

Computational Fluid Dynamics
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Module no. # 03

Template for the numerical solution of the generic scalar transport equation

Lecture no: 08

Topics

Spatial discretization of a simple flow domain

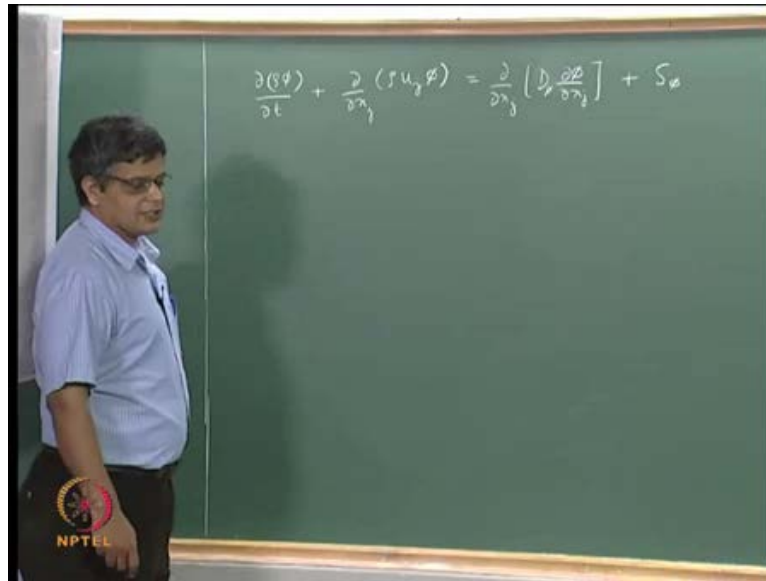
**Taylor series expansion and the basis of finite difference
approximation of a derivative**

Central and one-sided difference approximations

Order of accuracy of finite difference approximation

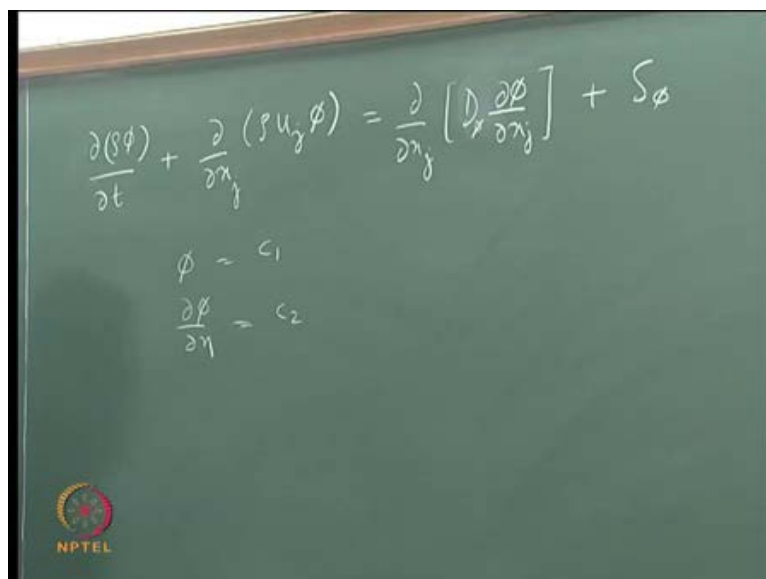
Well, we have derived the generic Scalar transport equation. Today, we will start looking at discretization of the equation to convert this back in to an algebraic equation on a structured grid on a simple grid. We are looking at the case of a flow domain which is described in terms of a Cartesian mesh, where the boundaries of the flow domain coincide with planes of constant x constant y and the constant z. And the same argument can be readily extended to cylindrical polar coordinates or spherical polar coordinates. Example: for a flow through a cylinder or a flow through an Annulus or some heat transfer in a sphere and such cases.

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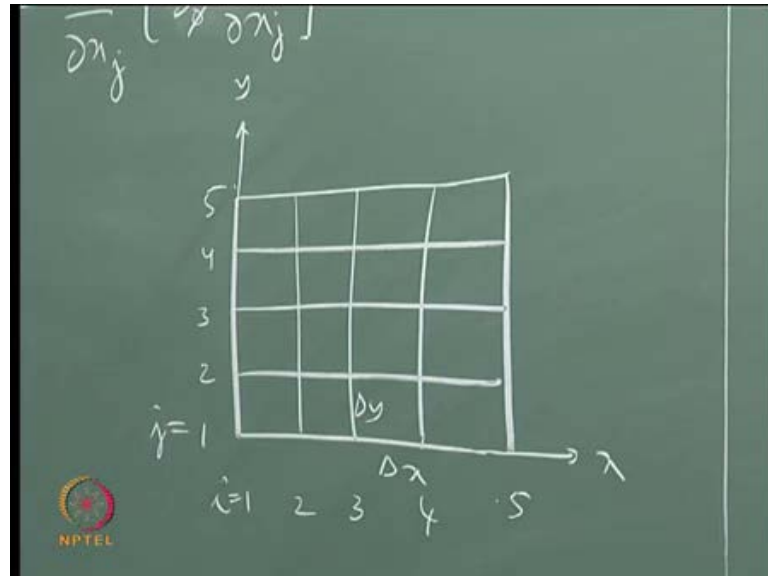
So, we are looking at a case of a scalar transport equation $\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u_j \phi)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[D_r \frac{\partial \phi}{\partial x_j} \right] + S_\phi$ where $\frac{\partial(\rho\phi)}{\partial t}$ is the accumulation term; $\frac{\partial(\rho u_j \phi)}{\partial x_j}$ is the advection term; $\frac{\partial}{\partial x_j} \left[D_r \frac{\partial \phi}{\partial x_j} \right]$ is the diffusion term; and S_ϕ is the source term.

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So, this is a general form of the equation that you want to solve subjective either at Dirichlet condition ϕ is a given value or a boundary or for example, $\frac{\partial \phi}{\partial n}$ equal to c two or a linear combination or any other combination.

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So, this is a problem that we have a, **a**, domain, which is right now we are considering it to be a regular domain which can be fitted in x and y coordinates. For example, this boundary coincides with constant y ; this boundary coincides with constant y ; this boundary coincides with constant x and this is constant x .

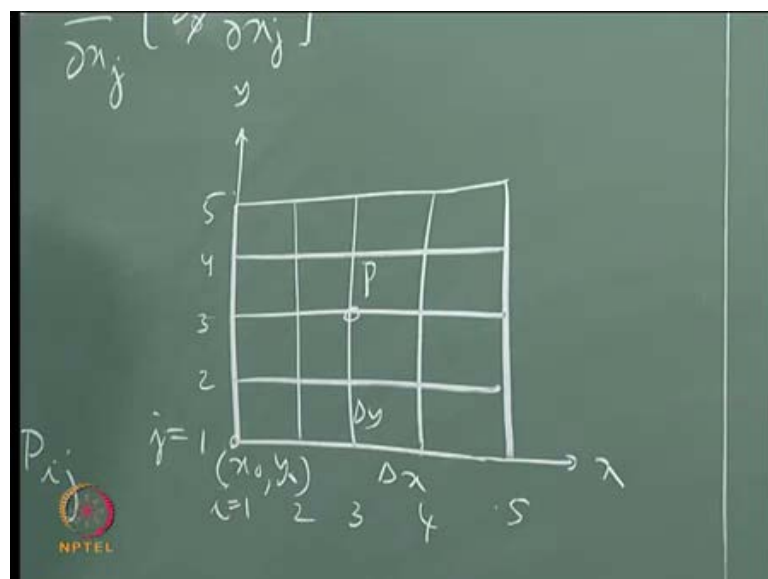
So, in such a case, we have said earlier that it is quite easy a trivial exercise to put a regular mesh in each of the coordinate direction with equal spacing for the sake of simplicity such that we have a spacing of Δx in the x direction and a spacing of Δy in the y direction. In such a case, each of these lines of constant x and constant y can be noted; can be given an index i and j i is constant x lines. So, this is i equal to 1 means this boundary 2, 3, 4, and 5 and j equal to 1 here is this 2, 3, 4, 5.

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In which case, the $x_i y_j$ corresponding to the same point p here can be written as x_i is equal to x_0 plus i minus 1 times Δx and y_j is y_0 plus j minus 1 times Δy - where x_0 and y_0 are the coordinates of this particular corner. So, in this way, we can identify the location of any point p which is at the intersection of the level of constant x and constant y with the corresponding grid index i and j in this way, and we can, we will refer to this point p at $x_i y_j$ at p_i, j or when there is no confusion, we can also write it as p_{ij} . So, and in the third three dimensions, we will have one more index z_k - where z_k will be given by z_0 plus k minus 1 times Δz .

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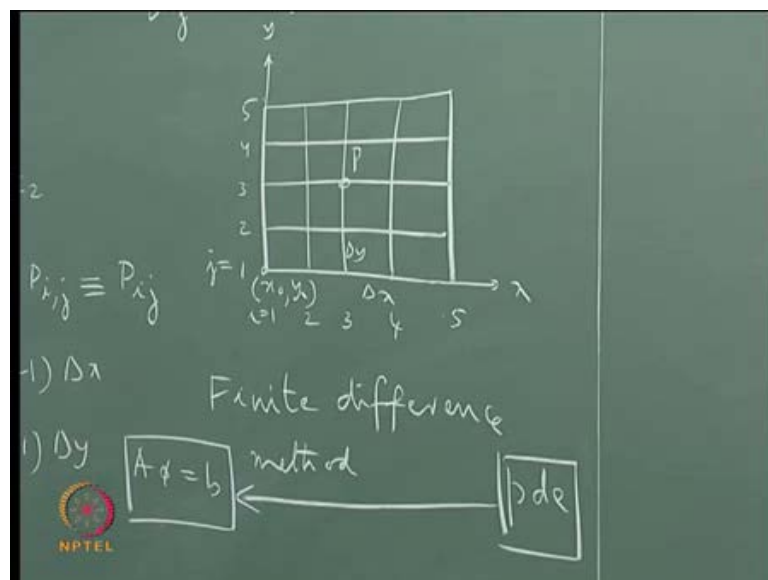


So, when you have a simple flow domain which is bounded by lines of constant coordinate planes, then it is a trivial exercise to fit a uniform grid of a given delta x chosen properly so that you can fit an integral number of coordinate planes within that, and then, accordingly, you can find out. You can discretize the whole flow domain into tiles like this and the objective would be to find the values of the variable at the intersection of these points. For example, like p here and a q maybe r and so on.

So, if we want to do this, then on a structured grid like this where every point here has four neighbors, four immediate neighbors in a two dimension case and six neighbors in the case of three dimension. Then, we can make use of finite difference, we can make use of finite difference, to convert this partial differential equation into an algebraic equation which is valid at every grid point and in so doing, we will be expressing the value of phi at this point in terms of the value at this point and the neighbouring points.

So, by doing that, systematically for all these points at which we want to have the value of phi. We will be able to convert this partial differential equation into a set of algebraic equations which can be written as a phi equal to b.

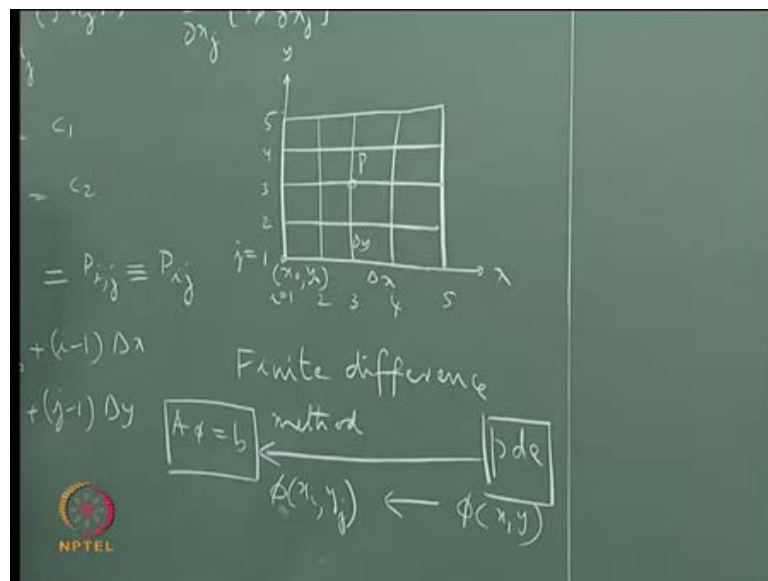
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So, using finite difference method, we convert p d e into an algebraic equation like this and this can be solved using any number of methods. So, the objective of the discretization of the equations, right now this is a continuous an equation expressed in terms of continuous variables, but in a CFD solution, we seek the solution at discrete pre determined points which are the points with are associated with the grid or the discretization of the flow domain and we want to have the values of phi which is the unknown variable here at the intersection of this constant lines of coordinate plane.

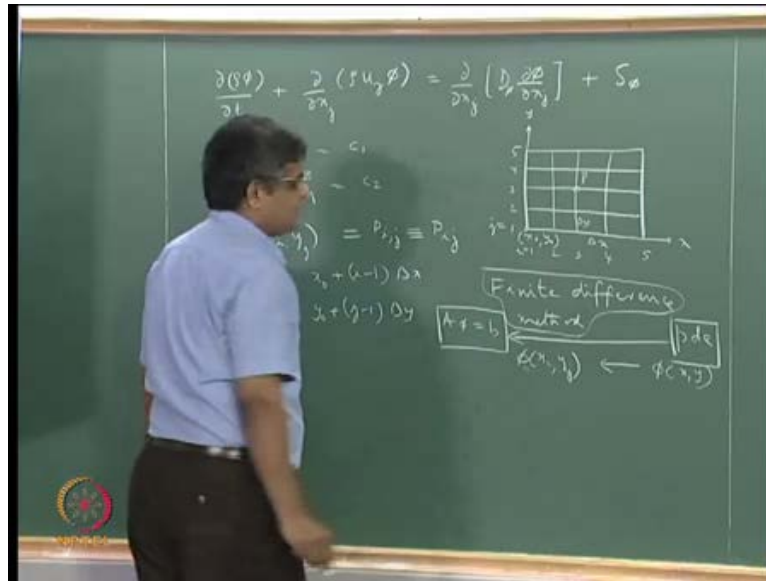
So, in this sense, this p d e which is expressed in terms of continuous variables is expressed now in terms is converted in to an algebraic expression in which the unknowns are the values of phi at all those grid points at which we want to find the solution. Here, we have no choice, but to find the value at all interior points, we cannot say we want to have the value only at this particular point. We can get the value of this, only at this point only when we find the value at all the other points also.

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So, the objective is to go from phi x y to phi x i y j so that to, in order to find these values, we need to solve only an algebraic equation, a set of algebraic equations, not a partial differential equation.

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So, in order to do this, we can make use of finite difference method, **finite difference method**, to systematically replace each derivative by an equal and finite difference approximation and so we need to see how we can, **how we can**, find a finite difference approximation for the given derivative.

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So, the idea is very simple. If you have phi of x, so, let us consider the case of one-dimension and we are looking at a function phi of x, and so, phi of x plus delta x, that is,

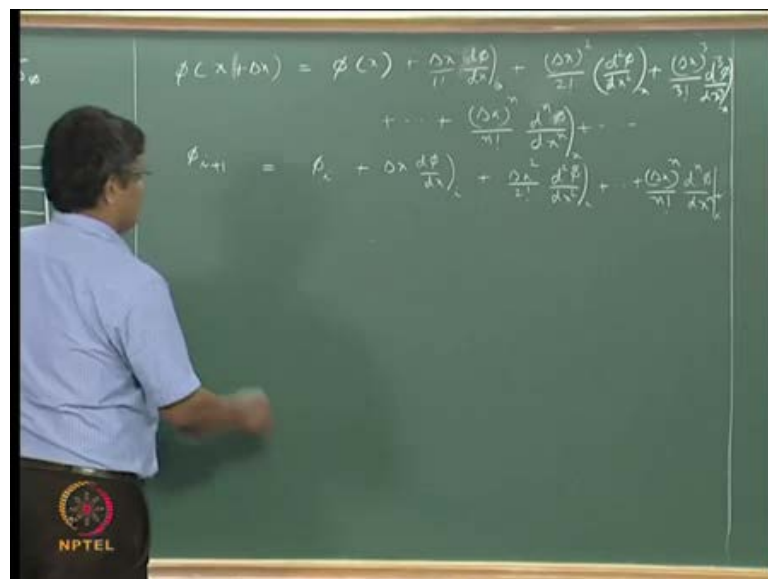
the value of the function at a point which is slightly displaced from x can be expressed in terms of the function at x in the following way using the Taylor series approximation.

We can write this as $\phi(x + \Delta x)$ as $\phi(x) + \Delta x$ times, we are looking at, let me just put it as $d\phi$ by dx at x plus Δx cube by factorial 3 and so on plus Δx raised to the power n by factorial n $d^n \phi$ by dx^n , that is all. This is the Taylor series function of the function ϕ at $x + \Delta x$ in terms of the function ϕ of x and its derivatives all defined at the same point x around which we are expanding this.

We note here that the first derivative is evaluated at x ; second derivative is evaluated at the third derivative, and n th derivative, all the derivatives are defined at particular x .

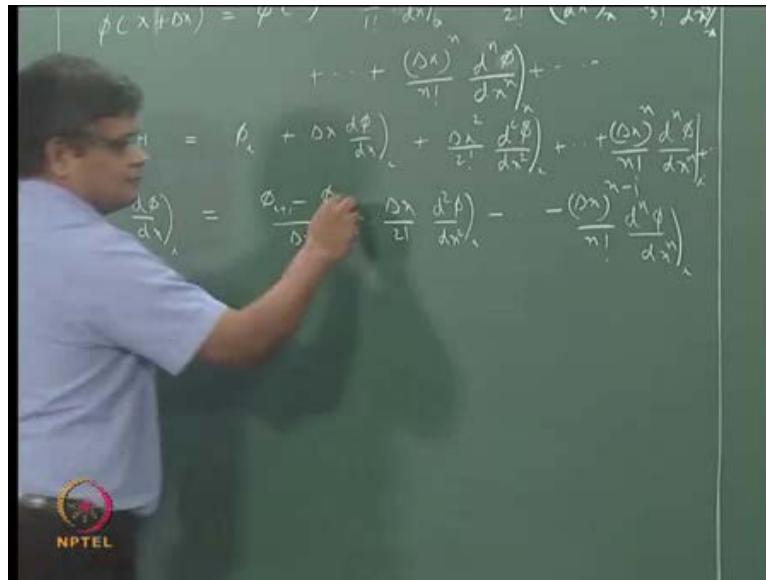
So, if we have an analytical expression for ϕ of x , then and if this function is continuously differentiable and all these derivatives are known, then we can find out the value of ϕ at a neighboring point only from the knowledge of the function at a particular point and at its derivatives. And this series has an infinite number of terms and this would converge for small values of Δx . And we can put this in our notation where we can say that x_i is x nought and i minus 1 Δx like this. We can say that, so, this is x plus Δx .

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So, we can say that, so, if ϕ of x is ϕ of i , then x plus Δx , that is, one grid point away can be expressed as ϕ of $i + 1$ is equal to ϕ of i plus Δx times factorial 1 and i plus Δx square by factorial two times d square ϕ by dx square at i plus Δx raised to the power n by factorial n d n ϕ by dx n evaluated at i and so on like this.

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So, from this, we can write an approximate formula for this. We can write therefore, from this, $d\phi$ by dx at i is equal to ϕ of $i + 1$ minus ϕ of i by Δx . So, I take all these things on to the left hand side and then I divide by Δx here minus Δx by factorial 2. This square here will cancel with this, so, I have d square ϕ by dx square at i minus, minus Δx n minus 1 by factorial n d n ϕ by dx n like this.

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The image shows a chalkboard with the following handwritten text:

$$\phi(x+\Delta x) = \phi(x) + \Delta x \frac{d\phi}{dx} + \frac{(\Delta x)^2}{2!} \frac{d^2\phi}{dx^2} + \dots + \frac{(\Delta x)^n}{n!} \frac{d^n\phi}{dx^n} + \dots$$
$$\phi_{i+1} = \phi_i + \Delta x \left. \frac{d\phi}{dx} \right|_i + \frac{\Delta x^2}{2!} \left. \frac{d^2\phi}{dx^2} \right|_i + \dots + \frac{(\Delta x)^n}{n!} \left. \frac{d^n\phi}{dx^n} \right|_i$$
$$\Rightarrow \left. \frac{d\phi}{dx} \right|_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\Delta x}{2!} \left. \frac{d^2\phi}{dx^2} \right|_i - \dots - \frac{(\Delta x)^{n-1}}{n!} \left. \frac{d^n\phi}{dx^n} \right|_i$$
$$\left. \frac{d\phi}{dx} \right|_i \approx \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

NPTEL logo is visible in the bottom left corner.

So, if I can neglect all these terms, then I can therefore write it as $d\phi$ by dx at i is roughly equal to $\phi_{i+1} - \phi_i$ divided by Δx .

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The image shows a chalkboard with the same handwritten text as the previous slide, but with the following additions:

$$\Rightarrow \left. \frac{d\phi}{dx} \right|_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\Delta x}{2!} \left. \frac{d^2\phi}{dx^2} \right|_i - \dots - \frac{(\Delta x)^{n-1}}{n!} \left. \frac{d^n\phi}{dx^n} \right|_i$$

The terms $-\frac{\Delta x}{2!} \left. \frac{d^2\phi}{dx^2} \right|_i - \dots - \frac{(\Delta x)^{n-1}}{n!} \left. \frac{d^n\phi}{dx^n} \right|_i$ are circled in red and labeled "higher order terms" in red handwriting.

$$\left. \frac{d\phi}{dx} \right|_i \approx \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

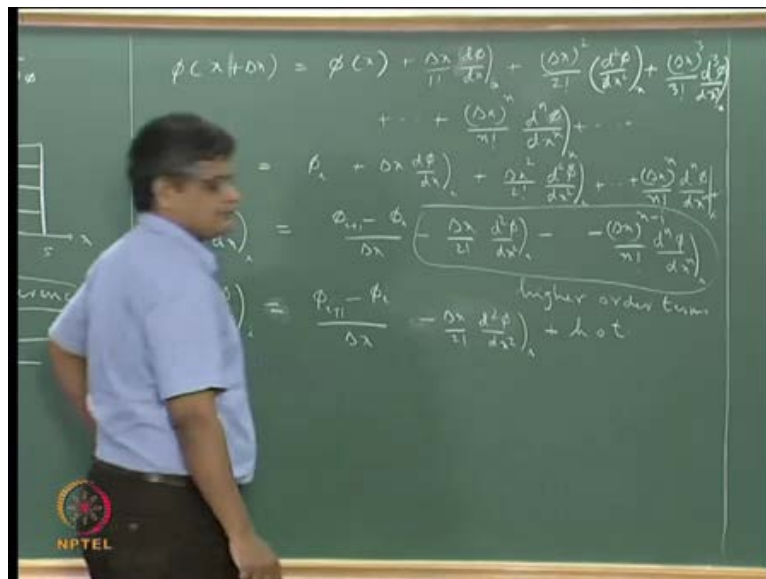
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So, in this approximation, we are neglecting all these terms. We call these as higher order terms. The idea being that when we do this expansion if Δx is very small and $\phi(x)$ is a smooth function, then we have, we can estimate the magnitude of each of these terms, and typically, when we have a continuous function, the magnitude of these terms will start decreasing may be after a few terms successively so that this term is smaller

than the next term and this is smaller and all these things. So, in that sense, so that eventually it will converge; the values will become so small that it will converge.

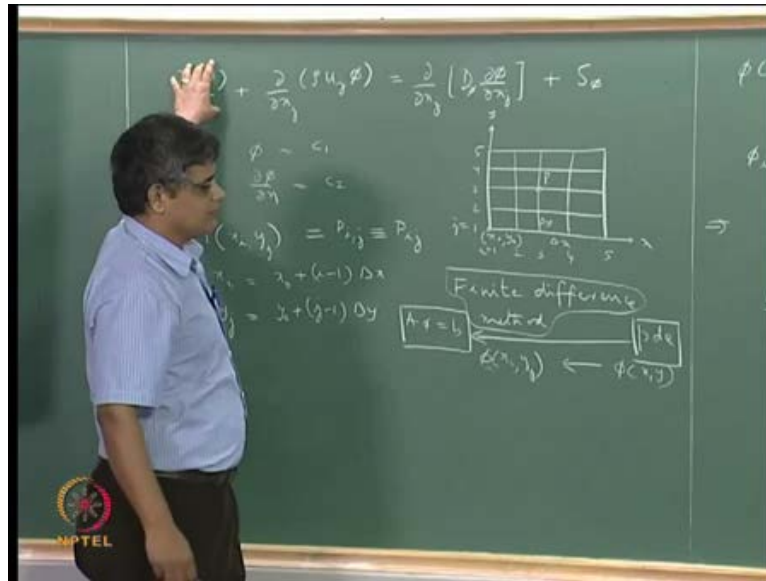
So, the idea is higher order terms - the terms which are coming later in this series - are smaller and smaller so that their contribution can be neglected. So, in that sense, you can write this approximately like this. It is not necessary that for a given function; this term is always less than this term or the next term is less than this, but in general, for provided Δx is very small and $\phi(x)$ is a smooth function, we may expect that significantly higher order terms are, **are**, successfully smaller and smaller in magnitude. So, there is some justification for writing it like this

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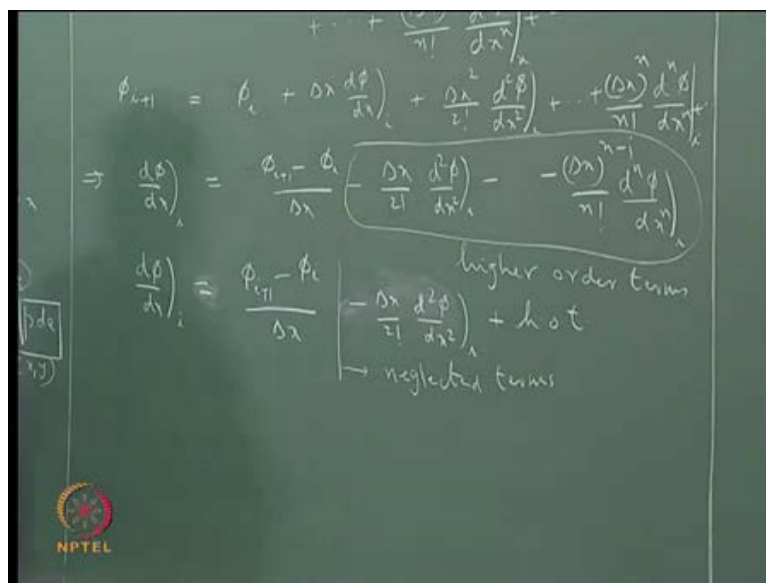


And So, we can say that this is equal to plus higher order terms h o t. And when we talk about the higher order terms, we characterize these higher order terms by putting the first term the leading term in the terms that are neglected. So, we can say that this is minus Δx by factorial two times $d^2 \phi$ by $d x$ square i plus higher order terms.

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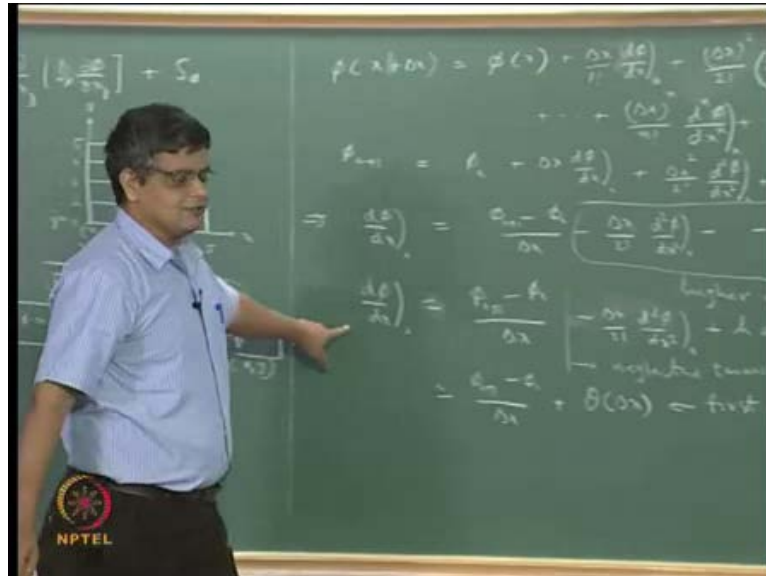


So, we can replace, for example, a derivative here, first derivative here with a corresponding expression like this and truncating this series at this point itself. So, all these terms are neglected and these are all the neglected terms.

By convention, the approximation, the order of this approximation is designated by the power of the delta x of the leading term that appears in the leading term. So, this is the leading term of the neglected terms, neglected series of terms, and in this term, the

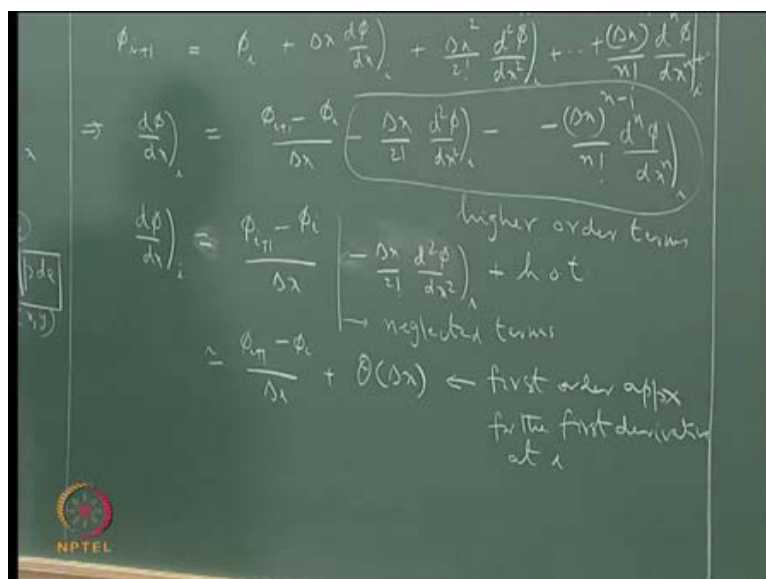
derivative here is multiplied by delta x raised to the power 1. So, this is called a first order approximation.

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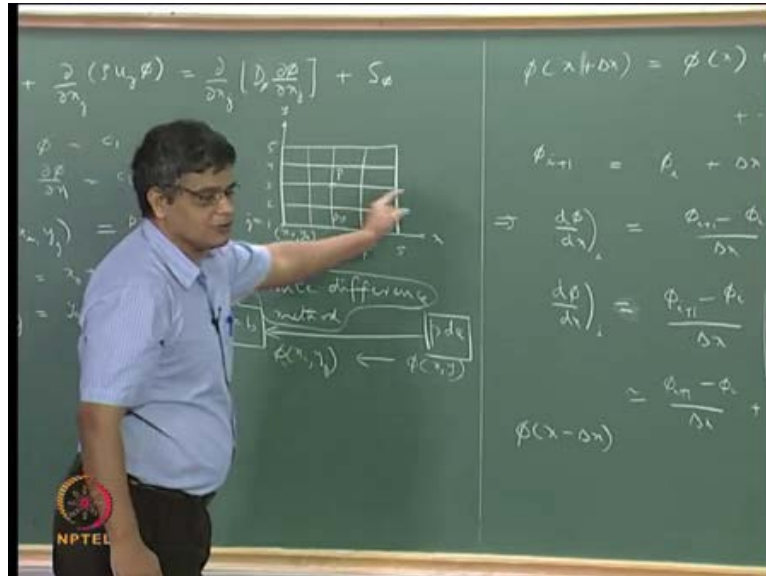
And we can write d phi by dx at i as phi i plus 1 minus phi i by delta x plus terms of the order of delta x. So, the power to which the delta x the spacing or the distance from x that is considered is this. So, this is a first order approximation. We call this as a first order approximation for the first derivative at i.

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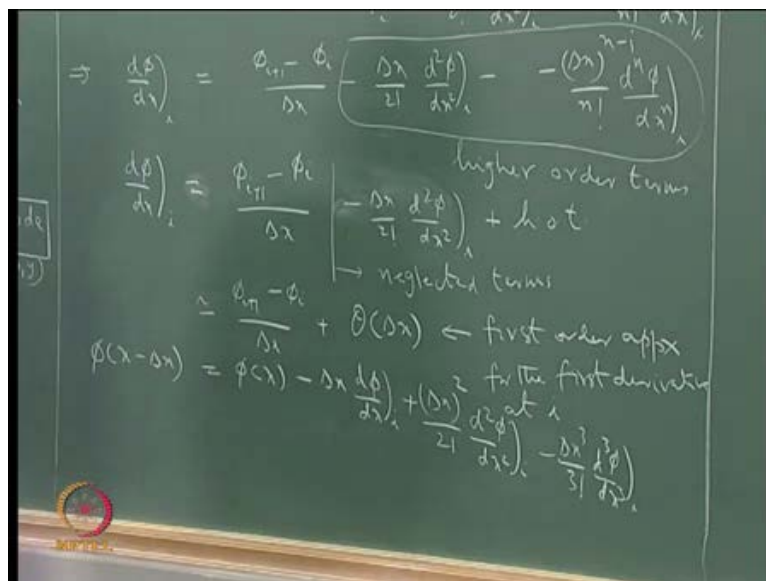
We can derive another expansion, another approximation for this by expanding not in terms of positive delta x. We can do it for a negative delta x.

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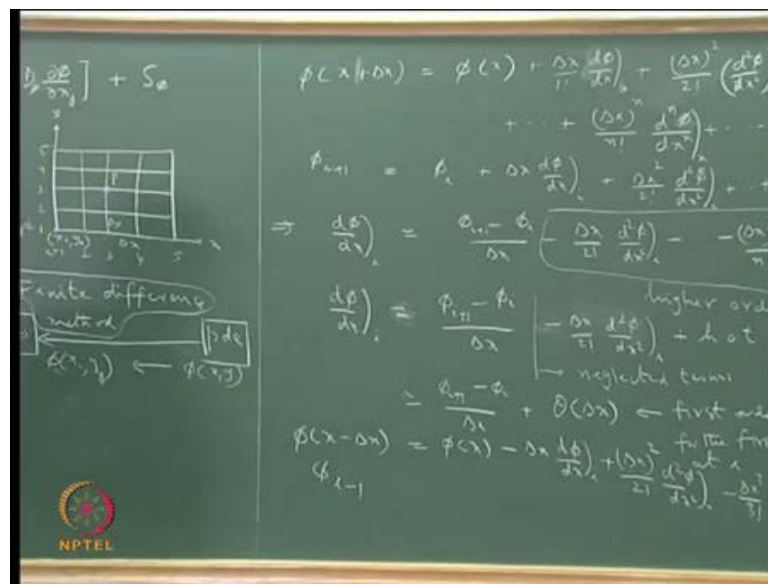
For example, we can write phi x minus delta x, that is, to the left of point i. So, we are going to plus delta x means we are going to the right of point i; we are going to the left of point i.

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And we can write phi of x minus delta x as a Taylor series expansion phi of x minus delta x by d phi times d phi by d x at i plus delta x square by factorial 2 d square phi by d x square minus delta x cube by factorial 3 third derivative at i and so on. And we can write a general expression in terms of minus 1 raised to the power of n and all this. So, wherever in this thing, wherever you have delta x, you put as minus delta x in order to get this approximation.

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Now, we can write it this x minus delta x is nothing but phi i minus 1. Here (()) convention which is like this.

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$$\Rightarrow \frac{d\phi}{dx}_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} - \left(\frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i - \frac{(\Delta x)^3}{3!} \frac{d^3\phi}{dx^3}_i + \dots \right)$$

$$\frac{d\phi}{dx}_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} - \left(\frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i + \text{h.o.t} \right)$$

higher order terms
neglected terms

$$\approx \frac{\phi_{i+1} - \phi_i}{\Delta x} + \mathcal{O}(\Delta x) \leftarrow \text{first order approx}$$

$$\phi(x - \Delta x) = \phi(x) - \Delta x \frac{d\phi}{dx}_i + \frac{(\Delta x)^2}{2!} \frac{d^2\phi}{dx^2}_i - \frac{(\Delta x)^3}{3!} \frac{d^3\phi}{dx^3}_i + \dots$$

$$\phi_{i-1} = \phi_i - \Delta x \frac{d\phi}{dx}_i + \frac{\Delta x^2}{2!} \frac{d^2\phi}{dx^2}_i - \frac{\Delta x^3}{3!} \frac{d^3\phi}{dx^3}_i + \dots + \text{h.o.t}$$

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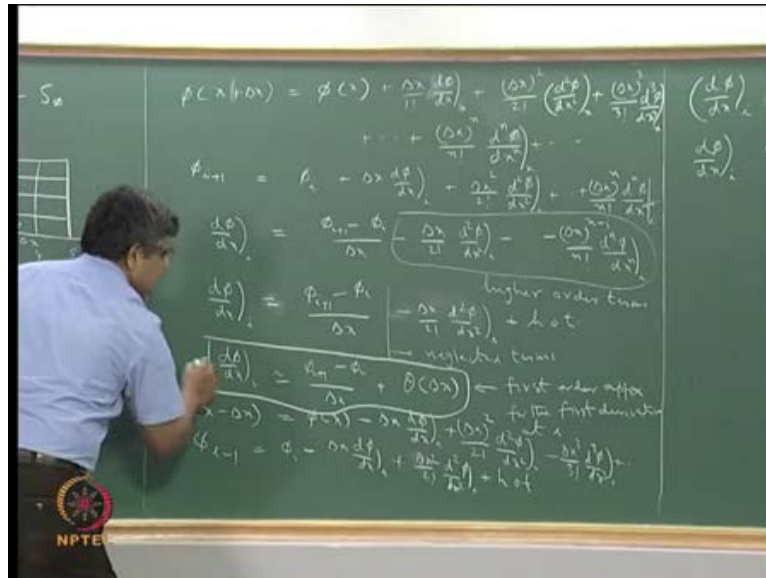
$$\left(\frac{d\phi}{dx} \right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i + \dots + \text{h.o.t}$$

$$\left(\frac{d\phi}{dx} \right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \mathcal{O}(\Delta x)$$

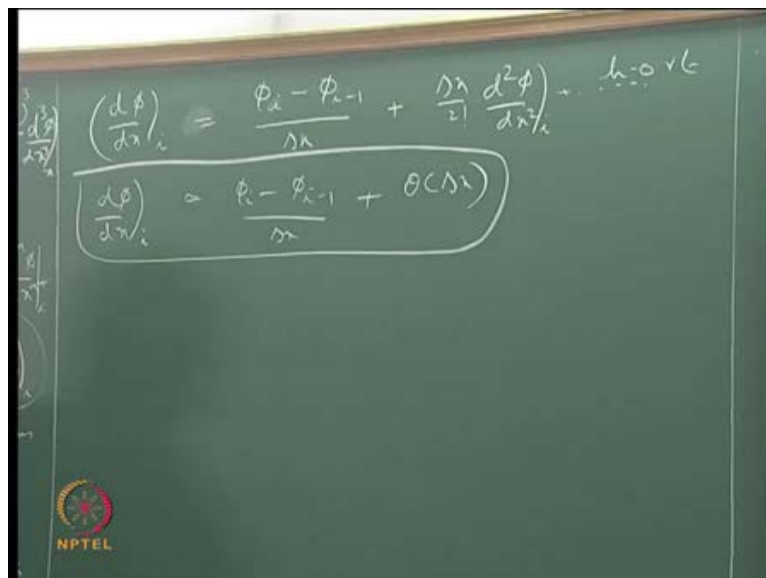
So, that is equal to phi i minus delta x d phi by dx at i plus delta x square by factorial two d square phi by dx square at i plus higher order terms, and using this expression, we can derive an approximate formula like this for the first derivative phi i minus phi i minus 1 by delta x plus delta x by factorial 2 d square psi by d x square at i plus so on plus higher order terms.

So, this is rewriting of this, and therefore, we can write this approximately as ϕ_i minus ϕ_{i-1} by Δx plus terms of the order of Δx . So, this is again a formula for an approximation for $d\phi$ by dx at i .

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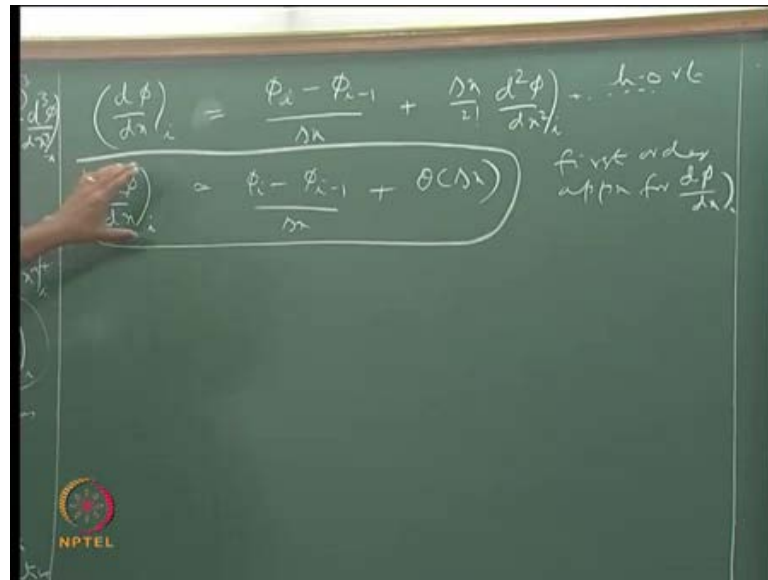
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Now, if you examine this formula and this formula both of them are first order approximation, because the leading term in the truncated series of terms is multiplied by Δx , is Δx times $d^2\phi$ by Δx^2 at i .

In one case, it is plus, and in the other case, it is minus. It does not really matter whether it is plus or minus or what is the value of the coefficient here and so on. What matters is that what is the delta x multiplicative term, which is there in the leading term and that defines whether it is first order or second order?

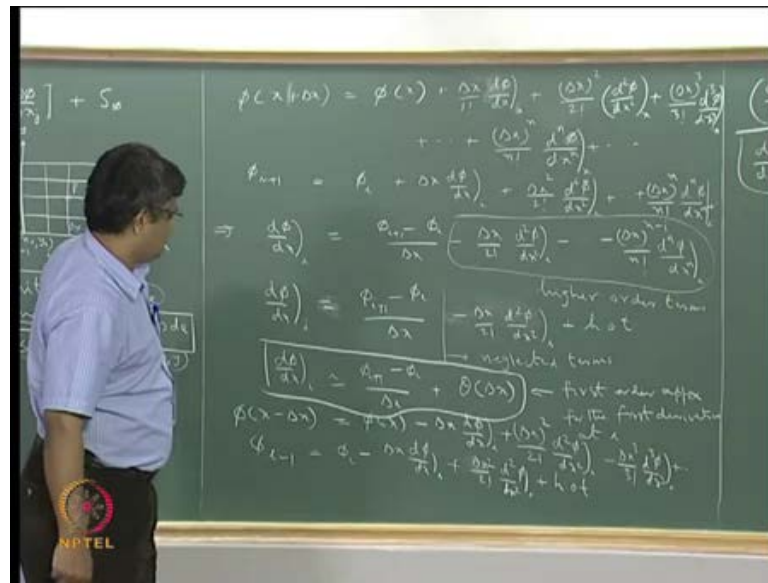
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What you mean by first order and second order approximation is that the accuracy of this approximation depends linearly with respect to delta x in this formula. And if you have delta x square, then it depends quadratically on that so that if you reduce delta x by a factor of 2, then the error is expected to reduce also by a factor of two provided delta x is very small.

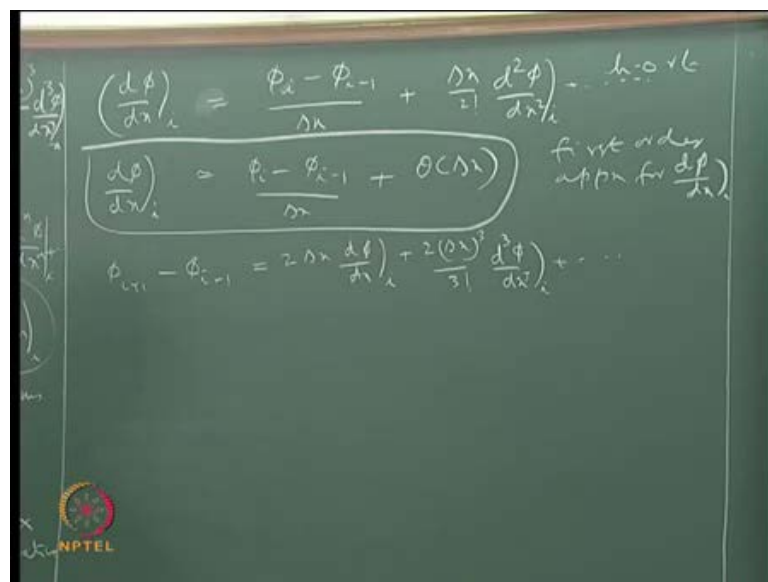
If you have large delta x, it need not there may be a number of terms which are increasing before you find the decrease later on. So, it is for small delta x, the error between the true derivative and the error obtained from this formula here will decrease linearly as delta x is decreased in a first order approximation.

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So, now, we can combine the two expressions here. We can take this expression and this expression and add the two; we can subtract the two. We can subtract this from this to get a difference approximation. If we do this, then this is phi i plus 1 minus phi i.

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So, we can say that phi i plus 1 minus phi i minus 1. If we do this, then this and this cancels out and we have delta x d phi by dx at i minus delta x minus delta x this. So, when we subtract this minus becomes plus. So, we can have we will have 2 delta x d phi

by dx at i and the next term here is delta x square by two factorial and here it is delta x square by two factorial.

So, when you subtract this from this, they cancel out and you will have no second derivative here, but the third derivative will appear as plus two delta x whole cube by factorial three third derivative at i plus so on like this.

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The image shows a chalkboard with several mathematical equations written in white chalk. The equations are as follows:

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i + \dots \text{h.o.t}$$

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + O(\Delta x) \quad \text{first order approx for } \frac{d\phi}{dx}$$

$$\phi_{i+1} - \phi_{i-1} = 2\Delta x \left(\frac{d\phi}{dx}\right)_i + \frac{2(\Delta x)^3}{3!} \frac{d^3\phi}{dx^3}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{2(\Delta x)^2}{2!} \frac{d^3\phi}{dx^3}_i + \dots \text{h.o.t}$$

In the bottom left corner of the chalkboard, there is a small circular logo with the text "NPTEL" below it.

So, using this, we can write an approximation again for d phi by dx at i as phi i plus 1 minus phi i minus 1 by 2 delta x minus 2 delta x square because this delta x and this delta x will cancel out by factorial two third derivative of phi with respect to x at i plus higher order terms.

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$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_i - \phi_{i-1}}{\Delta x} + O(\Delta x)$$
 First order approx for $\frac{d\phi}{dx}$

$$\phi_{i+1} - \phi_{i-1} = 2\Delta x \left(\frac{d\phi}{dx}\right)_i + \frac{2(\Delta x)^2}{3!} \frac{d^2\phi}{dx^2}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{2(\Delta x)^2}{2!} \frac{d^2\phi}{dx^2}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + O(\Delta x^2)$$
 Second order approx for the first derivative at i

Now, if you were to write it as a first order or a second order like this, we can see that we can therefore write $d\phi/dx$ at i roughly as $(\phi_{i+1} - \phi_{i-1}) / (2\Delta x)$ plus terms of the order of Δx square, because the leading term in the truncated series here has a square term associated with Δx . So, this is therefore, we call this as a second order approximation for the first derivative at i .

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So, we have here three different formulas for the same function $d\phi/dx$ at the same location i . It is expressed here as $(\phi_i - \phi_{i-1}) / \Delta x$ and it is expressed here in this formula $(\phi_{i+1} - \phi_{i-1}) / (2\Delta x)$.

as $i - 1$ minus $i - 1$ phi i minus phi $i - 1$, and here, it is expressed as phi $i + 1$ minus $i + 1$ phi i minus i . If you look at the order of the leading term in this case it is a first order and here also it is a first order. So, whereas here, it is a second order.

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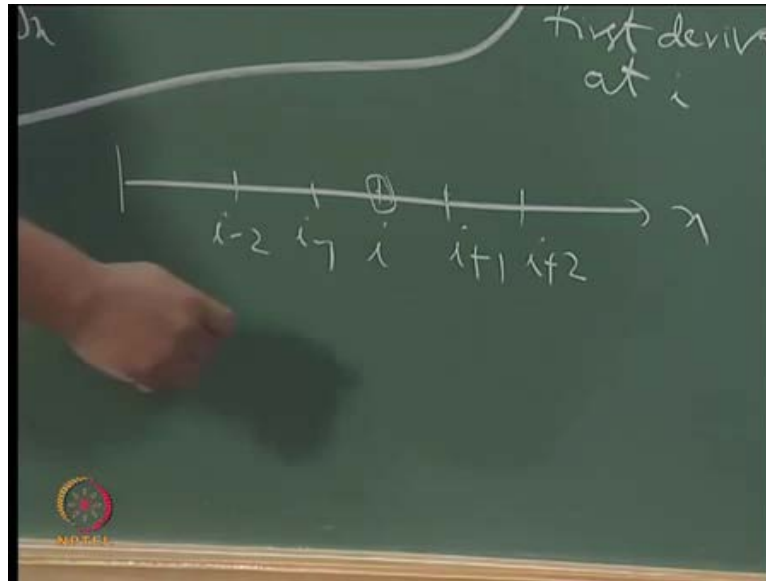
The image shows a chalkboard with handwritten mathematical derivations. At the top, the expression $\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{1}{2!} \frac{d^2\phi}{dx^2}_i \Delta x$ is written. Below this, a boxed equation states $\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_i - \phi_{i-1}}{\Delta x} + \mathcal{O}(\Delta x)$, with a note: "first order approx for $\frac{d\phi}{dx}$ ".

Next, the Taylor expansion for the function values is shown: $\phi_{i+1} - \phi_{i-1} = 2\Delta x \left(\frac{d\phi}{dx}\right)_i + \frac{2(\Delta x)^2}{3!} \frac{d^2\phi}{dx^2}_i + \dots$. This is used to derive the second-order approximation for the derivative: $\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{2(\Delta x)^2}{2!} \frac{d^2\phi}{dx^2}_i + \text{h.o.t}$.

Finally, a boxed equation states $\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2)$, with a note: "second order approx for the first derivative at i ".

In terms of accuracy when delta x is small, the error will become smaller if the power of the leading term if the order of the approximation is higher. Therefore, we expect this approximation to be a lot better than either this or this. We expect both of them, both the first one and the second to be about equally approximate, whereas, this is more accurate. And if we have an approximation which is third order, we expect that to be more accurate than the second order, but in all cases, we are expecting delta x is very small and we are deviating only very slightly from this so that we can claim that successive terms are progressively smaller and smaller.

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Now, when you look at this, what is the difference among these things? There is a clear difference. We are looking at a one-dimensional case; so, we are looking at x going like this and this is a grid point i . What we have on the right hand side is i plus 1 i minus 1 and i minus 2 and i plus two so on like this. We are looking at the first derivative approximation at this point. In the case of let us call this as formula a, in the case of formula a, it is given as i plus 1 ϕ the value of ϕ at this point minus this divided by 2, whereas, in this case, it is defined in terms of the difference between these two say taking a backwards step, and in the case of this, we are looking at the difference between this point and the other point. So, we are looking at the value of the function on both sides, whereas, in the first case, we were looking at forward point; in the other case, we are looking at backward point.

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$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\Delta x}{2!} \frac{d^2\phi}{dx^2}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_i - \phi_{i-1}}{\Delta x} + O(\Delta x)$$
 First order approx for $\frac{d\phi}{dx}$ backward differencing

$$\phi_{i+1} - \phi_{i-1} = 2\Delta x \left(\frac{d\phi}{dx}\right)_i + \frac{2(\Delta x)^2}{3!} \frac{d^2\phi}{dx^2}_i + \dots$$

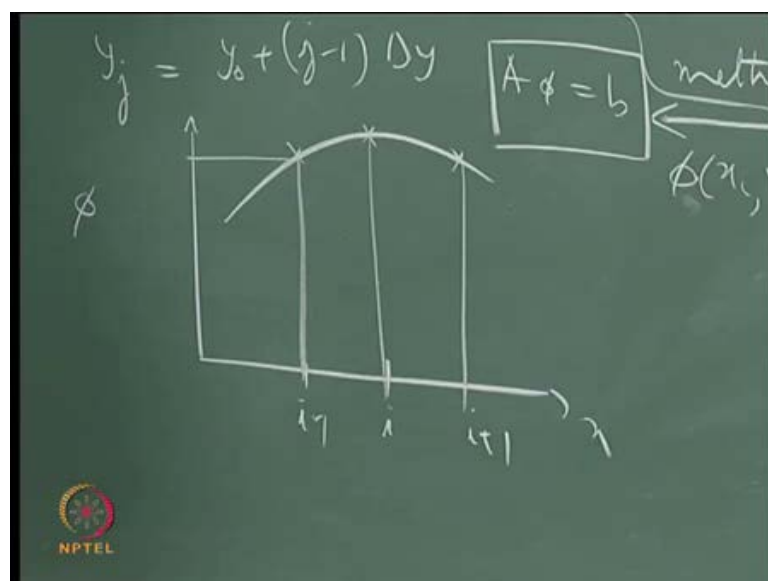
$$\left(\frac{d\phi}{dx}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{2(\Delta x)^2}{2!} \frac{d^2\phi}{dx^2}_i + \dots$$

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + O(\Delta x^2)$$
 Second order approx for the first derivative (central diff)

$$i-2 \quad i-1 \quad i \quad i+1 \quad i+2$$

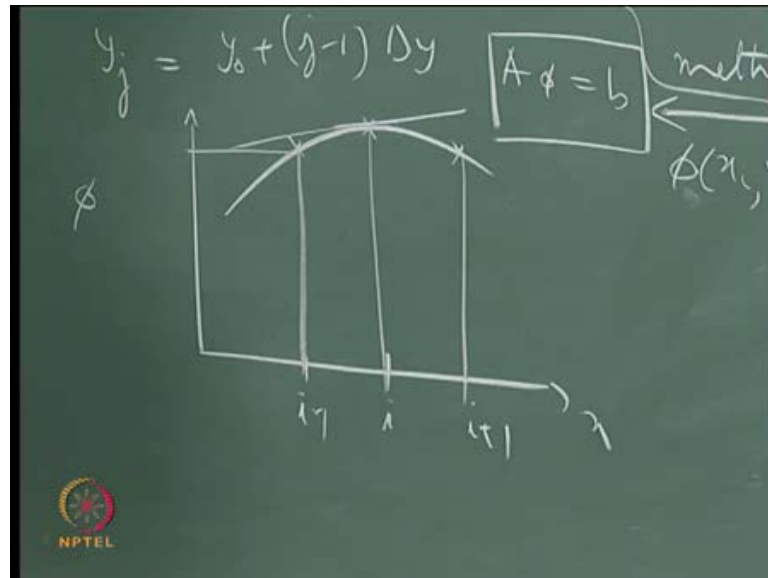
So, we call this as a forward differencing. So, a is forward differencing; this is backward differencing and this is central differencing. And we call either both the forward differencing and backward differencing as one sided formula, because in both the cases, only to one side of the point we take the functional values. So, it is to the left of this and in the forward differencing, it is to the right of this; whereas, in a central differencing, the value at a particular point is expressed in terms of points both to the left and to the right, and we can also express this graphically by considering this is x and phi is like this.

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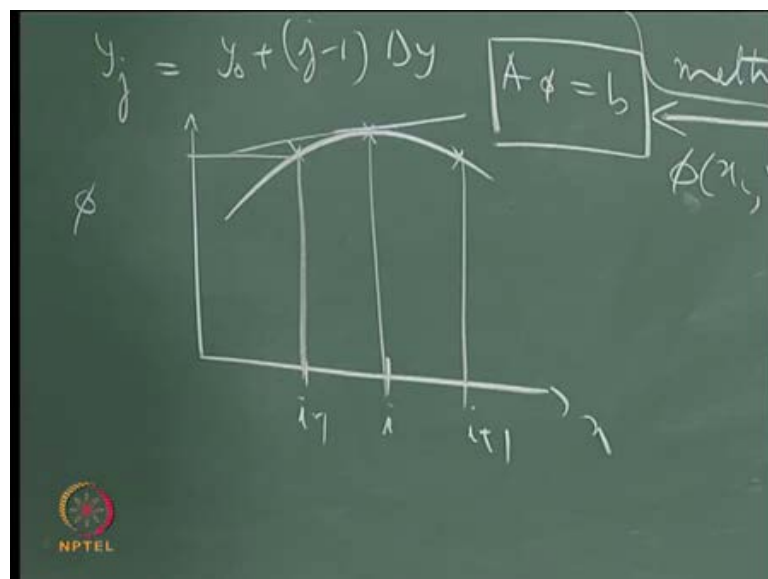
Let us say that this is the variation of phi with respect to x and we are looking at discrete points like i here i plus 1 and i minus 1. So, the value of phi, this is the value of phi i minus 1 and this is the value of phi i plus 1 and this is the value of phi at i and what we are interested is not specifically the value of phi, but d phi by dx.

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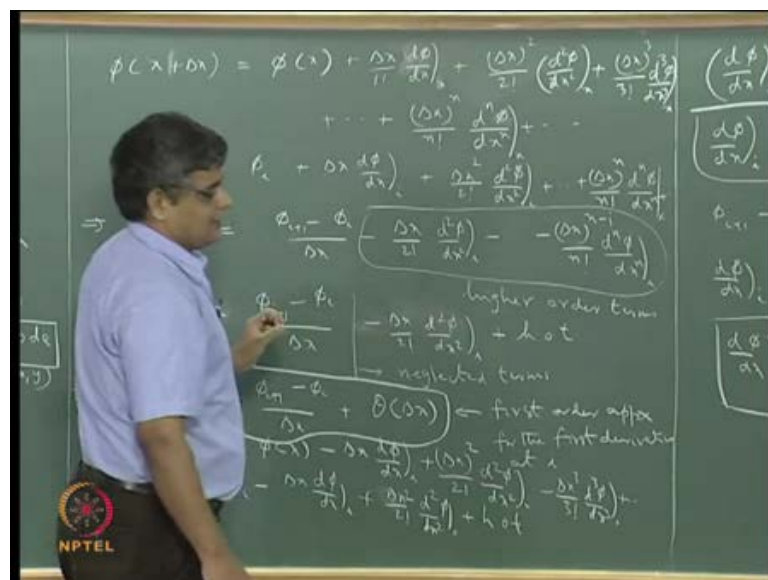
So, we are looking at the slope and the slope at this point is maybe something like. This, **this**, is a true slope by expressing in terms of i plus 1 minus i by delta x. We are evaluating a slope of a line which is passing through these points.

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So, this is the slope that we are getting from the forward difference approximation. With the backward, we are taking the two points - the point i and i minus 1. We are joining by a line here, and then, this is the slope of the line that we are approximating, that we are getting from the backward difference. And in the case of forward differencing, we take point i minus 1 and i plus 1, we join the two, and the slope of this line is what we are getting with central difference, and so, compared to the true slope here, we can see that the central one has a slope which more resembles this, this slope here than either the backward or the forward difference, but essentially what we are trying to do? In this particular case is to estimate the slope of the line which is what the first derivative $d\phi$ by dx is. Using points to the left or points to the right in the case of forward differencing or points to on either side of this, and in the case of first derivative, we are evaluating it just by drawing a line through these two points here. And one can see why a central differencing would give us a more accurate approximation, but when we go to higher order derivative or higher order approximations, then this kind of simplistic explanation will not be applicable, but for the simple case of first order, second order approximations for the first derivative at point i , this graphical interpretation is very useful.

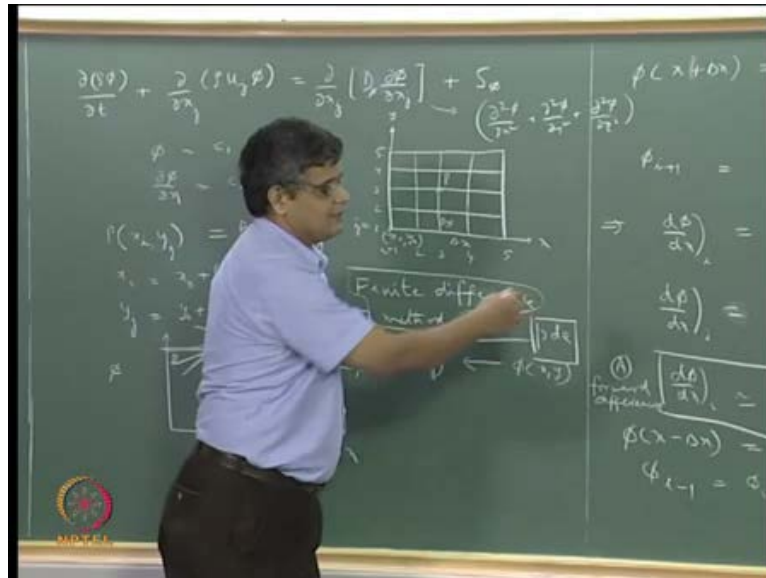
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But once you look at the error in the leading term of the truncated set of terms to find out what is the error and that qualifies that, that, characterizes the quality of the approximation that we are making for the derivative.

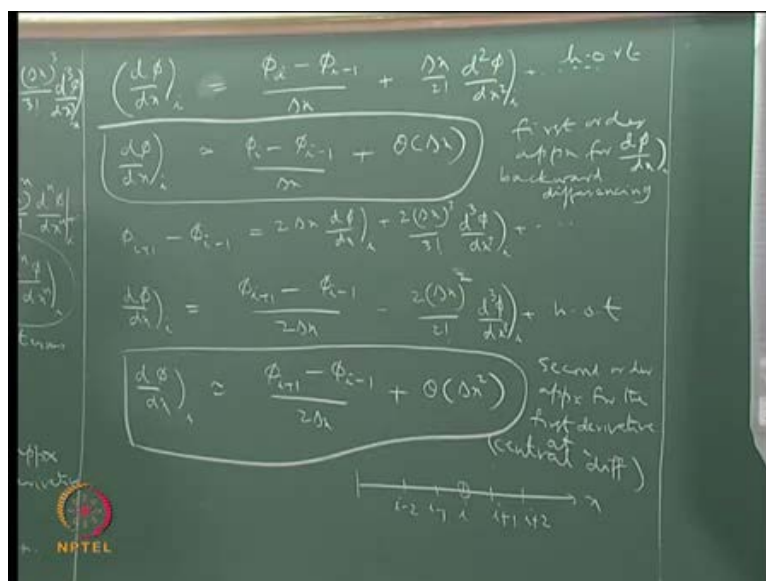
So, now, we have done for the first derivative, but in our equation, we not only have first derivative, we also have second derivative. For example, when d is constant, this becomes $d^2 \phi$ by dx^j at dx^j .

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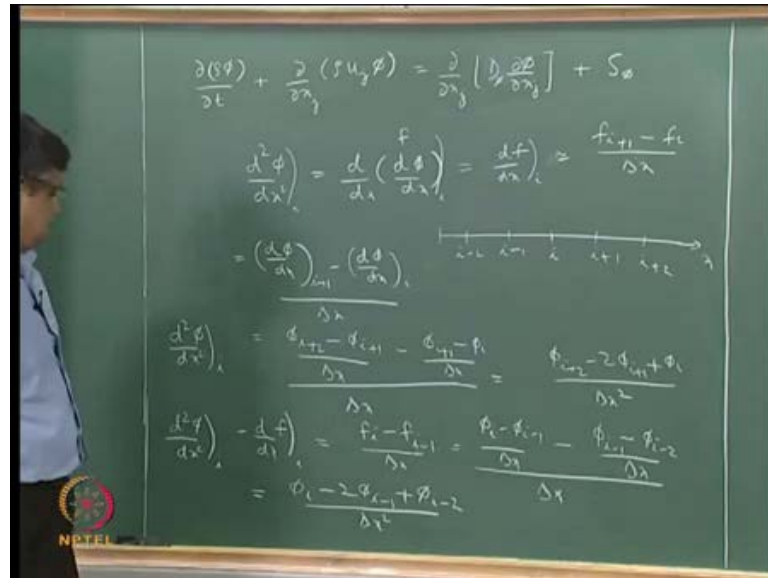
And since j is a repeated index, we will have $d^2 \phi$ by this term here will be $d^2 \phi$ by dx^2 plus $d^2 \phi$ by dy^2 plus $d^2 \phi$ by dz^2 . So, there are second derivatives.

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What, can we apply this method for second derivative? We can do that. For our second derivative, the approximation that we can make is very similar. We can take a second derivative as the first derivative of the first derivative.

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For example, we can say that a second derivative $d^2 \phi$ by dx^2 as d by dx of $d\phi$ by dx and we can write the derivatives here and we can evaluate it like this. Let us say that we have in a unidirectional coordinate x equal to 0 x varying in this direction. We have i here i plus 1 i minus 1 i plus 2 and i minus 2 and so on like this.

We are interested in evaluating the second derivative at point i . So, we can evaluate this like this, and now, we are looking at a first derivative of this function. Let us call this as f here. So, we can write this as $d f$ by dx at i .

We can make use of for example, forward differencing for this. We can say that f of i plus 1 minus f of i divided by Δx . We can write it roughly like this - where f itself is $d\phi$ by dx . So, we can write this as $d\phi$ by dx at i plus 1 minus $d\phi$ by dx at i divided by Δx . Now, we know what how we can write this? We can again make use of forward differencing for this and we can say that this is equal to ϕ i plus 2 minus ϕ i plus 1 by Δx and the forward difference approximation for this as ϕ i plus 1 minus ϕ i by Δx this whole thing divided by Δx .

So, since we are in the fortunate position of Δx being the same, we can write this as $\phi_{i+2} - 2\phi_{i+1} + \phi_i$ divided by Δx^2 . So, this is one approximation for $d^2\phi/dx^2$ at i . Now, this here, we can also make use of backward differences and we can write using that method as at i as $d^2\phi/dx^2$ at i , where f is ϕ here and we can use backward differencing.

We can write this as $\phi_i - \phi_{i-1}$ by Δx and f is therefore $d\phi/dx$ at i using backward differences will be, will be, ϕ_{i-1} by Δx minus the value of $d\phi/dx$ at $i-1$ using the backward differences is given by $\phi_{i-1} - \phi_{i-2}$ by Δx this whole thing divided by Δx , that is, this Δx . And this gives us a formula that that this is equal to $\phi_{i+1} - 2\phi_i + \phi_{i-1}$ by Δx^2 .

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$$\begin{aligned} \frac{d^2\phi}{dx^2}\bigg|_i &= \frac{d^2f}{dx^2}\bigg|_i = \frac{f_i - f_{i-1}}{\Delta x} = \frac{\left(\frac{df}{dx}\right)_i - \left(\frac{df}{dx}\right)_{i-1}}{\Delta x} \\ &= \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \end{aligned}$$

And we can use, **we can use**, we can, for example, do it in a different way $d^2\phi/dx^2$ at i is d^2f/dx^2 at i . For example, we can write this as f ; we have made use of backward differences here.

So, this by definition, this is approximate. This is by definition $d\phi/dx$ at i minus $d\phi/dx$ at $i-1$ by Δx , and at this stage, we can choose to make a forward difference approximation for this. So, we can write this as $\phi_{i+1} - \phi_i$ minus Δx , that is, forward difference approximation here, and here, we can make use of again forward difference approximation minus $\phi_i - \phi_{i-1}$ by Δx .

divided by delta x square. So, this will give us phi i plus 1 minus 2 phi i plus phi i minus 1 by delta x square.

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The chalkboard shows the following derivation:

$$\begin{aligned} \frac{d^2\phi}{dx^2} &= \frac{d}{dx} \left(\frac{d\phi}{dx} \right) = \frac{f_i - f_{i-1}}{\Delta x} = \frac{\left(\frac{d\phi}{dx} \right)_i - \left(\frac{d\phi}{dx} \right)_{i-1}}{\Delta x} \\ &= \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \\ \frac{d^2\phi}{dx^2} &\approx \frac{\phi_i - 2\phi_{i+1} + \phi_{i+2}}{\Delta x^2} \\ &\approx \frac{\phi_i - 2\phi_{i-1} + \phi_{i-2}}{\Delta x^2} \\ &\approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2} \end{aligned}$$

So, again, we have three formulae for the same d square phi by dx square at i being given by this formula here which is we will slightly write it. This is what we have from forward differences approximate and this is also approximately equal to phi i minus 2 phi i minus 1 plus phi i minus 2 divided by delta x square and d square phi by dx square using the final formula is phi i minus 1 minus 2 phi i plus phi i plus 1 by delta x square.

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The chalkboard shows the following derivation:

$$\begin{aligned} \frac{d^2\phi}{dx^2} &= \frac{d}{dx} \left(\frac{d\phi}{dx} \right) = \frac{f_i - f_{i-1}}{\Delta x} = \frac{\left(\frac{d\phi}{dx} \right)_i - \left(\frac{d\phi}{dx} \right)_{i-1}}{\Delta x} \\ &= \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \\ \frac{d^2\phi}{dx^2} &\approx \frac{\phi_i - 2\phi_{i+1} + \phi_{i+2}}{\Delta x^2} \\ &\approx \frac{\phi_i - 2\phi_{i-1} + \phi_{i-2}}{\Delta x^2} \\ &\approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2} \end{aligned}$$

So, we have three formulae. So, the second derivative at i is being given in the first one in terms of i , i plus 1 and i plus 2. So, it is all coming from these three points, and in the second case, it is coming from i minus 1 and i minus 2; it is coming from these three points. In the third case, it is coming from i minus 1 and i plus 1. So, it is coming from these two.

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So, this is the central differencing; this is backward differencing and this is forward differencing. And what will be the accuracy of the approximation? We can derive it systematically by taking Taylor series expansion.

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$$\frac{d^2 \phi}{dx^2} = \frac{d}{dx} \left(\frac{d\phi}{dx} \right) = \frac{f_i - f_{i-1}}{\Delta x} = \frac{\left(\frac{d\phi}{dx} \right)_i - \left(\frac{d\phi}{dx} \right)_{i-1}}{\Delta x}$$

$$= \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

$$\frac{d^2 \phi}{dx^2} \approx \frac{\phi_i - 2\phi_{i+1} + \phi_{i+2}}{\Delta x^2} \quad \text{forward diff} + \mathcal{O}(\Delta x)$$

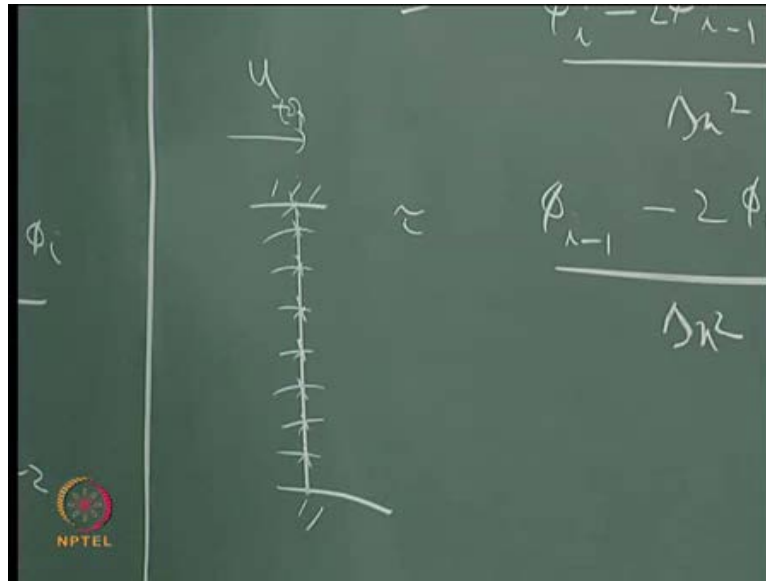
$$\approx \frac{\phi_i - 2\phi_{i-1} + \phi_{i-2}}{\Delta x^2} \quad \text{backward} + \mathcal{O}(\Delta x)$$

$$\approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2} \quad \text{central} + \mathcal{O}(\Delta x^2)$$

We will see how it can be done, but we can say that this will be typically first order accurate; whereas, this will be a second order accurate expansion. So, we have a second order expansion for central scheme using three points - the midpoint and the two neighboring points on either side, and three points going one way is the backward differencing of the first order; three points going the other way in the positive x direction is the forward differencing going this. Which of these three is correct? All the three are approximate.

One can say if delta x is small, then the central differencing is more accurate than the other two approximations; whereas, the other two approximations are equally approximate in the sense that if you reduce the delta x by a factor of 2, the error is expected to reduce by a factor of 2 for small values of delta x, Now, which of them is useful? Obviously, we would like to have an approximation which is more accurate than the 1 which is possibly to be less accurate, but each of them has got it is own use.

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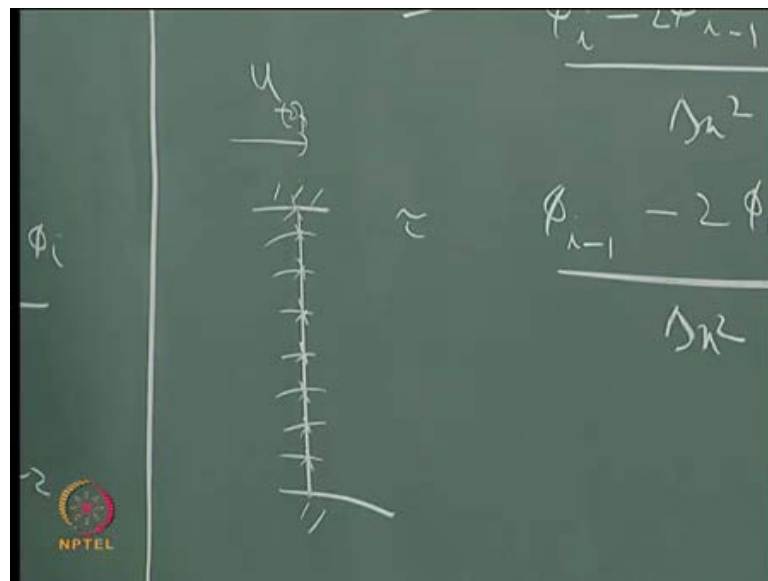
For example, if you are looking at one-dimensional domain, we have seen the case of fluid flow where we are looking at a domain which is going from the bottom wall which is stationary and a top wall which is moving at a velocity u top, and you add an equation which had to be discretized over this. Then you need to write, for example, if you had to write the second derivative approximation for this point, this point, this point, these points, then for all these interior points, we can make use of $i + 1$ and $i - 1$, because here, the two neighbouring points will be this and the two neighbouring points will be this like this, and when you come to the extreme point here, one may not be able to use all the three values. For example, here, if you are looking at, you may still be able to do this, but if you are looking at the point which is still here and if that happens to be a point which you need to evaluate, then you cannot write a finite central difference approximation for these two because this is going beyond the boundary.

So, typically, at the boundaries, if you want to have an approximation, if the boundary point is also one of the points that has to be determined, for example, if this is given with a normal boundary condition and not as a Dirichlet boundary condition, then in such a case, we need to evaluate the governing equation. Even after the governing equation here on the boundary condition at this point, which may require us to evaluate the derivative at this point. At that point under those conditions, we may not be able to write a central difference formula for the boundary point, because central difference formula requires

you to have a point on either side of the point at which we are writing the finite difference approximation.

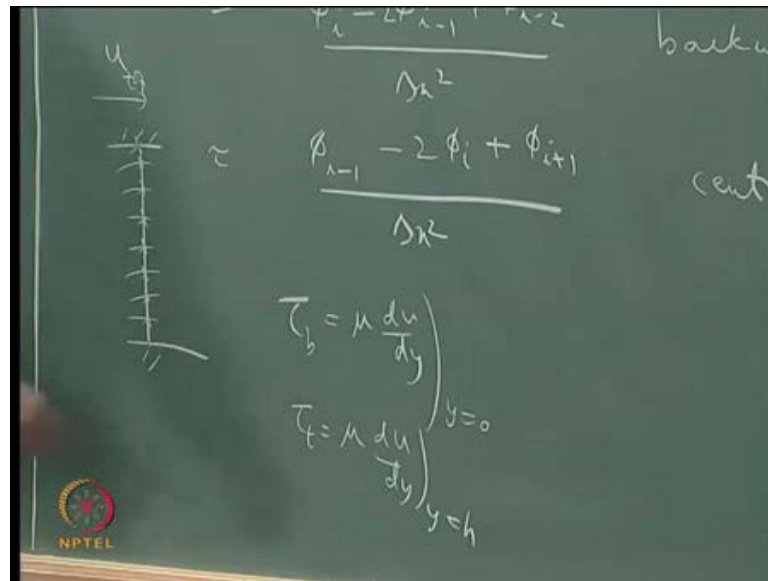
So, since we are already at one edge, we cannot find a point which is on the other side. So, in such a case, we may not be able to use a central difference approximation. We will have to use either a forward difference or a backward difference.

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For example, if you are looking at a derivative here, then we cannot use a forward differencing because the forward differencing points will be out of the domain. We have to use a backward differencing approximation here, and similarly, if you want to get a derivative here, then we cannot use a backward differencing or central differencing; we have to make use of a forward differencing point. So, why do we want to have to evaluate the derivatives here? As I mentioned, it may be as a part of the boundary condition or it may be that you have got the velocities here and you want to find the shear space.

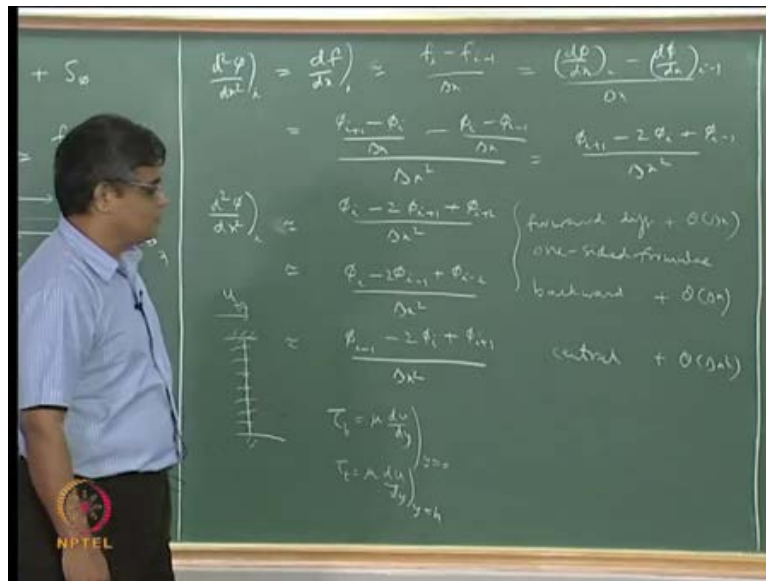
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So, we know that shear stress in this particular case is $\mu \frac{du}{dy}$ and we want to find out the shear stress at this wall and this wall. So, we have to evaluate shear stress at y equal to 0, and similarly, we may want to evaluate $\mu \frac{du}{dy}$ at y equal to h . So, this is the bottom wall and this is top wall. So, we are forced to evaluate $\frac{du}{dy}$ at y equal to 0. So, how can we define the value here? We cannot make use of the central difference formula, because that would mean you would need to have a value point here and here.

So, we will have to make use of forward differencing approximation for the first derivative at y equal to 0 in order to get the shear stress from computed velocity of this for the bottom wall. Similarly, at the top wall, we need to make use of the backward differencing formula in order to get an expression of $\frac{du}{dy}$.

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So, typically at the edges, at the boundary edges, we will have to evaluate the derivatives, derivatives using a 1 sided formula. So, both these things are one sided formulas for the first derivative or second derivative. So, as required by the problem at the boundaries, we will have to employ the one sided formulas for the derivatives, and in the interior, we can make use of central differencing formula to the extent that the points are available.

Now, having established the need for both one sided formula and the central formula and having established the need for, having expressed a desire for a more accurate formula. Then we see that if you have a domain like this, then for all the central differencing central points - the interior points which are not at the boundaries. We can make use of a second accurate formula for the central differential, but what about the edges? We are stuck with forward differencing formula, which are only first order accurate. Can we increase the order of the accuracy of the approximation?

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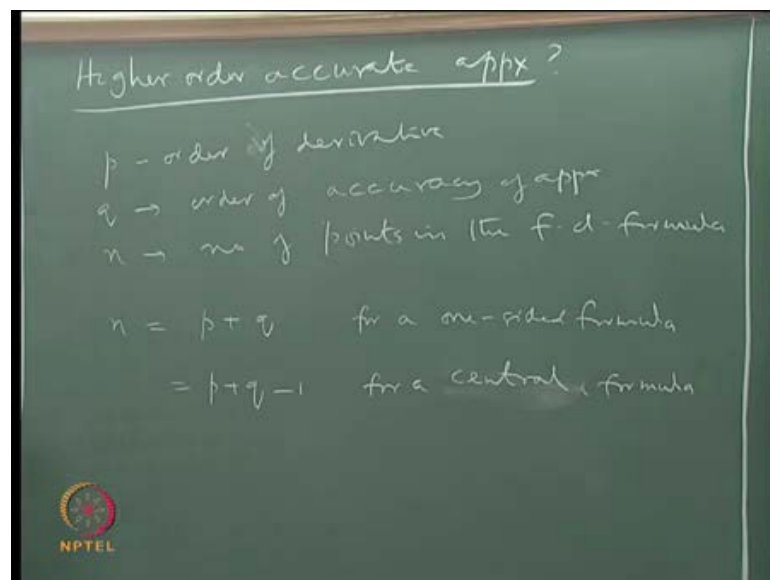
So, can we get a higher order approximation? The quick, the straight answer is - yes. In fact, it is possible to get for any derivative any order of approximation provided we take enough number of points. So, if you have for a first derivative, typically you need two points; in order to get, you need the point and then the immediate forward point or the backward point to get a one sided formula which is first order accurate. If you want to

have a second order accurate formula which is one sided, you need to take one more point. So, if you are looking at the forward differencing second order accurate formula for a first derivative, so, that it is $d\phi/dx$ at i expressed in terms of i , $i+1$, $i+2$ and so on. You need to have three points that is the value of ϕ at i , $i+1$ and $i+2$.

If you take one more point, that is, if you express your first derivative in terms of $i+1$ and $i+2$ and $i+3$, that is four points, then you get a third order accurate formula for derivative. Now, if you increase the order of the derivative, if we are looking at a second derivative, then you have to pay the penalty of having one more point in order to get the same accuracy.

So, that is, if you want to have a second order accurate expression for a second derivative using one sided formula, we need to have four points. So, that is, i , $i+1$, $i+2$ and $i+3$ and so on; whereas, with a central difference formula, it is sufficient to take one point on this side; one point from the left and one point to the right to get a second derivative, a second order accurate approximation for a second derivative.

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So, typically, if p is the order of derivative and q is the order of approximation, order of accuracy of approximation, then and if n is the number of points in the finite difference formula, then n is equal to p plus q for a one sided formula and is equal to p plus q minus

1 for a two sided formula, so, when we say two sided for a central differencing formula. So, let us just see whether this is valid.

In the case of a second derivative, we are saying that order of derivative p is equal to 2 and we are looking at a second order approximation. So, that is q is equal to 2. So, n is equal to p plus q minus 1, 2 plus 2 minus 1, that is three points, and we see here i minus 1 and i and i plus 1. So, this, **this**, thing is correct, and when we you look at this here, we have claimed that these are first order accurate approximations. So, this is again a second derivative p is equal to 2 and n is equal to 3 we have i i plus 1 i plus 2 or i i minus 1 and i minus 2. So, that is three here. So, n is 3; p is 2 and q is equal to therefore 1. So, that is why we get a first order problem and we have also seen for a first derivative and so on. This thing, this formula is valid on a uniform grid for any order of accurate accuracy of approximation and any derivative.

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p - order of derivative
 q - order of accuracy of approx
 n - no of points in the f.d. formula
 $n = p + q$ for a one-sided formula
 $= p + q - 1$ for a central formula

$$\frac{d^3 \phi}{dx^3} = \frac{a \phi_i + b \phi_{i+1} + c \phi_{i+2} + d \phi_{i+3} + e \phi_{i+4}}{\Delta x^3} + O(\Delta x^2)$$
 formula

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So, if we are looking at say expression for the d cube by the third derivative of ϕ at i here and if we want to have an order of approximation of Δx square, then we need to express this in terms of ϕ_i . We need to have how many points and we say that this is forward differencing. So, that is one sided formula. So, p is equal to 3 and q is equal to 2; so, we need to have five points. So, we need to write this as a ϕ_i $b \phi_{i+1}$ plus $c \phi_{i+2}$ plus $d \phi_{i+3}$ plus $e \phi_{i+4}$. So, that is five points - 1, 2, 3, 4, 5. For

dimension consistency, this must be divided by Δx^3 so that it is dimensionally consistent and this is the formula that we can expect.

So, we need to find out there is means of finding out what this coefficient a, b, c, d, e are such that we can get a second order forward difference formula for a third derivative. We will try to develop this general method, whereby, we can get for any derivative, any order of accuracy by choosing sufficient number of points on forward or backward or central in such a way that we can find the values of this a, b, c, d, e and get finite difference approximation. We will stop now.