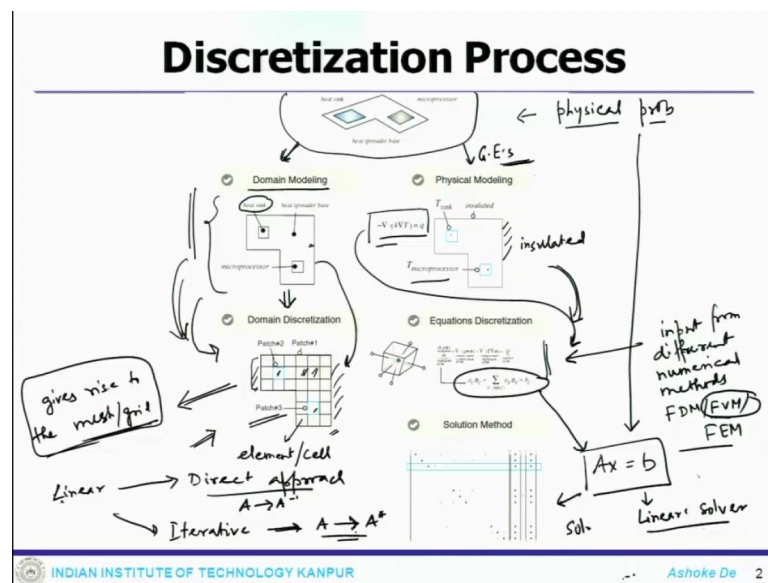


Introduction to Finite Volume Methods-I
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Lecture - 09

So welcome to the lecture of this Finite Volume Method. So, far if you recall what we have been discussing is the discretization process. How given a conditions you or a given a problem actually you discretize the system and reach to the particular linear system?

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So, if you recall from a previous lecture, this is a physical problem of interest that we are trying to solve. This is the physical problem. So, this physical problem we need to get a solution. So all along these process what we end up? Getting a linear system; that is $Ax = b$.

So, what you do? Given a problem in hand that could be of any kind in fluid flow system or heat transfer related problem. So, you convert them to a 2 different approach. One is that the governing equations that actually govern the system. So, for the problem that we had discussed is a problem of this kind of a heat, spread base; where you have a heat sink, where you have a microprocessor, which actually generates the heat. So, one case you have a heat source, one case heat sink and then the walls are sort of insulated.

And given that physical problem in hand, your first define the physical modelling which we called is a domain modelling or essentially this is the physical problem of interest. So, the physical problem you need to divide in such a fashion that your actual problem. So, this actual problem is completely replicated. Now from the actual problem to physical problem in one side, then you need to define the governing equations, the governing equation that actually govern this physical problem.

So, one hand we call it is a domain modelling; that means, the replication of the physical system. Other hand you call it a physical modelling, so that means, you write down the governing equations. For this particular problem we are solving the steady heat conduction equation. So, once you have this you then move to the next step of domain discretization. So, the domain modelling essentially take you to the domain discretization. So, domain discretization means, the particular physical problem that you have you discretize in the domain. So, these actually gives rise to lot of questions like kind of gives rise to the mesh or grid.

Why this is important? Because mesh or grid these are individual cell that because we have divided this particular problem in this kind of rectangular boxes which we call it a individual element or individual cell. Now once you divide them into and obviously, when while doing all these you take care of your physical system into account like patch 2, this essentially the heat sink; so that means, there will be a condition, which will be the boundary condition for the temperature, then patch 3 essentially the microprocessor. So, this will be the temperature for the microprocessor or source and then patch one which actually represents the outer boundary. So, these are all insulated outer boundary and then you get this different mesh.

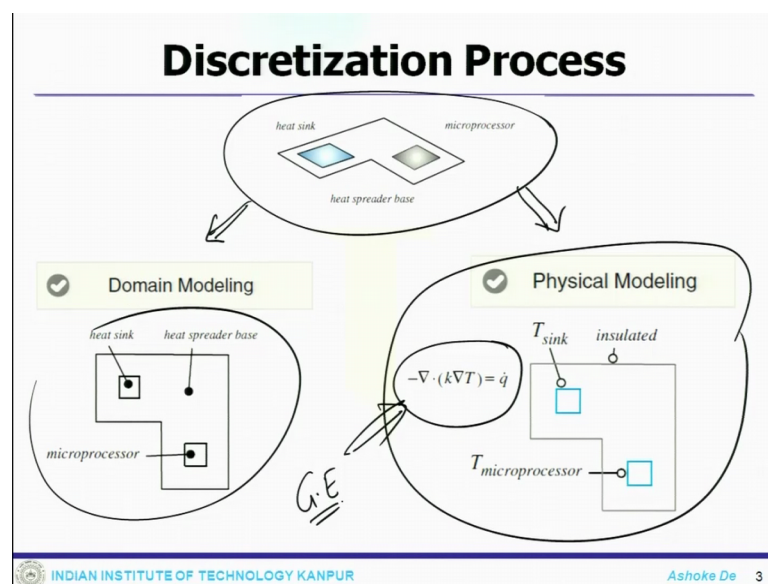
So and while talking about this we have also discussed that this is not the only way you can generate the mesh. You could have unstructured mesh and then whole idea is that the physical problem convert to the domain, then the domain leads to the grid or points or the elements or the cell; where your numerical equations or the governing equations would be solved. Now, the parallely from the physical modelling you come down to discretized equation.

So, this is the system of equations or the governing equation that we are solving for the heat transfer equation steady state heat transfer equation and the steady state heat transfer equations you discretize. Here you need the input from different numerical methods.

So, that means, like finite difference, finite volume, finite element so, these are the different methods. But particularly in our context we are talking about this. So, when we are talking about the finite volume, you discretize them and you get back these kind of system. Essentially that is the linear system you get. So, you get a system like Ax equals to b , once you get Ax equals to b you solve for it. And when you solve for that you get the final solution.

Now, while solving that Ax equals to b , also you need to have the different solvers or the linear solver. So, we have just talked about what kind of system, one approach is that the linear system, one can solve the direct approach; that means you get direct A to A inverse. That is one option another option is that iterative approach; that means, you get a solution for A to A exact through the iteration process. So, finally, you get the solution for the system, ok.

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So and if you look at that so you had this particular problem; so, one hand it is a domain modelling. So, you get these sort of things, one hand you have a physical modelling. So, you have get all the boundary conditions, along with the governing equations this is the governing equations that actually dictate the system and you solve for it.

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Discretization Process

✓ Domain Discretization

Patch#2 Patch#1
Patch#3

element / cell

K = solution

✓ Equations Discretization

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\mathbf{v}\phi) = \nabla \cdot (\Gamma\nabla\phi) + Q$$

∂(ρφ)/∂t
∇ · (ρvφ)
∇ · (Γ∇φ)
Q

$$a_C \phi_C + \sum_{F \in \text{NB}(C)} a_F \phi_F = b_C$$

Ax = b

✓ Solution Method

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And then you have the discretized domain. So, all these are individual element or cell and finally, you get the discretized equations, and this is particularly your Ax equals to b. And finally, you solve it the linear system. So, that gets you the solution, ok.

So, once you have the solution in this particular process, we just touched up on that this numerical methods using the finite volume, and get this linear system. So, there are few things that you have come across is the derivatives.

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Discretization Process

Derivatives \Rightarrow surface flux | FVM
& other derivatives

Numerical method \Rightarrow calculation derivative
error, accuracy, stability
- etc.

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So, even then there as surface fluxes and other derivatives. So, no matter what kind of approach you adopt, whether it is a finite volume or finite difference at the end when you come down to the algebraic system you need to get some sort of a derivative. Now this derivative calculation is another thing that leads to lot of errors. So, in the any numerical methods so, any numerical methods the important component is this calculation of these derivatives.

So, that leads to the errors, accuracy of the system, stability and all other associated stuff. So now, we need to know how you calculate these derivatives. So, which will be true for any other function any other variable. So, once we know that how you calculate that, then so the next step would be to look at this derivatives.

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Derivatives, Error, Accuracy

$$\frac{\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}}$$

$\frac{\partial f}{\partial x} \Rightarrow \frac{f(x+dx) - f(x)}{dx} = ?$

> Simple geophysical partial differential equations
 > Finite differences - definitions \Rightarrow
 > Finite-difference approximations to PDE's
 > Exercises
 > Acoustic wave equation in 2D
 > Seismometer equations
 > Diffusion-reaction equation
 > Finite differences and Taylor Expansion \Rightarrow
 > Stability -> The Courant Criterion
 > Numerical dispersion

flux calculation/derivatives

error, accuracy
 + stability

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So, when you look at this derivatives so, that would talk about the derivative from derivative, then we will look at this error of this discretization process. From there we look at the accuracy of the system.

Now, in a typical sense, if I have to get the derivative of this function of f of del f by del x, then you get the derivative like x plus x minus fx by dx. This is a definition of getting the derivative. Now this is a simple definition of the derivative that this is associated. Now how do you find out the function f x plus dx? If you know the function of fx, then how do you decide dx. So, still these are the associated question alongside the calculation of the derivative.

So, that will tell how the physically the differential equations are discretized. Because once we know this derivative then only would be able to discretize our differential equation. And while doing that here actually everything becomes finite difference approximation, even then you are using finite volume kind of approach. That is the conservative approach and once you have a self-conservative system, once you come down to calculate the derivative or the fluxes. So, either you call it the flux calculation or derivatives calculation, it requires some sort of a finite difference approximations.

And we were going to see how you can do that, and then we will look at certain example how the equations are derived and what are the conditions. So, essentially that lead to the stability and error calculation; so, error, accuracy and stability of the system. So, once we know that, then only we can I mean actually appreciate whether given a system when you bring down to a linear system it not necessary that always you are going to get an solution. Because that numerical system or the linear system they are associated with all these parameters.

So, given a condition, one should know what kind of error he has in his numerical approximation, what kind of accurate system he has in his numerical methods, what is the condition for his stability of the system, it is not guaranteed that if you have a given a system this is always going to be stable. So, you need to get all these details and that is possible when you get an look or have a look on this derivative calculation.

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Derivatives, Error, Accuracy

example $\partial_t^2 p = c^2 \Delta p + s$ $\xrightarrow{G.E}$

$\Delta = (\partial_x^2 + \partial_y^2 + \partial_z^2)$

P \rightarrow pressure
c \rightarrow acoustic wave speed
s \rightarrow sources

The acoustic wave equation

- seismology
- acoustics
- oceanography
- meteorology
- etc.

application

$\partial_t C = k \Delta C - \mathbf{v} \cdot \nabla C - RC + p$

C \rightarrow tracer (scalar) concentration
k \rightarrow diffusivity
v \rightarrow flow velocity
R \rightarrow reactivity
p \rightarrow sources

Diffusion, advection, Reaction

- geodynamics
- oceanography
- meteorology
- geochemistry
- sedimentology
- geophysical fluid dynamics

application

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Now, if you look at this simple example, this is an example, the example is the $\nabla^2 p$ by $\nabla t c^2$, this is the equation and this equation actually represents the acoustic wave equation. And these are the application of that, application of the system.

Seismology, acoustics, oceanography, meteorology, so all these areas there could be more all these area this is the applications, but the essential the governing equation this is the governing equations which actually represent this acoustic wave equations which is nothing but the second order pressure transient equations along with this. And what that ∇^2 stands for this nothing but the second derivative of the squares. And here p stands for pressure, c stands for acoustics wave speed and s stands for sources.

So, if I have a acoustics wave equation that can be represented by this kind of equations. Now our task is to get this equation solved through a numerical method. So, particularly we are talking about finite volume method. So, we should be able to get an solution using finite volume method of this equation. So, in a if I talk about in a sense, this is the governing equation then represent my physical problem, the physical problem is the solution of the acoustics wave equation for seismology or acoustics.

Now, this is the governing equations so the system is represented by these set of equations. And our numerical approach should be to get the solution of this particular system. Now while doing that we come across so when you have the system, the ultimate bottom line is that from this system you convert to the linear system. But in between that you have a mesh generation you have a discretizations and once you discretize that you come across derivative, you come across error you need to account for your accuracy, you need to account for your stability of the system all this would be the byproduct of that.

Similarly, if you have a reaction diffusion system, this is the application and these the area of applications. Geodynamics, oceanography, meteorology all these are the application area, and essentially this is the governing equations. So, that is a reaction diffusion system. And C is essentially or the C stands for the tracer. It could be any scalar. It could be any diffusion variable; it could be any non-reactive variable or tracer concentration. And there is a unsteady term, k is the diffusivity, v is the flow velocity, R is the reactivity and then p is the source term, ok.

. So, and the system that is represented by this equations are unsteady term, this is your variant term, convection term reaction term as a so again the idea is that this is a physical problem in hand, the governing equations is like this these, governing equations actually represents the reaction diffusion system. And then our numerical methods should discretize the system or the numerical approach that we use discretize the system to lead to a linear system, and we will get a solution. Once we get a solution that should again reflect back any physical problem that is dealt with this reaction diffusion system.

So, this is a some example where your derivative become really important.

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Derivatives, Error, Accuracy

Common definitions of the derivative of $f(x)$:

$$\partial_x f = \lim_{dx \rightarrow 0} \frac{f(x+dx) - f(x)}{dx} \quad \leftarrow (i+1) / (i-1)$$

$$\partial_x f = \lim_{dx \rightarrow 0} \frac{f(x) - f(x-dx)}{dx} \quad \leftarrow f_{i+1} - f_i$$

$$\partial_x f = \lim_{dx \rightarrow 0} \frac{f(x+dx) - f(x-dx)}{2dx} \quad \leftarrow \frac{f_{i+1} - f_{i-1}}{2dx}$$

These are all correct definitions in the limit $dx \rightarrow 0$.

But we want dx to remain **FINITE**

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Now, again coming back to the derivative calculation; so, underneath of all these are the calculation of the derivatives. So, how you calculate the derivatives? So, for a given a function $f(x)$; so, that $\frac{df}{dx}$ you can calculate like $\lim_{dx \rightarrow 0} \frac{f(x+dx) - f(x)}{dx}$. So, that is method one or approach 1, you can say approach 1. Or I can calculate $\frac{df}{dx}$ like $\lim_{dx \rightarrow 0} \frac{f(x) - f(x-dx)}{dx}$.

So, if you look at these 2 case, there is a slight difference. In these particular case, you are considering if I am trying to find out a derivative at a particular point in the domain. This is my i th point where I am trying to find out the $\frac{df}{dx}$. One case and let us say this is the distance between these points are dx , ok.

So, one case I am taking the points ahead of it. So, this essentially means f at $i + 1$ minus function at i . So, one case I am taking the function at this point, the second case I am taking the point at this point. Since, I am trying to find out the derivative at point i so that remains constant. Or alternatively this is the approach 3 or third approach, where you can find out the derivative considering the point here and considering the point here. So, one case it is essentially $f(i + 1) - f(i)$ divided by $2 \Delta x$. Because if this distance are Δx or dx , ok.

So, all these are the calculation of derivatives. What remains constant here is this Δx , ok. And the Δx also need to be finite and the calculation of these different methods are given different names. So, one case it is forward approach, other case is backward approach, third case is central approach.

Why we are saying all this? Because when you are trying to find out the derivative at i th location, invoking the point at $i + 1$ that it is actually become the forward approach. You are considering the point ahead of the point what you interested in. Second approach; when you are using or invoking the point, the behind of that interested point; that means, i and $i - 1$. So, that actually is a backward approach. That means, you are moving to these direction, one case you are going this direction, other case you are going the backward direction. And the third case you actually involve the point ahead of it which is $i + 1$ and the point which is behind it $i - 1$. But they are separated with a finite distance of 2 times of the difference between each point.

So, this actually takes some sort of a mean approach between around this point. So, if this point is sitting in the middle, as we said that dx , they need to be sort of uniform if, then it cause the central approach, ok. But no matter what adapt here the dx needs to be finite.

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Derivatives, Error, Accuracy

The equivalent **approximations** of the derivatives are:

$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}$	forward difference
$\partial_x f^- \approx \frac{f(x) - f(x-dx)}{dx}$	backward difference
$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$	centered difference

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Now, similarly equivalent approximation that as I said all these approximation that we have written so far so $\frac{\partial f}{\partial x}$. So, this plus sign means you go forward. As I said you are talking about this point i , you are having a point $i+1$, you are having a point $i-1$, and these are the distance which are considered to be uniform. So, these become $i+1$ minus i by like this. Backward you are moving backward. So, i minus $i-1$, and in the case of centered you use $i+1$ minus $i-1$.

So, essentially around this point you get some sort of a mean. So, the way you adapt the point, whether the point ahead of it, or the point behind it, or the point including both the upstream and the downstream point, then you call it a center. So, the depending on the point the derivatives are also given some sort of a name.

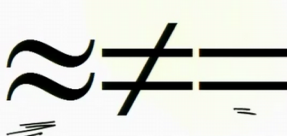
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Derivatives, Error, Accuracy

The **big** question

How good are the FD approximations?

\approx approx.




$\frac{\partial f}{\partial x} \approx \frac{\partial f}{\partial x}$

↑

error

This leads us to Taylor series....

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Now, the question which remains same, I mean is these are not equal to when we talk about this particular sign that means a lot. So, they are not necessarily equals to.

So, that means this is a approximation. So, what you can understand here or you can assume? That all this derivative that we are calculating whether using forward or backward all these derivative whether del f plus del f minus, all these are approximated. So, as soon as the term approximation comes into the picture, it is always or bound to associated with some sort of a errors. So, that is why we are going to discuss about errors which are associated while finding this derivative.

Now, when it is say these are approximated then how do you find out these derivatives. So, that leads to this famous theorem of the Taylor series which is A. How do you write that?

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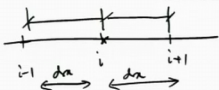
Derivatives, Error, Accuracy

Taylor series are expansions of a function $f(x)$ for some finite distance dx to $f(x+dx)$

$$f(x \pm dx) = f(x) \pm dx f'(x) + \frac{dx^2}{2!} f''(x) \pm \frac{dx^3}{3!} f'''(x) + \frac{dx^4}{4!} f^{(4)}(x) \pm \dots$$

$\underbrace{f(i \pm 1)}_{f_i \pm f'_i} \quad \underbrace{\frac{dx^2}{2!} f''(x)}_{f''_i} \quad \underbrace{\frac{dx^3}{3!} f'''(x)}_{f'''_i} \quad \underbrace{\frac{dx^4}{4!} f^{(4)}(x)}_{f^{(4)}_i} \pm \dots$
 What happens, if we use this expression for

$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx} \quad ?$



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So, again this are the point of interest. I have a point ahead of it. And they are of uniform distance. I have a point behind it also at a uniform distance. dx now if I write Taylor series expression, then I write x plus minus dx . So, essentially if I write i plus minus 1; that means, either I am writing for f i plus 1 or I am writing for f minus 1. And what you are writing for? f x so, that is evaluated at f i plus minus dx remain constant, because this is the distance between these 2 points.

So, i and i plus 1 this is the distance or i or i minus 1, ok. f prime i that means, f x plus dx into f prime i dx square by factorial 2 f prime double prime i plus minus dx cube by factorial 3 f triple prime i . So, all these at x means this is f 4 i all these are evaluated at the location of i . So, how do you find out these derivative using this Taylor series expression? So, essentially if I collect these terms and then write down that.

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Derivatives, Error, Accuracy


... that leads to :

$$\frac{f_{i+1} - f_i}{dx} = \frac{f(x+dx) - f(x)}{dx} = \frac{1}{dx} \left[dx f'_i(x) + \frac{dx^2}{2!} f''_i(x) + \frac{dx^3}{3!} f'''_i(x) + \dots \right]$$

$= f'_i(x) + O(dx)$
neglecting higher order terms
Taylor series expansion

The error of the first derivative using the forward/backward formulation is of order dx.

Is this the case for other formulations of the derivative?
Let's check!


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So, let us write that if $x + dx$ minus f_x . So, if you come back from these particular expression, and you collate the term f_{x+dx} by dx . So, which means $f_{i+1} - f_i$, then you get 1 by dx f'_i f''_i f'''_i , these are all evaluated at this i , ok.

Then if you take this terms into consideration, I can write $f'_i(x)$ and $O(dx)$; that means, I am not neglecting the higher order term. So, essentially the higher order terms are higher order terms. And this O stands for the order. So, if you divide by dx so any other term the highest order with dx . So, since dx is a small number, dx is a small number any other terms would be small. Because the third derivative will invoke dx^3 being dx is a small number dx^2 or dx^3 would be much smaller compared to dx . That is why you can it is relatively or reasonably fair enough to write that the other terms are kind of collected inside the order of dx .

So, what is the error? Essentially I am interested in this component and this component. So, this is an extra term, and these extra term is coming due to Taylor series expansion, ok. So, due to Taylor series expansion, you get this extra term and which essential is says the first derivative if you calculate using this forward formulation. This is the highest order of error is dx or in a reverse term sometime people say the first derivative using the forward formulation is of the order dx ; that means, the order of accuracy. Here this order

means a order of accuracy of the system. So, the order of accuracy of the system is in the forward formula is the first order.

So, the other formulations, this can lead to a different set of error or different set of order of accuracy. So, we can check what are them. Now for, but one point you can note here. So, this says that the order of accuracy is first order for forward formula. Now if you use the backward formula, for example, to calculate $f_i - f_{i-1}$. If you use like that, then that would be also first order derivative. So, whether it is a forward or backward they are first order accurate, but the same thing is not true for second order central system.

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Derivatives, Error, Accuracy


... with the *centered* formulation we get:

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

$= f'(x) + O(dx^2)$ ← truncation error

The error of the first derivative using the centered approximation is of order dx^2 .

This is an **important** results: it DOES matter which formulation we use. The centered scheme is more accurate!

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The centered system what it does? That it does you have the point i point $i + 1$ $i - 1$ and this is dx , then I am using this point and this point. The central if you collects the points you see the first derivative is order of dx square. So, essentially the center scheme gives you back a second order accurate system. Because these order or the highest ordered term which is actually associated with this discretization or the Taylor series expansion, they lead to the order of accuracy of the system.

And this is where when you say my numerical scheme is that order accurate or the these order accurate; that means, the value are calculating the derivative the highest order term, or the error which is associated with the highest order term which are actually left out of the truncated. This sometimes call it also the truncation error, ok.

And we will talk about that as we move forward with the lectures, because that is also an important quantity that we need to quantify and also discuss. So but for the time being this also given a name truncation error, why it is that? Because you are only interested in first order derivative and this the all higher ordered terms are truncated off. Since they are truncated off if you are collectively take them together the order which actually gets you back is the second order.

And since it is second order this is the order of accuracy of the system. So, the error now if you see interestingly this is dx square. So, when a system is second order accurate, and if your these dx nothing but my grid size for my numerical problem.

Now, if dx is small, if this is small, then you can think about the dx square root would be much smaller. So, these term actually the error term becomes negligible or these does not contribute to any numerical error; that is associated with your discretization scheme. But this is very, very important to note here that if you do not consider this things properly you may have a very stable system, but that does not guarantee that it you have a error free system or less error system. Now another important thing there if you use forward or backward compared to center this is always highest higher order accurate system.

So, what is recommended is that when you use any numerical scheme or calculation of the derivative that is what actually the key element of any numerical scheme, how you calculate the derivatives? Because the derivatives calculation will tell you what is the order of accuracy of the system. So, more and more or higher orders you have you have less error of these term, and that will have a more accurate system, ok. So, we will stop here today, and we will take from here in the follow up lectures.

Thank you.