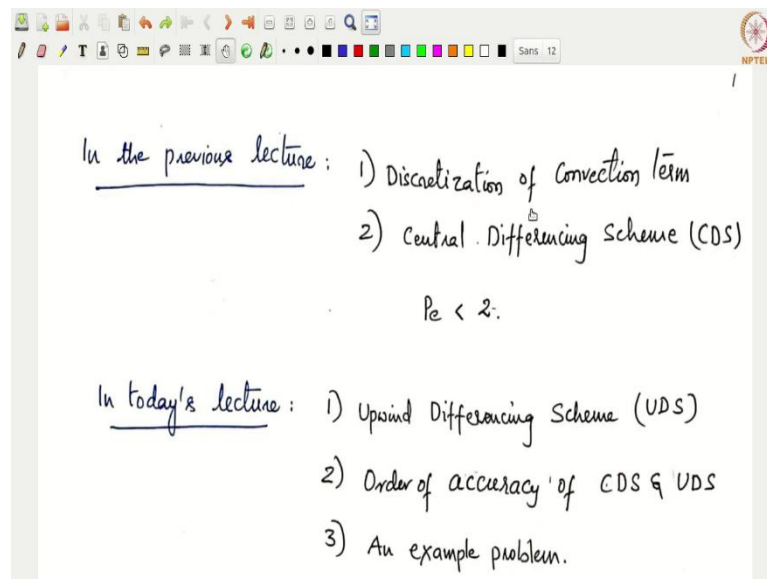


Computational Fluid Dynamics Using Finite Volume Method
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Lecture – 30
Finite Volume Method for Convection and Diffusion: Discretization of steady convection equation

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Hello everyone, welcome to another lecture as part of our ME 6151, the computational heat and fluid flow course. So, in the past lecture, in yesterday's lecture, we looked at how to discretize the convection term right; the $\rho u \bar{\phi}$ the convection term that we have learned how to discretize it.

And then we also looked at one particular scheme of discretization that we named it as Central Differencing Scheme that is CDS; basically where the face value of the dependent variable ϕ_e is expressed as a linear average or linear interpolation of the east and the primary faces, right.

We wrote ϕ_e equals ϕ_E plus ϕ_P by 2, right that is what we have done in order to come up with the value for the ϕ on the east face, and that is what we call it as a central differencing scheme in the literature. Now, we also saw that this central difference scheme produces negative coefficients. And in order to avoid getting these negative coefficients,

we have to choose our grid such that the cell Peclet number should be less than 2, less than or equal to 2 right; that is what we kind of discussed in the yesterday's lecture, alright.

So, in today's lecture we are going to look at an alternate scheme to the central difference scheme that is known as an upwind difference scheme which would not suffer from such a problem, ok. And after looking at how to kind of work with the upwind difference scheme; we are going to look at the order of accuracy of the central difference and the upwind difference schemes, ok.

We look at what is the spatial order of accuracy, which we have done for the pure diffusion equation, right. We have established the order of accuracy to be second order accurate in space; but we will do it for now for the convection terms that is basically with these particular two schemes, with the CDS and the upwind difference schemes.

Now, finally, we will also look at an example problem of solving a pure convection problem using both these schemes, both the central differencing and the upwind difference schemes, ok. So, that is the agenda for today's lecture. And so, let us move on with the upwind difference scheme.

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Upwind Differencing Scheme: (UDS)

Negative Coefficients in CDS were because of arithmetic avg.

CDS: $\phi_e = (\phi_E + \phi_P) / 2 \dots a_e = D_e - \frac{F_e}{2}$

$F_e = (\rho U)_e \Delta y$

$\phi_e = \begin{cases} \phi_P & \text{if } F_e > 0 \\ \phi_E & \text{if } F_e < 0 \end{cases}$

Determined by flow direction "upwind".

So, if you look at the central difference scheme that we had worked on yesterday; we note that there are negative coefficients and these were coming because of the arithmetic average, right. We wrote ϕ_e equals ϕ_E plus ϕ_P by 2 and only because of this, we were

getting negative coefficients; because the coefficient for here ϕ_E should be F_e by 2 and that would go in as to the a_E as D_e minus F_e by 2, right.

So, this is the reason we were getting the negative coefficients; if it was not a linear average then we would not probably have got negative coefficients like this, and further those constraints on the Peclet number would not have been there ok. So, in order to eliminate this kind of problem, people have proposed a different scheme, an alternate scheme that is known as upwind difference schemes; and which primarily works on the direction of the mass flow rate.

So, that means, let us consider this grid. So, we have our P cell, east cell and of course the west cell. And we have ϕ_P stored here and ϕ_E stored here, ok. Now, in the upwind difference scheme what we do is, depending on the direction of the mass flow rate; for example, let us say blue indicates arrow in the positive x direction, where the mass flow rate is greater than or equal to 0.

That means, the flow is going in this way; I mean essentially if you look at the definition of mass flow rate, it contains density, velocity and the Δy . Δy is positive, density is positive; so u_e . So, if the flow, if the u_e is positive; that means, F_e would be positive right, the flow is going this way. If u_e is negative, F_e would be negative and it will be going in the negative x direction; here shown using a red color arrow, right alright.

So, we have these two conditions. Now, what upwind difference scheme proposes is that, do not take the face value as the linear average as we have done here; rather take the face value as the corresponding cell value of the upstream direction.

For example, if F_e is greater than or equal to 0; that means, then consider this phi east equal to ϕ_P ok, this is the upwind direction. For example, as the flow is going this way; this would be the downwind direction; this would be the up of the wind, right. So, essentially up of the flow. So, that is the direction. So, calculate. So, assign ϕ_e equals ϕ_P if F_e is greater than or equal to 0, that is the first condition.

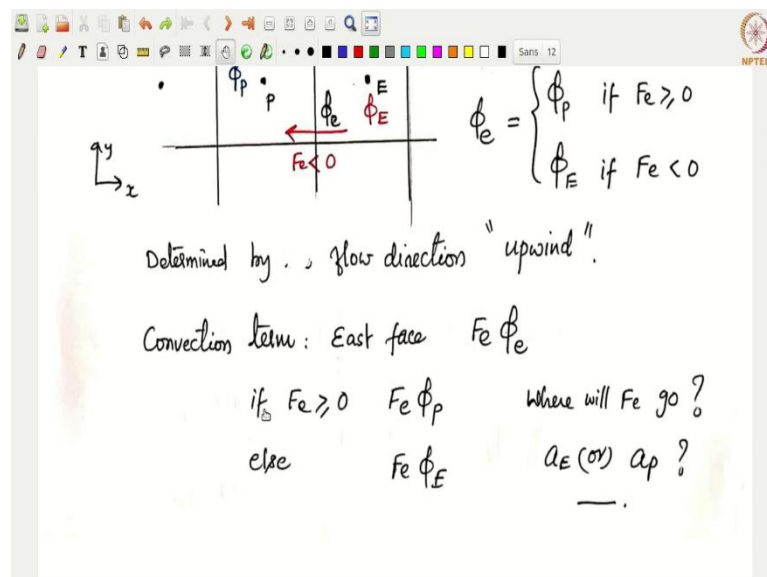
If F_e is less than 0, then take ϕ_e equals ϕ_E ; that means F_e is in this way, then take the up direction, the up direction for this would be this one, right. Because this would be the downside, this would be the upside right from where the upstream, from where the flow is

coming, right. So, essentially this would be the upstream for a flow like this and if the flow is going in the negative x direction, this should be the upside, right.

So; that means by definition the face value is approximated using the cell centroid value in the upstream direction, in the up upwind direction; that means ϕ_e equals ϕ_P if F_e is greater than or equal to 0, otherwise it will be equal to ϕ_E , ok. So, either ϕ_P or ϕ_E , purely determined by the flow direction of the upwind direction.

Now, you may have a question, ok. What about the diffusion, right? We might have had some diffusion by the time this phi might have reached this ϕ_e ; that is what we are actually neglecting here, right. If you we are not considering the diffusion of the scalar within this half the grid cell size, that is what is neglected in this particular, in this particular scheme.

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Now, given that this definition, as we can see we do not have essentially there is no linear average; it is just equal to the upwind cell center value. Now, so as we can see this is completely determined by the flow direction or the upwind direction. And the let us say if we consider the east face; we are only kind of focusing on the convection term and you consider the east face, the total convection term would come out to be $F_e \phi_e$, right.

In the case of CDS, we wrote this as $\frac{\phi_E + \phi_P}{2}$; whereas now what we would do is, we would write depending on the condition. So, we will have a conditional statement, that

is if F_e is greater than or equal to 0; then $F_e \phi_e$ would be equal to $F_e \phi_P$, otherwise it will be $F_e \phi_E$, ok. So, either this or this depending on the direction of the mass flow rate or the direction of the velocity on the face.

That means we would need to write four such conditions for all the four faces right, depending on whether F_e is positive or negative, you would get either of these coefficients; similarly depending on if F_w is positive or negative, you would get two conditions, and depending on F_n is positive or negative, you get two conditions and so on right, ok. Now, a logical question would be; where will F_e go? Where will F_e go? F_e will go to either a_E or a_P depending on the mass flow rate, right.

Because if, if F_e with the mass flow rate is positive, then F_e would kind of go into a_P right; because this is multiplying ϕ_P and if it otherwise F_e would go into a_E , right we understand that, alright.

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Diffusion:

$$a_P \phi_P = \sum a_{nb} \phi_{nb} + b$$

$$a_E = D_e = F_e \Delta y / \delta x_e$$

$$a_W = D_w = \dots$$

$$a_N = D_N = F_N \Delta x / \delta y_w$$

$$a_S = D_S = \dots$$

$$a_P = \sum a_{nb} - S_P \Delta V_P$$

$$b = S_C \Delta V_P$$

Convection ? : If $F_e \geq 0$ then

$$a_P = a_P + F_e$$

Then let us move on in terms of, how do we code this particular concept of upwind difference scheme, when we want when you want to solve a convection diffusion equation? So, one thing would be first of all discretize the equation as if there is no convection, right. First of all let us look at the diffusion part of the equation.

So, if you were to write a final equation as $a_P \phi_P = \sum a_{nb} \phi_{nb} + b$; then if the component from coming from the diffusion is the same as what we have studied before, right. So, that

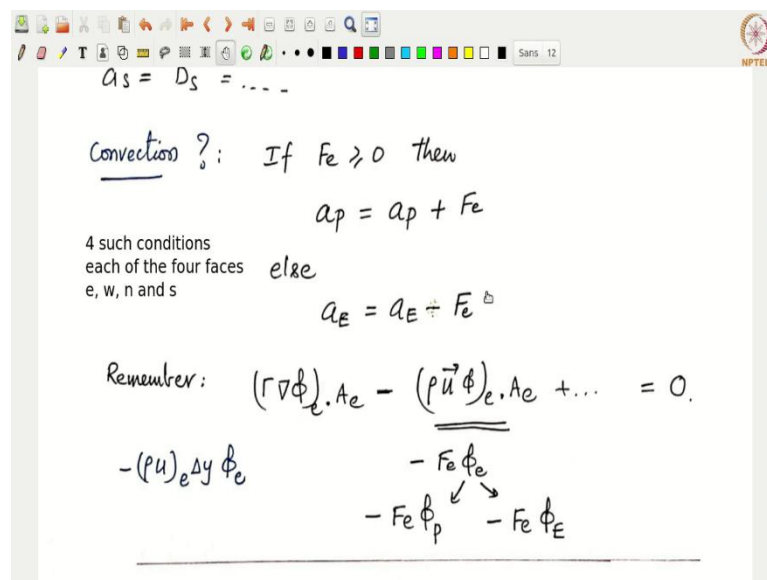
does not change; only the convection part would have now conditional statements, because of the mass flow rate coming into play.

So, what we can do is, we can first assign these a_{nb} 's only with contributions from the diffusion. So, a_E would be essentially $\frac{\Gamma_e \Delta y}{\delta x_e}$ right; that is nothing, but your D_e . Similarly, a_W would be D_w , that would be $\frac{\Gamma_w \Delta y}{\delta x_w}$. Similarly, a_N would be D_n which is given by $\frac{\Gamma_n \Delta x}{\delta y_n}$; and a south would be D_s that is $\frac{\Gamma_s \Delta x}{\delta y_s}$.

So far so good these are only a considering the diffusion part right; the contribution from convection needs to be still further added to a_E , a_W , a_N , a_S which we have not done at the moment up till here.

Now, what would be a_p ? a_p would be summation of all these neighbors that would be $\sum a_{nb}$ of course, the contribution coming from the source terms that is S_p times ΔV_p as well as b would be equal to S_C times ΔV_p , ok. So, that is what we have.

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This is, now, let us look at the convection part. So, the convection part; if F_e is positive, then what do we need to do? If F_e is positive, then you look at the original equation you have; you bring the convection term to the right hand side right, we have $(\Gamma \nabla \phi)_e \cdot A_e$ minus $(\rho \vec{u} \phi)_e \cdot A_e$. So, essentially we are only considering the east face; then we have diffusion term, the convection term brought to the right hand side, plus we have the source term.

Of course, we have four such terms corresponding to the three other faces west, north, south, ok. Now, what will happen if F_e is positive? F_e is positive, then essentially if you look at here; this is your F_e right, $\rho u_e \Delta y$, A_e in this particular case is positive i times Δy . So, this is, this term can be written as minus $\rho u_e \Delta y \phi_e$; essentially this will be minus $F_e \phi_e$ right, where F_e would be equal to $\rho u_e \Delta y$, alright.

So, that is your minus $F_e \phi_e$. Now, if F_e is positive; then ϕ_e equals ϕ_P right, then this will be minus $F_e \phi_P$ phi p. And if F_e is negative, if it is going in the negative x direction; then phi little e, the upwind direction upwind value for ϕ_e would be equal to ϕ_E , phi cell centroid value at the east cell that will be minus $F_e \phi_E$, right. So, this is essentially we are changing ϕ_e to either ϕ_P or ϕ_E .

Now, we have these two terms minus F_e or minus F_e , depending on whether this is positive or negative. Now of course, we know that if F_e is positive, this has to go to a_P and if it is negative, it has to go to a_E , right. But then what will be the signs; that is why we are kind of explaining all these concepts here. So, what will be the sign?

So, because this term is here, minus $F_e \phi_P$; remember when you when we have written this equations, we have sent the phi p terms to the right hand side, right. We leave the source terms and the A neighbors on the left hand side; we send the p terms to the right hand side here, right. That means, minus $F_e \phi_P$ would be a contribution to a p with a positive sign; so that means if F_e is positive, a_P would be equal to a_E plus F_e .

If F_e is negative, of course we know that this evaluates to, this entire thing evaluates to minus $F_e \phi_E$ right; because then we are replacing ϕ_e with ϕ_E , if F_e is negative. F_e itself is negative; but then you have minus $F_e \phi_e$.

So, what will be the, this contribution? This contribution of minus F_e would go into a east. So, a_E will be equal to a_E minus F_e ok, essentially this contribution; because it is getting retained on the left hand side here. Now, one thing you notice here is, because we have already populated the coefficients a neighbors and a_P with some values of the diffusion terms; we are now adding to the existing value whatever is the extra contributions here, right.

We are not writing a_P equals F_e that would be incorrect; because if you write a_P equals F_e , then all your contribution of the diffusion is gone, right. We are essentially solving for

pure convection problem that is not correct. So, a_p needs to take care of the original a_p , where the contribution from the diffusion is already there plus F_e right, which is the convection part.

So, we need to write a conditional statement such that we either such that either a_p or a_E get modified, because of the convection on the east face, right. So, we need to now write, how many such conditions? So, we need to write 4 such conditions right corresponding to each of the four faces right; that is basically east, west, north and south, ok.

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Similarly: If $F_w > 0$ then West face, w
 $F_w < 0$
 $a_p = a_p - F_w$
 else
 $a_w = a_w + F_w$

Remember: $(\Gamma \nabla \phi)_w \cdot A_w - (\rho \vec{u} \phi)_w \cdot A_w + \dots = 0$
 $+ (\rho u)_{ns} \Delta y \phi_w$ $+ F_w \phi_{ns}$ $\rightarrow + F_w \phi_p \quad F_w < 0$
 $\rightarrow + F_w \phi_{ns} \quad F_w > 0$

W | P | E

So, we need to write 4 such conditions. We will not write all the conditions here, rather I will look at the other face that is the west face here and I would leave the north and south for you to figure out. So, if you look at the west face here. So, if you are on the west face that is w; then what do we have here? We have if F_w is positive, then a_p is something I have written, else it will be blah blah blah right; either if F_w is positive, contribution has to go to a_p , if it is negative contribution has to go to a_w .

We will look into that. So, if we go back to the original equation, if I consider only the west face terms; that means I have $(\Gamma \nabla \phi)_w \cdot A_w$ minus $(\rho \vec{u} \phi)_w \cdot A_w$, right. So, this is the diffusion term, this is the convection term; plus we have three other terms like this corresponding to three different faces, plus we have the source term right, we have the source term plus equals 0, right.

So, essentially we brought the convection term to the right hand side to be on the same side as the diffusion term. Now, what is A_w here? A_w is minus Δy , right. That means, what would happen to this entire term of convection? This would become a plus because a w is now minus; this will become a plus $\rho u_w \Delta y \phi_w$ right, ϕ on the west face. So, what is $\rho u_w \Delta y$? This is F_w , so we can write this as plus $F_w \phi_w$.

Now, if F_w is positive, if F_w is positive; then what would be the upstream direction for F_w ? It would be, if F_w is positive; the upstream direction would be $F_w \phi_w$, right. This is the one, because, it has to be the, right. I think it has to be $F_w \phi_w$; is not it? Because you have west p and east; if F_w is positive, then it has to be $F_w \phi_w$ and if F_w is negative, then it has to be $F_w \phi_p$, right. It has to be $F_w \phi_p$, if F_w is negative, is that correct.

So, that means, what I am saying here is that; because if you see your mesh has w and then you have a p cell right and then you have the east cell, right. So, you have the w cell, the west cell. So, if F_w is positive, it is going this way right; that means your ϕ_w has to be, ϕ_w has to be ϕ_w , right. So, this is when it is positive and if F_w is negative, it is going this way; then your face value of ϕ_w has to be equal to ϕ_p right, that means what I have here.

So, this is when F_w is greater than or equal to 0, and this is when F_w is less than 0, right. If it is less than 0, ϕ_w would be equal to ϕ_p , alright. But both contributions are now plus values; I think this has to be changed, this is not correct. So, if F_w is positive right, then this is not correct; essentially this has to be, if F_w is positive, then a_w has to have a_w plus F_w right, because this contribution goes into a_w with a positive sign, right.

And if F_w is negative; so this is not correct here. So, you need to modify this, this is not correct; this is when F_w is, this is when F_w is less than 0; then the condition is that. If it is less than 0, then the contribution has to go to F_w ; this because it is multiplying ϕ_p it has to go to the right hand side. So, it has to go to the right hand side that is why there is a minus. So, a_p would be equal to a_p minus F_w and otherwise if F_w is greater than or equal to 0; then your $F_w \phi_w$ would be equal to $F_w \phi_w$ for the west, that means the contribution is going to a_w .

So, you need to fix this one, but otherwise this is fine. I hope you understand this part here, alright. So, now, you need to of course write two more such expressions; one for the north

face and one for the south face which I am not going into it right now as such, but you can reduce it and write it the same way alright, ok. Now, alright; so this is one way to implement the convection diffusion equation.

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A General Algorithm for UDS: Define Max function:

$$\text{Max}(a, b) = \begin{cases} a & \text{if } a > b \\ b & \text{otherwise} \end{cases}$$

$$a_p \phi_p = \sum a_{nb} \phi_{nb} + b$$

$$a_E = D_e + \text{Max}(-F_e, 0)$$

$$a_W = D_w + \text{Max}(F_w, 0)$$

$$a_N = D_n + \text{Max}(-F_n, 0)$$

The other way to implement is basically to get rid of all these if else statements; you can write one particular general algorithm for the upwind difference equation by defining, by defining a Max function. What is a Max function? Max function is something that finds a maximum of two variables, this is very much available in either c or in Fortran's.

So, this is or in C plus plus. So, Max a, Max of a, b if where a and b are two real numbers; then it would give you a, if a is greater than b or it will give you b, if not. So, essentially whichever is the maximum will be returned by the Max function. Now, this can be a very good tool to compactly write the upwind difference scheme rather than writing so many if else statements, ok. So, instead of writing so many if else statements, we can just write a very compact method for the upwind difference team using this Max function, alright.

So, I am going to kind of tell you what it is and then you have to double check; you have to verify whether it is correct or not, ok. So, essentially we seek to write a p phi p equals sigma a n b phi n b plus b, ok.

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$$a_E = D_e + \text{Max}(-F_e, 0) \phi_P$$

$$a_W = D_w + \text{Max}(F_w, 0) \phi_P$$

$$a_N = D_n + \text{Max}(-F_n, 0) \phi_P$$

$$a_S = D_s + \text{Max}(F_s, 0) \phi_P$$

$$a_P = \sum a_{ub} - S_p \Delta V_p + (F_e - F_w + F_n - F_s)$$

$$b = S_e \Delta V_p$$

And our a neighbors, a capital E is now D east right; this is basically what is D is? This is coming from your diffusion, right. These, these components are coming from your, coming from your diffusion right; these are all coming from your diffusion and then this is the convection part, right.

So, we would not worry about these things, which is basically same as before. Now, in the convection part what we say here is that, in the convection part; we know that depending on the direction of F_e , the contribution will either go to a_E or it will go to a_P , ok. So, what we do is, let us say if your F_e is positive, if F_e is positive; that means it is in the positive x direction, then the contribution has to go to a_P , right. That means, if F_e is positive, Max of minus F_e comma 0 would return what? This would return how much? This would return a 0, right.

Because F_e is positive, minus of positive and 0 maximum is 0. So, 0, that means a_E will have no contribution; because the contribution of positive F_e has to go to; has to go to what? F_e times ϕ_P right; because ϕ_e is now ϕ_P , because F_e is positive, that means F_e has to go into the contribution for a_P right, it has to go into contribution for a_P .

So, as a result, we add F_e here in the a_P equation, ok. So, basically this is bringing in only D_e . So, the D_e goes in here minus $S_p \Delta V_p$ plus F_e , ok. I am only focusing on right now on the east face. So, I am only looking at a east this guy and the a_P , alright. Now, that is fine

if your F_e is positive. What if F_e is negative? Then the contribution has to be added to a east and there should be no contribution to a p.

But because we have written it here, this may not be correct. So, let us check that. So, if F_e is negative, what will be returned with maximum of minus F_e comma 0? What will this function return, if F_e is negative? F_e is negative, this function will return minus F_e right; because F_e is negative, this will return minus F_e is not it, because minus F_e would be greater than will be bigger than 0,

So, if minus F_e comes into play, your a_E equals D_e minus F_e ; would that be the same as what we had before, right? So, if F_e is negative a_E equals a_E minus F_e , that is correct; that means this is fine. But what will what is the contribution for a_p ? a_p has to be 0. So, this brings in a east brings in D_e minus F_e . So, we have D_e minus F_e here plus we have this F_e .

So, F_e gets cancelled with this extra F_e minus F_e coming and then we essentially have D_e ; that means there is no contribution of F_e going into a_p . Do you see how it is working; yes, alright. The same is the case for F west. Let us say if F west is positive, F_w is positive; that means what will this be? This will be F_w is positive; so this would what will be returned would be F_w and this term would evaluate to F_w , because it is positive, the upwind direction would be phi w, right.

So, essentially the contribution has to go into a_w , right. Contribution has to go to a_w ; that means F_w is positive, Max of this would be F_w and it would read $F_w \phi_w$. So, essentially a_w will have a contribution. So, but when that a_w gets added here; this will be D_w plus F_w , but there is a minus F_w . So, as a result, there is no contribution to a_p , ok. Now, what about if you have F_w is negative? This is let us say minus F_w is negative; then what will be returned by this Max of F_w comma 0, 0, right.

F_w is negative. So, Max of F_w comma 0 will return 0, right; that means there is no contribution to a_w . Because if F_w is negative; then what will be the total value? $F_w \phi_p$ right; that means there is a contribution going to a_p , isn't it? Ok. So, that means, a west will have no contribution; but when you come here, there is a contribution of, there is nothing that is coming into $\sum a_{nb}$ through these guys, but there is minus F_w . Minus F_w , because it will be gone to the other right hand side.

So, that means, minus $F_w \phi_P$ and then $F_w \phi_W$ is that correct of what we had; if F_w is positive, then the contribution has to go to W which is a_W plus ϕ_W and if it is negative, it has to go to minus F_w . So, this is correct, fine. So, what we discussed is collaborates with this function. Now, I am not doing it for these two quantities here.

So, you have to do it yourself for the north face and for the south faces. So, for the north face and for the south face you have to do it yourself; verify whether this is working or not. As a result what we have is, we have a nice compact algorithm without having all these if else statements; we just have a Max function, we code it up and then both the diffusion and convection parts come into play here.

So, we have a_E, a_W, a_N, a_S and a_P would be equal to $\sum a_{nb}$ minus $S_P \Delta V_p$ plus F_e minus F_w plus F_n minus F_s ok, this is required and b equals $S_C \Delta V_p$, alright ok.

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$$a_p = \sum a_{nb} - S_p \Delta V_p + (F_e - F_w + F_n - F_s)$$

$$b = S_c \Delta V_p$$
 What about the coefficients now? a_{nb} are all +ve.
 If $S = 0$ and $\nabla \cdot \vec{u} = 0$ then $a_p = \sum a_{nb}$.
 Scarborough criterion?
 Roundness behaviour?

That is kind of very compact thing than the if else statements. What about the coefficients now? So, if you look at the coefficients; what is the property you have? All the coefficients are now positive, isn't it? If F_e is like, the diffusion coefficients are always positive, these are always positive. What about the convection parts coming into play? If this is negative, this will become positive, it will be returned; if this is positive, this will be 0 right, either this is always positive or 0 that is what is happening.

That means, all a east, a west, a north, a south would always be either 0 or positive right; that means, we will have 0 or positive contribution coming from the convection terms, that means a_{nb} are all positive. Now, what repercussions does it have on the Scarborough criteria and on the boundedness if they are all positive? We are happy; because if they are all positive, we can satisfy some of these properties. Let us say if there is no source S equals 0 and the and for the incompressible flow, it satisfies continuity equation.

So, if the underlying flow field that is given to us; let us say satisfies the continuity equation, right it satisfies the mass conservation. That means, if it satisfies mass conservation; what will happen to this term here? That we have the $F e$ minus this entire term would be; would be what? Would be equal to 0; because it satisfies mass continuity and the source term is also 0. So, this term is also not there, right.

In that context, what would be your a_p ? a_p equals $\sum a_{nb}$ right; if there is no source term and the given flow field satisfies continuity equations, then a_p equals $\sum a_{nb}$. We also note that all the a_{nb} 's are positive, all the a_{nb} 's are positive; that means $a_p = \sum a_{nb}$ and also we have $a_p \phi_p = \sum a_{nb} \phi_{nb}$.

So, essentially it is satisfies Scarborough criteria. So, Scarborough criteria is satisfied right, in equality, satisfied in equality.

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If $S=0$ and $\nabla \cdot \vec{u} = 0$ then $a_p = \sum a_{nb}$.

Scarborough Criterion ? Satisfied, Equality

Boundedness behaviour ? Boundedness is guaranteed

UDS, can, however smear discontinuities even when $\Gamma=0$...

Example problem; diffusive, High-order UDS

CDS UDS

What about boundedness? Of course, it is also boundedness is guaranteed right; because $a_p \phi_p = \sum a_{nb} \phi_{nb}$, so boundedness is also guaranteed, alright. So, what we see is that, we have now developed a new scheme which satisfies this Scarborough criteria as well as boundedness, which is much better than what we had before and they seems to be there is no condition on the coefficients, right.

And mesh can be taken to be anything, right. Unlike central difference scheme, where the mesh size is kind of restricted by the cell Peclet number that we have. So, far so good, but it turns out that the upwind difference scheme is quite diffusive ok; it is very very diffusive and even with we are taking say finer grids, this can actually smear out the discontinuity.

So, if there is a discontinuity in the problem and there is no diffusion given; let us say gamma equal to 0 and there is a discontinuity in the solution of phi, then it can actually smear the discontinuities. So, it turns out to be very diffusive. This we will explore this behavior with an example problem little later.

So, that because of this UDS is can be used as an initial solution, but it is quite diffusive. As a result we will look for some of the high order upwind difference schemes which are better in terms of not having such high diffusion, such as the UDS.

So, we look for some higher order schemes as well little later in the course. As of now we have learned these two schemes. So, one is the central difference scheme, the other is the upwind difference scheme, ok. So, both of them we have looked at in terms of their properties and how to implement them in a particular code.

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Order of accuracy of CDS and UDS:

Uniform mesh,
1D
uniform properties

Diagram showing a 1D uniform mesh with nodes W, P, e, E and cell boundaries. The distance between nodes is Δx .

Expand ϕ_P about ϕ_e

$$\textcircled{1} \phi_P = \phi_e - \left(\frac{\Delta x}{2}\right) \frac{d\phi}{dn}\bigg|_e + \frac{1}{2} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dn^2}\bigg|_e + O(\Delta x^3) \dots$$

Let us move on to the next concept, that is basically we have not actually looked at what will be the order of accuracy of these central difference scheme and the upwind difference scheme.

So, the order of accuracy, again for this I would resort to a basically a uniform mesh and I would also look at a 1 dimensional problem with let us say uniform properties in order to look at the order of accuracy. So, we have a 1 D problem with uniform mesh that is Δx is it is the same for all the cells and then we have the P cell, E cell, W cell and the east and west faces here. Now, as usual I would use the Taylor series expansion here.

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Expand ϕ_p about ϕ_e Taylor series expansion

$$\textcircled{1} \phi_p = \phi_e - \left(\frac{\Delta x}{2}\right) \frac{d\phi}{dx}\bigg|_e + \frac{1}{2} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dx^2}\bigg|_e + O(\Delta x^3) \dots$$

Expand ϕ_E about ϕ_e

$$\textcircled{2} \phi_E = \phi_e + \left(\frac{\Delta x}{2}\right) \frac{d\phi}{dx}\bigg|_e + \frac{1}{2} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dx^2}\bigg|_e + O(\Delta x^3) \dots$$

From eq. ①;

$$\phi_e = \phi_p + O(\Delta x) \dots$$

So, use Taylor series expansion and then using this, expand ϕ_p about ϕ_e ok; that means ϕ_p is ϕ_e and the distance is minus $\Delta x/2$. So, this will be minus $\Delta x/2 \frac{d\phi}{dx}\bigg|_e$ at the east face plus $\frac{1}{2!} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dx^2}\bigg|_e$ on the east face plus order Δx^3 and so on.

Similarly, let me expand ϕ_E about ϕ_e , ok. So, this would be at a distance of plus $\Delta x/2$. So, ϕ_E would be ϕ_e plus $\Delta x/2 \frac{d\phi}{dx}\bigg|_e$ on the east face plus $\frac{1}{2!} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dx^2}\bigg|_e$ and so on you get all positive coefficients here; you get a negative here and this also has to be a negative, fine.

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$$\textcircled{2} \phi_E = \phi_e + \left(\frac{\Delta x}{2}\right) \frac{d\phi}{dx}\bigg|_e + \frac{1}{2} \left(\frac{\Delta x}{2}\right)^2 \frac{d^2\phi}{dx^2}\bigg|_e + O(\Delta x^3) \dots$$

From eq. ①;

$$\phi_e = \phi_p + O(\Delta x) \dots$$

For UDS, if $F_e \geq 0$ $\phi_e = \phi_p$... Only first-order accurate.

$(\text{Eq. ①} + \text{Eq. ②})/2 \Rightarrow$

$$\phi_e = \left(\frac{\phi_E + \phi_p}{2}\right) - \frac{(\Delta x)^2}{8} \frac{d^2\phi}{dx^2}\bigg|_e + \dots$$

Now, from one of these equations, we can write let us say ϕ_e equal to ϕ_P plus some order Δx , right. If you send these guys to the left hand side, then ϕ_e equals ϕ_P . Now, what are we doing? We are saying in the upwind difference scheme; let us say if your F_e is positive; we are saying take ϕ_e equal to ϕ_P .

So, what does that mean? That means, by this approximation, what is the order of accuracy of the scheme? Order of accuracy is only order Δx right, it is only order Δx . So, that means, if upwind difference scheme is only first order accurate. Similarly, if F_e is less than 0; we say that ϕ_e equals ϕ_E that also gives you an order Δx for the downwind for the upwind direction right, if the mass flow rate changes.

So, upwind difference scheme is only first order accurate in space ok, that needs to be kind of understood. Then, what about the central difference scheme? Central difference scheme what we are doing is that, we are saying ϕ_e equals ϕ_P plus ϕ_E by 2.

Then let us add these two equations and divide by 2; that means add equation 1 and equation 2 divided by 2. Then we can write what is ϕ_e equals; ϕ_E plus ϕ_P by 2 and there is a 2 times ϕ_E by 2. So, this will be ϕ_e , this term gets cancelled; because we are adding and this term becomes $\Delta x^2/8$ here and 8 here.

So, this will be $\Delta x^2/4$; but then we are dividing by 2, so this will be $\Delta x^2/8$.

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$$(E_e \cdot ① + E_e \cdot ②) / 2 \Rightarrow$$

$$\phi_e = \left(\frac{\phi_E + \phi_P}{2} \right) - \frac{(\Delta x)^2}{8} \frac{d^2 \phi}{dx^2} \Big|_e + \dots$$
 CDS
$$\phi_e = \left(\frac{\phi_E + \phi_P}{2} \right) + O(\Delta x^2)$$
 second-order accurate.

And when we send to the right hand side, what we get is a minus $\Delta x^2 / 8 \left. \frac{d^2 \phi}{dx^2} \right|_e$ and the next term here would be order Δx^4 , ok. That means, in a central difference approximation; when we say ϕ_e equals ϕ_E plus ϕ_P by 2, the truncation error we are making is basically order Δx^2 , right.

So, this is the truncation error we are making, this is only this is about second order accurate, ok. So, what we see is that, although CDS is second order accurate, it comes with a condition on the simulation on the mesh refinement; whereas upwind difference scheme is only first order accurate, but it has no condition.

However, upwind different schemes are very diffusive. We will also see that the central difference schemes kind of are kind of dispersive or basically they produce oscillations; if you do not meet the Peclet number criteria, ok.

So, essentially the question remains is; then how do I solve for convection? What we are saying is that if you use CDS, there is too much restriction and if you use upwind difference scheme, then there is too much diffusion; what do I do? Then the answer is you go for a higher order scheme, that is constructed based on the upwind difference schemes ok, that is the kind of answer.

So, look for higher order schemes which we will learn in little while into the course ok, in the few more lectures in the course, alright.

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An example problem: Pure Convection

No source, no diffusion

$$\vec{u} = 1 \hat{i} + 1 \hat{j}$$

$$\Gamma = 0.$$

Cell Peclet no. = $\frac{\rho |\vec{u}| \Delta x}{\Gamma}$

$$\text{Peclet no.} = \frac{\rho |\vec{u}| L}{\Gamma} \rightarrow \infty.$$

What should be Delta x? CDS $Pe < 2$

The diagram shows a square domain of side length L. A diagonal interface separates the domain into two regions: a blue region where the concentration $\phi = 0$ and a red region where $\phi = 1$. A velocity vector \vec{u} is shown pointing from the bottom-left towards the top-right. The x and y axes are indicated at the bottom-left corner.

Let us look at this then the final part of today's lecture, that is basically an example problem. So, what we want to discuss is, let us look at pure convection ok; that means we are setting gamma equal to 0, there is no diffusion, there is no source term.

So, basically no source and no diffusion, ok; so, it is only pure convection; that means the equation and it is also steady. So, what we are solving for is basically $\nabla \cdot (\rho \vec{u} \phi) = 0$ ok, just convection. And the given velocity field is basically is something that is flowing at 45 degrees right; we have $1\hat{i} + 1\hat{j}$. So, it is flowing at theta equal to 45 degrees from the x axis.

So, this is the flow field, it kind of goes this way and leaves the domain. We are also considering a square domain with dimensions L by L, that is what we are considering and there is no diffusion; but we are interested in how does the scalar get transported. So, we have the scalar given a value of ϕ equals 0 on this vertical boundary, ok. So, it is basically given a value of ϕ equals 0, if I were to draw it with blue.

So, the value of ϕ on this vertical boundary is 0 and the value of ϕ on the horizontal boundary is given as 1. So, we are interested in if there is no diffusion; how does this 1 value and this 0 value get convected into the domain because of this flow field? Well, it is very simple, if you essentially release some dye here; this dye is going to convect and it is not going to diffuse, because there is no diffusion.

So, that means, everything and because the flow is angled at 45 degrees; everything that originates from here would go and this would, this entire thing would get filled up with ϕ equals 1. So, this entire thing would be ϕ equals 1 and whatever is on the top would be ϕ equals 0, right. So, essentially this entire thing would be filled with ϕ equals 0 and right this entire thing would be filled with ϕ equals 0.

But then there is no diffusion, that is why you will see an abrupt jump in the; along the diagonal you would see an abrupt jump between ϕ equals 1 and ϕ equals 0 right, there is an abrupt jump. However, if there was some diffusion; then there will be a kind of a layer that gets formed between these two right, which would in which the value of ϕ would change from 1 to 0 through some diffuse layer.

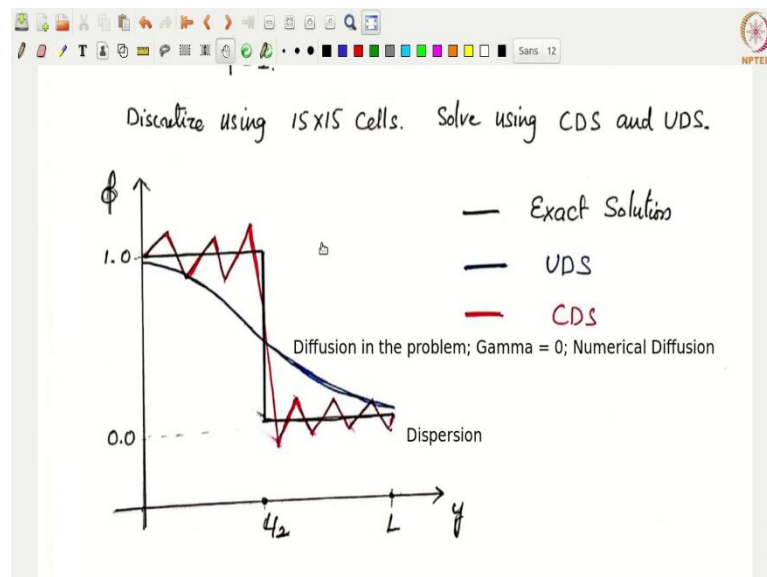
Now, the thickness of this layer would depend on the amount of diffusion you have. If you have larger diffusion, this layer would be thicker and thicker or in limit of gamma equal

to 0, this will also be 0, right. So, this layer kind of thing would exist in which the ϕ value will change from 1 to 0 in this particular dial on the diagonal.

But for the present problem, we do not have this gamma. So, as a result there is no such layer, ok. So, this is the exact solution. Now, if you were; if you were to calculate the cell Peclet number, which is given by $\frac{\rho|u|\delta x}{\Gamma}$; what would this value be?

This will be infinite or if I write a Peclet number for the entire domain, instead of calculating the length scale as δx ; if I take the length scale as capital L, this entire thing would come out to be also infinite.

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So, the Peclet number is infinite; then what does that mean? Peclet number is infinite; then the cell, then what would be the, what should be δx right? What delta x should I take; if I am using central difference scheme, what delta x should I take? There is no δx I can take, because which satisfies this problem; because Peclet number is infinite, that means δx has to be 0.

So, even if I take smaller and smaller mesh, it will never satisfy this condition of Peclet number less than 2 right; because gamma itself is 0, as a result δx has to be also 0. But then that is impossible; that means for any δx that we take, we are going to see some kind of oscillations if you solve this problem using a central difference scheme.

And we will see that if you solve this problem using an upwind difference scheme; then what you see is that, you see some kind of an artificial diffusion which is not there in the original problem specification, right.

So, let us say if I were to travel along this vertical line ok; I go from y equals 0 to y equal to L , what will be the solution ϕ change look or look like? So, ϕ would be equal to 1 all the way to y by 2 and it will be equal to 0 from y by 2 to y L , is not it? So, this will be 0 to L by 2, ϕ would be equal to 1 and L by 2 to L , ϕ would be equal to 0.

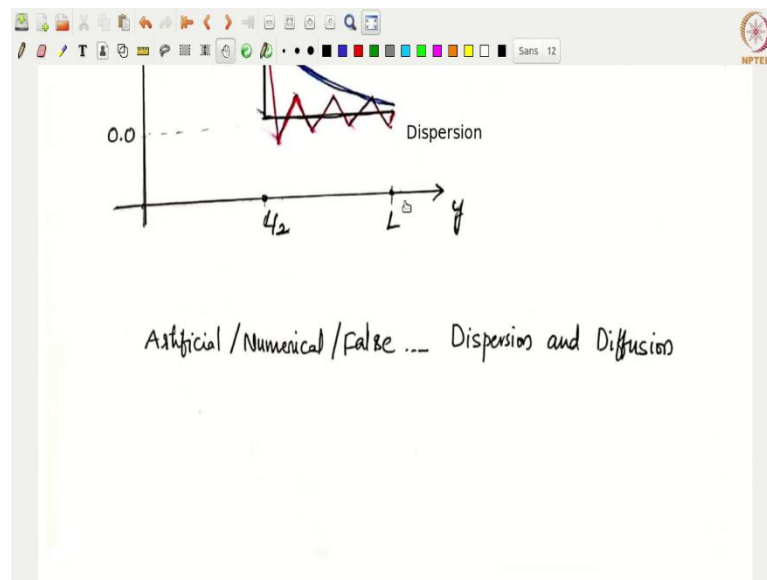
So, essentially we see a step function with 1 here and 0 here; that would be the exact solution that is expected from this problem, ok. We would kind of draw that. So, the exact solution is given by as we go along y axis; if I plot the ϕ , then the exact solution is ϕ equals 1 until I reach L by 2 and then it will suddenly drop to 0 and it will come to some value here.

Now, if you solve this problem using let us say 15 by 15 cells using both the central difference scheme and the upwind difference scheme; what you notice is that, with the central difference scheme the results are shown in red here. What you get is, you can you get some kind of an oscillations, ok. So, you see these artificial oscillations are false dispersion; this is what we call it as this behavior of oscillation we call it as dispersion.

And if you had solved this using upwind difference scheme; what you see is that, you essentially get a smooth curve right that kind of goes like this, which shows there is some diffusion in the problem, right. But however, there is no diffusion right; but we know that the γ is equal to 0, right. So, what we see here is basically some kind of a numerical diffusion that is basically an artifact of the upwind difference scheme, ok. So, that is what we see here.

So, as a result this is not; this is not, none of these things kind of give an exact solution, ok. So, that is the behavior. Now, these two behaviors are known as either artificial numerical or false dispersion, which is this one, the oscillations, the Gibbs phenomena we see here and then the artificial or numerical dissipation which is given by the upwind difference scheme.

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Now, these two is what we will elaborate in the next lecture; but it is good to know that this kind of behavior exists, when you try to solve a pure convection problem with any of these schemes, ok. Now, one question you may have is; what if there is some diffusion that is given in the problem statement, instead of taking gamma equal to 0?

Now, depending on the value of gamma you have, the upwind difference scheme will still produce some more diffusion. Now, depending on the value of gamma you have and depending on the δx that you take to particularly satisfy Peclet number less than 2; you may or may not see these oscillations coming because of the central difference scheme.

So, that is the answer. We will see depending on how it goes; we probably we will solve one assignment problem on this convection diffusion problem also. Then, I am going to stop here; because that is kind of the end of whatever we want to discuss for today, then I will talk to you in the next lecture, alright.

Thank you.