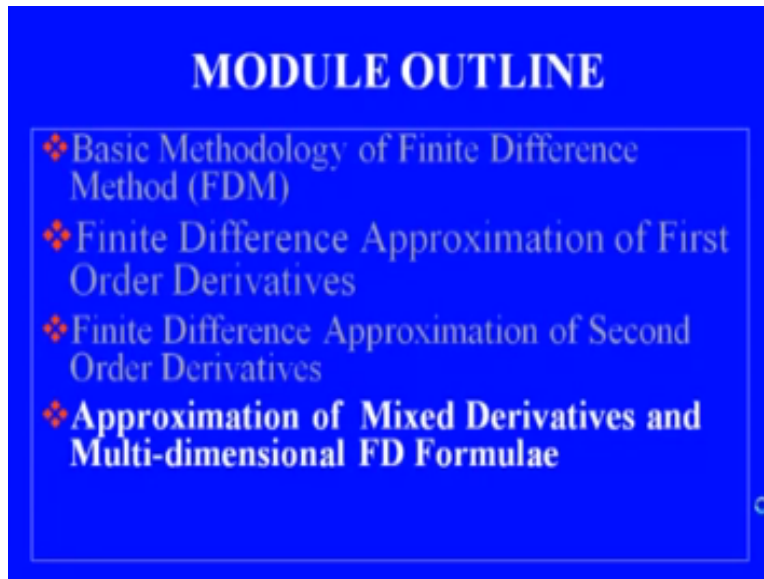


Computational Fluid Dynamics
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Lecture – 14
Approximation of Mixed Derivatives and Multi-Dimensional F.D Formulae

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Welcome to the next lecture in module 3 on finite difference method is get back to an outline; we had covered the basic methodology of finite difference method. We also finished our discussions on finite difference approximation of first order derivatives and second order derivatives. Today, we are going to focus on approximation of mixed derivatives and multidimensional finite difference formulae.

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Recapitulation of Lecture III.4

In previous lecture, we discussed:

- ❖ Approximations based on Taylor Series Expansion
 - ❖ General Procedure on Uniform Grids
- ❖ Polynomial Fitting

for FD approximation of Second Order Derivatives.

And then later on we would take up applications of finite difference method; tis scalar transport problems, just a recap of recapitalisation of what we did in lecture 5. In previous lecture, we discussed approximation based on Taylor series expansion specifically the one based on the general procedure on uniform grades and we discussed our derived formula using polynomial fitting for finite difference approximation of second order derivatives.

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LECTURE OUTLINE

- ❖ Approximation of 2nd Order Derivative in Scalar Transport Equation
- ❖ Multi-dimensional Formulae
- ❖ Approximation of Mixed Derivatives
- ❖ Implementation of Boundary Conditions
- ❖ Finite Difference Algebraic System

Today, that is the fifth lecture in this theory; we were look at approximation of mixed derivatives and multidimensional finite difference formulae. So, outline of todays lecture, let us have a look at the approximation of second order derivatives of mixed type in the scalar transport equation then we will have a look at how do we extend the formulae which we derived so for; for single

variable or in one dimension to multidimensional situation because for this, we would need in practical CFD combinations.

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SECOND ORDER DERIVATIVE IN GENERIC TRANSPORT EQUATION

The diffusion term in the generic conservation equation involves a second order derivative of the form $\partial(\Gamma \partial \phi / \partial x) / \partial x$.

- ❖ If Γ is constant, this term becomes $\Gamma (\partial^2 \phi / \partial x^2)$
 - ❖ Use approximations derived earlier for 2nd order derivatives.
- ❖ Otherwise, use formulae derived earlier for 1st order derivatives for outer and inner ' ' derivatives.

We will look at approximation of mixed derivatives next, then we also look at implementation of boundary conditions in finite difference method and if time permits, we will look at the algebraic system of equations we get from finite difference discretisation. So, let us have a look at the second order derivatives which occurs in generic transport equation. It is slightly different from the simple second derivative, which we have seen so far.

And others occurs in the diffusion term; the diffusion term in the generic conservation equation involves a second order derivative of the form; $\partial/\partial x$ of γ times $\partial \phi / \partial x$, where γ is a diffusivity or diffusion coefficient. Now, if γ were constant that is to say it were independent of y and x , then it can be taken out of the bracket and this diffusion term becomes γ times $\partial^2 \phi / \partial x^2$.

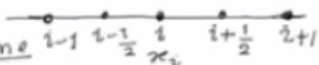
Now, we have already learn, we have already derived various formulae for approximation of $\partial^2 \phi / \partial x^2$, so we can use these approximations derived earlier for second order derivatives for finite difference approximation of this diffusion term but in case if γ were not a constant, then we have got 2 derivatives; outer derivative and an inner derivative. So, we have to use the formulae derived earlier for first order derivative for outer and inner derivatives.

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FD approximation for diffusive term in generic scalar transport equation

$$\left[\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) \right]_i \approx ?$$

Central difference scheme



- Assume a uniform grid for sake of simplicity (Let relax this condition, and first go for a general grid).

CDS approximation of outer derivative:

$$\left[\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) \right]_i \approx \frac{\left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i+1/2} - \left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i-1/2}}{\Delta x}$$

Now, let us see one simple way of doing this on both. So, we want to find out the finite difference approximation for diffusive term in or generic scalar transport equation and as we noted that this term at a grid node I, focus on one dimension for the sake of simplicity, so it is grid node I at the coordinate location x_i and we would like to find out a finite difference discretisation of $\frac{\partial}{\partial x}$ of Γ times $\frac{\partial \phi}{\partial x}$ at this grid location.

So, you want to find out what would be their suitable approximation or suitable finite difference approximation for this second order derivative. Let us try a simple scheme based on central difference approximation. So, we are going to derive or I will try to derive a scheme based on central differences, so we have a grid node I, to the right of it we have the grid node $i+1$, then to the left will have the grid node $i-1$. For the time being, for the sake of simplicity, let us assume a uniform grid; uniform grid for sake of simplicity, okay.

These are our midway nodes, let us call them as $i+1/2$ and $i-1/2$, so we can derive the approximations of both uniform as well as non uniform case or else okay, let us relax it; relax this condition and first go for a general grid, then what would happen to our outer derivative, so CDS approximation of outer derivative; the outer derivative means the first one which occurs outside, $\frac{\partial}{\partial x}$, so we have got $\frac{\partial}{\partial x}$ of Γ times $\frac{\partial \phi}{\partial x}$ over Δx .

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Central difference scheme $i-1 \quad i-\frac{1}{2} \quad i \quad i+\frac{1}{2} \quad i+1$

- Assume a uniform grid for sake of simplicity (Let relax this condition, and first go for a general grid).

CDS approximation of outer derivative:

$$\left[\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) \right]_i \approx \frac{\left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i+\frac{1}{2}} - \left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i-\frac{1}{2}}}{(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}})}$$

$$\begin{aligned} x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}} &= \frac{1}{2} (x_{i+1} + x_i) - \frac{1}{2} (x_i + x_{i-1}) \\ &= \frac{1}{2} [x_{i+1} - x_{i-1}] \\ &= \frac{1}{2} [(x_{i+1} - x_i) + (x_i - x_{i-1})] \\ &= \frac{1}{2} (\Delta x_i + \Delta x_{i-1}) \end{aligned}$$

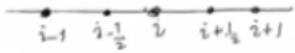
We want to evaluate it at grid point i and we can approximate it in terms of the values at this midway nodes at $i + 1/2$ and $i - 1/2$, so we can take the value of $\gamma \frac{\partial \phi}{\partial x}$ at these nodes again okay and there by obtain the approximation of this derivative at the central node, i using a central difference approximation. So, we can write this as $\gamma \frac{\partial \phi}{\partial x}$ at grid node $i + 1/2 - \gamma \frac{\partial \phi}{\partial x}$ at the grid node $i - 1/2$ divided by spacing between these half nodes that as we can write it as $x_{i+1/2} - x_{i-1/2}$.

Now, let us try and simplify the terms which are involved in numerator and denominator. First, let us have a look at grid spacing difference terms which occurs in denominator, can we write it in terms of usual grid spacing Δx_i , so $x_{i+1/2} - x_{i-1/2}$; $x_{i+1/2}$ is basically is midway between i and $i+1$ when it is note; $1/2$ of x of $i+1 - x_{i-1/2}$ of $x_i - x_{i-1}$ sorry $x_{i+1/2}$; the coordinate of $x_{i+1/2}$ will be the average of the coordinates of x_i and x_{i+1} . Similarly, $x_{i-1/2}$ would be considered middle point.

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... Diffusive Term

CDS for inner derivatives



$$\begin{aligned}
 \left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i+\frac{1}{2}} &= \Gamma_{i+\frac{1}{2}} \left(\frac{\partial \phi}{\partial x} \right)_{i+\frac{1}{2}} \\
 &\approx \Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{(x_{i+1} - x_i)} = \Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{\Delta x_i} \\
 \left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i-\frac{1}{2}} &\approx \Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{(x_i - x_{i-1})} = \Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{\Delta x_{i-1}} \\
 \left\{ \frac{\partial}{\partial x} \left[\Gamma \frac{\partial \phi}{\partial x} \right] \right\}_i &\approx \frac{\Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{\Delta x_i}}{\Delta x_i} - \frac{\Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{\Delta x_{i-1}}}{\Delta x_i}
 \end{aligned}$$

So, $1/2$ of x_{i+1} , take the $1/2$ outside, so what we have got is $x_{i+1/2}$; sorry x_{i+1} , this x_i and x_i , they get cancelled out, $x_{i+1} - x_{i-1}$ or we can reintroduce x_i coordinate; $x_{i+1/2} - x_i = x_i - x_{i-1/2}$. So, that leads to $1/2$ of $\Delta x_i + \Delta x_{i-1}$. Next now, let us use the central difference approximation for the inner derivative. So, we are dealing with the diffusive term, so use of CDS for inner derivatives, this straight we draw it again, so $i, i+1, i+1/2, -1, i-1/2$.

So, inner derivatives are to be evaluated at the mid nodes between nodes $i+1$ and $i-1$, so $\partial \phi / \partial x$ at $i+1/2$, this is multiplied with Γ . So, this is simply Γ at $i+1/2$ $\partial \phi / \partial x$ at $i+1/2$; $i+1/2$ is the central node or is a midway node between $i+1$, so we can use the value at nodes $i+1$ and i to obtain the CDS approximation of $\partial \phi / \partial x$ at $i+1/2$, so it becomes $\Gamma_{i+1/2} * (\phi_{i+1} - \phi_i) / (x_{i+1} - x_i)$, so denominator is simply Δx_i .

Similarly, the second term which we had, $\Gamma \partial \phi / \partial x$ at $i-1/2$, and for this derivative, $\partial \phi / \partial x$ at mid node $i-1/2$, we can use value of this nodes $i-1$ and i , this can be written as, $\Gamma_{i-1/2} \text{ times } (\phi_i - \phi_{i-1}) / (x_i - x_{i-1})$ that is $\Gamma_{i-1/2} (\phi_i - \phi_{i-1}) / \Delta x_{i-1}$. So, now we substitute the expressions, the expressions of these inner derivatives that is $\Gamma \partial \phi / \partial x$ at $i+1/2$ and $\Gamma \partial \phi / \partial x$ at $i-1/2$.

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$$\begin{aligned}
& \approx \Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{(x_{i+1} - x_i)} = \Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{\Delta x_i} \\
\left(\Gamma \frac{\partial \phi}{\partial x} \right)_{i-\frac{1}{2}} & \approx \Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{x_i - x_{i-1}} = \Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{\Delta x_{i-1}} \\
\left\{ \frac{\partial}{\partial x} \left[\Gamma \frac{\partial \phi}{\partial x} \right] \right\}_i & \approx \frac{\Gamma_{i+\frac{1}{2}} \frac{(\phi_{i+1} - \phi_i)}{\Delta x_i} - \Gamma_{i-\frac{1}{2}} \frac{(\phi_i - \phi_{i-1})}{\Delta x_{i-1}}}{\frac{1}{2} (\Delta x_i + \Delta x_{i-1})} \\
\Rightarrow \left[\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) \right]_i & \approx \frac{\Gamma_{i+\frac{1}{2}} (\phi_{i+1} - \phi_i) \Delta x_{i-1} - \Gamma_{i-\frac{1}{2}} \Delta x_i (\phi_i - \phi_{i-1})}{\frac{1}{2} (\Delta x_i + \Delta x_{i-1}) \Delta x_i \Delta x_{i-1}} \\
\text{On uniform grid, } \Delta x_i &= \Delta x_{i-1} = \Delta x \\
\left[\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right) \right]_i & \approx \frac{\Gamma_{i+\frac{1}{2}} (\phi_{i+1} - \phi_i) - \Gamma_{i-\frac{1}{2}} (\phi_i - \phi_{i-1})}{\Delta x^2}
\end{aligned}$$

So, these 2 expressions which you derived into the expressions for outer derivative which we written in previous page that will give us final expression for diffusive term, this is given by; in numerator we have gamma i+1/2 times phi i +1-phi i/ delta xi – gamma of i-1/2 times phi i –phi of i -1/delta x i-1 and our denominator, xi +1/2 –xi-1/2, we have derived earlier, this is equivalent to 1/2 of delta xi+delta xi-1.

Let us simplified further and then we can write a final expression for the diffusive term is del/del x of gamma del phi/del x at I, this can be approximated by gamma i+1/2 phi of i+1 – phi I * delta xi -1- gamma i – 1/2 delta xi phi I – phi of i-1/1/2 delta xi+delta xi-1* delta xi delta x i-1. If our grid spacing were uniform we would get a simpler formula. On uniform grid that is delta xi = delta xi -1 = delta x, because we can simplify 6% and write it as del phi/del x of gamma del phi/del x of I, can be approximate gamma i+1/2 phi i+1-phi i- gamma i-1/2 phi of i- phi of i-1.

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... Diffusive Term

Variation Γ

- If $\Gamma = \Gamma(x) \Rightarrow \Gamma_{i \pm 1/2} \equiv \Gamma(x_{i \pm 1/2})$
- If $\Gamma = \Gamma(\phi, x)$
 - \Rightarrow Approximate $\phi_{i \pm 1/2}$ by a simple average of neighboring nodes, i.e.
 - $\phi_{i \pm 1/2} \approx \frac{1}{2} (\phi_{i+1} + \phi_i)$

$$\Gamma_{i+1/2} = \Gamma \left[\frac{1}{2} (\phi_{i+1} + \phi_i), \frac{1}{2} (x_{i+1} + x_i) \right]$$

$$\Gamma_{i-1/2} = \Gamma \left[\frac{1}{2} (\phi_i + \phi_{i-1}), \frac{1}{2} (x_i + x_{i-1}) \right]$$

In denominator simplifies to delta x square, the half will vanish because delta x+, i +delta x i-1, that will give us 2 delta x, so the factor half vanishes and one delta x gets cancelled from delta x in numerator. So, this simplified expression is on a uniform grid. This one is small thing which is still left here, we have what these terms gamma i+1/2 and gamma i-1/2. So, what do we do with these terms? If gamma was simply a function of the spatial coordinates, absolutely no problem we just evaluate.

We can have 2 cases regarding variation of gamma, gamma exist a function of spatial coordinate, so we got no problems whatsoever or gamma i+1/2 is basically the function value 1+-of this; we can obtain and these nodes xi+-1/2 but what happens if gamma were function of the variable phi itself? So, if gamma were a function of phi and x both, so in this case how do we find out and suitable numerical approximation.

So, in this case you would approximate phi i+1/2 by a simple average of neighbouring nodes that is our phi of i+1/2, this would be approximated as 1/2 of phi i +1+ phi i and then we would evaluate gamma i+1/2 as this function; gamma at 1/2 phi i+1+ phi I and similar is spatial coordinate, 1/2x +1+xi. In the similar way of gamma i-1/2 would become given by function; gamma 1/2 phi i+phi of i -1 and x coordinate is 1/2 of xi+xi+1. So, that is how we would evaluate this diffusivity values which we require at the mid node locations i+1/2 and i-1/2.

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$$\phi_{i+\frac{1}{2}} \approx \frac{1}{2} (\phi_{i+1} + \phi_i)$$

$$\begin{aligned} \Gamma_{i+\frac{1}{2}} &= \Gamma \left[\frac{1}{2} (\phi_{i+1} + \phi_i), \frac{1}{2} (x_{i+1} + x_i) \right] \\ \Gamma_{i-\frac{1}{2}} &= \Gamma \left[\frac{1}{2} (\phi_i + \phi_{i-1}), \frac{1}{2} (x_i + x_{i-1}) \right] \end{aligned}$$

Exercise: (1) Derive similar approximations for the diffusive term $\frac{\partial}{\partial x} \left(\Gamma \frac{\partial \phi}{\partial x} \right)$ using FDS/BDS.

- (2) Find out the order truncation error in scheme obtained using (i) CDS, (ii) FDS/BDS

FDS \equiv Forward difference scheme
BDS \equiv Backward difference.

So, what we write? we derived in a scheme which is based on CDS that is only one choice, so I would leave as an exercise tips would be a nice exercise, so derive similar approximations for the diffusive term $\frac{\partial}{\partial x}$ of Γ times $\frac{\partial \phi}{\partial x}$ using forward difference scheme or backward difference scheme and there is exercise which you can try is find out; find out the order of truncation error in the schemes obtained using CDS that is the one which we derived in the class.

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- (2) Find out the order truncation error in scheme obtained using (i) CDS, (ii) FDS/BDS

FDS \equiv Forward difference scheme
BDS \equiv Backward difference scheme
CDS \equiv central difference scheme.

And second is FDS, BDS hope you, by now you are familiar with these terms FDS BDS and CDS, just in case we missed out, let discuss them out once again. This FDS; this is stands for forward difference approximation or forward difference scheme, BDS stands for backward

difference scheme and CDS stands for central difference scheme. So, please do remember these acronyms because we are going to use them very often.

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**MULTIDIMENSIONAL FINITE
DIFFERENCE FORMULAE**

$$f_{i,j,k} \equiv f(x_i, y_j, z_k)$$

First order derivative using FDS are

$$\left(\frac{\partial f}{\partial x} \right)_{i,j,k} = \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x} + O(\Delta x)$$

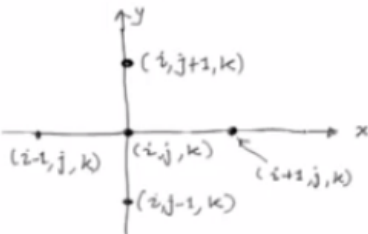
$$\left(\frac{\partial f}{\partial y} \right)_{i,j,k} = \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y} + O(\Delta y)$$

$$\left(\frac{\partial f}{\partial z} \right)_{i,j,k} = \frac{f_{i,j,k+1} - f_{i,j,k}}{\Delta z} + O(\Delta z)$$

So, far we had confined ourselves to obtaining the expressions for one dimensional derivative, now we want to extend these formulae in multi dimension. So, how do we extend this one dimensional formula to multi dimensional situations that is what we would require in most of the CFD applications? For that, let us have a look at a simple grid and see in which way we can extend our one dimensional formulae.

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Multi-dimensional Formula

$$f_{i,j,k} \equiv f(x_i, y_j, z_k)$$


$$\left(\frac{\partial f}{\partial x} \right)_{i,j,k} \stackrel{\text{FDS}}{\approx} \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x}, \quad O(\Delta x)_{\text{TE}}$$

$$\text{CDS} \quad \left(\frac{\partial f}{\partial x} \right)_{i,j,k} \approx \frac{f_{i+1,j,k} - f_{i-1,j,k}}{2 \Delta x}, \quad O(\Delta x^2)_{\text{TE}}$$

$$\left(\frac{\partial f}{\partial y} \right)_{i,j,k} \stackrel{\text{FDS}}{\approx} \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y}, \quad O(\Delta y)_{\text{TE}}$$

So the multidimensional formula; let us draw a planar grid for the sake of simplicity, there is all the points in this plane, we will have the same k index, so the centre point is identified as i, j, k , we have used usual grid combinations xy plane, so the node, top of this node along the y grid line which is of the j grid line, this index would be given by $j-1$ sorry $j+1$, the one towards the bottom is the j index would be one smaller $j-1, k$.

Similarly, the nodes which are to the right on x grid line, this index would be given by $i+1, j, k$ and a node to the left of i, j, k , next y plane on x line, this index is $i-1, j, k$ and let us remember the sorting notation which we introduced earlier that we will use the symbol f_{ijk} to indicate the function value at a grid point x_i, y_j, z_k . Now, if you want to find out, let us say first order derivative $\Delta f / \Delta x$ at i, j and k , we want to find out x derivatives that means or interesting variation only long x direction.

So, this has to be approximated in terms of the neighbouring values on x line, for instance, if we use forward difference approximation FDS, we have to use the function values at the grid point $i+1$ and grid point i , so this can be simply written as f of $i+1$ remaining indices will remain the same as j, k - f of ijk / Δx . Suppose, you want to an instant use a CDS on an uniform grid, so in that that case the values involved would be at $i+1$ jk node and $i-1$ jk node.

So, $\Delta f / \Delta x$ ijk using central difference approximation, this can be expressed as f of $i+1, j, k$ - f of $i-1, j, k$ divided by the grid spacing between two nodes that is $2 \Delta x$. In the case of FDS, first order Δx , in the case of central difference approximation it is the order of Δx square. Now, this is the expressions for the derivatives in x . How about derivative in y ? That is $\Delta f / \Delta y$ at ijk , suppose once again we want to approximate it using a forward difference scheme.

So, we need to consider a node on y grid line which is towards increasing y location that is at $j+1$ of node at i will take the function value at the node $i, j+1, k$ and at the node ijk , take the difference of that, so f of $i, j+1, k$ - f of ijk / Δy and of course this is scheme has got the accuracy of first order that is order Δy , these are truncation error. So, we already noticed what you all that we have done to obtain this multidimensional formula is that just vary the indices.

Or changed the indices along the direction with respect to which we are finding out derivative difference and we want to find a derivative with respect to x, we just need to change the I indices in the function values, remaining indices are left unchanged. Similarly, to obtain the y derivative, we just changed the j indices in our corresponding one dimensional formulae which we derived earlier and that is all, remaining indices were left unchanged.

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$$\begin{aligned} \left(\frac{\partial f}{\partial x}\right)_{i,j,k} &\stackrel{\text{FDS}}{\approx} \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x}, \quad \underbrace{O(\Delta x)}_{\text{TE}} \\ \text{CDS } \left(\frac{\partial f}{\partial x}\right)_{i,j,k} &\approx \frac{f_{i+1,j,k} - f_{i-1,j,k}}{2\Delta x}, \quad \underbrace{O(\Delta x^2)}_{\text{TE}} \\ \left(\frac{\partial f}{\partial y}\right)_{i,j,k} &\stackrel{\text{FDS}}{\approx} \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y}, \quad \underbrace{O(\Delta y)}_{\text{TE}} \\ \text{Similarly, expression z-derivative} \\ \left(\frac{\partial f}{\partial z}\right)_{i,j,k} &\stackrel{\text{FDS}}{\approx} \frac{f_{i,j,k+1} - f_{i,j,k}}{\Delta z} + O(\Delta z) \\ \left(\frac{\partial f}{\partial z}\right)_{i,j,k} &\stackrel{\text{CDS}}{\approx} \frac{f_{i,j,k+1} - f_{i,j,k-1}}{2\Delta z} + O(\Delta z^2) \end{aligned}$$

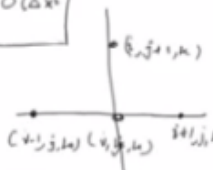
So, keeping that in mind, now we can easily write the expression for z derivative; del f over del z ijk, if we use FDS, this will remain; ij would remain same, we just need to change k index k +1-f of ijk divided by delta z+let us have a different truncation , let us have an order a scenario which would be of the order delta z or if you want to use a CDS approximation, so del f/del z ijk using CDS, we can write it as fi, j, k +1 – fi, j, k -1 divide by 2 delta z, we are trying as an order delta z square.

So, these are our expressions for the z derivative, so to support a summary which I have put first order derivative using FDS del f/del x ijk is = fi +1, j, k-fi jk divide by delta x, del f/del y ijk, fi, j+1k-fi jk divide by delta y and del f/del z is f of i, j, k +1 -fi jk divided by delta z, just to reinforce you again, let us see which indices we need to change or which subscript we need to change in a formula.

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Second order Multidimensional derivatives

CDS (on uniform grid)

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


$$\left(\frac{\partial^2 f}{\partial x^2} \right)_{ijk} = \frac{f_{i+1,j,k} + f_{i-1,j,k} - 2f_{i,j,k}}{\Delta x^2} + O(\Delta x^2)$$

$$\left(\frac{\partial^2 f}{\partial y^2} \right)_{ijk} = \frac{f_{i,j+1,k} + f_{i,j-1,k} - 2f_{i,j,k}}{\Delta y^2} + O(\Delta y^2)$$

If you are dealing with x, change would be in i index, if you are dealing with y, we need to change only j index, other two indices remain the same, if you are dealing with z, change the k index, so the other indices i and j would remain the same. Now, these were the approximations of the formulae for first order derivative. What happens to the second order derivative? Second order multidimensional derivatives.

This is to do a CDS and for the sake of simplicity will take the example using the CDS on uniform grid. Let us write our reference formula for the second derivative $\frac{\partial^2 f}{\partial x^2}$, this was given by $f_{i+1} + f_{i-1} - 2f_i$ divided by Δx^2 , so this for the reference one dimensional finite difference approximation which had a truncation error of Δx^2 .

And now let us write down in multidimensional setting ijk , $i+1jk$, $i-1jk$ in the top nodes $ij+1,k$ and $ij-1,k$ okay, for derivatives along x, what do we do? $\frac{\partial^2 f}{\partial x^2}$ at node ijk , we would only change i indices, i indices will take the value; $i+1$, $i-1$, other two indices would remain fixed. So, $f_{i+1,j,k} + f_{i-1,j,k} - 2f_{i,j,k}$ divided by Δx^2 and truncation error is of the order; Δx^2 .

So, that is the simple formulae or simple formula for second derivative with respect to x, derivative with respect to y, what do we need to do? Once again, we have 3 terms in the numerator and remember now since we are taking derivative with respect to y, we need to

change only j indices, I and k would remain fixed in all the terms, so the first term would be $f_{i,j+1,k}$, next term is $f_{i,j-1,k}$ - twice of f_{ijk} divided by Δy square and truncation error is of the order Δy square.

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$$\left(\frac{\partial^2 f}{\partial x^2} \right)_{ijk} = \frac{f_{i+1,j,k} + f_{i-1,j,k} - 2f_{ijk}}{\Delta x^2} + O(\Delta x^2)$$

$$\left(\frac{\partial^2 f}{\partial y^2} \right)_{ijk} = \frac{f_{i,j+1,k} + f_{i,j-1,k} - 2f_{ijk}}{\Delta y^2} + O(\Delta y^2)$$

$$\left(\frac{\partial^2 f}{\partial z^2} \right)_{ijk} = \frac{f_{ijk+1} + f_{ijk-1} - 2f_{ijk}}{\Delta z^2} + O(\Delta z^2)$$

Exercise Write down formulae for second order derivative $\frac{\partial^2 f}{\partial x^2}$, $\frac{\partial^2 f}{\partial y^2}$, $\frac{\partial^2 f}{\partial z^2}$ for a non-uniform grid

Similarly, a formula for z derivative $\frac{\partial^2 f}{\partial z^2}$ at ijk , this would be, now we did do vary only k index, keep I and j indices is fixed, so $f_{ijk+1} + f_{ijk-1}$ - twice of f_{ijk} divided by Δz square at truncation error is of the order Δz square, so these are which we have formulae which we have written using uniform grid spacing, we already derived one dimensional formulae for both uniform and non uniform grid spacing, okay.

And how like you to do the simple exercise write down, you just need to write down this basically this no need to derive these formulas, the formula we have already derived one dimensional that is x dimension, all that we need to do is append appropriate subscripts to f depending on which direction we want to take or with respect to which variable x, y or z, we are taking the derivatives.

So, write down formulae for second order derivatives $\frac{\partial^2 f}{\partial x^2}$, $\frac{\partial^2 f}{\partial y^2}$, $\frac{\partial^2 f}{\partial z^2}$ for a non uniform grid, so just rewrite once again that getting the formula is very simple, write down your base formula or the basic formula which we derived with x as your reference variable, okay use that formula and just vary the appropriate indices,

this is an appropriate grid spacing, first you are dealing with x derivative, just write down $i+1$ $i-1$ and i and remaining 2 indices are j and k divide by Δx square.

If you are dealing with that second order derivative with respect to y , keep i and k fixed and then write $j+1$ $j-1$ and j in these 3 terms of variables appearing in a formula divide by appropriate grid spacing in y direction. Similarly, if we want to find out derivative with respect to z coordinate, keep i and j subscripts on function variable everywhere same, only change k variables as per this formula and grid spacing changing from Δx to Δz , Δz_{i-1} and so on as the case may be.

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APPROXIMATION OF MIXED DERIVATIVES

In thermo-fluid problems, mixed derivatives are encountered in a few situations, e.g.

- ❖ Heat conduction in an anisotropic medium
- ❖ The transport equations expressed in non-orthogonal coordinate systems.

Next, we take up the case of mixed derivatives; mixed derivative means, we have so far we deal with only the $\frac{\partial f}{\partial x}$, $\frac{\partial^2 f}{\partial x^2}$ that is $\frac{\partial^2 f}{\partial y^2}$ and so on, the derivatives were only with respect to a single variable but there are certain thermo fluid problems which involve mixed order derivatives. For example, if you are dealing with heat conduction in anisotropic medium, we will get the terms like $\frac{\partial^2 T}{\partial x \partial y}$.

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...APPROXIMATION OF MIXED DERIVATIVES

Mixed derivatives can be treated by combining one dimensional approximation in the same way as discussed earlier for second order derivative.

❖ The mixed derivative ($\partial^2 f / \partial x \partial y$) can be re-written as

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y} \right)$$

❖ Use of CDS for outer as well inner derivatives gives

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

Similarly, if the solvent transport equations in non orthogonal coordinate system, which will arise if you want to use body fitted grids, see in both situations, we need mixed derivatives. So, how do we obtain expression for mixed derivatives? Now, this mixed derivatives that they can be treated by combining one dimensional approximation in the same way as you have discussed earlier for second order derivative.

In particular, the way today we discussed the case of $\partial f / \partial x$ of gamma, $\partial f / \partial x$ for the generic transport equation, so remember in this case suppose we want to deal with the mixed order derivative $\partial^2 f / \partial x \partial y$, this we can simply written using a basic calculus that $\partial^2 f / \partial x \partial y = \partial / \partial x$ of $\partial f / \partial y$, so now you got 2 derivatives here; the outer derivative with respect to x and the inner derivative with respect to y.

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outer derivative:

$$\left(\frac{\partial^2 f}{\partial x \partial y}\right)_{ij} \approx \frac{(\partial f / \partial y)_{i+1,j} - (\partial f / \partial y)_{i-1,j}}{2 \Delta x} + O(\Delta x^2) \quad (2)$$

CDS in y-direction for inner derivative

$$\left(\frac{\partial f}{\partial y}\right)_{i+1,j} \approx \frac{f_{i+1,j+1} - f_{i+1,j-1}}{2 \Delta y} + O(\Delta y^3) \quad (3)$$

$$\left(\frac{\partial f}{\partial y}\right)_{i-1,j} \approx \frac{f_{i-1,j+1} - f_{i-1,j-1}}{2 \Delta y} + O(\Delta y^3) \quad (4)$$

Substitute (3) and (4) in eq.(2):

$$\boxed{\left(\frac{\partial^2 f}{\partial x \partial y}\right)_{ij} \approx \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{4 \Delta x \Delta y}}$$

\uparrow CDS approximation TE $\sim O(\Delta x^2, \Delta y^2)$

Ex Derive FD approximation for $\frac{\partial^2 f}{\partial^2 x}$

And we can use our own judgement or choices for both of these derivatives and now let us try and derive one approximation using CDS for this mixed derivative. Let us get back to board and find out the next present for mixed derivative, so finite different approximation for mixed derivatives, for reference let us draw a simple 2 grid with a xy plane, the centre grid, the grid point is ij; i+1, j to the left we have got, i-1,j and similarly the bottom side we got grid point ij-1, on top we got the grid point ij+1.

We want to find out an approximation for the derivative $\frac{\partial^2 f}{\partial x \partial y}$ at grid point ij. So, now we will first write this as $\frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right)$ at grid point ij. Let us use CDS in x direction; x direction for the outer derivative. So, if you do that, then we simply get the $\frac{\partial f}{\partial x}$ at grid point ij, this can be approximated as $\frac{\partial f}{\partial x}$ at the grid point i+1, j - $\frac{\partial f}{\partial x}$ at the grid point i-1, j, we are using central different schemes, so we would use the values at grid point i+1 and i-1 along the x direction.

And let us assume that we are dealing with uniform grid, so grid spacing, we can simply write it as 2 delta x. So, here for the sake of simplicity, we have assumed uniform grid in both x and y direction. Now, the truncation error of course in this scheme what would be of the order? Delta x square and approximation of this is outer derivative. Now, we have got 2 derivatives with respect to y, which was called inner derivative and let us use CDS again.

CDS in y direction for 2 inner derivatives which we have got, so our $\frac{\partial f}{\partial y}$ at grid point $i+1, j$ this can be approximated using CDS as f of $i+1, j+1$, we are dealing with a derivative with respect to y direction, so I subscripts would remain the same only J subscripts would vary, the 2 terms; if $i+1, j+1 - f$ of $i+1, j-1$ divided by $2 \Delta y$, truncation of the order Δy square. Similarly, $\frac{\partial f}{\partial y}$ at $i-1, j$, this is equal to f of $i-1, j+1 - f$ of $i-1, j-1$ divided by $2 \Delta y$ truncation of the order Δy square.

This number at the equations at 3 and 4 and the previous equation was 2, so substitute now 3 and 4 in equation 2; substitute 3 and 4 in equation 2 and once we do the substitution and we can easily simplify, so that would yield our approximation for mixed derivative $\frac{\partial^2 f}{\partial x \partial y}$ at point ij using CDS approximation. This would be f of $i+1, j+1 - f$ of $i+1, j-1 - f$ of $i-1, j+1 + f$ of $i-1, j-1$ divided by $4 \Delta x \Delta y$, so this is our approximation obtained using CDS in both x and y direction and truncation error is of the order Δx square Δy square, okay.

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$$\left(\frac{\partial f}{\partial y}\right)_{i+1,j} = \frac{f_{i+1,j+1} - f_{i+1,j-1}}{2 \Delta y} \quad (3)$$

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

Substitute (3) and (4) in eq.(2):

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

\uparrow CDS approximation TE $\sim O(\Delta x^2 \Delta y^2)$

Ex Derive FD approximation for $\frac{\partial^2 f}{\partial x \partial y}$ on a non-uniform grid using

- (i) CDS
- (ii) FDS/BDS.

So, we have done one set of derivations, I would like to give you some exercise here and this derivation, i have used a uniform grid can extend it using non uniform grid, so derive the formulae or derive finite difference approximations for $\frac{\partial^2 f}{\partial x \partial y}$ on a non uniform grid using let say we just extend the way, we use CDS and you can also use a combination of forward difference and backward difference scheme.

So, this lecture we stop here. In the next lecture, we would discuss implementation of boundary condition in finite difference method, we will also take up the case of how do we write the discrete finite difference equations at EC grid node and when can be collect it, what sort of system algebraic equations we get? How to you store that system, so different storage aspects and we would also take up the case of ordering aspects in what way we have to order of nodes and the corresponding indices in our standard linear system of equations.

So, these two topics will discuss in the next lecture. We will also take up some applications will apply finite difference method to solve some simple one dimensional problems.