

Introduction to Finite Volume Methods-II
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Lecture – 29
Discretisation of the Source Term, Relaxation and Other Details-I

So, welcome back to the lecture series of Finite Volume; and we will start a discussion on a new topic. So, essentially where we have stopped we have looked at discretization of the diffusion equation pure diffusion equation, then we have looked at convection diffusion equation, then we discussed about high resolutions higher order scheme. And their formulation implementation in the finite volume framework and then we have also discuss the unsteady or transient formulation. So, up to this we are done.

Now, before moving ahead and discussing about the fluid flow problem which has slightly different level of complexity; we want to discuss few more issues or rather small issues which are associated with the discretized equation. One of them would be source term then we can also talk about certain iterative methods where the under relaxations are used.

So, all this relevant things which will be pertinent to the complete finite volume solver or a linear solver that we will discuss and after that discussion gets over we will straightway move forward for discussion of the fluid flow problem; where we will start discussing the Navier Stokes equation. And as I said why it brings the extra level of complexity that because in the Navier Stoke solver, it has all the unsteady term convection term diffusion term source term as well as it has the pressure gradient term.

So, so far what we have discussed while discussing even the unsteady convection diffusion system. We have not looked at how to discretize the pressure gradient up or rather the coupling between flow field and the pressure gradient. So, that beings the extra bit of complexity while looking at the fluid flow problem through Navier Stokes equation. So, that is the idea and that should be the towards the end of the course. Now, as I said let us start looking at the source term discretization.

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Other discretization details

Element 'c': $a_c \phi_c + \sum_{F \in NB(c)} a_F \phi_F = Q_c V_c$

$Q_c = f(\phi_c)$
C.A. / relatively small → may not be a big issue
 Large variation → slower convergence rate

$Q(\phi_c) = Q(\phi_c^*) + \left(\frac{\partial Q}{\partial \phi_c}\right)^* (\phi_c - \phi_c^*)$
 $= \underbrace{\left(\frac{\partial Q}{\partial \phi_c}\right)^* \phi_c}_{\text{Implicit part}} + \underbrace{Q(\phi_c^*) - \left(\frac{\partial Q}{\partial \phi_c}\right)^* \phi_c^*}_{\text{Explicit part}} \leftarrow \text{based on values from previous iteration}$

$a_c V_c = \iint_{V_c} Q \, dV = \iint_{V_c} \left(\frac{\partial Q}{\partial \phi_c}\right)^* \phi_c \, dV + \iint_{V_c} \left(Q_c^* - \frac{\partial Q}{\partial \phi_c} \phi_c^*\right) \, dV$

Diffusion, Convection, Source/Sink, Transient

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So, now one see this is a particular element which we have been considering throughout a lecture I mean typical element where you see the centre of this element is C. And so it has a source term of Q and it is associated with 5 different faces F 1 different six different elements and six different phases. So, F 1, F 2, F 3, F 4, F 5, F 6 and these are the corresponding connecting phases.

So, we need to calculate the; so, the once you do the integration over these elements C. So, for element C the discretized equation we are not going in the detailed derivation of this because we have done enough throughout the lectures; how we start from the equation take an volume integral, then convert that to surface integral and get back the I mean initially the semi discretized form and from there to the discretized from.

So, will now to some extent as we go along with the lectures; now onwards we will straightway start writing the discretized system because we hope that this time by this time you are comfortable with that kind of things. So, for element C the discretized equation should look like $a_c \phi_c + \sum_{F \in NB(c)} a_F \phi_F = Q_c V_c$. So, that is a standard generic discretized form where the source term Q_c for this particular element.

Now, typically this source term is a function of ϕ_c which would be a function of this variable. So, if it is a function of that kind of then it can be explicitly calculated based on the available information of this ϕ value at the cell centre. But which in an iterative

process could be a representation from the previous iteration. Though we can calculate it explicitly, but the information will come from the previous iteration.

Now if the source term is constant or relatively small then the and the variation of Q_c is large in comparison with other terms in the equation; the rate of convergence can be negatively affected; in that kind of situation to improve the rate of convergence. So, essentially what it means that if it is smaller constant may not be a problem, but if the variation is large; then there is a problem because the it can add to the stiffness to the system.

So, the convergence rate of the iterative solver. So, may not be a big issue, but large variation, this can lead to slower convergence rate and that could be a big hit in the iterative process. So, what one can do that time to reduce the stiffness of the system; one can use some sort of an Taylor series kind of expression liberalize the system.

So, for example, let us say if one writing Q_{ϕ_c} you can write $Q_{\phi_c}^* + \frac{\partial Q}{\partial \phi_c} (\phi_c - \phi_c^*)$ into $\phi_c - \phi_c^*$; which is a I mean taking only the first term not considering any other higher order term. So, this one can write Q_{ϕ_c} into $\phi_c + Q_{\phi_c}^* - \frac{\partial Q}{\partial \phi_c} (\phi_c - \phi_c^*)$. So, this is the implicit part and this guy could be explicit part and this can be calculated based on the values from the previous iteration. So, this is based on values from previous iteration.

So, this is easily possible to calculate like that. So, one component comes as implicitly, other component comes as explicitly and one can actually calculate that. Now once you look at in the control volume context you have a term which is sitting there as a $Q_c V_c$. So, the $Q_c V_c$ which is nothing, but the volume integral of $Q dV$ which one can now write $V_c \frac{\partial Q}{\partial \phi_c} (\phi_c - \phi_c^*) + \text{second component } V_c Q_c^* - \frac{\partial Q}{\partial \phi_c} (\phi_c - \phi_c^*) dV$.

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Other discretization details

$$a_c V_c = \left(\frac{\partial a_c^* V_c}{\partial \phi_c} \right) \phi_c + \left(a_c^* - \frac{\partial a_c^* \phi_c^*}{\partial \phi_c} \right) V_c = \text{Flux}_C \phi_c + \text{Flux}_V V_c$$

$$\left[a_c - \text{Flux}_C \right] \phi_c + \sum_{F \in \text{NB}(C)} a_F \phi_F = \text{Flux}_V V_c$$

To have diagonal dominance $\text{Flux}_C < 0$

Iterative solvers \rightarrow performance \leftarrow
 \rightarrow Under-Relaxation

$A\phi = b \rightarrow$ slowly converges towards actual solution

Explicit Under-Relaxation: $\phi_c^{\text{new, used}} = \phi_c^{\text{old}} + \lambda \left(\phi_c^{\text{new, pred.}} - \phi_c^{\text{old}} \right)$

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So, using this we get the integration done and once you do the integration it will like to $Q_c V_c$ equals to $\frac{\partial Q_c^*}{\partial \phi_c} \phi_c + Q_c^* - \frac{\partial Q_c^* \phi_c^*}{\partial \phi_c} V_c$. So, that is what you get which you can think about the two coefficients linearization like $\text{flux}_C \phi_c + \text{flux}_V V_c$; so that way one can think about that. Now once you put this back in the algebraic equation that looks $\text{minus flux}_C \phi_c + \sum_{F \in \text{NB}(C)} a_F \phi_F = \text{flux}_V V_c$; so that is what it get you back.

So, you take now in this particular formulation the implicit part of that flux_C which is here; this required to be negative to guarantee the diagonal dominance. From here one can see to have diagonal dominance of the iterative solver this guy has to be negative or else the stabilities carry over criteria may not be fulfilled which can lead to the divergence of the iterative solver. So, this is an restriction that to have diagonal dominance this flux_C must be less than 0; otherwise there would lead to a problem.

Now, top of that the when the value of ϕ is positive definite the explicit part which is here $\text{flux}_V V_c$; must be positive to ensure the positive prediction of ϕ ; so, these are some information which one can think about. Now the other think that when you talk about this iterative solvers; so, essentially here we are only talking about the performance of the iterative solver so that essentially the important quantity is the performance of that

solver. Now performance has to do with 2 condition I mean all sort of convergence stability all this would come under that.

But essentially what is important is that when you talk about the iterative solver as we have seen in details; they are they are some sort of a under relaxation is very much necessary. Now one can now see also why is that required and probably as we moving ahead with the discussion in this lecture; you can see when we start doing the Navier Stokes equation or the fluid flow problem and that time you can see why this become so, important to get and convert solution using some iterative process.

Because the here only were talking about a source term and that can make the system really stiff. And if the system is stiff exactly is the prime example sitting here; you got this coefficient matrix which will finally, you linear system is like that. And this A will have some coefficients from the guy and there is a restriction on flux C_c ; so, that has to have certain properties.

If they do not satisfy, but this is a simplicity part which actually comes from the linearization calculations of the source term and which uses the values which are available in the nodes or the elements. So, this is not having something that user has too much of control; it may be dependent on the physical problem how it evolves in the system and that can lead to certain issues, but while it is evolving this kind of conditions like the as we stated here they need to be satisfied.

If that does not happened this guy will no more remain diagonal dominance; so that will have a hit on the iterative solver. Now, so one more thing also people do that is or heavily used in often in the CFD codes is or the rather codes which are dependent on finite volume approach and along with the iterative solvers they use it under relaxation. And so what it effectively does? It reduces the stiffness of the system and the solution slowly convergence; convergence towards the actual solution. So, that is why it becomes very important.

Now, since it is important we can see how we do this kind of system; for example, you can start with an explicit under relaxation. So, when you say that explicit under relaxation, then the method at end of every iteration the new solution is obtained and the new solution is actually not modified with the completely the one which is obtained. So, certain percentage of the new solution is updated with the old one.

So, after the new solution is obtained all cells in the computational domain are revisited and the predicted value which is; let us say the new value which is phi new and that predicted. So, that can be used to modify let us say phi c; new used will be phi c old value which was sitting there plus some lambda factor multiplied with phi c, new predicted which you obtained from the solution minus phi c old.

So, the difference between the newly obtained solution and the old value and certain percentage of that this lambda is called the relaxation factor it now it could be for both explicit and implicit relaxation can be interpreted according to this.

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Other discretization details

Notes: (i) $\lambda < 1$: under-relaxation, (ii) $\lambda = 1$, (iii) $\lambda > 1$: over-relaxation

Implicit Under-Relaxation Methods

(a) Patankar's Under-Relaxation

$$\phi_c = \phi_c^* + \lambda (\phi_c^{\text{new, it.}} - \phi_c^*) \quad : \phi_c^* = \text{value from previous iter.}$$

$$\phi_c = \phi_c^* + \lambda \left[\left(\frac{-\sum a_f \phi_f + b_c}{a_c} \right) - \phi_c^* \right]$$

$$\frac{a_c}{\lambda} \phi_c + \sum_{f \in \text{NN}(c)} a_f \phi_f = b_c + \frac{(1-\lambda)}{\lambda} a_c \phi_c^*$$

↳ modifies the diagonal coeff. - RHS

$\lambda < 1$:

$\phi_c^{\text{new, used}} = \phi_c^{\text{old}} + \lambda (\phi_c^{\text{new, pred}} - \phi_c^{\text{old}})$

Now, there are certain things one needs to note. First is that a lambda less than 1, which will essentially becomes a under relaxation system. And this may slow down the speed of the solution or the convergence, but it increases the stability of the calculation. So, it decreases all sort of a possibility of small or spurious oscillations which can lead to the divergence of the solution.

Second lambda could be 1 which corresponds to no relaxation; if this is applied then the complete predicted value is going to be used because lambda 1 means; the old part gets cancelled. So, the predicted value would be updated one and this case one can use the same value what is predicted for the next iteration, but there is a issue associated with that this can lead to instability and finally, the divergence of the solver.

And lambda greater than 1 which could lead to over relaxation; now in that case sometimes it is used to accelerate the convergence, but usually decreases the stability. So, one case is increases the stability slow down the convergence when lambda less than 1 and when lambda greater than 1; it actually increases the convergence rate it accelerates, but the same time it reduces the stability

. So, it is kind of a 20/20 case; 20/20 situation where you have to be careful, but more often most of the flows it is a under relaxation it is used for unless there is a specific kind of problem where over relaxation is required. Now explicit under relaxation as I said used for under relaxing the pressure in your fluid flow problem; we will see when you move to discussion of the fluid flow problem. And then, problem where the fluid properties depends on the solution and which will essentially promote the convergence. Now also if a fluid is exposed to highly turbulent conditions; there also sometimes I mean the under relaxations are used.

Now, the second one is implicit under relaxation. So, there are different methods and these methods are sort of proposed by the person known as Patankar; who is one of the pioneer scientist in this field who got people introduce this finite volume method for the fluid flow systems. So, one of the one this is named as Patankar's under relaxation. So, that is; now equation that we are using is the same. So, that is our equation remain ϕ_c new which is to be used; use ϕ_c old plus lambda ϕ_c new predicted minus ϕ_c old; so, that is the equation that we are using. Now, in this case lambda can be explicitly specified or expressed.

To simply use the notation in Patankar's under relaxation the this particular equation gets modified like ϕ_c equals to ϕ_c^* plus lambda ϕ_c new iteration minus ϕ_c^* ; so, where ϕ_c^* is values from previous iteration. Now ϕ_c iteration in this particular expression is replaced by an equivalent expression, which looks like. Then ϕ_c is equals to ϕ_c^* plus lambda which will look like minus summation $F_N B C a F \phi_c$ plus bc by ac minus ϕ_c^* .

. So, once you rearrange this; this will get you ac by lambda ϕ_c plus summation $a F_N B C a F \phi_c$ equals to bc minus 1 by lambda divided by lambda bc plus ac ϕ_c^* . So, the discretized equation actually now gets this lambda sitting in place. So, the relaxation factor lambda it actually here; when you look at these modifies the diagonal

coefficient show on the right hand side. So without changing the governing equations or the changing the discretized equation mathematically.

Since lambda less than 1 under relaxation, it increases the diagonal dominance of the algebraic system it enhances the stability of the integrative solver. So, this is one of the advantage of using compared to an explicit approach; this implicit under electrician brings out that advantage because it modifies the coefficients or the diagonal coefficients of the linear solver; which due to the under relaxation it enhances the stability and the convergence become faster.

So however, one may note that the implicit relaxation applies a relation that is proportional to the diagonal coefficient. Thus the relation relaxation will be larger for a larger diagonal coefficient which translates into a larger relaxation of higher importance for smaller control volumes. So, one we can see how that affects.

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Other discretization details

(b) E-Factor Relaxation : $a_c \phi_c = b_c - \sum_{F \in \text{NB}(c)} a_F \phi_F$ } λ is used to modify RHS

$$a_c \phi_c = \lambda \left(b_c - \sum_{F \in \text{NB}(c)} a_F \phi_F \right) + (1-\lambda) a_c \phi_c^*$$

$$\lambda = \frac{E}{1+E} \quad \left| \quad a_c \phi_c = \frac{E}{1+E} \left(b_c - \sum_{F \in \text{NB}(c)} a_F \phi_F \right) + \left(1 - \frac{E}{1+E} \right) a_c \phi_c^*$$

$$\left(a_c \left(1 + \frac{1}{E} \right) \phi_c + \sum_{F \in \text{NB}(c)} a_F \phi_F = b_c + \frac{1}{E} a_c \phi_c^* \right)$$

time step = Δt , v_c is small
 $E \Delta t^* = \Delta t$ \downarrow rate of convergence \downarrow
 $\Delta t^* = \frac{\rho_c v_c}{a_c}$ $\left| \quad E = \frac{1}{1-\lambda} \right.$
 $E \equiv \text{CFL number}$ \downarrow $A=10, \lambda=0.9$

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Now, the second one we can think about E factor relaxation. So, that is E factor relaxation it in this method the Patankar's formulation that we have just seen it is modified. And what it is done we get it by rewriting the equation $a_c \phi_c$ equals to b_c minus $\sum_{F \in \text{NB}(c)} a_F \phi_F$. So, by rewriting the equation in this following form and we use the under relaxation to get an system like $a_c \phi_c$ equals to $\lambda (b_c - \sum_{F \in \text{NB}(c)} a_F \phi_F) + (1-\lambda) a_c \phi_c^*$ which is a F if plus 1 minus lambda ac; phi c star.

So, this gets modified or the relaxation factor only applied to right hand side; λ is used to modify right hand side of the discretized system. And once that is used, so one can replace this under relaxation factor by some ratio like $\lambda = \frac{E}{1 + E}$; then this equation becomes $a_c \phi_c = \frac{E}{1 + E} b_c - \sum a_f \phi_f$; $a_f \phi_f + 1 - \frac{E}{1 + E} a_c \phi_c$.

So, you rearrange this and you will get $a_c; \frac{1}{1 + E}; \phi_c + \sum a_f \phi_f$; $a_f \phi_f - b_c + \frac{1}{1 + E} a_c \phi_c$. So, that is what you get after doing the modification. And now this formulation the under relaxation effect can be readily interpreted in terms of some artificial transient time scale; which can advance ϕ_c at each solver iteration. Now if your time step is Δt then characteristics time interval Δt^* can be obtained which will be related as $E \Delta t^* = \Delta t$. So, the Δt^* is $\frac{\Delta t}{E}$; $\frac{\Delta t}{E} = \frac{\rho_c}{b_c}$.

Now, in this particular expression where you characteristics Δt^* is calculated is uses the volume of the cells centre. So, this uses the time required to diffuse and convective scalar ϕ_c across the element. So, one can think about this E factor is equivalent to some sort of an CFL criteria or number CFL equivalent to some sort of an CFL number; so that one may think of in that fashion.

So, now from here you can see what is happening the time step advancement of this E factor relaxation is dependent on the cell volume and the with the solution is smaller element can advance slowly than in a costal element. So, this could be a detrimental to the convergence because if your cell size if b_c is small; then the rate of convergence also goes down; so, that is the problem.

. So, this is very common use highly stretch elements with small volumes near boundary; thus forcing a critical region in the computational domain to advance a very small time step compared to the remainder of the domain. So, this the straightway this applicability is that where you have a small cells and highly skewed close to the boundary, you can use this to improve the convergence.

So, this is also a characteristics of the Patankar relaxation method now between E and λ ; the relation between E and λ that we have obtained is that the $E = \frac{1}{1 - \lambda}$ which essentially gives $\lambda = \frac{E}{1 + E}$. So, typically this range of E is

between 4 to 10; so correspondings lambda would be somewhere 0.72 or 75 to 0.9; so that is a typical values what one can use.

So, we will stop here today and we will take from here in the follow up lectures.

Thank you.