

Introduction to Finite Volume Methods- I
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Lecture – 32
Discretization of Diffusion Equation for non-orthogonal systems-III

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Diffusion Equation

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

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

Anisotropic Diffusion : semi-discretized diffusion eqn.

$\sum_{\text{faces}(c)} (-\Gamma \cdot \nabla\phi)_f \cdot S_f = S_c V_c$

Γ = varying in space
 Γ = 2nd order symmetric tensor

Assuming a general 3-D situation,

$$(-\Gamma \cdot \nabla\phi)_f \cdot S_f = - \begin{bmatrix} \Gamma_{11} & \Gamma_{12} & \Gamma_{13} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} \end{bmatrix}_f \cdot \begin{bmatrix} \frac{\partial\phi}{\partial x} \\ \frac{\partial\phi}{\partial y} \\ \frac{\partial\phi}{\partial z} \end{bmatrix}_f \cdot S_f$$

So, welcome to the lecture of this Finite Volume Method. Now, moving ahead we may look at one more important topic is that anisotropic diffusion.

So, we have done some discussion on these when we are looking at the variation of the diffusion coefficient gamma over space and sale to sale when there is a variation we have looked at it, but now, we are looking at it in more details. So, what it happens is that if there is a anisotropy in the diffusion coefficient or semi discretized equation. So, the semi discretized diffusion equation that will look like now, f equals to all these places minus gamma dot del phi f. Here one can think about this gamma is like an dot S f equal to S c V c. Here gamma is varying in space.

So, what happens? This, gamma here can be treated as this is also a second order symmetric tensor which will actually represent the anisotropic tensor. So, now, if you assume a general, so assuming a general 3-D situation, so which can be boils down to 2-D and a 1-D. So, what one can write this left hand side? If you assume a general 3-D situation the left hand side which is essentially minus gamma dot del phi at phase f dot S

f which will be essentially looking like an tensor, which will be gamma 11, gamma 12, gamma 13, gamma 21, 22, 23, gamma 31, 32, 33 at f here you have del phi by del x, del phi by del y, del phi by del z, phi dot S f. So, the in a 3 dimensional system, generic 3 dimensional system gamma is an tensor. So, the gamma would look like that.

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Diffusion Equation

Matrix calculation:

$$\begin{aligned} (-\nabla \cdot \nabla \phi)_f \cdot S_f &= - \begin{bmatrix} \Gamma_{11} \frac{\partial \phi}{\partial x} + \Gamma_{12} \frac{\partial \phi}{\partial y} + \Gamma_{13} \frac{\partial \phi}{\partial z} \\ \Gamma_{21} \frac{\partial \phi}{\partial x} + \Gamma_{22} \frac{\partial \phi}{\partial y} + \Gamma_{23} \frac{\partial \phi}{\partial z} \\ \Gamma_{31} \frac{\partial \phi}{\partial x} + \Gamma_{32} \frac{\partial \phi}{\partial y} + \Gamma_{33} \frac{\partial \phi}{\partial z} \end{bmatrix} \begin{bmatrix} S_x \\ S_y \\ S_z \end{bmatrix}_f \\ &= - \begin{bmatrix} \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} & \frac{\partial \phi}{\partial z} \end{bmatrix}_f \begin{bmatrix} \Gamma_{11} & \Gamma_{12} & \Gamma_{13} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} \end{bmatrix} \begin{bmatrix} S_x \\ S_y \\ S_z \end{bmatrix}_f \\ &= - (\nabla \phi)_f \cdot [(\Gamma)^T \cdot S]_f = - (\nabla \phi)_f \cdot S'_f \end{aligned}$$

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

$$\Gamma = 1$$

isotropic diffusion.

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So, if you do the matrix calculation what you get, minus gamma dot del phi at f dot S f equals to minus sum gamma 11 del phi by del x plus gamma 12 del phi by del y, gamma 13 del phi by del z. Second row is gamma 21 del phi by del x gamma 22 del phi by del y plus gamma 23 del phi by del z. 31 del phi del x, 32 del phi by del y, 33 del phi by del z. And you have S x, S y, S z at phase f. So, that is also the component of this surface vector S f.

Now, if you do further manipulation this would give me back del phi by del x, del phi by del y, del phi by del z at phase f into write down that 11, 12, 13, 21, 22, gamma 23, 31, 32, 33 at f S x, S y, S z at f which further simplification can get me minus del phi f dot gamma transpose dot S f which is one can think it is del phi S f dot S prime f. So, if you substitute this particular expression in this particular equation, so now, if you substitute that one there what we get is summation of phases minus del phi f dot S prime f Q c, V c. So, this is what you get as semi discretized system.

Now, once or one can expand this one and get the full discretized system from here. Now, one can simplify from here that gamma 2, if you apply instead of tensor to be 1 and

is f prime equal to $S f$. So, the same thing can be used for both isotropic discretization and anisotropic discretization. So, this is the special case for isotropic diffusion.

So, again reiterating that fact the beauty of this finite volume lies here, you see a generic expression for the diffusion which contains the anisotropy. Now, from anisotropy if you just replace with this coefficient that will bring down the whole system to a isotropic diffusion system and which is again a special case of anisotropy diffusion system. So, that again ends or closes the thing in that fashion such a fashion that if you have a generic equation derived for a generic system, like when we derive the discretized equation from non-orthogonal unstructured system the special case is the orthogonal system. The cross diffusion goes away and we can get back the normal orthogonal system. Again when you consider the diffusion anisotropic diffusion, the isotropic diffusion is one special case, and one can always achieve things from there.


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Diffusion Equation

Iterative Process (Relaxation \rightarrow under/over)
 $\Pi = f(\phi)$, Non-orthogonal grid \rightarrow Large cross diffusion term \Rightarrow
 \downarrow
 Large variation in ϕ
 \leftarrow Large source term \leftarrow Large variation in ϕ
 Linear solver } Leads to divergence
 (due to non-linearity of coeffs & cross diffusion term)

To promote convergence & stabilize the solver: Underrelaxation of variable
 \downarrow
 slow down the changes of ϕ'

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


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Now, the part which actually like to discuss in that, now we bought this discretized equation for the solution there are some iterative process which are involved and they are you need to do some sort of a relaxation, whether it could be under or it could be over depending on the situation. And why that happens? That happens essentially your any generic variable that ϕ , so the γ , so the γ is a function of ϕ and also it can possibly happen then you have an non-orthogonal grid.

So, if you have a non-orthogonal grid which actually means you have a cross diffusion term or rather large cross diffusion term or contribution. So, if you have a non-orthogonal grid we have a large cross diffusion term. So, if you have a large cross diffusion term again it will have a large variation ϕ . So, it actually getting towards a system where you have a non-orthogonal grid which actually leads to some sort of a large cross diffusion term, large cross diffusion term lead to a large variation of ϕ , so which means large source term and which may possibly if you have a large source term which can possibly the leads to some sort of a divergence. So that means, the code can be unstable and it can be divergence. So, this is essentially related to your linear solver, where it can be diverged.

And why that happens? Primarily because of all these if you have a variable Q dot orthogonal grid which can lead to some sort of a cross diffusion term, cross diffusion term can be large variation of the variable because the cell, large variation lead to the source term positive source term which can lead to the divergence of the solver. And that essentially one can think about due to non-linearity of coefficients and cross diffusion term. So, due to that that primarily happens.

So, what is the remedy? Remedy here is that since, that happens and all these diffusion equations they are kind of lead to a system where one has to solve the linear system. So, this becomes and pertinent issue or pertinent problem. Though we will come back and discuss this is a part of our discussion of linear solver. When we talk about the linear solver we will do the discussion, but since some understanding of this kind of situation is required we are doing the discussion preliminary discussion here so that you can appreciate what can happen in non-orthogonal system which leads to the large cross diffusion term and lead to this kind of situation.

So, one has to do two things, mostly basically to, in order to promote convergence one has to convergence as well as stabilized the solver. So, one has to do some sort of a under relaxation of variable. So, you need to slow down, so which means essentially slow down the changes of variable ϕ . So that means, when you go from one step to another step and another to another step, so you slow down the variation or the changes so, that you move towards your final solution slower. It is not with 100 percent weight you update the solution and move from one step to another. So, this is called under

relaxation. And that is very much required in order to have better convergence and also to have a stable system.

So, once we can one can look at the general discretized equation which you have a ϕ_c plus $F_{NB(c)}$, a $F \phi F$ equals to b_c . So, this is true for any system what we have discussed so far. Orthogonal, non-orthogonal, non-orthogonal unstructured, orthogonal, Cartesian everything, non-Cartesian orthogonal this is a unit equation that works for everybody.

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Diffusion Equation

$$\phi_c = \frac{-\sum_{F \in NB(c)} a_F \phi_F + b_c}{a_c} \quad \left| \begin{array}{l} \phi_c^* = \text{value of} \\ \phi_c \text{ from} \\ \text{previous} \\ \text{iteration.} \end{array} \right.$$

$$\phi_c = \phi_c^* + \left(\frac{-\sum_{F \in NB(c)} a_F \phi_F + b_c}{a_c} - \phi_c^* \right)$$

⇒ the change in ϕ_c produced by the current iteration

$$\phi_c = \phi_c^* + \lambda \left(\frac{-\sum_{F \in NB(c)} a_F \phi_F + b_c}{a_c} - \phi_c^* \right)$$

$$\frac{a_c}{\lambda} \phi_c + \sum_{F \in NB(c)} a_F \phi_F = b_c + \frac{(1-\lambda)b_c}{\lambda} \phi_c$$

$\phi_c = \phi_c^*$ (Converged) $0 < \lambda < 1$: under relaxed $\lambda > 1$: over relaxed

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Now, while doing this iterative process one may do some sort of an algebra and can write from their ϕ_c equals to, one can write like minus F goes over all this $a_F \phi_F$ plus b_c divided by a_c . So, let us define ϕ_c^* which is value of ϕ_c from previous iteration. So, ϕ_c is added to or subtracted from the right hand side of this equation. So, ϕ_c^* I can add or subtract. So, let us see I will do the addition then I will have minus $a_F \phi_F$ plus b_c , where F goes $NB(c)$, a_c minus ϕ_c^* . So, I have just done a from here to here one hand I have added ϕ_c subtracted ϕ_c^* .

Now, if you look at this expression within the parenthesis it is essentially represents the change in ϕ_c produced by the current iteration. So, essentially the element or the value within this parenthesis this shows the change in ϕ_c produced by this current iteration. Now, one can write by introducing an another extra variable called lambda and I can write down this particular equation ϕ_c equals to ϕ_c^* plus lambda and I will write

everything within this parenthesis like that which is $\frac{a \phi F + b c}{a c - \phi c}$ or one can do $a c$ by $\lambda \phi c$ plus summation of F goes to $NB c a F$ ϕF equals to $b c + 1 - \lambda$ into ϕ star $a c$ $1 - a c \lambda \phi c$. So, that is what it turns out.

Now, here you get an expression which one has to look at it carefully. Now, when that convergence ϕc is actually become ϕc star will the system is converged. So, if you have converged then they will become ϕc equals to ϕc star, and value of the relaxation factor it will become actually independent of this relaxation factor λ which is used.

So, this you can see from this equation what now; another thing is that depending on the value of the λ one may have if λ lies between 1 to 0, this is called under relaxed or if λ is greater than 1 it is over relaxed. So, depending on the value of λ one can have a system which is either under relaxed or should be over relaxed.

So, most of the time actually in normal CFD calculation or most of the CFD calculation the under relaxation factor is used because that leads to a; but it is also not very generic that always you need to use under relaxation. It all depends on the particular equation or the physical problem that one is solving for.

Now, that having said that a value which λ closed to 1 such that you need very little under relaxation, or closed to 0 means you have heavily under relaxation. That means, someone is talking λ equals to 0.001; that means, your system is heavily under relaxation and someone is using λ equals to 0.99 which is almost close to using very little relaxation. Now, the optimum under relaxation factor is problem dependent as I said and is not essentially governed by generic rule, so which means, so λ or the value of λ value depends on problem and it is not governed by any general rule.

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Diffusion Equation

$\lambda = \text{value} \nabla \text{ depends on prob.}$

$\hookrightarrow \text{depends on experience of user}$

$$a_c \leftarrow \frac{a_c}{\lambda}$$

$$b_c \leftarrow b_c + \frac{(1-\lambda)a_c \phi_c^*$$

\rightarrow Solution of Iterative process can be improved / made faster

\rightarrow " " " " " stable

at different location in domain

- vary iteration to iteration

\Rightarrow key role in stabilizing the solution of non-linear prob.

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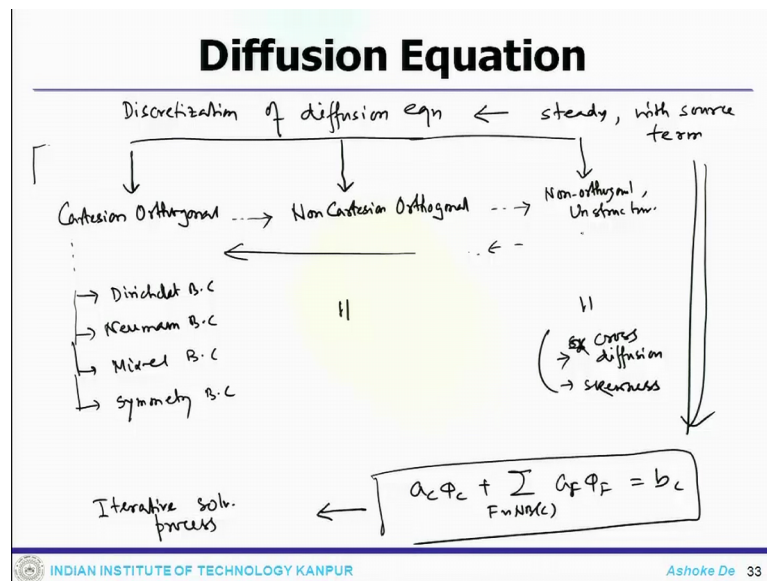
So, the factor which effects lambda value include the type of problems solved as I said size of the equation system that means, number of grid point, degrees of freedom, grid spacing and all the other iterative procedures. So, all these are the issues which will be involved in choosing the value of lambda. Also lambda is essentially assigned or how one can use this lambda value. It also depends on to some extent the depends on experience of user, because this is heavily dependent on your problem definition, in your comparison grid, degrees of freedom, grid spacing iterative solver and all these things. Moreover it is not very necessary to use the same under relaxation value throughout the computational domain.

So, one can actually also vary a different value of under relaxation at different location in domain. So, that is also possible and the lambda can also vary iteration to iteration so that means, from one physical time step to another physical time step one can vary the lambda. So, to promote better convergence or stability also different location one can use different values of lambda in the domain. Now, these equation if we rewrite in a slightly different form, so my a c which one can say a c by lambda and the source term which is added as b c plus 1 minus lambda divided by lambda a c phi c star. Now, this particular method of under relaxation plays an very very key role or important role in stabilizing the solution of non-linear problem.

So that means, what we see here that is the different kind of lambda can be used, the lambda can be varied from iteration to iteration and then once we use this kind of under relaxation. That actually, whether depending upon lambda though under relaxed or over relaxation the system can be used in more stable fashion the iterative solver can be converged or solution the solution of iterative process can be improved or may be can be made faster number 1.

Number 2, solution of the iterative process can be stable so, the discretized equation or the governing equation they do not get unstable of the linear solver does not get unstable. So, it can be also solved stability. So, these are things which are essentially important when you talk about the solution of this iterative process. But this is just to give you an idea when you have the discretized diffusion equation like this and then what kind of iterative process one can use and what are the certain issues. But more detailed discussion will follow well we will be talking about very specifically on linear solver.

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So now, that brings down to the important discussion that what we have done while talking about the discretization of diffusion equation. What we have considered here? We have considered here the steady and with source. So, that is what we have done.

And the way we have approached to that first we have looked at a simplest system that means, first Cartesian orthogonal system. Then from there while we are talking about the orthogonal system Cartesian system orthogonal system, we have talked about (Refer

Time: 28:02) boundary condition, the implementation of Dirichlet boundary condition, Neumann boundary condition, mixed boundary condition, symmetry boundary condition. So, all we have done. Then the system we have taken is the non-Cartesian orthogonal. So, still the orthogonality is maintained.

So, this is a one step improvement and same thing we have repeated. We have looked at the implementation of bounded condition, because essentially from here the discretization process will actually give us back a discrete equation which is in a generic form. That means, this gives us back the equation of $a_c \phi_c + F_{NB} c$, $a_c \phi_c = b_c$ that is the generic equation that we get. So, when you talk about the one orthogonal we have done that. Then finally, got non-orthogonal unstructured here also we have done the detailed discussion of this implementation of the boundary condition. So, that is where things where, when you talk about the non-orthogonal system we came across the important term cross diffusion term which is a important contribution, then skewness.

And then finally, for this we have talked about the iterative solution process or the convergence and the stability of the process. And our non-orthogonal system is one which is essentially if you go back in this direction, this is a generic case and the special case can be obtained in all these direction. So, non-orthogonal with a special correction can get you back the simplest one in the orthogonal system. So, we will stop here, and then the other discussion will follow up in the next lecture.

Thank you.