

Introduction to Finite Volume Methods-I
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Lecture – 12

(Refer Slide Time: 00:15)

Derivatives, Error, Accuracy

• Second derivatives: f''

* Central difference: f''_{i+2}

If $\Delta x_i = \Delta x_{i+1} = \Delta x$, then

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

* Forward difference:

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

* Backward difference:

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

$f_{i+2} = f_i + (2\Delta x)f'_i + \frac{(2\Delta x)^2}{2}f''_i + \dots$

→ uniform spacing.

$f_{i+1} = f_i + \Delta x f'_i + \frac{\Delta x^2}{2} f''_i + \dots$

$f_{i-1} = f_i - \Delta x f'_i + \frac{\Delta x^2}{2} f''_i - \dots$

$f_{i+1} + f_{i-1} = 2f_i + \Delta x^2 f''_i$

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So, welcome to the lecture of this Finite Volume Method. Now, similarly if you look at the second derivative that means, f double prime. Now f double prime you look at in again 3 different ways and you see what happens. So far we have been talking about only f prime, f double prime if you look at central differences so, this can be written as del 2 f by del x 2. So, my stencil is like this. I have i, I have i plus 1, I have i minus 1 and these are all delta x; that means, essentially uniform spacing.

So, if that is there, so, similarly I evaluate second order derivative del 2 f by del x 2. It just like writing all these Taylor series expansion, f i plus delta x f i prime delta x square by 2 f double prime, ok and f i minus 1 equals to f i minus delta x f i prime plus delta x square by 2 f i double prime. If you add and take this out then this guys goes off and you take them together. So, you get an expression f i plus 1 plus f i minus 1 equals to 2 f i plus delta x square by 2 f i double prime.

So, if you take that and the terms which are written there, so, third derivative would be plus and minus. So, they will cancel up and the term which will be written is order of x

square; that means, even using 3-point stencil, the second derivative using central scheme is second order accurate, ok. But at the same time if you use this 3 point and try to capture the forward difference, then you use not only $i + 1$ and $i - 1$ you use one point ahead of it $i + 2$. So, $i + 2$ would be like if I try to write $i + 2$ this is nothing but $i + 2 \Delta x f'(i + 2 \Delta x) + \frac{1}{2} (2 \Delta x)^2 f''(i + 2 \Delta x) + \dots$ and so on. If you take that, so, essentially $f(i + 2 \Delta x) - 2f(i + \Delta x) + f(i)$, but important thing is there.

Similarly, for backward difference you use $i - 2$, but important point is here. So, irrespective of that stencil; first derivative or second derivative if you use whether 3-point stencil or 2-point stencil they remain in forward and backward difference scheme. They are always first order accurate. At the same time, central difference scheme is always second order accurate, whether we use 3-point stencil or 5-point stencil. This is always second order accurate. So, this is an important thing to note how you evaluate your derivative and then you get your schemes, ok.

(Refer Slide Time: 04:31)

Derivatives, Error, Accuracy

Mixed derivatives:

* Taylor series expansion:

$$f(x + \Delta x, y + \Delta y) = f(x, y) + \Delta x \frac{\partial f}{\partial x} + \Delta y \frac{\partial f}{\partial y} + \frac{(\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(\Delta y)^2}{2!} \frac{\partial^2 f}{\partial y^2} + 2 \frac{(\Delta x)(\Delta y)}{2!} \frac{\partial^2 f}{\partial x \partial y} + o[(\Delta x)^3, (\Delta y)^3]$$

* Central difference:

$$\left(\frac{\partial^2 f}{\partial x \partial y} \right)_{i,j} = \frac{f_{i-1,j+1} - f_{i-1,j-1} - f_{i+1,j+1} + f_{i+1,j-1}}{4(\Delta x)(\Delta y)} + o[(\Delta x)^2, (\Delta y)^2]$$

* Forward difference:

$$\left(\frac{\partial^2 f}{\partial x \partial y} \right)_{i,j} = \frac{f_{i+1,j+1} - f_{i,j+1} - f_{i+1,j} + f_{i,j}}{(\Delta x)(\Delta y)} + o[(\Delta x), (\Delta y)]$$

* Backward difference:

$$\left(\frac{\partial^2 f}{\partial x \partial y} \right)_{i,j} = \frac{f_{i,j} - f_{i-1,j} - f_{i,j+1} + f_{i-1,j+1}}{(\Delta x)(\Delta y)} + o[(\Delta x), (\Delta y)]$$

$f(x, y)$
 $f(x + \Delta x, y)$

$f_{i+1, j+1} = f(x + \Delta x, y + \Delta y)$
 $f_{i-1, j+1} = f(x - \Delta x, y + \Delta y)$
 $f_{i+1, j} = f(x + \Delta x, y)$
 $f_{i-1, j} = f(x - \Delta x, y)$

2nd order accurate (Central difference)
1st order accurate (Forward/Backward difference)

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Now, since we are trying to find out the derivatives one can find out the mixed derivatives. Like, again that through that Taylor series expansion. It is essentially retaining the terms both x and y . So, your function which is essentially at certain location is x and y , then x plus Δx and y plus Δy it would be $f(x, y)$; that means, the function at a given point, now I am going to do it is x plus Δx and y . And I am going in

this direction where $x \Delta y$. So, this distance is Δy this distance is Δx ok. So, $f(x + \Delta x, y + \Delta y)$; that means, it would be $f(x, y) + \Delta x \frac{\partial f}{\partial x} + \Delta y \frac{\partial f}{\partial y} + \frac{1}{2} \Delta x^2 \frac{\partial^2 f}{\partial x^2} + \Delta x \Delta y \frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2} \Delta y^2 \frac{\partial^2 f}{\partial y^2} + \dots$. So, this is the term in the first derivative term then Δx^2 by factorial 2 $\frac{\partial^2 f}{\partial x^2}$. So, this is term retaining second derivative, then this retain the cross derivative then the higher order terms or the truncation terms, truncated terms.

So, mixed derivative, you get an Taylor series expansion like this. $f(x, y) + \Delta x \frac{\partial f}{\partial x} + \Delta y \frac{\partial f}{\partial y} + \frac{1}{2} \Delta x^2 \frac{\partial^2 f}{\partial x^2} + \Delta x \Delta y \frac{\partial^2 f}{\partial x \partial y} + \frac{1}{2} \Delta y^2 \frac{\partial^2 f}{\partial y^2} + \dots$ Now if you use central difference scheme to find out $\frac{\partial^2 f}{\partial x \partial y}$, then that uses $f(i+1, j+1) - f(i+1, j) - f(i, j+1) + f(i, j)$. So, $f(i+1, j+1) - f(i+1, j) - f(i, j+1) + f(i, j)$ is nothing but $f(x + \Delta x, y + \Delta y) - f(x + \Delta x, y) - f(x, y + \Delta y) + f(x, y)$, $f(i+1, j+1) - f(i+1, j) - f(i, j+1) + f(i, j)$ equals to $f(x + \Delta x, y + \Delta y) - f(x + \Delta x, y) - f(x, y + \Delta y) + f(x, y)$, ok. And divided by 4 into this, but as expected central difference is second order. Even for mixed derivative central difference is second order. While you look at forward difference and backward difference, that will retain $f(i+1, j+1) - f(i, j+1) - f(i+1, j) + f(i, j)$, but it is first order accurate system. When you look at $\frac{\partial^2 f}{\partial x \partial y}$ using backward $f(i, j) - f(i-1, j) - f(i, j-1) + f(i-1, j-1)$ divided by this again this is first order accurate.

So, the bottom line here is that if you use forward or backward difference scheme they are always first order accurate. So, that is true for first derivative, that is true for second derivative, that is true for f' , that is true for f'' , that is true for f''_{xy} even mixed derivative. And central difference scheme is always second order accurate. So, that is true for first derivative, second derivative, higher derivative or the mixed derivative. So, this is what is expected.

(Refer Slide Time: 09:23)

Derivatives, Error, Accuracy

High-order approximations

Taylor series
+ stencil \Rightarrow weights

1st $\Rightarrow \left(\frac{\partial u}{\partial x}\right)_i = \frac{2u_{i+1} + 3u_i - 6u_{i-1} + u_{i-2}}{6\Delta x} + \mathcal{O}(\Delta x)^3$

1st $\Rightarrow \left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 6u_{i+1} - 3u_i - 2u_{i-1}}{6\Delta x} + \mathcal{O}(\Delta x)^3$

1st $\Rightarrow \left(\frac{\partial u}{\partial x}\right)_i = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + \mathcal{O}(\Delta x)^4$

2nd $\Rightarrow \left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12(\Delta x)^2} + \mathcal{O}(\Delta x)^4$

backward difference } 3rd order accurate } 4th stencil

forward difference }

central difference } 4th order accurate }

central difference } 5th stencil

Pros and cons of high-order difference schemes

- ⊖ more grid points, fill-in, considerable overhead cost u_{i-2}
- ⊕ high resolution, reasonable accuracy on coarse grids

✓ Criterion: total computational cost to achieve a prescribed accuracy \leftarrow

$\Delta x = \text{small} \downarrow$
 less truncation error.

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Now, you can always using this kind of Taylor series expansion you estimate the higher order approximation. So, the baseline of that is Taylor series, and you define a stencil then find out the weights, ok. And once you do that you can always get back the higher order terms. For example, let us say someone wants to find out $\frac{\partial u}{\partial x}$, that is a first derivative, this is first derivative. First derivative but using backward difference scheme, ok. And the order of accuracy of this is third order. So, I am trying to find out first derivative using backward scheme so far we have seen that first derivative is using backwards scheme always give back the first order accurate system.

But if you use higher order approximation, this is very important to note if you use higher order approximation then the weights are different this become third order accurate. And if you look at the weight of this points they are different. So, this is my i th point i plus 1 i plus 2 i minus 1 i minus 2. So, it uses all these information of i plus 1 i minus 1 i minus 2 and get a third order system this is same thing for forward difference. It uses i plus 2 i plus 1 i minus 1 and it gets you back the third order accurate system.

Now, interesting to note here that number of points which are involved to find out this derivative, so, here we are interested to find out the derivative at location i . And using forward and backward difference scheme the points which are involved for backward difference the point which are involved are essentially these 4 points. i plus 1 i minus 1 i

minus 2, when you go to forward difference it involved $i - 1$, $i + 1$, $i + 2$ so, it involves these 4 points. So, that actually requires 4 point stencil, ok.

Now, same thing if you use these things for the central difference scheme, if you use these for the central difference scheme, and still you are trying to find out the first derivative. And the points which are involved so, I am trying to find out the first derivative at i and this is central so, I need $i + 1$ I need $i + 2$ I need $i - 1$ and $i - 2$, and if I write down the Taylor series expression and then find out the weights these becomes 4th order accurate, ok.

Now, at the same time using all these 5 points, if I find out the second derivative, using central different scheme, this is also 4th order accurate. But the points which is required, now for the central difference scheme you need 5-point stencil ; that means, 2 point ahead of the interested point of the desired point, 2 point downstream of it. So, you get and if you look at this weights using Taylor series expansion you can easily find out these weights or like the matrix method we have discussed, you multiplied with you find out u_{i+1} you find out u_{i+2} you find out u_{i+1} you find out u_{i-2} u_{i-1} u_{i-2} multiplied each of this expression a b c d and find out these weights, ok.

But some advantage some disadvantage of this higher order schemes. What you can immediately see even for backward and forward differences you need 4 points. So, more grid points are required; that means, the stencil size is higher. Fill in is more considerable overhead cost; that means, your computing overhead would be higher. So, every time instant the number of floating point calculation would be higher, but advantage high resolution even it is reasonably accurate on coarse grid. Because, few minutes back we have been talking about the discretization error or the truncation error and that one way to reduce is that Δx to be small even here; if it is small, this leads to less truncation error.

But what here we say high resolutions that higher order scheme or higher order approximation, that on even coarse are grid; that means, Δx is not very small, you have reasonably accuracy on the; so, what is the primary criteria? Primary criteria is that total computational cost to achieve a prescribed accuracy. So, you need to calculate the computational overhead, and make an tradeoff that whether you really need a higher

order scheme, or you can afford to have a lower order scheme, and uses better grid spacing and reduce those errors.

(Refer Slide Time: 16:50)

Derivatives, Error, Accuracy

In many situations, questions arise regarding the **round-off** and **truncation errors** involved in the numerical computations, as well as the consistency, stability and the convergence of the finite difference scheme.

Round-off errors: computations are rarely made in exact arithmetic. This means that real numbers are represented in "floating point" form and as a result, errors are caused due to the rounding-off of the real numbers. In extreme cases such errors, called "round-off" errors, can accumulate and become a main source of error.

Handwritten notes:
- variable definition \leftarrow double precision? \Rightarrow Reduce the round off errors
do have proper machine precision

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So, what I just said if you put them together; that means, in many situations, the questions arise regarding the round off, and truncation errors involved in the numerical computation as well as the consistency, stability and the convergence of the scheme, ok. So, this is very, very important questions that brings to our table, that all these error how do they accumulate. And so, as I again repeat back the round off errors. So, the computations are really made in exact arithmetic. This means, that real numbers are represented in floating point from and as a result errors are caused due to the rounding off the real numbers. In extreme cases such errors called round off errors.

And this becomes one of the main source of errors; that means, your variable definition must be double precision so that it uses an do have proper machine precision. In combination of these 2 you can always reduce the round off errors ok.

(Refer Slide Time: 18:48)

Derivatives, Error, Accuracy

❖ The accuracy of a numerical solution is determined by its total error, which is the sum of the round-off error and truncation error

Total error = Round-off error + Truncation error

- ❖ Round-off error is directly proportional to the total number of arithmetic operations
- ❖ The total number of arithmetic operations is inversely proportional to the step size
- ❖ Round-off error is inversely proportional to the step size
- ❖ Truncation error is directly proportional to the step size

Variation of round-off error, truncation error, and total error with step size

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Now, if you look at the complete picture of that so, total error would be the sum of the round off error and the truncation error, ok. And how they vary if this is my error plot in this direction, this is my grid spacing.

So, if grid size or the step size increases my truncation error goes up; which is obvious because the order of scheme would be the our higher the terms which are truncated off from the Taylor series they will lead to the more error. But round off error can come down. And if grid size is small truncation error comes down, but so it is always between a optimum zone where your total error is minimized. So, round off error is directly proportional to the total number of arithmetic operations. And on the other side, the total number of arithmetic operation is inversely proportional to the step size. So, these 2 kind of lead to this picture of round off errors. So, this becomes inversely and truncation error is directly proportional to the step size. So, you need an optimum bandwidth where your total error would be minimal and uses that for your calculation.

(Refer Slide Time: 20:37)

Derivatives, Error, Accuracy

- ❖ To get the most accurate solution, one has to perform a grid independence test.
- ❖ The test is carried out by experimenting with various grid sizes and watching how the solution changes with respect to the changes in grid sizes.
- ❖ A stage will come when changing the grid spacing will not affect the solution. In other words, the solution has now become independent of grid spacing.
- ❖ Grid sizes are changed discretely, one does not get an exact minimum, but a range of grid sizes for which total error remains more or less unchanged. (This is called **grid independence test**.) ✓
- ❖ Below the lower limit and above the upper limit of the grid independent region, total error increases. The largest value of grid spacing for which the solution is essentially independent of step sizes is chosen so that both the computational time and effort and the round-off error are minimized.

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Now, another thing when you say our solution has converged, or solution does not change or we have reached to a steady solution that means actually nothing or sometime that means a lot. Because to get an accurate solution you always need to perform a grid independence test; that means, I should Δx should vary, ok. And check how so this is the numerical error and the solution. So, this line correspond to the error, this line correspond to the solution and this is the choice of Δx that one requires.

So, one need to have solution at multiple grids and see if the solutions are not changing with the grid; that means, the solution becomes or rather independent of grid spacing. If that happens; that means, the solution has becomes independent of grid spacing and you can take that an optimal size of the grid and move forward. So, this essentially one needs to be carried out, and how solution changes with respect to the grid size. At some point of time when the solution become independent of grid spacing so; that means, it will not affect the solution any other I mean anymore.

So, you can say the solution is now independent of grid spacing. Now once grid sizes are changed discretely one does not get an exact minimum, but a range of grid size for which that total error remains more or less unchanged. This is when you call is the grid independence test; that means, when I am varying the grid spacing and getting a solution so, solution one to solution 2 and solution 2 to solution 3, the error percentage when that becomes independent of grid size then we can call it as a grid independence test.

So, below the lower limit and above the upper limit of the grid independent region, total error increases. So, the largest value of the grid spacing for which the solution is essentially independent of step sizes is chosen. So, that computational time and effort both are sort of minimized.

(Refer Slide Time: 23:42)

Example

$$\partial_t^2 p = c^2 \Delta p + s$$

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

P	pressure ✓
c	acoustic wave speed ✓
s	sources ✓

Problem: Solve the 1D acoustic wave equation using the finite Difference method.

Solution:

$$p(t + dt) = \frac{c^2 dt^2}{dx^2} [p(x + dx) - 2p(x) + p(x - dx)] + 2p(t) - p(t - dt) + s dt^2$$

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Now, the example that we have taken that if you look at it that wave equation; that solve the 1D acoustic wave equation using some. The governing equations is this where delta is the Laplacian, p stands for pressure, c is the wave speed, s is source and solution would be of this nature, p t plus delta t and x plus dx and all these.

(Refer Slide Time: 24:18)

Example

$$p(t + dt) = \frac{c^2 dt^2}{dx^2} [p(x + dx) - 2p(x) + p(x - dx)] + 2p(t) - p(t - dt) + sdt^2$$

Stability: Careful analysis using harmonic functions shows that a stable numerical calculation is subject to special conditions (conditional stability). This holds for many numerical problems. (Derivation on the board).

$c \frac{dt}{dx} \leq \varepsilon \approx 1$

⇒ stability

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Now, what happens when you try to see the solution? There is a restriction on the wave speed and dt. And actually the careful analysis shows that the restrictions comes on this guy $c dt$ by dx which must be less than 1. So, this has to do with the stability of the solution. So now, so far we have been talking about the accuracy of the solution, order of accuracy of the solution round off error truncation error now we come across a new term the stability of the solution. And one has to make sure the solution that you obtain that is stable enough. And that has some restriction, but this is an example we will have these criteria more and more in details.

(Refer Slide Time: 25:17)

Example

$$p(t + dt) = \frac{c^2 dt^2}{dx^2} [p(x + dx) - 2p(x) + p(x - dx)] + 2p(t) - p(t - dt) + sdt^2$$

less dispersion error

Dispersion: The numerical approximation has artificial dispersion, in other words, the wave speed becomes frequency dependent (Derivation in the board). You have to find a frequency bandwidth where this effect is small.

The solution is to use a sufficient number of **grid points per wavelength**.

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Now, if you look at the solution at different time step with these, and if you plot this is some representative plots there are some things called dispersion. So, the numerical approximation has some artificial dispersion. In other words, the wave speed becomes frequency dependent. So, your solution also needs to have less dispersion error. And that means, one hand you must have stable solution and which will have a criteria to bandwidth, other case you have a less dispersive solution. So, that also for this particular case if you use sufficient larger number of grid points per wavelength then you can actually reduce this dispersion error, ok.

(Refer Slide Time: 26:23)

Derivatives, Error, Accuracy

Higher order terms that is retained in truncated terms

Accuracy: Refers to the correctness of a numerical solution when compared to an exact solution. In most cases, we do not know the exact solution. It is therefore more useful to talk of the *truncation error* of a discretization method. The truncation error associated with the grid size. Thus, if we refine the mesh, we expect the truncation error to decrease. The *order* of a discretization method is n if its truncation error is $O(\Delta x^n)$. It is important to understand that the truncation error tells us how fast the error will decrease with mesh refinement, but is not an indicator of how high the error is on the current mesh. Thus, even methods of very high order may yield inaccurate results on a given mesh. However, we are guaranteed that the error will decrease more rapidly with mesh refinement than with a discretization method of lower order.


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So, that is a solution one can and if you look at the velocity is this would these are some representative things. Now coming back to the accuracy; so, accuracy of the system is that your truncation order or the order of the truncation error, how accurate that is; so, more useful to talk about the truncation error or the discretization error. So, the order of accuracy of the system will depend higher order terms; that is, retained in truncated during or truncated terms, ok.

So, essentially this has to do the order of accuracy of the system. So, if you refine the mesh, we expect the truncation error to decrease. Because the order of discretization method is order of Δx to the power n , but one has to also understand that how fast the error decrease with the mesh refinement. But it is not a indicator of how high the error is on the current mesh. So, even the methods of very high order may yield inaccurate

results on a given mesh; however, we are guaranteed that the error will decrease more rapidly with mesh refinement than with a discretization method of lower order.

(Refer Slide Time: 28:06)

Derivatives, Error, Accuracy

Consistency: A *consistent* numerical method is one for which the truncation error tends to vanish as the mesh becomes finer and finer. (For unsteady problems, both spatial and temporal truncation errors must be considered). We are guaranteed this if the truncation error is some power of the mesh spacing Δx (or Δt). Sometimes we may come across schemes where the truncation error of the method is $O(\Delta x/\Delta t)$. Here, consistency is not guaranteed unless Δx is decreased faster than Δt . Consistency is a very important property. Without it, we have no guarantee that mesh refinement will improve our solution.

Stability: The previous two properties refer to the behavior of the discretization method. Stability is a property of the *path to solution*.

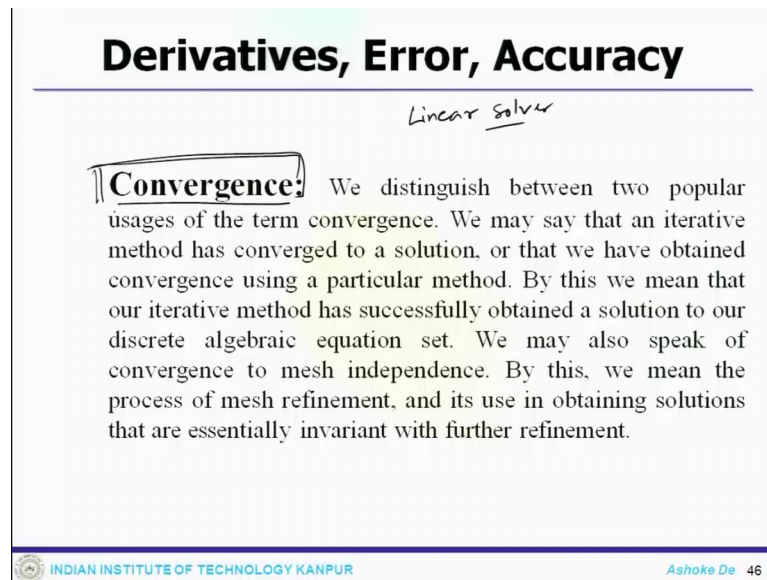
stable/unstable

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Second point is the consistency a consistence consistent. Numerical method is one which the truncation error tends to vanish as mesh becomes finer and finer. So, the truncation error is of the power of mesh spacing and delta t. So, sometime we may come across schemes where the truncation error of the method is delta x by delta t. So, consistency is not guaranteed unless delta x is decreased faster than delta t. Consistency is a very important property without it we have guaranty that mesh refinement will improve our solution.

So, accuracy then consistency of the solution, then the stability, that we already come across with that example that the path of the solution. If I want the solution from here to there, the path of the solution whether it is stable or unstable. So, your numerical scheme must be stable enough to get you a solution.

(Refer Slide Time: 29:17)



Derivatives, Error, Accuracy

Linear solver

Convergence: We distinguish between two popular usages of the term convergence. We may say that an iterative method has converged to a solution, or that we have obtained convergence using a particular method. By this we mean that our iterative method has successfully obtained a solution to our discrete algebraic equation set. We may also speak of convergence to mesh independence. By this, we mean the process of mesh refinement, and its use in obtaining solutions that are essentially invariant with further refinement.

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Finally, convergence so, convergence has to do so, there are 2 types of convergence. One may say that how my linear solver has converged; that means, the convergence of the linear solver. Others may say that when I keep on refining the grid so solution has converged.

So, both the cases you can actually say the convergence of the solutions. So, when you say convergence, it can be meant for both the cases. Solution of the linear solver or solution of the your mesh refinement or the grid refinement test. So, your scheme should have all these properties. And so, today we will stop here and carry forward in the next lecture.

Thank you.