

**Introduction to Finite Volume Methods-I**  
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**Lecture – 31**  
**Discretization of Diffusion Equation for non-orthogonal systems-II**

So, welcome to this particular lecture. And what we are discussing right now on the diffusion equation or rather the discretized equation for the diffusion term. So, what we have done so far just to give you a brief idea before we begin with the exact lecture for today is that, we have taken the diffusion equation for Cartesian orthogonal grid, then we have done the non-orthogonal system and right now we are dealing with the non-orthogonal unstructured system.

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### Diffusion Equation

$$\sum_{f \in \text{nb}(c)} (J_f^p \cdot S_f) = \underbrace{\left( \sum_{f \in \text{nb}(c)} \text{Flux}_G \right) \phi_c} + \underbrace{\left( \sum_{f \in \text{nb}(c)} \text{Flux}_{F_f} \right) \phi_F} + \underbrace{\sum_{f \in \text{nb}(c)} (\text{Flux}_{V_f})}$$

↓ expand, ⇒ final form

$$a_c \phi_c + \sum_{f \in \text{nb}(c)} a_f \phi_f = b_c$$

F: stands for elements  
Discretized eqn

$$a_f = \text{Flux}_{F_f} = -\Gamma_f D_f$$

$$a_c = \sum_{f \in \text{nb}(c)} \text{Flux}_G = - \sum_{f \in \text{nb}(c)} \text{Flux}_{F_f} = \sum_{f \in \text{nb}(c)} \Gamma_f D_f$$

$$b_c = a_c v_c - \sum_{f \in \text{nb}(c)} (\text{Flux}_{V_f}) = a_c v_c + \sum_{f \in \text{nb}(c)} \left[ (\Gamma \nabla \phi)_f \cdot \mathbf{T}_f \right]$$

⇒ 0 (Ortho gen)  
Cross-diffusion

So, if you look at what we have obtained in the last class is, this is what we obtained and stopped for the unstructured grid system or the non-orthogonal grid system. So, this is the final discretized equation that we obtained. And if you look at this particular equation, this particular equation it looks exactly similar to your orthogonal system or non-orthogonal non-Cartesian orthogonal system. So, the equation system actually looks similar.

So, that is for one of the advantage for this finite volume formulation, that you can have a similar kind of discretized equation. So, only one discretized equation like the one which is shown here, so that would work for.

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### Diffusion Equation

$$a_c \phi_c + \sum_{F \in \text{NB}(c)} a_f \phi_f = b_c$$

→ Cartesian - Orthogonal

→ Non-Cartesian "

→ Non-orthogonal, Unstructured

$(a_c, a_f)$

$Ax = b$

Cross-Diffusion term →  $(b_c)$

$$S_f = E_f + T_f$$

↙

ortho

↘

Non-ortho

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So, essentially whatever system you have you end up getting a  $c \phi_c$  plus  $F$  goes over all the elements neighboring element equals to  $b_c$ . So, that is one equation that works for everybody. It works for my Cartesian orthogonal system, non Cartesian orthogonal system, non-orthogonal unstructured system. So, for each of this system the end discretized equation exactly similar; where it differs? It differs in calculation of this coefficients of this  $a_c a_f$  here  $F$  goes for neighbor elements.

So, essentially the elements which are surrounded of that particular elements  $c$ , where the discretization has been taken place or the discretization is being carried out. And the contribution from all these neighboring elements are going to come in the discretized system. This is the algebraic system which will finally, lead to  $Ax$  equals to  $b$ . And while you compare all these different- different kind of systems you only get different coefficients. But, once you come down to non orthogonal system there will be one more extra term, which is very important term is called the cross diffusion term.

So, this contribution from this particular term goes in the source term. So, this is an added contribution which comes due to non orthogonality and that bone has to take here while doing the non orthogonal grid system or the unstructured system. And we have

already seen that the surface vector which is the surface normal vector having two different component  $E_f$  plus  $T_f$ ; that means, one component provides you or gets you back the orthogonal contribution other compute to the non orthogonality.

So, this is where all these system will differ from each other and the contribution would show up in the calculation of the coefficient. So, this is where we stopped. And now what is important is that when we dealing with the Cartesian system or the non-Cartesian orthogonal system, we have seen how to implement the boundary condition. Similarly non orthogonal unstructured system also will work out how to implement the boundary condition. And once you have worked out the boundary condition because as I keep on reiterating the fact these particular equation is valid for any interior element or cell this is not valid anything which actually exit at the boundary or anything which is associated with the boundary phase.

So, for the boundary phase or the boundary element, some special treatment is required all though the governing equation is going to be the same or the rather the discretized equation is going to be the same, only contribution due to boundary treatment they will turn up.

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### Diffusion Equation

Non-orthogonal grid

1: Dirichlet  $B_c$

$$J_b^p \cdot S_b = -\Gamma_b (\nabla \phi)_b \cdot S_b = -\Gamma_b (\nabla \phi)_b \cdot (E_b + T_b)$$

$$= -\Gamma_b \left( \frac{\phi_b - \phi_c}{d_{cb}} \right) E_b - \Gamma_b (\nabla \phi)_b \cdot T_b$$

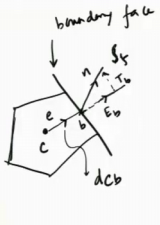
$$= \text{Flux}_{Cb} \phi_c + \text{Flux}_{Vb}$$

$$\text{Flux}_{Cb} = \Gamma_b D_b$$

$$\text{Flux}_{Vb} = -\Gamma_b D_b \phi_b - \Gamma_b (\nabla \phi)_b \cdot T_b$$

$$a_f = \text{Flux}_{Ff} \quad , \quad a_c = \sum_{f \in \text{nb}(c)} \text{Flux}_{Cf} + \text{Flux}_{Cb}$$

$$b_c = Q_c V_c - \text{Flux}_{Vb} - \sum_{f \in \text{nb}(c)} \text{Flux}_{Vf}$$



\* Need to account for cross-diffusion term

$$S_f = E_b + T_b$$

$$D_b = \frac{E_b}{d_{cb}}$$

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So, will set that will now look at this non orthogonal systems. Non orthogonal grid we will look at the first type of boundary condition is the prescribed boundary condition or Dirichlet boundary condition ok. So, this is where you have given the phi.

So, if you consider a surface like that this is a surface like that or element like that, where it is center is  $c$  it goes to this boundary which is  $b$  and this vector is  $e$  then you have a normal vector in this direction which is the direction of the surface vector and this is the connecting distance and this distance should be  $dc$  small  $b$  and that is the boundary phase. So, this is the element which we are interested in and that is the centroid  $c$  and this is the connecting line between the point  $b$ , and there is a surface vector which is acting here along this direction  $n$ .

So, now we implement, but one thing one has to note here even while you implement the Dirichlet boundary condition or Neumann condition, you need to account for the cross different diffusion term. So, essentially important point is that need to account for cross diffusion term which is also arises at the boundary phases. Now this happens whenever the surface vector which we are looking at here they are not collinear along the connecting lines. So, cross diffusion term will appear.

So, now the term the system which we are dealing with at the boundary is  $J_b \cdot S_b$  which is  $\gamma_b \nabla \phi_b \cdot v \cdot S_b$  which one can write minus  $\gamma_b \nabla \phi_b \cdot E_b$  plus  $T_b$ ; that means, my surface vector at the boundary having two component  $E_b$  plus  $T_b$  and if one has to look at it this should be the direction of  $E_b$  and this is how it is going to be  $T_b$ . So, that is the decomposed or the components of that.

Now, if i write that it is  $\gamma_b \phi_b$  minus  $\phi_c$  by  $dc_b E_b$  minus  $\gamma_b \nabla \phi_b \cdot T_b$ . So, which in terms of coefficients it is flux  $C_b \phi_c$  plus flux  $b$ . Now flux  $C_b$  where is equal to  $\gamma_b D_b$ .  $D_b$  is as you have defined so, far  $D_b$  is the geometric diffusion coefficient and this would be  $\gamma_b, D_b \phi_b$  minus  $\gamma_b \nabla \phi_b \cdot T_b$  and our  $D_b$  is nothing, but  $E_b$  divided by  $dc_b$ .

So, once you put this things back and the system, you get your if you put these things back in this particular equation you get back a  $F$  equals to flux  $F_a$  a  $c$  equals to small  $mbc$  flux  $f$  flux  $C_b$  and  $b_c$  equals to  $Q_c V_c$  minus flux  $b_b$  minus  $nbc$  flux  $V_f$ . So, given a specified boundary value one can get all this final coefficients.

Now, once you get that the second kind of boundary condition would be Neumann type of boundary condition.

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## Diffusion Equation

II: Neumann B.C  $\Rightarrow$  follows exactly like orthogonal grids  
 flux = user-specified  $\Rightarrow$

III: Mixed B.C. ( $\phi_b = \text{specified}$  & flux = specified)

$$J_b \cdot S_b = -\Gamma_b \left( \frac{\phi_b - \phi_c}{d_{cb}} \right) E_b - \Gamma_b (\nabla \phi)_b \cdot T_b$$

$$= -h_{\infty} (\phi_c - \phi_b) S_b$$

$$\phi_b = \frac{h_{\infty} S_b \phi_c + \frac{\Gamma_b E_b}{d_{cb}} \phi_c - \Gamma_b (\nabla \phi)_b \cdot T_b}{h_{\infty} S_b + \frac{\Gamma_b E_b}{d_{cb}}}$$

Boundary for  $\phi = \text{specified}$   
flux = 0

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So, Neumann boundary condition it is thing is that in this particular case this follows exactly like orthogonal grids. So, the Neumann case one can follow the procedure in this case. So, flux is user specified. So, one can follow the procedure exactly that we have derived for orthogonal system.

So, if you do that just the extra term which is going to be added at the source term. Now the third kind is the mixed boundary condition. Now for mixed boundary condition you have both specified value phi specified and flux  $E q$  is also specified. So, both of them are specified. So, in this case also one can derive that boundary condition.

So, once should do that we use the similar kind of example like what we have drawn right now that the element is there, and you have that boundary phase where you get the this is  $e b$  this is where the  $sf$  and  $n$ . And here at this phase this is the boundary phase you have both phi specified and you have both flux specified. So, you can derive the system like  $J_b \cdot S_b$ , which is going to be now  $\gamma_b \phi_b - \phi_c d_{cb} E_b - \gamma_b \nabla \phi_b \cdot T_b$ .

So, again your surface vector is having two component one is  $E_b$  another is  $T_b$ . So, this is essentially  $E_b + T_b$ . So, that is what it shows up here which is  $h_{\infty} \phi_b - \phi_c S_b$ . Now from here you get  $\phi_b$  which is  $h_{\infty} S_b \phi_c + \gamma_b E_b / d_{cb} \phi_c - \gamma_b \nabla \phi_b \cdot T_b$  and denominator you get  $h_{\infty} S_b + \gamma_b / d_{cb}$  divided by.

So, that is what you get for phi b at the boundary. So, once you get that you use this in this particular equation. So, now, you put in back in that particular equation and you get now your Jb dot S b is.

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### Diffusion Equation

$$J_b \cdot S_b = - \underbrace{\left[ \frac{h_c S_b \Gamma_b E_b}{h_c S_b + \Gamma_b E_b} \right]}_{a_b} (\phi_x - \phi_c) - \underbrace{\frac{h_c S_b \Gamma_b (\nabla \phi)_b T_b}{h_c S_b + \Gamma_b E_b}}_{S_b^{CD}} \quad \text{CD} \equiv \text{cross diffusion}$$

$$= \text{Flux } C_b \phi_c + \text{Flux } V_b$$

$$\text{Flux } C_b = \frac{h_c S_b \Gamma_b E_b}{h_c S_b + \Gamma_b E_b} \quad \rightarrow 0$$

$$\text{Flux } V_b = - \text{Flux } C_b \phi_x - \left( \frac{h_c S_b \Gamma_b (\nabla \phi)_b T_b}{h_c S_b + \Gamma_b E_b} \right)$$

So, it will get slightly involved now, because you will have some cross diffusion term associated with this calculation which was not present in the case of orthogonal systems. But again the non orthogonal system is more generic in the sense the special case of this is the orthogonal system. Now you get h infinity S b gamma b del phi b dot T b divided by h plus gamma b E b divided by dcb.

So, one can think about this is my coefficient of a b, and this one can write S b comma due to cross diffusion CD here essentially represents cross diffusion. So, I will represent this one is in more compact form by flux C b phi c flux flux b V b. And if you equate the coefficients you will get by equating the coefficients between these two you get flux C b equals to h infinity S b gamma b E b divided by dcb h infinity S b gamma b E b and what you get for flux V b V b is minus flux C b phi infinity minus h infinity S b gamma b del phi b dot T b divided by.

So, this is what you get for these coefficients. Now the thing is that since this is for the non orthogonal system if the cross diffusion coefficient is zero. That means, from here you can always get back the similar thing for orthogonal system and that is a special case

of non orthogonal system where this particular term actually goes to 0, then everything else look exactly similar for orthogonal system now.

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### Diffusion Equation

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modified co-eff. in discretized eqn  $\Rightarrow$

$$a_f = \text{Flux } F_f - \Gamma_f \frac{E_f}{\Delta x_f}$$

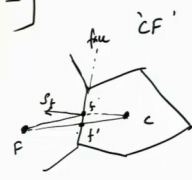
$$a_c = \text{Flux } C_b + \sum_{\text{faces}(c)} \text{Flux } C_f$$


$$b_c = Q_c V_c - \text{Flux } V_b - \sum_{\text{faces}(c)} \text{Flux } V_f$$


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Spurious : Estimate the value at face -  
- Linear variation - ]

To keep the accuracy of discretization method, integration needs to taken place at pt. 'f'




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So, the modified coefficients in that system of the discretized equation: so the modified coefficient in discretized equation look like a F would be flux F f minus gamma f E f by dcf and a c equals to flux C b plus f goes from all the phases flux C f and b c which is the source term it will be Qc V c minus flux V b minus c flux V f. So, that is what you get when you apply all the boundary condition. So, essentially what you get when you deal with all this orthogonal or non orthogonal system your equation discretized equation looks same then when you come down to the boundary element as per your boundary condition.

So, you use that boundary condition and get this modified coefficient as we have derived for all these cases individually whenever you have a specified feed value at the boundary phase. That means, the Dirichlet boundary condition, you obtain the different coefficients when you have the Neumann condition that time the flux is specified. So, you obtain the flux condition then when you have a mixed condition you get the coefficients modified accordingly.

And non-orthogonal system is more generic in the sense because if you get these term of the cross diffusion term which are the contribution due to T b if a are 0 it essentially becomes orthogonal system. Now there would be one important thing to discuss is that

skewness. So, that is something which will be very important to discuss because your discretized equation you need to have or it is very much necessary to estimate the value at the phases.

Now, when you estimate the value at the phases: so essentially you estimate the value at phase. Now that could be of average value or it could be in a different value. At different steps of the discretization process linear variation of the variables are essentially assumed. So, that is the most common that which we have discussed linear variation at the variable which are essentially assumed. Now if this linear variation is extended for the other cases then there are certain issues for specific cases.

So, that time we can avoid this linear variation and come up with something else. So, the common practice is essentially is that you do a linear interpolation profile to estimate the phase value. So, that is the common practice. Now when the grid is essentially as long as you have no problem with the grid there is no issues with this linear interpolation and you can get an very good estimate, but if there is a small skewness for example, let us say you have an element like this and that is your connecting element. So, you have c here you have f here.

So, they would be connected with this line. So, this is  $F'$  and there would be another point which is essentially going from there which is  $f$  and this is also connected and the surface vector will act as  $S_f$ . So, if you look at this particular element or the example which we have drawn right now, where the intersection point of segment of  $C$  and  $F$  that intersection point is  $F'$  which does not coincide with the phase centroid of that  $f$ .

So, essentially this is my phase and the phase center actually lies at this point  $f$  and the connecting line between the centroid of  $C$  and the neighboring element  $F$  they lie at  $f'$ . So, they do not lie at the same location. So, there is a offset or essentially this is the skewness. Now, in order to keep the accuracy or in order to maintain the accuracy of the discretization method: so in order to do that maintain that accuracy of the discretization methods. So, all phase integration need to take place at point  $f$ . So, essentially the integration needs to be taken place at point  $f$  ok.

So, what happens a correction for the interpolated value at  $f'$  is needed in order to get the value at  $f$  why? Because the connecting line between  $c$  and  $f$  there are not




collinear or they do not lie on the same point  $f$  and  $f'$  are essentially different point. So, the skewness correction can be derived.

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### Diffusion Equation

Skewness correction:  $\phi_f = \phi_{f'} + (\nabla\phi)_{f'} \cdot d_{f'f}$

$d_{f'f}$  = vector from the intersection pt  $f'$  to the face Centre  $f$



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So, this is the skewness and the skewness correction can be derived for  $\phi_f$  at point  $\phi_f$  is that  $\phi_{f'}$  plus  $\Delta\phi_{f'}$  dot  $d_{f'f}$ , so which essentially the distance of these two between these two point  $f$  and  $f'$  and considering the value at  $f'$ . So, this is a skewness correction and  $d_{f'f}$  is the vector from the intersection point  $f'$  to the phase center  $f$ . So, that is the correction that one has to do.

So, with that correction one can interpolate the value at this point. So, this is very natural when you have some sort of a skewness or skewness in the grid this kind of small skewness correction needs to be taken place so.

Thank you, we will discuss or other things in the next lecture.