times fi+16*fi+1-fi+2/12 delta x square. Now these equations which we have derived or which we have written for these coefficients a1, a2, a3, and a4, you can also find out and I would leave as an exercise.

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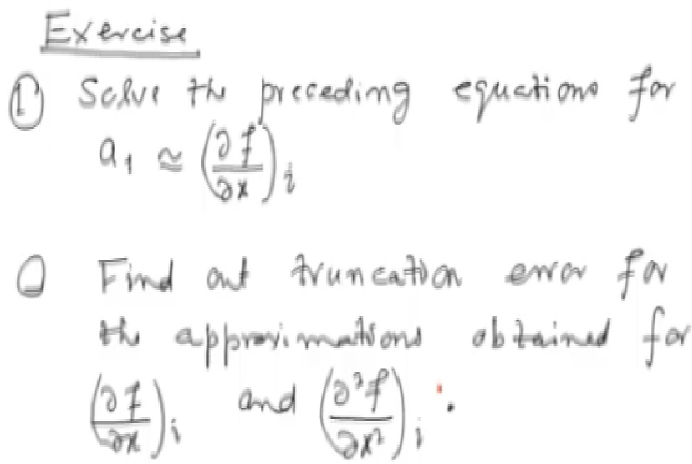

This is an exercise, solve the preceding equations for a1 and if you solve for a1 that is an approximation for del f/del xi. So this is one exercise and the second exercise, which I would like you to do is find out truncation error for the approximations, which we have obtained for del f/del xi and del 2f/del x square i. Use Taylor series expansions to find out your results. Now there is something which I would like to note here, which you can try and verify from your results on truncation error.

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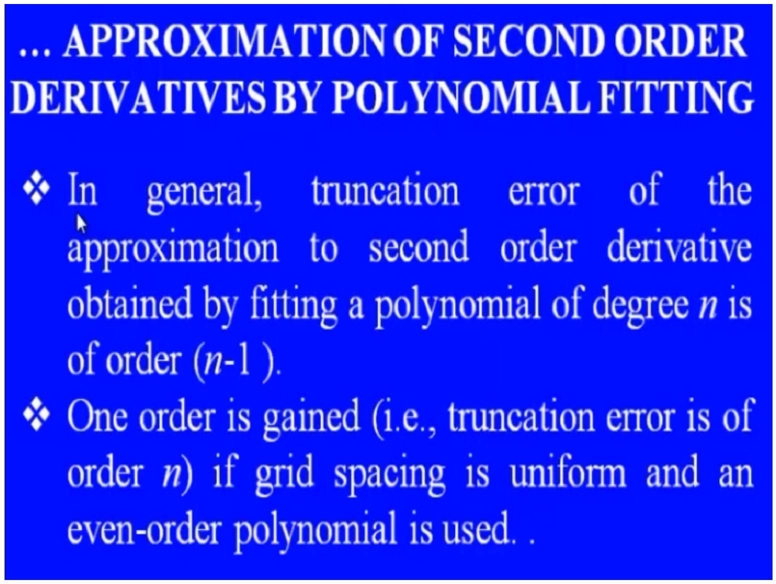

We have already made similar comments on the approximation of first order derivative by polynomial fitting and what happens in the case of second order derivatives. In general truncation error of the approximation to second order derivative obtained by fitting a polynomial of degree n is of order n-1. However, one order is gained that is truncation error is of order n. If grid spacing is uniform, this is the first condition and an even order polynomial is used.

So in just discussed example, we had taken uniform grid spacing and polynomial of order 4. So this observation says that you truncation error should be of order 4. Now please verify from your derivations. Today, in this lecture, we stop here as for the approximation of second order derivatives is concerned and in the next lecture, we will have further look at finite difference approximations for the second order derivative occurring in generic transport equation and for mixed derivatives.

We will also take up the case of multidimensional problems, so how do we obtain the approximation for the derivatives occurring in the partial differential equations in 2 and 3 dimensions and thereafter we will take up few applications in the next lectures.