

**Introduction to Finite Volume Methods-I**  
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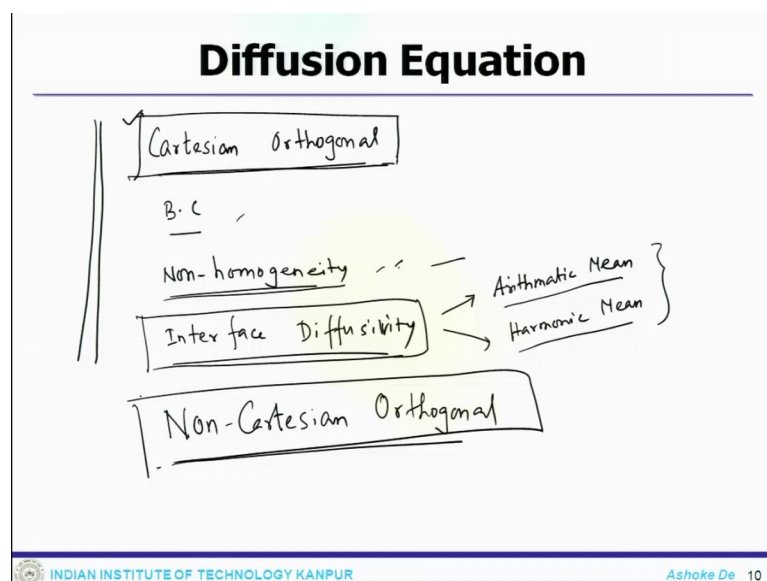
**Lecture - 29**

**Discretization of Diffusion Equation for non-Cartesian orthogonal systems-I**

So, welcome to this particular lecture on, we will continue our discussion what we have been doing so far. So, we started doing the Discretization for Diffusion equation. So, we started with steady state diffusion equation and whatever so far we have done in the front of numerics is that we have considered the orthogonal Cartesian grid system and derived our discretized equation for the diffusion equations; steady state diffusion equation and in the process of doing so, we have looked at the individual term how to calculate the fluxes, how to convert the governing equation to the final discretized equation and then we looked at the implementation of boundary condition.

And when we looked at the boundary condition implementation that time we have come across three to four different kind of boundary conditions like we have used the Dirichlet boundary condition, we have considered Neumann boundary condition, we have considered mixed boundary condition, we also considered symmetry boundary condition. And for all this respective cases, we have looked at the formulation and the numerics part like the discretized equation.

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So, in top of that what we have also done is that we when we considered the Cartesian system, we also took care of the non homogeneity of the diffusivities. And to do the calculation for the Non-Homogeneity, we have come across the formulations or different methodology how to take care of the differences of the non homogeneity. And then finally, what we have discussed or rather stopped in our last lecture is the calculation for the Interface Diffusivity. And interface diffusivity is an important parameter. When you have the variation of the diffusivity coefficient along the space, then there is a non homogeneity and you need to take care of that. And then, we can calculate the interface diffusivity thorough different approach.

One simple approach was to consider the arithmetic mean and the second approach that we have considered the harmonic mean. So, these are the two approach that we have discussed. And both of them do have certain advantage and certain limitations of the applications. Like in top of the non homogeneity; if there is a sharp gradient of the diffusivity coefficients across the cell interface, then the arithmetic mean may lead to a erroneous result; in that case if it is more preferred to use some kind of a harmonic mean. So, and that is where we have discussed these two things. And now once we have done all these though we will move to the next level of discussion for the formulation on Non-Cartesian Orthogonal system.

So, what we have done Cartesian orthogonal? So, everything is restricted to the discretization of the diffusion equation. So, after we conclude or wrap up this diffusion equation, we will move to the next set of system is the convection diffusion. So, in this context, we have done the Cartesian orthogonal system which is probably the simplest of the system because here you have all the points which are orderly placed, the cells are orderly placed. And you can actually track the local indexing and global indexing in a simple fashion. And then from Cartesian orthogonal system, we will move to the non-Cartesian orthogonal system.

So, that will be the next level to do that, in order to do that and that case also we have to implement the boundary conditions. We need to take care of the diffusivity coefficients which is varying along the space. So, what just; let us consider an example of a non-Cartesian system; this is the example of a non-Cartesian orthogonal grid system.

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## Diffusion Equation

*discretized indexing*

$S_f = \text{surface vectors}$   
( $f: e, n, s, w$ )

$\nabla \cdot \mathbf{J}_c = Q$

$\sum_{f \in \text{faces}(c)} -(\nabla \phi)_f \cdot \mathbf{S}_f = Q_c V_c$

$(\Delta x)_C = (\Delta x)_E = (\Delta x)_W$   
 $(\Delta y)_C = (\Delta y)_S = (\Delta y)_N$

$d_{e,n} = (\Delta x)_n$   
 $\|d_{e,n}\| = (\Delta x)_n$

$S_n = \|S_n\| \mathbf{n}$   
 $S_w = -S_n$   
 $\|S_n\| = (\Delta y)_n$   
 $S_s, S_e$

Example of non-Cartesian orthogonal grids

Similar to our Cartesian system

$$\mathbf{J}_c^T \cdot \mathbf{S}_c = -\nabla_c \cdot (\nabla \phi \cdot \mathbf{n})_{S_c} = -\nabla_c \cdot \left( \frac{\partial \phi}{\partial \mathbf{n}} \right)_{S_c}$$

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So, here why we call it non-Cartesian because if you look at the grid pattern, the important thing to note here is that the discretizing indexing which is shown here these are all discretized indexing. And discretized indexing, they follow the similar pattern like the direction pattern that we have adopted for this particular class.

So, this is what or rather one can say that. This is more a standard notation for any finite volume formulation. So, you consider a element C and then ahead of that element is a standard notation of that element is east element, then the top of that or in the northern side is the north element. Then behind that element is the west side element and the underneath or the down of that element is the south element and respective surfaces are identified like E N W S. And all other  $S_f$  are surface vectors. So, these are all standard where f stands for small e w n and s.

So, these are all standard notations that we are using and, but now this system is non-Cartesian. The reason is if you look at it this is our standard reference frame x and y system and this has been opted by an angle theta. Now if you that is why it is a non-Cartesian system, but still this is orthogonal. The reason is that when you consider a particular elements C, then all the surface vectors or the other elements like the surrounding elements; they are nicely ordered. Only difference is that the whole grid system has been shifted by a offset or by an angle theta. So, that is why it is a non-Cartesian system, but still it remains in the orthogonal mode. And the so, that allows to

calculate the fluxes and all these things in a simpler fashion that like what we have done for our orthogonal system Cartesian orthogonal system.

Now, to come back to the system, we consider the one row of element. So, that if you look at it; essentially it is in a two dimensional system here. It is a two dimensional Cartesian system or two dimensional orthogonal system. So, from here you come down to 1D system and if you come down to 1D system, here you see the element C sitting here. And then, east is only one element, west one element. These are the normal vectors surface normal vectors and then along this direction you have a normal vector and there will be a tangential component of the vector. The reason is all these stencil. It has been offset by your standard reference frame. And the other definition like the distance between the cell is  $\Delta x$  E in the y direction  $\Delta y$  c and also even non-Cartesian system the  $\Delta x$  E; if this is let say  $\Delta x$  E, they are equal.

So,  $\Delta x$  C must be equal to  $\Delta x$ . So, that uniformity is maintained only thing it is different from our previous Cartesian orthogonal system is that it has been tilted by an angle. And if you consider the this also this would be also same. So,  $\Delta y$  C must be same with  $\Delta y$  south or  $\Delta y$ , this is  $\Delta x$  west. So, that maintains the uniformity. And now if you look at this distances, the distance between c and e which is  $D_{CE}$ ; so, that is essentially the distance with a normal vector. So, that will get you that thing and similarly you get the surface vector  $S_e$ , you get the west opposite in sign. So, you get both these things and since its one dimensional, we can get in a two dimensional similarly  $S_n$  and  $S_s$ .

So, that will follow the standard procedure that we have adopted. So, the now if you look at the discretized equation, so this would be essentially look similar to our Cartesian system and we can derive that. So, how we can derive that? We will start with our equation. So, that is our standard equation  $\Delta \cdot J$  equals to  $Q$ . Now this would be once you write over the elements C, this will turn out to be the surface integral where  $f$  goes from  $N_b c$  minus  $\gamma \Delta \phi$   $f \cdot S_f Q c V c$ . Now each face we need to calculate the fluxes

So, once you try to calculate that  $J_e \cdot S_e$ , this would be minus  $\gamma_e \Delta \phi$  dot  $n_e S_e$ . So, that will be essentially now minus  $\gamma_e \Delta \phi$  by  $\Delta n$  at east face with  $S_e$  ok.

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## Diffusion Equation

$(\nabla \phi \cdot \mathbf{n})_e = \left( \frac{\partial \phi}{\partial n} \right)_e \rightarrow$  gradient of  $\phi$  at face 'e' along the 'n' direction.

Assume, the linear variation in the profile of  $\phi$

$\left( \frac{\partial \phi}{\partial n} \right)_e = \frac{\phi_E - \phi_C}{d_{CE}} \Rightarrow$  orthogonality is still there

\* Rest of the calculation are exactly similar as we have obtained for Cartesian - Orthogonal system

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Diffusion eq. (Discretized)

Cartesian Orthogonal ✓

Non-Cartesian " ✓

Non-Orthogonal Unstructured

elements    faces    nodes

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Now importantly here this delta dot delta phi dot n at this east face is, but del phi by del n at east face. Now this is the gradient of phi at face e along the n direction. Why we say it is n direction? If you look at this the picture here, this is the n direction; that means, the normal direction and this is the tangential direction. So, normal and tangential directions are estimated. So, again what one can do the simplest of the thing that you one can assume the linear variation in the profile of phi.

So, if you assume the linear variation of the profile, then you can get the del phi by del n at surface e is phi E minus phi C divided by d C E ok. So and why this is possible? Because this is possible for the reason the orthogonality is still there. Now rest of the calculations for finally, obtaining the discretized equation. So, rest of the calculation are exactly similar as we have obtained for Cartesian system Cartesian orthogonal system. So, this is the important point.

So, rest of the derivation one can basically reproduce the as we have done for this case. Now so, what we have looked at this moment is that two important thing. One is that we have got our discretization of the diffusion equation. So, essentially we are getting diffusion equation the discretized one using our numerical approximations. So, while doing that we got it for Cartesian orthogonal system. So, you have got it in details, then we got it for non-Cartesian orthogonal, then we can go to non orthogonal unstructured system.

Now, when we move to non orthogonal unstructured system, the things would be different, why? Because in the Cartesian system as long as they are orthogonal, they are actually easy to handle because the elements or the cells they are nicely ordered. As soon as we go to unstructured that we have already come across or seen looking at the finite volume means that they are not nicely ordered. They are rather randomly spaced. So, one has to keep track of lot of information starting from its elements, faces, nodes and among them the connectivity through local indexing and global indexing ok.

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### Diffusion Equation

Non-Orthogonality  
 $\text{gradient} = f_f(\phi_C, \phi_F, \dots)$

orthogonal grid: (gradient in the direction normal to the face)  
 $(\nabla \phi \cdot n)_f = \left(\frac{\partial \phi}{\partial n}\right)_f = \frac{\phi_F - \phi_C}{\|r_F - r_C\|} = \frac{\phi_F - \phi_C}{d_{CF}}$   
 ( bcs,  $CF$  &  $n$  are aligned ... )

$e =$  represents the unit vector along the direction defined by the line connecting 'C' & 'F'

$$e = \frac{r_F - r_C}{\|r_F - r_C\|} = \frac{d_{CF}}{d_{CF}} \quad \text{gradient along 'e'}$$

$$(\nabla \phi \cdot e)_f = \left(\frac{\partial \phi}{\partial e}\right)_f = \frac{\phi_F - \phi_C}{\|r_F - r_C\|} = \frac{\phi_F - \phi_C}{d_{CF}}$$

$n =$  unit normal vector to  $f$

Non-orthogonal mesh

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So, once we go to unstructured system. So, these are non orthogonal unstructured grid. First we consider the Non-Orthogonality. So, you first consider the non-orthogonality and to deal that the essential component would be the gradient calculation. So, let us consider these system for non-orthogonality. So, let us consider one particular elements C. So, this is in non orthogonal mesh ok. So, we have just considered one cell and then the neighbouring cell F. Now here they are not orthogonal. So, at the face the surface vector  $S_f$ , this is the surface vector which goes in the normal direction to the face. So, this is my face and this  $n$  is perpendicular to that  $f$ . And along the face, this is the tangential direction. So, this is my normal direction this is my tangential direction.

So, at the face we got two different directions. So, one along this and the connecting points between these two cell centres are connected through the line that is the distance between these two cell  $d_{CF}$ . Now these lines which are also going through the point F at

the face. So, initially we consider they are actually sitting on the line or rather they are going to be sort of collinear. Then the normal vector is offset by an angle  $\theta$  from this line. So, as it clearly shown this is going by an angle  $\theta$ . And now so, writing the gradient in this case as a function of these information show the gradient still would be a function of  $\phi_C$ ,  $\phi_F$  and some other component because due to the normal orthogonality.

So, now one has to write the exact expression for this connecting centres and the for element C. So, orthogonal grid what do we have obtained if you just recall from the orthogonal grid, what do we have got. So, if it is the gradient in the normal direction, so, orthogonal grid the gradient in the direction normal to the face. So, what we have got  $\nabla \phi \cdot \mathbf{n}$  at face equals to  $\nabla \phi \cdot \mathbf{n}$  at f which is  $\phi_F - \phi_C$  divided by sort of  $r_F - r_C$  which is one can write  $\phi_F - \phi_C$  divided by  $d_{CF}$ . So, essentially this is the distance vector between these two cell centres.

So here, why we can write that? We can write here because  $C-F$  and  $\mathbf{n}$ ;  $\mathbf{n}$  is the unit normal vector which is the  $\mathbf{n}$  is one can say that  $\mathbf{n}$  is unit normal vector to f the face. So,  $C-F$  and  $\mathbf{n}$  are aligned ok. So, that is why we can write these things and connecting the points C and F, we can obtain these things. Now, if  $\mathbf{e}$  which represents the unit vector along the direction defined by the line connecting C and F, so,  $\mathbf{e}$  actually defines the normal vector or unit vector along the line C and F which are joined along that. So,  $\mathbf{e}$  actually represents the unit vector.

So, once we do that we can actually define the  $\mathbf{e}$ ;  $\mathbf{e}$  would be  $r_F - r_C$  that is the difference between the radius vector minus  $r_C$  which is  $d_{CF}$  divided by small  $d_{CF}$  ok. So, that is what it is. So, essentially this is the mod of that. Now you can find out the gradient along the direction. So, the gradient along  $\mathbf{e}$ ; so, this would be  $\nabla \phi \cdot \mathbf{e}$  at face is  $\nabla \phi \cdot \mathbf{e}$  at face which is  $\phi_F - \phi_C$  divided by  $r_F - r_C$  which also one can write that  $\phi_F - \phi_C$  divided by small  $d_{CF}$ . So, that is the vector.

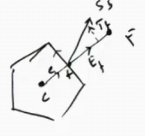
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## Diffusion Equation

Linearize the flux :  $S_f = E_f + T_f$  |  $E_f =$  in the direction of CF

$$(\nabla\phi)_f \cdot S_f = \underbrace{(\nabla\phi)_f \cdot E_f}_{\text{orthogonal contribution}} + \underbrace{(\nabla\phi)_f \cdot T_f}_{\text{non-orthogonal contribution}}$$

like:  $= E_f \left(\frac{\partial\phi}{\partial c}\right)_f + (\nabla\phi)_f \cdot T_f$

$$= E_f \left(\frac{\phi_F - \phi_C}{dcf}\right) + (\nabla\phi)_f \cdot T_f \Rightarrow \text{cross-diffusion term}$$


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Now, if we linearize the flux, so linearize the flux in this particular system in this non orthogonal system, then the surface vector which was defined here the surface vector  $s_f$  the  $s_f$  will have two component. So, surface vector will be decompose in two component one is the  $E_f$  plus  $T_f$ . So, these are the two component that one needs to essentially decompose this surface vectors. And then what happens that I can write down the total surface vector in that fashion where one can think that  $E_f$  would be in the direction of CF and; that means, they are connecting these two point. So, if you look at this  $S_f$ , one component will go along this which will be  $S_f$  some sort of a  $\cos \theta$  component, then other one will go along the tangential component which will be the  $\sin \theta$  component.

So, there are two components. So, now if I write down my diffusion flux, so there will be  $\nabla\phi_f \cdot E_f$  that component plus because  $s_f$  is the sum of these two component. So, it would be  $\nabla\phi_f \cdot E_f$  plus  $\nabla\phi_f \cdot T_f$  ok. So, if you look at it this is along the direction of the CF. So, these part or this guy is nothing, but my some sort of  $n$ . So, now, I have connected these two points C and F and the component which is going the surface vector has two components: one going along these direction, another is going along tangential direction. So, this one, the one which will go along this direction  $e$ , they will be similar to our orthogonal like orthogonal contribution.

One can think about in that fashion because this is my cell which was connected CF. They are connected from here this is goes my  $S_f$ . This goes my  $E_f$  this goes my  $T_f$ . So,



that is how the components are decomposed. So, this one can think about along this line which is the line connecting between centre C and centre F, this will be looking like a orthogonal contribution. Now what about this term? This term is another term which will look like an or non orthogonal contribution. So, this is the first term first term will look like an our orthogonal contribution which actually the component of the surface vector goes along this unit vector of e, other one goes along this direction which is the non orthogonal contribution.

Now, if you compare to our orthogonal system, this is where the non orthogonal system starts debating from that. You do not have any contribution from the non orthogonal system. So, one can write or expand this term in a slightly more detail  $E_f$ . This would be  $\nabla \phi$  by  $\nabla e_f$  plus  $\nabla \phi_f \cdot T_f$ . So, this one can write  $E_f \phi_F$  minus  $\phi_C$  by  $d_{CF}$  plus  $\nabla \phi_f \cdot T_f$  ok. So, these component actually involves the information of these two cells centre C and F and this is exactly looking like our contribution which we do get in our orthogonal system.

But this extra term which was not present, sometime this is also referred called the cross-diffusion term. In some text book they call it an orthogonal contribution, some textbooks call it a cross diffusion term or cross diffusion contribution. So, this is where the difference starts appearing between the orthogonal system and a non orthogonal system. When you have a purely orthogonal system, you just get these contribution and when you have a non orthogonal system, you get this contribution and plus this contribution. So, this is the difference.

Now, one can think about in a other way the orthogonal system is a special case of non orthogonal system, why? Because if the non orthogonal system, this contribution goes off then it turns out to be an orthogonal system; that means, essentially one can derive and discretize equation for a non orthogonal system. And then can be used for both non orthogonal system and a orthogonal system by assigning that term like the non orthogonal contribution term to be zero.

So, that is the one of the beauty of finite volume method that things can be more generic in nature and once we go along with the complexity, you can see that the higher level things can be always simplified to the lower level one. Though we are starting from the

orthogonal system, then moving to a non orthogonal system; the non orthogonal system can be boiled down to orthogonal for a special case as it is here ok.

Now, the point comes how do you decompose this  $S_f$ ? When you decompose this  $S_f$  or if you put back the  $S_f$  you get this particular equation. So, we will stop here and.

Thank you.