

Introduction to Finite Volume Methods I
Prof. Ashoke De
Department of Aerospace Engineering
Indian Institute of Technology, Kanpur

Lecture – 30
Discretization of Diffusion Equation for non-orthogonal systems-I

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Diffusion Equation

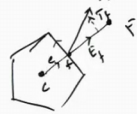
Linearize the flux : $S_f = E_f + T_f$ | $E_f =$ in the direction of CF

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

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

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

Decomposition of S_f :



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So, welcome to this particular lecture on; we will continue our discussion what we have been doing so far. Now that decomposition of S_f so, there are different ways multiple ways one can do that.

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Diffusion Equation

Minimum Correction approach
 to keep the non-orthogonal correction
 as small as possible
 (Minimize T_f Contribution)
 if non-orthogonality $\uparrow \rightarrow \phi_e, \phi_F \downarrow$

$$E_f = (e \cdot S_f) e = (S_f \cos \theta) e$$

$$S_f = E_f + T_f$$

 Decomposition
 of S_f
 through min.
 Correction method

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So, let us start with let us have this cell connected which is let us look at this picture. So, this is a approach called minimum correction approach. So, this is for the decomposition of S_f through minimum correction method or approach.

So, you have these two points or the cell centre connected along the line $D C f$, this is the e unit vector e along this surface point this is the direction of the surface vector then we have got two component. Now in this case the idea is that the way it is done to keep the non-orthogonal correction. So, the non-orthogonal corrections or the contribution for the non-orthogonal distribution is as small as possible.

So, that is why we call it a minimum correction approach so; that means the contribution due to. So, S_f will have two component; one is E_f one is T_f this is like an orthogonal contribution, this is our non-orthogonal contributions.

So, idea is that you sort of minimize T_f contribution as much as possible ok. And, but what happens if non-orthogonalities increases, non-orthogonality, increases if that increases so, the contribution to the diffusion flux from ϕ_F and ϕ_C this contribution will start decreasing ok. Now in this case it would be simple to compute the E_f is $e \cdot S_f$ which is nothing, but $S_f \cos \theta$ so, that is a simple way one can do that. Now, this is approach one of the approach one can do that.

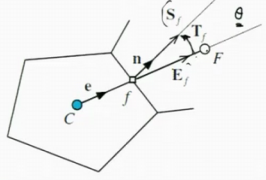
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Diffusion Equation

B Orthogonal Correction Approach

$$E_f = S_f e$$

Φ_F & Φ_C same as
orthogonal mesh -



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Then one can do second way of doing that that is called orthogonal correction approach. So, what you do here again you get this particular two elements, they are connected as usual and the component of the surface vector one would be along this line, if this is theta and the other one would be along this line the perpendicular one ok.

So, there also contribution comes from both phi F and phi C so, here what you do? You define E_f again $S_f e$ so, that is our orthogonal correction approach. Now, that is exactly like what kind of I mean contribution that we take it essentially, keeps the contribution of the term involving phi F and phi C same as orthogonal mesh, irrespective of the degree of non-orthogonality.

So, this is why it is called the orthogonal correction approach, you just take a contribution like that, where it will involve the information of these two cell centres as we have done for the orthogonal mesh irrespective of the degree of non-orthogonality. Once you do that this may not be an very acceptable approach because, if your theta increases this can create trouble.

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Diffusion Equation

\approx Over-Relaxed Approach

ϕ_F, ϕ_C

$$E_f = \left(\frac{S_f}{\cos \theta} \right) e = \left(\frac{S_f^2}{S_f \cos \theta} \right) e$$

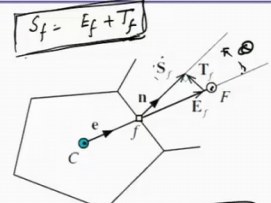
$$= \frac{S_f \cdot S_f}{e \cdot S_f} e$$

$(\nabla \phi)_f \cdot T_f = (\nabla \phi)_f \cdot (S_f - E_f)$

\downarrow
(orthogonal)

$$= \begin{cases} (\nabla \phi)_f \cdot (n - \cos \theta) S_f & \text{--- min. correction} \\ (\nabla \phi)_f \cdot (n - e) S_f & \text{--- normal correction} \\ (\nabla \phi)_f \cdot \left(n - \frac{1}{\cos \theta} e \right) S_f & \text{--- over-relaxed} \end{cases}$$

$S_f = E_f + T_f$



Cross-diffusion term

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Now, another option one can have the over relaxed approach ok. So, what you do here? The vectors and everything look similar the corrections vectors and the components S_f will have as usual E_f plus T_f cell centres are connected along e through the surface. So, here the terms which are very important here is ϕ_F and ϕ_C . Now how we do that or mathematically one can achieve this calculation we can get E_f equals to S_f by $\cos \theta$ e which is S_f square divided by $S_f \cos \theta$ e one can write S_f dot S_f divided by e dot S_f .

So, to summarize what we are doing it here the diffusion flux at an element face of non-orthogonal grid cannot be written surely in terms of the values which are connecting through the cell centres or the nodes which are connecting through the cell centres. So, what it require a term which will account for this non-orthogonality? So, you need a term which will account for the non-orthogonality or this sort of angle θ .

So, that is the degree of I mean the degree of non-orthogonality. So, the term which accounts for the non-orthogonality needs; to be added and which is called the so, called cross diffusion term. So, that is very very important term for non orthogonal grid system.

So, if we put together everything what we have looked at it, then one can see that what we are doing is at the gradient calculation at the faces. So, this was the component so, this $\nabla \phi_f \cdot S_f$ minus E_f . So, we are trying to see the contribution from the cross

diffusion term, which was essentially one is that $\nabla \phi \cdot \mathbf{n} \cos \theta e S_f$, this was the case when you have minimum correction.

Then another option is that $\nabla \phi \cdot \mathbf{n} \cos \theta e S_f$ which is normal correction and the last option that is that $\nabla \phi \cdot \mathbf{n} \cos \theta e S_f$ so, this is over relaxed. So, theoretically what we are doing it we know the surface vector or the surface vector will have two component. Now the component which is going along the line that connecting the cell centres that is along \mathbf{e} or the normal that is easy to obtain.

And then, that involves the information of ϕ_C and ϕ_F and once you obtain that information then you can actually using this information of the vector algebra we get the contribution for the cross diffusion term. So, instead of going directly to calculate $\Delta \phi$ so, if you go back and see there are two component for my flux discretization, one is like our orthogonal contribution which can be directly computed using the information of the connecting cells. And the distance connecting between these two cell centres and then there is a contribution which comes from the cross diffusion term.

Now this cross diffusion term instead of calculating directly what we do, we calculate the corrections for E_f and then using that E_f we get back the other component. So, what happens is that as we said the cross diffusion component, this component it is absolutely 0 for orthogonal system.

So, that actually brings back the non-orthogonal system to be a orthogonal system or the behaviour of the non-orthogonal system; when you assign this cross diffusion term to be 0 that becomes an orthogonal system.

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Diffusion Equation

Cross-Diffusion term \rightarrow Cannot be expressed using the nodal values

Gradient Computation: Diffusion flux \neq $f_n(\text{nodal values})$

Discretized system \leftarrow Non-orthogonality

Gradient theorem $\Rightarrow \int_V \nabla \phi \, dV = \oint_{\partial V} \phi \, dS$ ds: outward pointing interface surface vector

$$\overline{\nabla \phi}_V = \frac{1}{V} \int_V \nabla \phi \, dV \quad \left| \quad \overline{\nabla \phi}_C = \frac{1}{V_C} \oint_{\partial V_C} \phi_f S_f \right.$$

$$= \frac{1}{V_C} \sum_{\text{funcs}(C)} \phi_f S_f$$

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Now the things come how do we treat this cross diffusion term that is an very important issue because this cross diffusion term cannot be so, if you look at it the cross diffusion term, they cannot be actually this cross diffusion term cannot be expressed using the nodal values.

So, the point here is that when you calculate this component along e or the sort of pseudo orthogonal component, you can use the information of this two cell or the information of this nodal values and can find out that $E \cdot f$. But or $\Delta \phi \cdot E \cdot f$, but cross diffusion term the problem arises this cannot be straight away expressed through the nodal values.

So, due to this, this some kind of corrections approach is required and some sort of a calculation is required. One of this that how do you calculate the essentially we can look at it the first the gradient computation. And then, we will see in a non-orthogonal system how do we actually derive this cross diffusion term?

So, gradient computation so, the point here is that in non-orthogonal domain as we have already come across the non-orthogonal domain the computation of the diffusion flux itself is complex. Because, it cannot be linearized and so, the diffusion flux cannot be linearized in a straight cut way or straight forward way and also cannot be written directly with the function of nodal values.

So that means, the non orthogonal system gives rise to some sort of a challenge for the engineers or the scientists to get this computation done in a perfect fashion. So, which on the other way round it means the gradient calculation or the gradient has to be evaluated in order to incorporate is non-orthogonal contribution in the discretization system.

So, essentially my discretized system must have the information of non-orthogonality so, which gives rise to the cross diffusion term. And the cross diffusion term cannot be calculated using nodal value so, that is where the problem lies. So, what we can use for calculating the flux actually? We can use some gradient theorem, if we use the gradient theorem what it gives you that which we have done $\text{del } \phi \text{ d } v$ is the surface integral of $\phi \text{ d } s$ ok.

And this is actually the ds is outward pointing interfacial vector, inter or you can say outer pointing surface vector ok.

So, what one can get the average gradient how do we got it $\text{del } \phi \text{ v}$, the average gradient we got the $\text{del } \phi \text{ d } v$. Now once you combine this two what you get for a system that $\text{del } \phi \text{ c}$ average value is 1 by $v \text{ c}$ surface integral $\phi \text{ f } S \text{ f}$ ok. So, once you integrate over the cell faces, this will lead to 1 by $v \text{ c}$ summation $n \text{ b c}$ $\phi \text{ f } S \text{ f}$.

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Diffusion Equation

$$\nabla \phi_f = g_c \nabla \phi_c + g_f \nabla \phi_f$$

$$\sum_{\text{fnd}(c)} (\mathcal{D}_f \cdot S_f) = \sum_{\text{fnd}(c)} [-(\nabla \phi)_f \cdot (E_f + T_f)]$$

$$= \underbrace{\sum_{\text{fnd}(c)} [-(\nabla \phi)_f \cdot E_f]}_I + \underbrace{\sum_{\text{fnd}(c)} [-(\nabla \phi)_f \cdot T_f]}_II$$

$$= \sum_{\text{fnd}(c)} \left[-\mathcal{D}_f E_f \frac{(\phi_f - \phi_c)}{d_{cf}} \right] + \sum_{\text{fnd}(c)} [-(\nabla \phi)_f \cdot T_f]$$

$$= \sum_{\text{fnd}(c)} \mathcal{D}_f \mathcal{D}_f (\phi_c - \phi_f) + \sum_{\text{fnd}(c)} [-(\nabla \phi)_f \cdot T_f]$$

ϕ_c, ϕ_f
= nodal/cell center values

$S_f = E_f + T_f$
↑ ↑

I: Orthogonal linearized part

II: Non-orthogonal linearized part

$\mathcal{D}_f = \frac{E_f}{d_{cf}}$

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Now what one can do the gradient at the face can have two contribution; one at $g_c \Delta \phi_c$ plus $g_F \Delta \phi_F$ where ϕ_c , ϕ_F are the nodal or cell centre values. So, you use the information of the cell centre values to get this particular information.

Now, once we use this cell centre value and then we can sort of short of linearize the system using the information of that. Now if you look at the whole summation term over the cell so which is essentially J_f for the diffusion term S_f . Now this term is going over all the face minus $\gamma \Delta \phi_f \cdot E_f$ plus T_f .

So, this comes as we have seen this will be a two component one is E_f one is T_f and this is giving rise to cross diffusion term or rather non-orthogonal correction term, this is my sort of orthogonal correction term ok. Once we do that then I can write this one expanding and I will write this one as minus $\gamma \Delta \phi_f \cdot E_f$ plus summation over all the faces minus $\gamma \Delta \phi_f \cdot T_f$ ok.

So, what it does this is a term, this term is I and this is the second term; term II term I is the orthogonal linearized part or contribution or term II is due to non-orthogonal non-orthogonal linearized part ok. So, we get two different contribution as expected. Now if you expand it further so, this would be over f if I write down this would get me back that minus $\gamma_f E_f \phi_F$ minus ϕ_C by $d_c f$ plus summation over all the faces and we get minus $\gamma \Delta \phi_f \cdot T_f$.

So, we written the second term as it is for the time being. Then again we simplify the first part and what we get is that $\gamma_f D_f \phi_C$ minus ϕ_F plus over the all the faces we written $\gamma \Delta \phi_f \cdot T_f$. Here that D_f is the again the similarly as we have defined for the orthogonal system it is the geometric diffusion coefficient which would be E_f divided by $d_c F$ so, that is the definition of D_f .

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Diffusion Equation

$$\sum_{\text{funs}(c)} (J_f^D \cdot S_f) = \underbrace{\left(\sum_{\text{funs}(c)} \text{Flux}_G \right) \phi_c}_{\text{Ortho}} + \underbrace{\left(\sum_{\text{funs}(c)} \text{Flux}_{F_f} \right) \phi_F}_{\text{Ortho}} + \underbrace{\sum_{\text{funs}(c)} (\text{Flux}_{V_f})}_{\text{Cross-diffusion}}$$

↓ 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

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

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

$$b_c = Q_c V_c - \sum_{\text{funs}(c)} (\text{Flux}_{V_f}) = Q_c V_c + \sum_{\text{funs}(c)} \left[(\Gamma \nabla \phi)_f \cdot T_f \right] \Rightarrow 0 \text{ (Ortho)}$$

κ
Cross-diffusion

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Now if you take it slightly more or expand it slightly more so, what we are having at the left hand side is the flux going for all the faces and after decomposition or expanding we get now summation over all the faces it is flux C f phi c plus summation over all the faces flux F f phi f ok. And so, this you can put it in the bracket plus summation of f going over c you have flux v f.

So, all these things are written in this coefficient format what we use to do for the orthogonal system. Here once you write down this if you expand these things, now if you expand and these things, the final form of my discretized equation would be like phi c a c plus summation F going over NB c a F phi F b c. Again here F stands for elements or rather neighbouring elements so, where you get all this information.

So, if you look the discretized system, they look exactly similar to our orthogonal system. And again I am repeating or reiterating the fact this is one of the beauty of the finite volume method, that what you get at the end the discretized equation or rather this is my sort of discretized equation.

So, whether it is a orthogonal system or non-orthogonal system the discretized equation looks pretty similar. So, mathematically they looks similar only differences will come in this coefficients. So, what that makes you to do or allow you to do that you can have a discretization pattern or discretized equation which looks similar and can be applied to all sort of system.

Then it is much easier for computing purposes. Now before we talk about that in more we just look at the coefficients here for this case which is going to be now flux F_f which is nothing, but $\gamma_f D_f$ and my b_c is $Q_c V_c$ minus summation of n_{bc} flux v_f equals to $Q_c V_c$ plus summation of f these things to $\gamma \Delta \phi_f \cdot T_f$

So, this is the contribution which come as a source term in the non orthogonal this is cross diffusion term. So, as I was mentioning the discretized equation looks exactly same for your orthogonal non-orthogonal system. It start so, you can be on a one single frame work and then, one can do the programming and that is the advantage of finite volume method that it actually gets you back a same system of equations which can be applied to both orthogonal and non-orthogonal system.

Only thing is that what you need to take care of this coefficients? So this coefficients are only going to change from one case to another case and for non-orthogonal system you come across this cross diffusion term, which is a extra contribution come as a source term.

If this term goes to 0 that will become the orthogonal system and the other things will look exactly similar. So, that is where the advantage lies that we can have a same discretized system for both orthogonal and non-orthogonal system and can be used with different coefficients.

So thank you we will discuss all other things in the next lecture.