Computational Fluid Dynamics
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Lecture - 11
Finite Difference Method Approximation of First Order Derivatives

Welcome back to the second lecture in module 03 Finite Difference Method. In the first lecture we covered basic methodology finite difference. In this lecture we are going to focus on obtaining finite difference approximation of first order derivatives.

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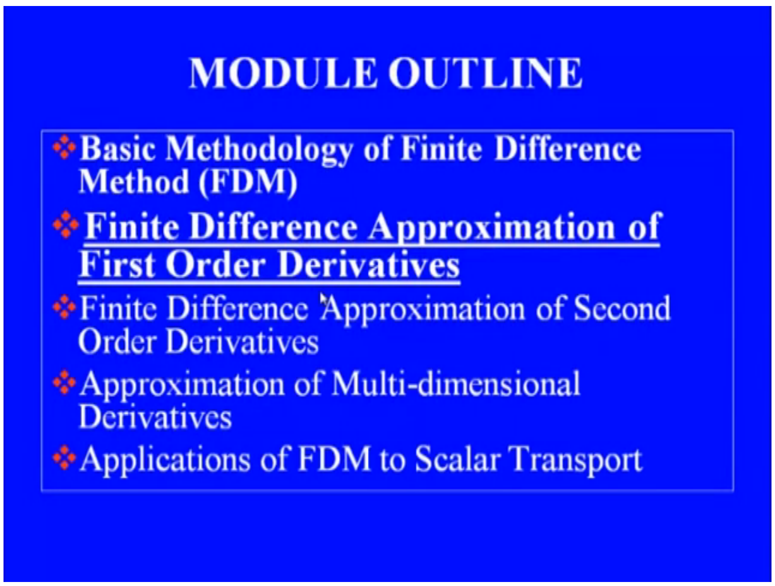

And thereafter, we will go to obtain approximation for second order derivatives, and followed by approximation for multi-dimensional derivatives and applications to scalar transport. Let us have a brief recap of what we did in the last lecture. We discussed basic features of finite difference method for the features which make it very attractive for CFD applications.

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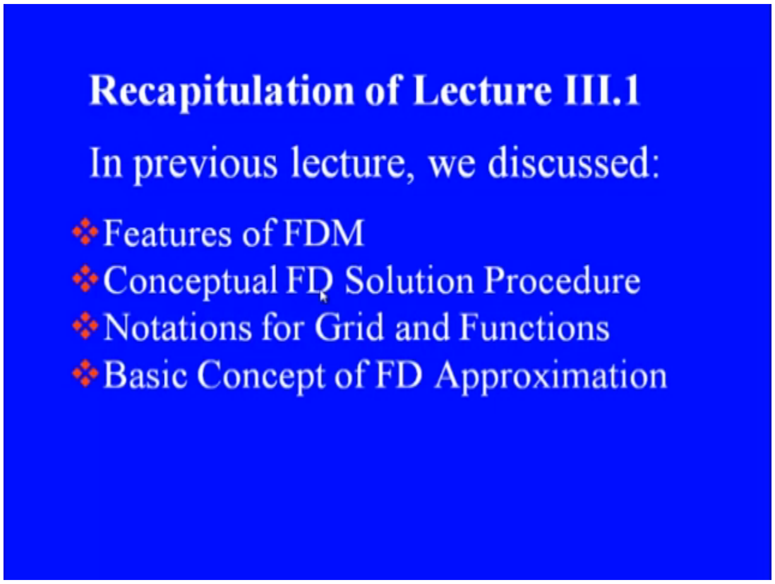

And then we described conceptual framework of obtaining finite difference solution for a flow problem, and we discussed the basic conventions or notations which we use for representing finite difference grid points and functions, and reiterated the basic concept behind finite difference approximation which is based on the basic definition of a derivative. So in this lecture we would now focus on we continue from there and we would obtain the finite difference approximation of first order derivatives.

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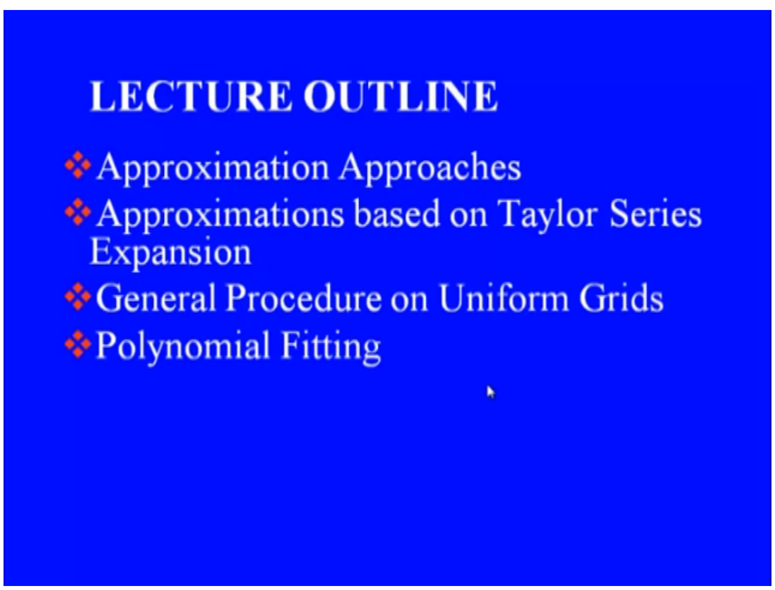

The outline of this lecture we will first have a recap of the approximation approaches which can be used to obtain in the finite difference approximation of partial derivatives, and then we would focus on approximation based on Taylor series expansion, in particular we will look at a general procedure for obtaining finite difference approximation for first order derivative on uniform grids, and then you will have a look at a generic method called polynomial fitting method to obtain an expression of finite difference approximation of first order derivative.

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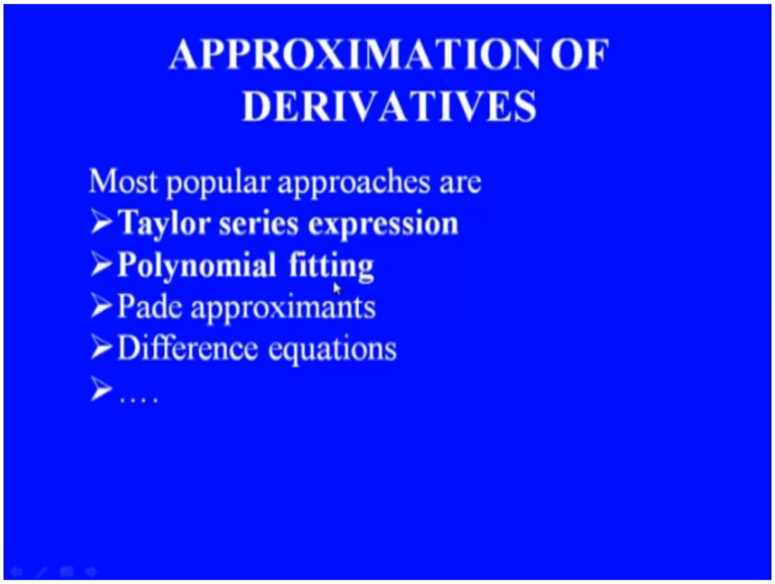

Now we have already seen that most popular approaches Taylor series expression, polynomial fitting, pade approximants, difference equations, there are few other approaches. We would focused primarily on Taylor series expansion and polynomial fitting. So now let us have a look at what is Taylor series expansion.

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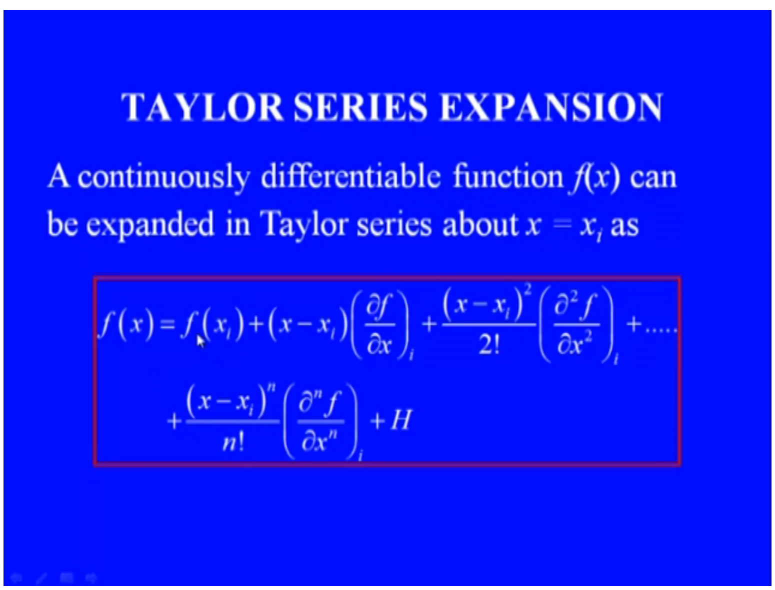

Suppose, we are dealing with a continuously differentiable function f(x) define on the real line, so f(x) can be expanded in Taylor series about x=xi as fxi=value function at point xi+x-xi the first derivative of f at point xi+ x – xi square/2! and the second derivative of f at point xi+ other derivatives+ x-xi to the power n/n! nth derivative of f at point xi+ higher order terms. Now let us use this Taylor series expansion to obtain different expressions or different approximations for first order derivative.

This summary slide will come back to it after we would finish the derivations.

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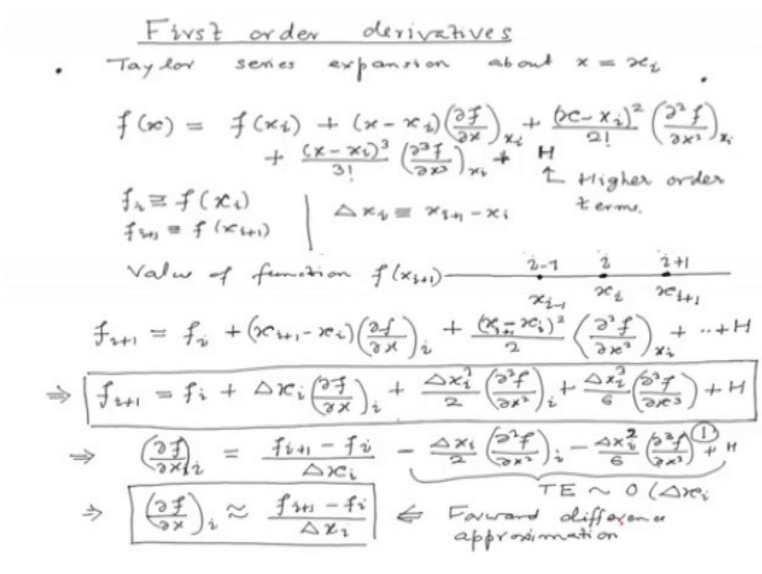

So let us do the formal derivation, so we are interested in finding out approximations for first order derivatives based on the Taylor series expansion, so let us rewrite what we just saw in the previous slide. So Taylor series expansion about x=xi, so at point x in the neighborhood of our grid point xi the value function can be expressed in terms of the function value at the grid point i that is f of xi+ +x-xi del f/del x at point xi+ x-xi squared/2! second derivative of f at point xi+ x-xi cube/3! the third derivative+ so on.

So we can express the reminder terms by symbol H where refers to our higher order terms okay, so now let us draw our one-dimensional grid we are at point xi we have got 1 node to the right of xi which we will called it as xi+1, the indices of these nodes are i, i+1 and then the grid point to the left of xi is xi-1 and its index is i-1. Now we can write the function values at the two neighboring points in terms of the Taylor series expansion.

So let us use the value function at point x= xi+1 function f at xi+1, so now let us switch over to our shorthand notation that is fi+1 which is stands for f of xi+1, this would be =f of i we have now used fi for f of xi, so let us just have recap of the shorthand notation which we have introduced earlier, this fi is stands for fxi, fi+1 we would use this in place of function value at the node xi+1 and so on okay. So now fi+1=fi+ x of i+1-xi*del f/del x at the grid point i+ xi+1-xi whole square/2 del 2 f/del x square xi+ higher order terms.

Now these differences xi+1 and x-xi we can write in terms of delta symbols, so we can write in a compact form that fi+1=fi+ delta xi where remember we have used a symbol delta xi to denote the difference xi+1-xi, so fi+1 it becomes f of i+ delta xi del f/del x at i+ delta xi squared/2 del 2 f/del x square at point i+ delta xi cube/6 del cube f/del x cube + so higher order terms, so this is function value at point xi+1 in terms of the function value at node xi, and the difference between two node points the distance delta xi let us call this as equation 1.

Now we can straight away get a difference approximation by just transferring the fi terms on one side, so this gives us our first expression for del f/del x at point i=f of i+1-fi/delta xi-delta xi/2 del 2 f/del x square at i-delta xi square/6 del cube f/del x cube+ higher order terms, so we can retain the first term on the right hand side agenda or approximation, so we can write an approximation for first order derivative at node i as f of i+1-fi/delta xi, and the remaining terms they become what we call as our truncation error.

So if you look carefully this truncation error is of order delta xi, and here we have used the value at the node forward or to the right of point xi so this is our celebrated forward difference approximation.

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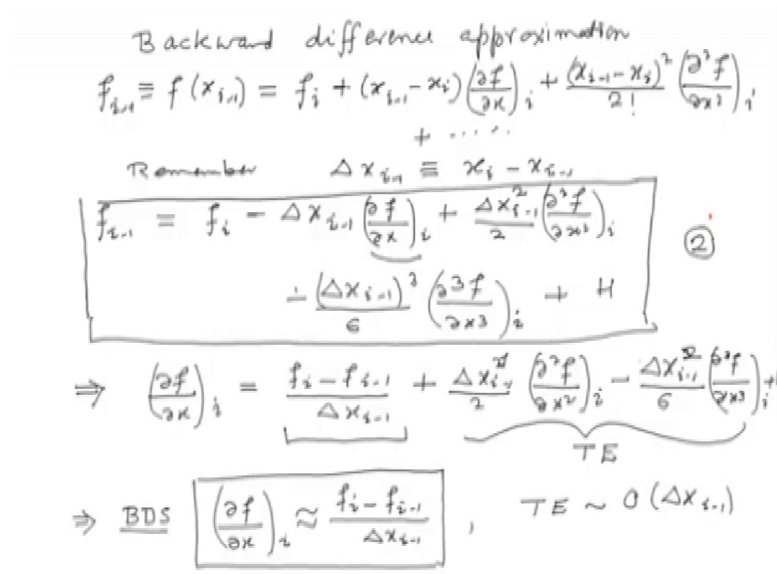

Next, what we can do is to use the function value at the left node and that will give us what we called as our backward difference approximation, so fi-1 which is transfer the function value at point xi-1 this can be expressed by our Taylor series as f of i+x of i-1-xi del f/del x at i+ x of i-1-xi squared/2! The second derivative del 2 f/del x square at point i+ higher order terms. Let us write it more compactly by introducing our delta x terms.

So remember that delta xi-1 this is xi-xi-1, so in terms if you introduce this delta symbol we get a f of i-1=fi-delta of xi-1 del f/del x i+ delta xi-1 squared del 2 f/del x squared at i- delta xi-1 cube/6 del cube f/del x cube at point i+ higher order terms. So if we rearrange this equation that will give us the value of the derivative at point i or rather approximations for that, so del f/del x i this can now be written as fi-f of i-1/delta xi-1+delta xi-1square/2 del 2 f/del x square at point i-delta xi-1 cube/6 del cube f/del x cube at i+ higher order terms.

So we can retain this first term on the right hand side for our approximation of the derivative and remaining terms they will become what we call our truncation error, so we straight away get our BDS approximation scheme backward difference scheme del f/del x at grid point i can be approximated in terms fi-f of i-1/delta xi-1, and once again what we can say this truncation error for this scheme this is of the order of sorry this is of the order of delta xi-1. So both forward difference and backward difference approximations they give us a scheme of first order.

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Central Difference Approximation

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

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

$$\text{CDS}: \left(\frac{\partial f}{\partial x}\right)_i \approx \frac{f_{i+1} - f_{i-1}}{\Delta x_i + \Delta x_{i-1}}, \quad \boxed{TE \sim O(\Delta x_i - \Delta x_{i-1})}$$

$$(TE)_{CDS} < (TE)_{FDS} \text{ or } (TE)_{BDS}$$

$$\text{On uniform grid,} \quad \boxed{(TE)_{CDS} \sim O(\Delta x^2)}$$

Now we can also obtain what we referred to as the central difference approximation, now the central difference approximation can be obtained by combining the two expansions which we had written earlier, one on the previous page which we wrote as an expansion at point xi+1, and the second one which we wrote as Taylor series expansion at point xi-1. So let us subtract the equation 1 from 2.

So what do we get? f of i+1-f of i-1 fi gets cancelled and we get delta xi+ delta xi+1*delta delta f/delta x at i+ delta xi square-delta xi-1 square/2 del 2 f/del x square at i+ delta xi cube+ delta xi-1 cube/6 del cube f/del x cube at point i+ remaining higher order terms. Now this can be rearranged to yield the value of the first derivative, so del f/del x i= f of i+1-f of i-1/delta xi+delta xi-1 + delta xi square-delta xi-1 square/2 del 2 f/del x square at i+ delta xi cube+ delta xi-1 cube/delta xi+delta xi-1 del cube f/del x cube at point i+ higher order terms.

So now let us retain the first term on the right hand side as the approximation of our derivative, the remaining terms that is the one which just put in curly braces they represent our truncation error, so we get the series approximation of central difference approximation for first order derivative as del f/del x i=f of i+1-f of i-1/delta xi+ delta xi-1 so this is the approximation which we get, now truncation error is in this case this is of the order of delta xi-delta x-1.

So formally the truncation error for the series on an non-uniform grid it is still of order one, but if you say it is a difference of two grid spacings, so this truncation error for series TE series this will always be<TE of truncation error of forward difference scheme or backward difference scheme. Moreover, if you have uniform grid then what happens on an uniform grid this the leading term in truncation error vanishes.

so for on uniform grid TE series this now becomes of the order of delta x square, so that is why we say that look the second order accurate our central difference scheme is second order accurate. So let us go back to a slide and say the summary of what we just derived.

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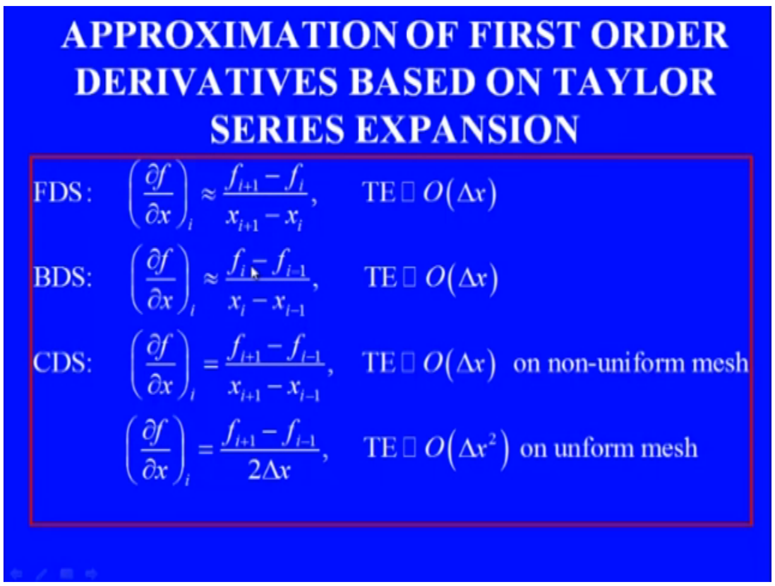

So we derived a forward difference approximation del f/del x at point i=f of i+1-fi/xi+1-xi which is stands for delta xi and truncation error is of the order of delta x, backward difference scheme by using values at the point left towards current point so del f/del x at point I approximately=fi-fi-1/xi-xi-1truncation error is still of the order x. So both of these schemes are first order accurate.

Next, we had obtained an expression for central difference scheme series del f/del x at point i=f of i+1-fi-1/xi+1-xi-1 this what we get when we expand the terms delta xi+delta xi-1, and this scheme is normally first order accurate a sort of delta x on non-uniform mesh, but has a much smaller error co-efficient or truncation error value compared to our forward difference truncation error or backward difference truncation error.

And if a mesh spacing is uniform we get a very simple expression for the derivative del f/del x at point i=f of i+1-fi-1/2 delta x, and in this case truncation error is an order of delta x square that should say our difference approximation is second order accurate on uniform mesh. It is also possible for us to derive a central difference formula for first order derivative which would be second order accurate on any grid and for that we have to do a bit more jugglery or algebra with respect to the 2 expansion or Taylor series expansion which we wrote earlier.

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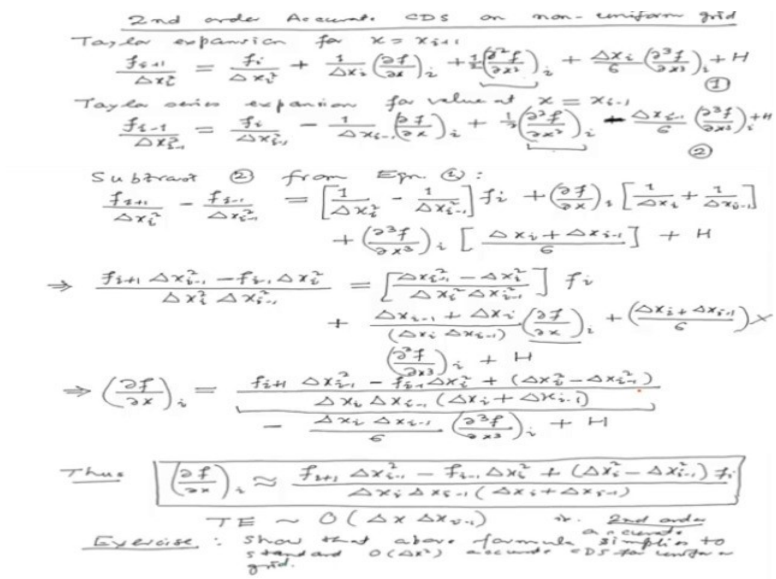

So now let us derive a second order accurate central difference approximation or CDS on non-uniform grid for this you rewrite our previous Taylor series expansions by dividing by the square of the mesh spacing or main purpose would be to eliminate the second order derivative from the expansions. So let us write our Taylor series expansion for x=xi+1, so this we can write it as fi+1/delta xi squared, we just dividing the entire expression which we written earlier by delta xi square.

So this will become fi/delta xi square+1/delta xi del f/del x at point i+1/2 del 2 f/del x square at point i+ delta xi/6 del cube f/del x cube at point i+ our higher order terms. Similarly, let us rewrite our Taylor series expansion for value at x=x of i-1 in terms of a mesh spacing and if we can write f of i-1/delta xi-1 square= fi/delta xi-1 square-1/delta xi-1 del f/del x at point xi+1/2 del 2 f/del x square at i- delta xi-1/6 del cube f/del x cube at i+ higher order terms.

Now if you subtract the bottom equation from top one, we would be able to eliminate the second order derivative that is what we wanted, let us call the first equation top equation as 1, and the bottom equation as 2, subtract 2 from equation 1. So what we get on LHS? We will have f of i+1/delta xi squared- f of i-1/delta xi-1 square on the right hand side the first term would be let us take fi common, so 1/delta xi squared-1/delta xi-1 squared*fi.

Similarly, for the second term let us take del f/del x i common so del f/del x at point i and we are left with 1/delta xi+1/delta xi-1, sorry this small correction here this term has to be negative, the third terms they cancel del 2 f/del x square half of it is in top equation and the same in the bottom equation so these 2 would cancel out, so next term which we get is del cube f/del x cube at i delta xi+ delta of xi-1/6 + higher order terms.

Now let us simplify the terms a little bit, so on the left hand side we will have f of i+1 delta xi-1 squared-f of i-1 delta xi squared/delta xi squared delta xi-1 squared on the right hand side similarly, we will get delta xi-1 squared- delta xi squared/delta xi squared delta xi-1 squared this becomes multiplied by fi+ delta xi-1+ delta xi/delta xi delta xi-1*del f/del x at i+ delta xi+ delta of xi-1/6 this is multiplied by the third order derivative del cube f/del x cube at i+ higher order terms.

So now we can rearrange to obtain an expression for a first order derivative, so del f/del x at point i so this would be = f of i+1 delta xi-1 squared-f of i-1 delta xi squared+ delta xi squared-delta xi-1 squared whole thing/delta xi delta xi-1* delta xi+ delta xi-1-delta xi delta xi-1/6 del cube f/del x cube at point i+ higher order terms. So now you can clearly say that we have by eliminating the second derivative del 2 f/del x cube.

We now get 1 series approximation by retaining the first term which would be second order accurate irrespective of the grid spacing. So thus, we can write our series approximation as, and truncation error this is of the order of delta x*delta xi-1 that is this is scheme is second order accurate irrespective of the mesh spacing. if a mesh is uniform you can do a simple algebra, so that I would leave as an exercise to you.

So exercise show that above formula simplifies to standard series delta x square accurate series for uniform grid. Now so for what we did we wrote a Taylor series expansion and we used our own ingenuity to eliminate few terms and obtain the difference approximation for the first order derivative. Now the procedure was intuitive, so we had to guess which equation to subtract and which one to multiply by fort and then do the subtraction.

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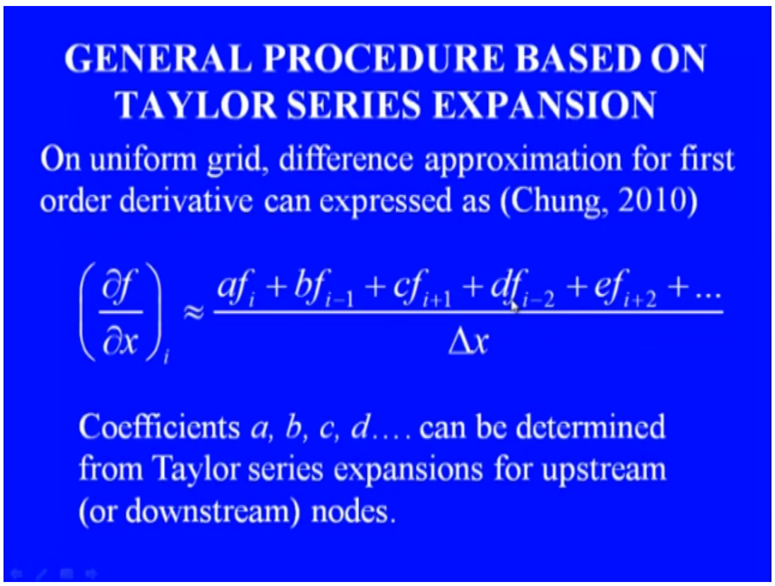

Now if you are dealing with uniform grid Chung proposed a general formula that if you have got uniform grid difference approximation for first order derivative can be expressed by the simple generalized formula, that remember for uniform a grid on the denominator we will have this delta x anyway and that numerator will contain the function values at different grid points multiplied by some numerical multipliers.

So just using this simple logic as Chung proposed this formula del f/del x i is approximately= afi+ bfi-1+ cfi+1+ df1-2+ efi+2 and so on, so we can choose as many number of the neighboring grid points as we would like to have to derive or to obtain a difference approximation for the first order derivative order, and to obtain the values for this a, b, c, d this coefficients they can be determined from Taylor series expansion for upstream nodes that is our nodes i+1, i+2 so on or downstream our nodes i-1, i-2 so on.

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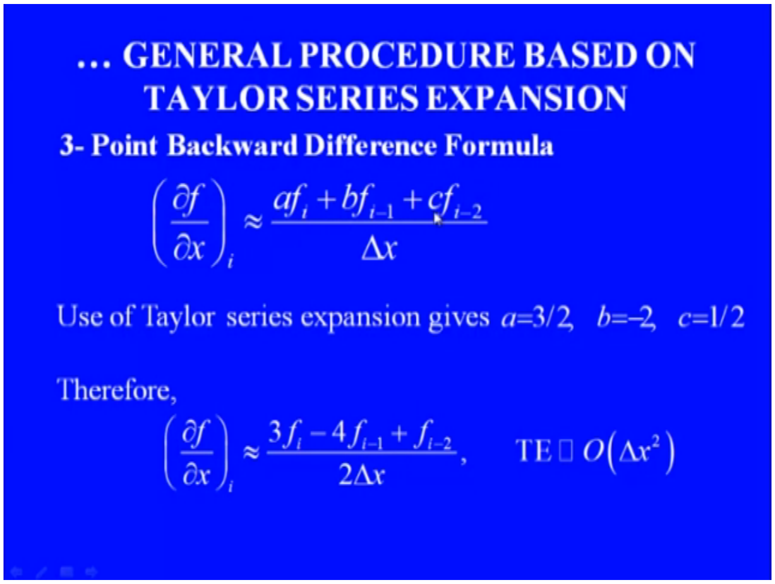

So one simple example of this 3 point backward difference formula that if you want to use values at to downstream nodes or backward nodes, in addition to the function value at point xi so afi+ bfi-1+ cfi-2/delta x this would give us difference approximation to the first order derivative at del f/del x i. Now let us try and get the values of these coefficients by performing a simple Taylor series expansion.

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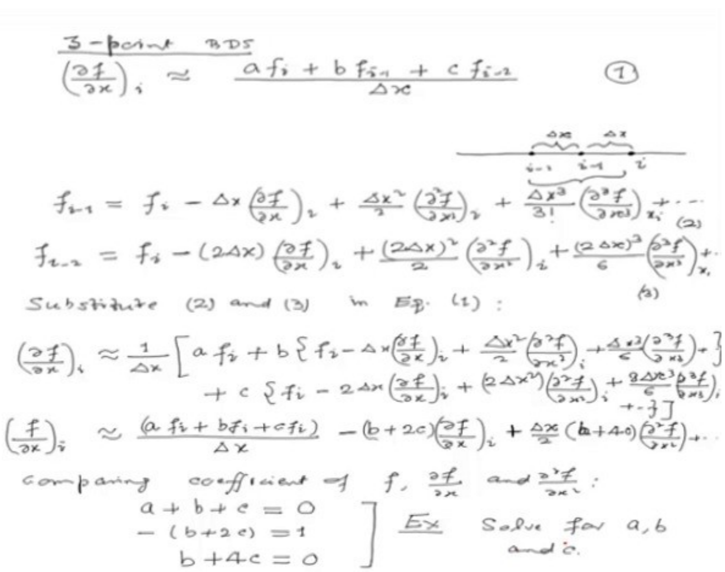

So 3 point BDS, so we had written as this del f/del x i is approximately =afi+ bfi-1+ cfi-2/delta x, now please remember our grid spacing which is uniform, let us say this is our point i delta x to the left of it we have got the point i-1, and this point i-2 this is further at is distance delta x from the node xi-1. So the function value at point xi-1, if you use Taylor series expansion this would become fi-delta x del f/del x at i+delta x square/2 del 2 f/del x square at point i+delta x cube/3! del cube f/del x cube at point xi and + so on remaining higher order terms.

Similarly, the function value at the grid point i-2 in terms of Taylor series can be written as fi-2=f of i-2 delta x because fi-1 node this is situated at the distance of twice of delta x left of point xi, so 2 delta x times del f/del x at point i+2 delta x squared/2 del 2 f/del x square at i+2 delta x whole cube/6 del cube f/del x cube at xi+ so on. Now let us substitute these expressions in our formula 1, so let us call that is 1, the expansion fi-1 let us call it as expression 2 and the expansion for i-2 let us it as expression 3.

To substitute 2 and 3 in equation 1, so if you do this substitution what do we get? On left hand side we have got del f/del x at i, on the right hand side what do we get? let us take 1/delta x common let us collect the term one by one so afi that remains as such afi+ b times fi-delta x del f/del x i+ delta x square/2 del 2 f/del x square at i+delta x cube/6 del cube f/del x cube+ the higher order terms+ the c times fi-2 delta x del f/del x of i+2 delta x whole square that becomes 4 delta x square/2 so that gives us 2 delta x square del 2 f/del x square at i+8 delta x cube/6 del cube f/del x cube of i+ H.

Now let us collect the terms together, so what do we get? the terms which correspond to the function values so we will get a of fi+ b of fi+ c of fi/delta x-b+2c del f/del x of i+ delta x/2*b+4c del 2 f/del x square+ so on, so now let us compare the terms on left hand side and right hand side, on the left hand side we have got only del f/del x and its coefficient is 1, so the coefficient of fi on the right hand side that must be 0.

So comparing these coefficients of f, del f/del x and del 2 f/del x square what do we get a+b+c=0, -b+2c=1 and b+4c this would be = 0. So now can we solve these equations to get the values, so I would leave this that is a simple exercise, exercise solve for a, b and c and once we have obtained the values of a b and c we will get our expression for the first order derivative using our generalized expression on a uniform grid.

So that is what we get we should get a=3/2, b=-2 and c=1/2. so therefore, we get this 3 point backward difference formula is del f/del x i= 3 of fi- 4 of fi-1+ f of i-2/2 delta x and if you can substitute the values of a, b and c into the terms which the coefficient of del cube f/del x cube you will find out the truncation error of this scheme is of order delta x square, that is this 3 point backward difference formula is second order accurate.

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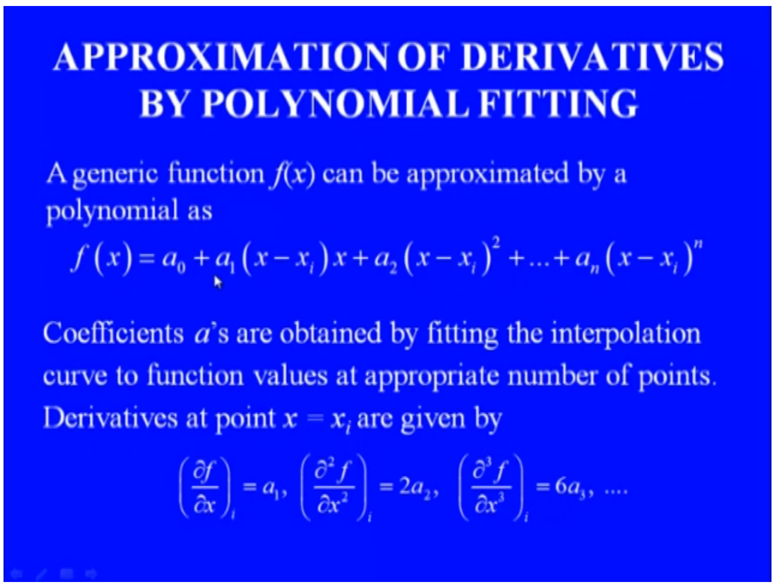

Now next, let us move on to the approximation of derivatives by polynomial fitting, so if you have any generic continuous function let us call this function f(x) it can be approximated by a polynomial as, now we have taken the polynomial expansion around the point xi to simplify the algebra for obtaining finite differences expressions f(x) can be written as a0+ a1 times x-xi+ a2 times x-xi whole square+ and so on up to an x-xi to the power n.

Now these co-efficient a's a0, a1, a2 and an they can be obtained by fitting this interpolation curve to function values at appropriate number of points, and once you have obtained this approximation or this interpolation curve how do we obtain the derivatives? That was simple let us just differentiate this interpolation function, so if we differentiate it once what do we get? del f/del x i that will simply be the coefficient a1, differentiated twice so we get del 2 f/del x square = twice of a 2.

Similarly, third derivative at point xi this will become 6 times a3 and so on. So once we have obtained this interpolation we should be able to obtain any order derivative up to order n-1 using this. As an example let us find out using polynomial fitting a 3 point finite difference approximation which we would need a quadratic polynomial at grid point i-1, i and i+1.

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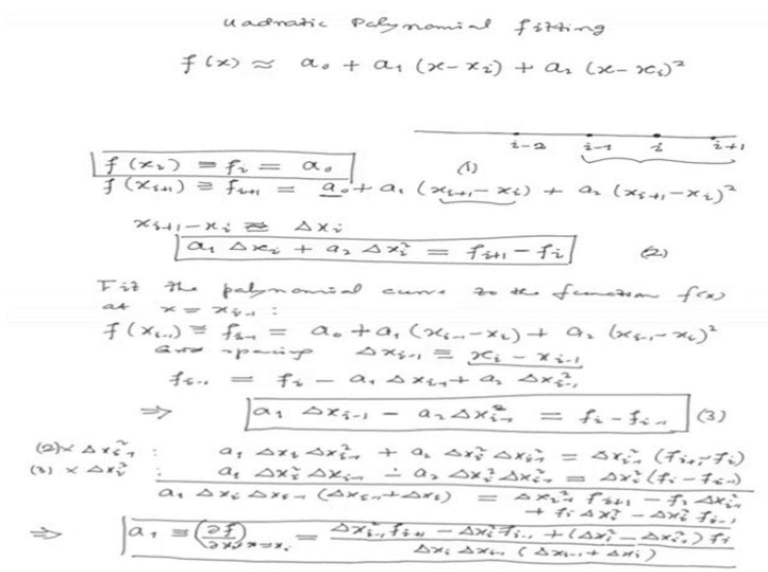

We want to have a quadratic polynomial fitting, so f of x that is would be approximate by the polynomial a0+ a2 times x-xi+ a2 times x-xi whole square, so here we have got 3 unknown coefficients a0, a1 and a2 and these we would determine by using function values at point i, i-1 and i-2 or rather let us take a centralized difference formula, let us use the values at i, i-1 and i+1. So they are 3 node points.

So what is the function value at point xi that is our fi this would simply be=a0 because remainder terms if you substitute x=xi they vanish, so this becomes our first equation f at xi+1 what will this be we denoted by xi+1=a0+ a1 times xi+1-xi + a2 times xi+1-xi square. Now let us make use of shorthand notation for the grid spacing, so xi+1-xi we would use the symbol delta xi so therefore, we get an expression of this form a1 times delta xi+ a2 times delta xi squared= fi+1-fi.

Where we have substituted the values for a0, a0=f of i, so this becomes our second equation, now let us fit this polynomial at point i-1. So fit the polynomial curve to the function f(x) at x=xi-1, then what we will get? fxi-1 which we would denote by f subscript i-1=a0+ a1 times xi-1-xi + a2 times xi-1-xi whole square, introduced the grid spacing delta notation, so delta xi-1 this is stands for xi-x of i-1.

So in terms of this grid spacing which is a positive quantity, the previous expression would be f of i-1=fi substitute as fi the value of a0- a1 times delta xi-1+ a2 times delta xi-1 whole square, so if you rearrange what do we get? We get a1 times delta xi-1- a2 times delta xi-1 whole square=fi-f of i-1, so this is our third equation. Now you have got 3 equations for 3 unknowns 1,2 and 3, the first equations straight away gives us the value of a0.

We are interested in finding out the value of a1, so we can solve equation 2 and 3 to get the value of a1. There are 2 simple linear equations and it should be pretty straight forward to eliminate this a2, so how do we eliminate a2? Multiply equation 2 by delta xi-1 squared, and equation 3 by delta xi. so what we get equation 2*delta xi-1 square, so this will give us a1 times delta xi delta xi-1 squared+ a2 times delta xi squared delta xi-1 whole square= delta xi-1 squared times f of i-1-f of i.

Equation 3 times delta xi squared that will give us a1 times delta xi squared delta xi-1- a2 times delta xi squared delta xi-1 squared= delta xi squared times fi-f of i-1 just add these 2 equations and thereby you would be able to eliminate a2, so we get a1 times delta xi delta xi-1*delta xi-1+ delta xi=delta xi-1 squared f of i+1-fi times delta xi-1 squared+ fi times delta xi squared-delta xi squared times f of i-1.

So if you rearrange the terms we straight away get expressions for a1 and this a1 is nothing but the derivative which we wanted del f/del x at point I or x=xi= delta xi-1 squared f of i+1- delta xi squared times f of i-1+ delta xi squared- delta xi-1whole squared fi/delta xi delta xi-1 delta xi-1+ delta xi. So now we have obtained an expression for first order derivative using polynomial fitting.

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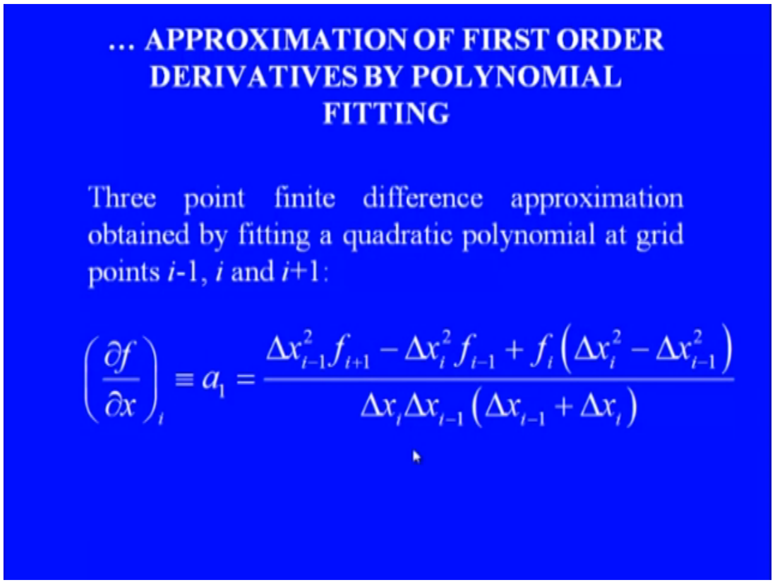

And if you want you can go back and compare you have obtained same expression earlier using Taylor series expansion. So that confirms that the two approaches can give us identical results, so we can either use polynomial fitting approach or Taylor series expansions to obtain the expression for the first order derivative, and how about the accuracy you can find out or workout the truncation error term by putting the Taylor series expansion.

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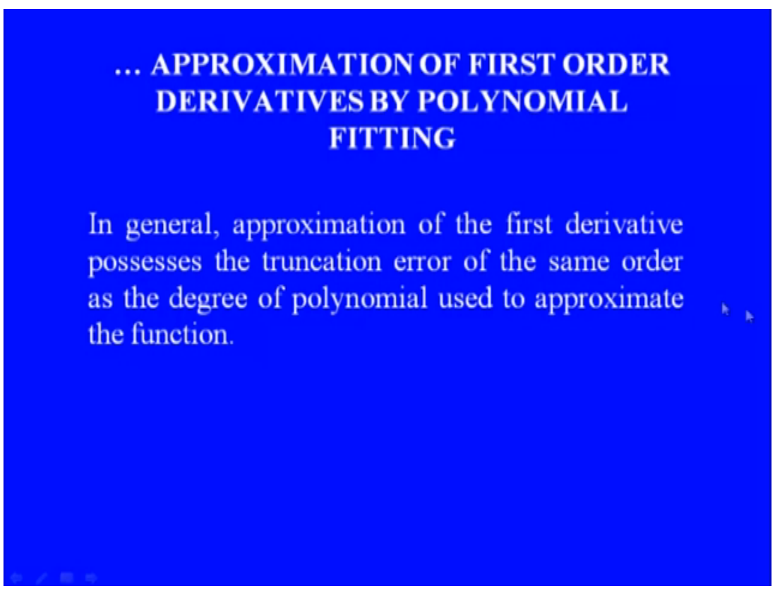

And this is general observation, that in general approximation of the first derivative but this is the truncation error of same order, for instance if you just use the quadratic polynomial fitting which was second order polynomial and that approximation which we got that was second order accurate. So in general the approximation of the first order derivative produces truncation error of the same order either degree of polynomial used to approximately function.

So this where we are going to stop today, and the next lecture we will take up the finite difference approximations for second order derivatives.