

Computational Fluid Dynamics Using Finite Volume Method

Prof. Kameswararao Anupindi

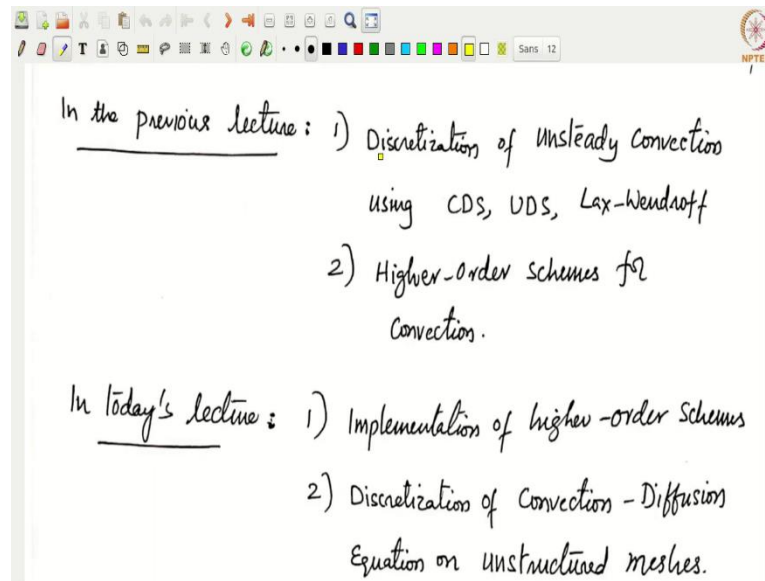
Department of Mechanical Engineering

Indian Institute of Technology, Madras

Lecture – 33

Finite Volume Method for Convection and Diffusion: Discretization of convection-diffusion equation on unstructured mesh

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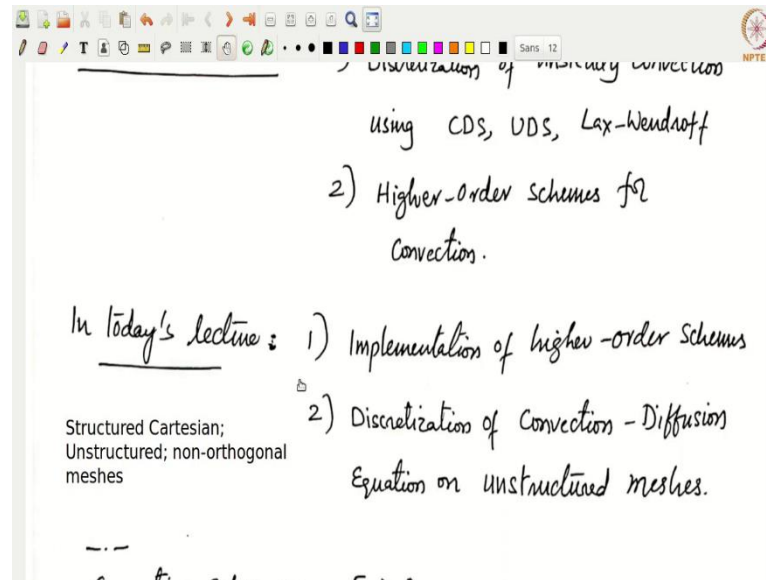


Hello everyone, let us get started. So, in the previous lecture, we looked at discretization of unsteady convection equation using the central difference scheme upwind difference scheme and a Lax Wendroff scheme right, which was affix for central difference scheme, isn't it? Alright. So, we looked at discretization and looked at the several properties associated, and how the exact solution compares with the solutions obtained from these schemes.

In addition, we also looked at couple of higher order schemes; one was the second order accurate upwind scheme, and the another one was the third order accurate upwind scheme, which we call it as the quick scheme right, the quadratic upwind interpolation for convective kinetics, right. So, that is what we looked at the previous lecture. In today's lecture, we are going to look at implementing this, these higher order schemes. So, how do we actually go about implementing them in a code?

And, we will then kind of switch gears and then look at Discretization of convection-diffusion equation on unstructured meshes, right. Because, till now we only looked at how to discretize on essentially on a structured Cartesian meshes only we have looked at.

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So, today we are going to look at unstructured and essentially non-orthogonal meshes, so we are going to look at that in today's lecture. And depending on the time, we will also look at how do we, how can we actually extend these higher order schemes to unstructured meshes ok; that is something we have not, we have of course not done, ok. So, these are the kind of topics for today's discussion.

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Convection Schemes: $F_e \geq 0$, $u_e \geq 0$

UDS: $\phi_e = \phi_p$

CDS: $\phi_e = (\phi_E + \phi_P) / 2$ central second-order

second-order upwind scheme: Fromm Scheme $\phi_e = \phi_p + \left(\frac{\phi_E - \phi_W}{4}\right)$

backward difference formula Beam-Warming Scheme $\phi_e = \phi_p + \left(\frac{\phi_P - \phi_W}{2}\right)$

Third-order upwind scheme:
 QUICK: $\phi_e = \phi_p + \frac{1}{6} (\phi_E - \phi_W) (\phi_E + \phi_W - 2\phi_P)$

So, let us get started. So, let us kind of review the convection schemes, where you have looked at in the last class. So, essentially the convection schemes are, if your flow rate on the east face is greater than or equal to 0; the way this is basically defined is, if your u_e is greater than or equal to 0, then your F_e , the flow rate on the east face would come on to be 0.

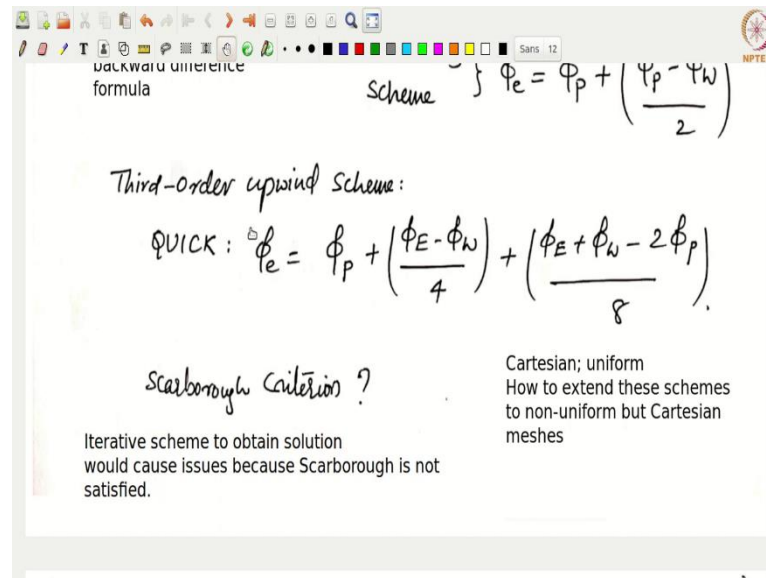
In under such conditions, we have defined the upwind difference scheme as something that assigns the value of the face value right, ϕ_e as the upwind value that is ϕ_p right; because, because F_e is positive, so it is going in the positive x direction. So, ϕ_e would be taken as ϕ_p right, that is what we have. And then, if it is a central difference scheme, then the face value of phi would be taken as of course arithmetic average of the east and the P cells.

So, we have $(\phi_E + \phi_P) / 2$, alright. Then if you, we have also looked at the second order upwind scheme in which the phi or the face ϕ_e is written as $\phi_p + \left(\frac{\phi_E - \phi_W}{4}\right)$, right. So, this was obtained using an approximation for the first derivative, right. The first derivative essentially is evaluated, the $\left.\frac{\partial \phi}{\partial x}\right|_p$ is evaluated using a central second order accurate formula right; that you obtained essentially the Fromm scheme.

And, if you had used the for expanding the first derivative and using a backward difference right, backward difference formula; then you essentially obtained a scheme that is known

as Beam Warming scheme, right. Basically you had the Taylor series expansion and ϕ_P plus $\frac{\partial \phi}{\partial x} \Big|_P$ that is where we have used these two definitions for the first derivative, ok.

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Going on extending the same concept, if you start including higher order terms, that is $\frac{\partial^2 \phi}{\partial x^2} \Big|_P$ as well and then use a central difference formula for both the first derivative and the second derivative; then the Δx that we have got cancelled and then we essentially obtained something known as the quick scheme, where ϕ_e equals $\phi_P + \left(\frac{\phi_E - \phi_W}{4} \right) + \left(\frac{\phi_E - 2\phi_P + \phi_W}{8} \right)$, right.

These are basically the central difference formulae for the first and the second derivatives; of course in doing all this we have assumed that, we are essentially working with a not only with a Cartesian mesh, but the mesh is also uniform. So, it is probably a good idea for you to ponder on, how do I extend? So, how to extend these schemes to non-uniform, but let us say still Cartesian meshes, that is something I want you to kind of think about and see how do you extend these schemes. So, what are the changes you have to make, and things like that, alright.

Now, we looked at all these schemes, but all do all these schemes look ok, or are there any issues that you see right away? Yes we do see some issues; if it is upwind scheme, we do not have any problem, because $\phi_e = \phi_P$. So, this either ϕ_P or ϕ_E depending on the direction of the flow rate. So, there is no problem; because all the coefficients would come

out to be positive. As we have seen in the context of the central difference scheme, there is a possibility for central difference scheme to have negative coefficients and those can be avoided using these by maintaining the cell, Peclet number to be less than 2 right that is what we have already discussed.

Now, of course, if you are working with any of these higher order schemes; again, you see that there are these neighboring coefficients which are the ϕ_{west} and ϕ_p here, which have which is essentially carry a negative coefficient, right. So, these negative coefficients are not good; because, essentially this is not good and of course this is also not good, because this is making the central value ϕ_p to go to a smaller value right. You have minus one-fourth here coefficient, which makes the central value a P to go down right, ok.

So, essentially these negative coefficients are not good; because, they do not satisfy Scarborough criterion, right. The moment you have these negative coefficients, your Scarborough criterion may not be satisfied; essentially, the diagonal dominance would not be respected, right. As a result, if we use an iterative scheme to solve for the solution, then we would run into trouble, right. Using an iterative scheme to obtain solution would cause issues; because, the Scarborough is not satisfied, right.

As a result, we need to find a way of getting around this problem ok, so that we can still satisfy Scarborough criteria. But, we will not any issue; we will not have any issues in converting the solution using some iterative scheme, ok. So, I am going to, we are going to look at one particular method and after that I want you to think and see if there is, if there could be any other method that you can do this in a different way, ok.

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Implementation of Higher-Order Schemes;

To satisfy Scarborough criterion we use deferred correction approach. Legacy codes that were originally UDS -- work for high-order schemes

UDS always satisfies Scarborough...

Consider $F_e \phi_e$ for $F_e \geq 0$

UDS : $F_e \phi_e = F_e \phi_P$

HOS : $F_e \phi_e = F_e(\phi_{Ho})$

Deferred Correction: $e \quad e \quad | \quad e \quad e \quad |$

So, let us get started. So, implementation of higher orders schemes. So, you will see, how do we get about this problem. So, essentially to satisfy Scarborough criteria, we use something known as a deferred correction approach, ok. So, this was proposed essentially to make some of the kind of legacy codes that were originally written using the upwind difference solutions, ok.

So, in order to kind of make these work for high order schemes, a deferred correction approach is proposed. This also not only to make these codes work with very simple with small changes, but also to make any of these iterative solvers also to work, because then they will start satisfying these Scarborough criteria, ok.

So, essentially the method is same as what we have learned till now; this is basically deferred correction approach, in which we like the way we have done it for the source terms and the way we do it for any of the non-linear terms. So, what we do is, we know that if we take a simple upwind scheme, that is basically the first order upwind difference scheme; this always satisfies Scarborough criteria, because everything is positive coefficient, either it is going into the a P term or to the a and b terms and you have no problem in obtaining the solution, ok.

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UDS always satisfies Scarborough...

consider $F_e \phi_e$ for $F_e \geq 0$

UDS : $F_e \phi_e = F_e \phi_p$

HOS : $F_e \phi_e = F_e (\phi_{HO})$

Deferred correction : $F_e \phi_{HO} = F_e \phi_p + (F_e \phi_{HO} - F_e \phi_p)$

So, what we do is, essentially we take that point, and then if you consider the convective scheme; the discretized value is nothing, but $F_e \phi_e$ yeah right, this is what you would get after discretization. So, $F_e \phi_e$ and if I assume that F_e is positive and F_e is greater than or equal to 0. Then, for a upwind difference scheme, what we do is, if F_e is positive, then $F_e \phi_e$ would translate into $F_e \phi_p$ right, essentially this F_e would go into the coefficient of a P right or a east, if this was negative, this will go into a capital east, ok.

Now, what about the higher order scheme? Let us say if you take some higher order scheme, which I would like to write it as HO, Higher Order scheme. So, $F_e \phi_e$ would become F_e times phi higher order. Now, phi higher order is basically what? It is not just ϕ_p , but it is basically all this entire thing right; phi higher order is ϕ_p plus blah blah blah or it is this thing or this thing right, it is basically a big expression that contains not only ϕ_p , but also contains several other neighboring values, which is given by the higher order scheme.

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$\tau e^{\psi_{H_0}} = \tau e^{\tau p} (\tau e^{\psi_{H_0}} - \tau e^{\tau p})$
 known values -- starred values $= F_e \phi_p + (F_e \phi_{H_0}^* - F_e \phi_p^*)$
 What happens at convergence?
 What about Scarborough now?
 $F_e \phi_{H_0} = F_e \phi_p + F_e (\Delta \phi_{H_0}^*)$
 $\Delta \phi_{H_0}^* = (\phi_{H_0}^* - \phi_p^*)$
 a_p ? b term ?
 Example: QUICK scheme

Now, we know that if I use directly this, it is not going to satisfy Scarborough; because, it is going to cause trouble with the coefficients. So, as a result what we do is, we look at deferred correction approach. So, what we do here is that, we write $F_e \phi_{H_0}$, the Higher Order scheme as, we add and subtract the upwind difference component that is $F_e \phi_p$. So, I would add $F_e \phi_p$ to $F_e \phi_{H_0}$ and then I will subtract $F_e \phi_p$ ok, so essentially this is same as what we have on the left hand side.

Now, what we do is that, now in the deferred correction approach; we will evaluate everything that is there in this parenthesis ok, using the previous iteration value. So, we are going to put a star here for these two terms, ok. So, whatever we have here, this will be evaluated using the previous iteration values, ok. So, these are basically $F_e \phi_{H_0}^*$ star minus $F_e \phi_p^*$ star, ok.

Now, this is something that is not the same as what we have written in the previous step; but we understand that by writing it this way, we have now changed few things, right. Of course, what did we change? We have changed that, excuse me. So, we have changed that, at convergence what will happen here; at convergence ϕ_p equals ϕ_p^* as a result, this term gets canceled, essentially this term gets canceled right with this term and we kind of recover back our ϕ_{H_0} right, that is what we would recover.

And now, what about Scarborough criterion? Now, because this term is written F_e as $F_e \phi_p$ and these two terms are evaluated at the star level, that is the current iterate level or known

values right are the starred values; then where does, where do these terms go, right. So, if we have written it like this $F_e \phi_{HO}$ equals $F_e \phi_P$ plus F_e times. If I want to write this as $\phi_{HO}^* - \phi_P^*$ as some $\Delta\phi_{HO}^*$ ok, some difference between the higher order value and the ϕ_P value, essentially the upwind value; then, where will these coefficients go? This coefficient will go into, into where? This will go into your a P.

And, where will this term go; because this is star values, these will not go into a w, a neighbors, this will go into the b term, ok. As a result, now your Scarborough is now satisfied; because, it is basically similar to your upwind difference scheme, except that these are going into the source terms, right. So, your Scarborough is now satisfied. As a result, for every iteration or the outer iteration that you have, your Scarborough is always satisfied and you have no problem right, you can implement any higher order scheme in this particular way, alright.

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a_P $\Delta\phi_{HO}^* = (\phi_{HO}^* - \phi_P^*)$
 $b \text{ term}$
 Example: QUICK scheme

$$F_e \phi_{QUICK} = F_e \phi_P + F_e \left(\phi_P^* + \left(\frac{\phi_E^* - \phi_W^*}{4} \right) + \left(\frac{\phi_E^* + \phi_W^* - 2\phi_P^*}{8} \right) - \phi_P^* \right)$$

$$= F_e \phi_P + F_e \left(\left(\frac{\phi_E^* - \phi_W^*}{4} \right) + \left(\frac{\phi_E^* + \phi_W^* - 2\phi_P^*}{8} \right) \right)$$

Now, let us take an example of the quick scheme and see how do we go about implementing it. So, if you look at the quick scheme; what we have is, $F_e \phi_e$ would read as $F_e \phi_{QUICK}$ equals $F_e \phi_P$ plus, ok. So, this particular thing, entire expression here is the ϕ_{QUICK} right; that is what we have for ϕ_{QUICK} minus ϕ_P^* .

So, essentially we have added $F_e \phi_P$ and subtracted it here F_e times ϕ_P , and everything in the parenthesis we have, we are starting evaluating at star values. Of course, there could

be a different way of doing this, because there is already a ϕ_p^* here, but I would like to follow with what we have written up here, ok.

So, that means $F_e \phi_p$ equals , so this basically equals $F_e \phi_p$ plus F_e times ϕ_p^* now gets canceled. So, what you get is, you get this remaining term, ok. So, essentially again now this entire thing would go into the b term and this entire thing here would go into the a P term, ok. So, as a result this Scarborough is now satisfied, alright. So, this is how you would implement it. Now, what about another way of implementing it? Let us say, is there it another way of implementing it, if you do not want you use a different deferred correction approach? Yes, you can do it.

Essentially, what you have to do is, if you want to do in another way, what we are losing here is the diagonal dominance right, your Scarborough would not be satisfied. So, you can make it satisfy diagonal dominance or Scarborough by using some kind of relaxation, right. If you have a relaxation factor, you can make it go up right; you can make it an under relaxation factor or something and then, you can or, and then you can make it this Scarborough satisfied or diagonal dominance, ok. So, that is another way.

But in in our particular course, we will use this deferred correction approach; because, it is much simpler and also you can make, you can write a code for let us say the upwind difference scheme and make any other scheme work as well in a very simplified way, because all you have to change is basically the b term, right. Once you change that, you essentially are doing a higher order differencing, alright.

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Overall Equations for Higher-Order Scheme: upwind scheme

$$a_p \phi_p = \sum_{nb} a_{nb} \phi_{nb} + b$$

$$a_E = D_e + \text{Max}(-F_e, 0)$$

$$a_W = D_w + \text{Max}(F_w, 0)$$

$$a_N = D_n + \text{Max}(-F_n, 0) \quad \text{UDS}$$

$$a_S = D_s + \text{Max}(F_s, 0)$$

$$a_p = \sum_{nb} a_{nb} - S_p \Delta V_p + (F_e - F_w + F_n - F_s)$$

Let us see now how do we, when we concatenate all the equations, let us look at the overall equations, if you have let us say a higher order scheme, essentially we are talking about a higher order upwind scheme, ok.

So, that means what we have is, if you kind of concatenate all the equations what you get is the discrete equation is $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$ ok, where your a_E is we have already seen this as the diffusion component D_e plus max of minus F_e comma 0. And, a_W equals D_w plus max of F_w comma 0. Notice that there is a minus and a plus here; this is because, we have defined the flow rate as simply $\rho u_e \Delta y$ here, and we have defined it here simply as $\rho u_w \Delta y$, ok.

So, we have not defined these as the dot product of $\rho \vec{u} \cdot \vec{A}_f$ ok, rather we have simply written it as the rho density times velocity times area. As a result we got this minus plus problem right, minus plus issue. And similarly, a_N would be D_n plus max of minus F_n comma 0 and then a_S would be D_s plus max of F_s comma 0, ok. So, this is if we have already known about all these things, this is basically your first order upwind difference scheme, right. If you are asked to write code for upwind difference scheme, this is the algorithm.

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$a_s = D_x + \max(F_x, 0)$
 zero; \bar{u} satisfied cont.
 $a_p = \sum_{nb} a_{nb} - S_p \Delta V_p + (F_e - F_w + F_n - F_s)$
 $b = S_C \Delta V_p - F_e \Delta \phi_{HO,e}^* + F_w \Delta \phi_{HO,w}^* - F_n \Delta \phi_{HO,n}^* + F_s \Delta \phi_{HO,s}^*$
 UDS; high-order scheme
 Cartesian; Structured meshes
 Only change when compared to UDS
Convection - Diffusion on Unstructured non-Orthogonal meshes:

Now, what about the higher order scheme? Essentially, the higher order scheme would contribute to the b term. So, as a result, your a_p is also the same as before. So, you have a_p equals $\sum a_{nb}$ minus the source term that is $S_p \Delta V_p$ plus we have F_e minus F_w plus F_n minus F_s , right. Essentially, this term is comes into play to counteract the upwind scheme whether it is going into a_p or a_E right, only for that this is coming into play.

And again, we know that the term here in the parentheses would evaluate to zero; if your under line flow field that is the \vec{u} , let us say if it satisfies continuity, right. If it satisfies continuity equation; then, the mass flux that is coming in and going out would be balanced. As a result, this parentheses term would go to zero, alright.

What about b term? b term, now contains $S_C \Delta V_p$ and then we would contain if F_e is positive; you would get a F_e times, you would get $\Delta \phi_{HO,e}^*$ term evaluated at star value, right. Delta here is, because we have phi higher order minus phi upwind right, and this is evaluated on the east face and everything is evaluated at this star value, alright.

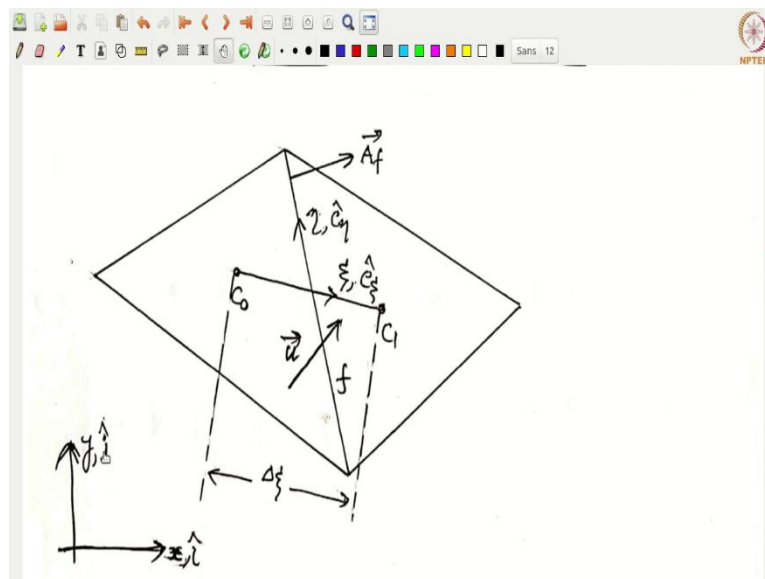
Now, why is there a minus here? There is a minus, because your term is basically F_e times; $F_e \phi_p$, alright. Because F_e is positive, then the contribution will go into a_p . And so, F_e is positive, then this will go into $F_e \phi_p$; but this is being sent to the other side, so we have a minus $F_e \Delta \phi_{HO,e}^*$, alright. But if F_e is negative, then this would turn out to be going into a_E , right. Is this correct? Maybe you need to check for the sign here; if is this correct or not,

ok. Then, we have plus $F_w \Delta \phi_{HO,w}^*$ on the west and then minus $F_n \Delta \phi_{HO,n}^*$ star on the north plus $F_s \Delta \phi_{HO,s}^*$ for the south on the star, ok.

So, this extra term is basically the only change when compared to the upwind difference scheme, ok. So, this is the only change; because, we have used the deferred correction strategy, ok. So, as a result this is the only change; so, that means if you write a code for upwind difference scheme, it is very easy to modify to use any higher order scheme using this deferred correction strategy, alright.

Then, let us move on to now something different; because, up till now we have been only looking at the Cartesian or we have been only looking at the structured Cartesian meshes right, and then, we have seen how to discretize the convection diffusion equation as well as the unsteady convection equation, ok. Now, what about unstructured non orthogonal meshes? How do I solve for convection diffusion equation on unstructured non orthogonal meshes, ok. So, this is something we take up now, alright.

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So, as usual we have our two cells; let us say this is the C_0 cell and this is the C_1 cell and the vector connecting them would be the ξ direction, and the direction along the face would be your η direction. And, we have these two unit vectors that is e_ξ and e_η and we of course, have the global coordinates that is x y and \hat{i} and \hat{j} and the face normal vector is \vec{A}_f .

And in addition we have now because of convection, we have some velocity field \vec{u} , let say this is the velocity vector that is in the flow field and this is known ok, now this is known, alright. Then, how do I now go about calculating convection diffusion in an unstructured mesh like this that is also non orthogonal, ok. So, that is the question.

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Easily
$$\frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \vec{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi$$

Applying FVM:
$$\sum_f (\Gamma \nabla \phi)_f \cdot \vec{A}_f - \sum_f (\rho \vec{u} \phi)_f \cdot \vec{A}_f + \bar{S}_\phi \Delta V_0 = 0$$

$$A_f \quad F_e = (\rho u)_e \Delta y ; \quad F_f = (\rho \vec{u})_f \cdot \vec{A}_f$$

$$F_w = (\rho u)_w \Delta y ;$$

$$(\Gamma \nabla \phi)_f \cdot A_f = \frac{\Gamma_f}{\Delta x} \frac{A_f \cdot A_f}{\Delta x} (\phi_i - \phi_n) + (S_d)_f$$

Our governing equation is the same as before right, we start off with the general scalar transport equation that is $\frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \vec{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi$, right. For now, we would only look with, work with the just look at the convection diffusion equation.

So, we will not study convention diffusion equation. So, as the result we would check the unsteady part to 0 and of course, this is something that can be drawn easily. So, you can see how do extend this to be in cooperate the unsteady equation, which we have already seen in the context of structured meshes for convection diffusion, ok.

So, if I apply now finite volume method to the convection diffusion equation, of course we can write this by getting this term to the right hand side. As $(\Gamma \nabla \phi)_f \cdot \vec{A}_f$ minus $(\rho \vec{u} \phi)_f \cdot \vec{A}_f$ plus $\bar{S}_\phi \Delta V_0$ equal to 0, ok. So, this is basically you apply a integrate it on a finite volume and then convert the volume integrals into surface integrals using Gauss divergence theorem and then replace the surface integrals with summation ok, that is what. And then, we already know how to discretize the first time here, this is the diffusion flux $(\Gamma \nabla \phi)_f \cdot \vec{A}_f$.

And, we also know how to discretize the $\overline{S_\phi} \Delta V_0$ right; essentially, we make a linearize the source, write the $\overline{S_\phi}$ as $S_C + S_P \phi_P$. Now, only thing that we do not know is this part that is the convection term right, which is $(\rho \vec{u} \phi)_f \cdot \vec{A}_f$, ok. Remember for the structured meshes, we have defined for the east face, west face and so on; we have clubbed $\rho \vec{u}$ and \vec{A}_f together, we call that as some kind of flow rate right, because it is kind of multiplying density times velocity times the area, the scalar area.

So, this was $\rho u_e \Delta y$, we defined it as F_e right that is the mass flow rate through the east face. Similarly, we defined $\rho u_w \Delta y$ as the mass flow rate through the west face, ok. Remember, while defining these things, we did not consider the area vector direction, ok. We have only used the area magnitude, ok. So, as a result we got this plus minus in the definition of the upwind schemes, so right that is the consequence of that.

Whereas, now what I would like to do is, I would like to define our flow rate as $(\rho \vec{u})_f \cdot \vec{A}_f$, ok. So, now this e is, this takes into account the plus minus automatically depending on the face we are; of course, \vec{A}_f is now pointing out of the cell that we have focused on, ok. So, that means F_f is the flow rate which is basically $(\rho \vec{u})_f \cdot \vec{A}_f$ ok; that means, this term can be written as $F_f \phi_f$ right for each of the faces, alright.

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The image shows a whiteboard with handwritten mathematical derivations. At the top, there is a small equation: $\tau_w = \rho u_w \Delta y$. Below it, the convection term is discretized as follows:

$$(\rho \vec{u} \phi)_f \cdot \vec{A}_f = \frac{\Gamma_f}{A_f} \frac{A_f \cdot A_f}{A_f \cdot e_f} (\phi_1 - \phi_0) + (s_a)_f$$

Under the fraction $\frac{\Gamma_f}{A_f}$, there is a bracketed term D_f . Below this, the text "know about the diffusion discretization" is written. The equation is then simplified to:

$$= D_f (\phi_1 - \phi_0) + (s_a)_f$$

Below this, the convection term is further simplified to:

$$(\rho \vec{u} \phi)_f \cdot \vec{A}_f = F_f \phi_f$$

At the bottom, the text "discrete equation:" is written.

If we go about the diffusion flux that we have, diffusion term is $(\Gamma \nabla \phi)_f \cdot \vec{A}_f$; bar is missing here equals; this, basically has two components; if it is a non-orthogonal mesh, one was the primary derivative, the other one was the secondary derivative.

So, the primary derivative was $\frac{\Gamma_f A_f \cdot A_f}{\Delta \xi A_f \cdot e_\xi} (\phi_1 - \phi_0)$ right; essentially, $(\phi_1 - \phi_0)/\Delta \xi$ is coming from your $\frac{\partial \phi}{\partial \xi}$ on the face, plus we had some term which is basically your $\frac{\partial \phi}{\partial \eta}$ on the face, this we call it as a secondary gradient, ok. So, that is coming from the diffusion on the unstructured non orthogonal meshes, alright.

Now, just like what we have done in the structured examples, we would like to call this entire coefficient as some D_f , ok. Remember we have defined something called D_e , which was $\Gamma \Delta y / \delta x_e$. So, on similar lines we would like to define this entire coefficient as D_f ok, D_f , this is D_f times $\phi_1 - \phi_0$ plus secondary gradient of f , this is fine, this is we already know about the diffusion discretization. So, there is nothing new here.

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$(\rho \vec{u} \phi)_f \cdot \vec{A}_f = F_f \phi_f$

Discrete equation:

$$\sum_f D_f (\phi_1 - \phi_0)_f + (S_w)_f - F_f \phi_f + (S_c + S_p \phi_0) \Delta V_f = 0$$

CDS: Recall $\phi_e = \frac{\phi_E + \phi_P}{2}$ Similarly $\phi_f = \frac{\phi_0 + \phi_1}{2}$

What about the convection term? The convection term if we write that is $(\rho \vec{u} \phi)_f \cdot \vec{A}_f$, with our definition of $(\rho \vec{u})_f \cdot \vec{A}_f$ as F_f ; this term evaluates to F_f times ϕ_f , right. Now, notice the similarity, here this is basically similar to your F_e times ϕ_e ok; of course, in definition of F_e is different here slightly, because it does not consider the direction here, alright.

So, then we have F_f times ϕ_f . Now, can we write the complete discrete equation? Yes, we can write essentially, that is basically you go back and substitute for each of these terms and then write the summation on the f that basically gives you D_f times $\phi_1 - \phi_0$ for f .

So, that means either this is $\phi_1 - \phi_0$ or $\phi_2 - \phi_0$, and the corresponding things depending on the which face we are looking at plus you have secondary gradient of f minus you have F_f time ϕ_f , right. So, this is basically you are coming from the convection flux, plus we have the source term that is $S_C + S_P \phi_0$ times ΔV_0 equal to 0, ok. So, that is the full equation. Now, just like what we have done in the structured mesh case, we now have to apply a particular discretization scheme for our convective term right, our convective term is basically ϕ_f , F_f times ϕ_f .

Now, we need a some kind of profile assumption or some kind of value for our ϕ on the face f , ok. So, if we apply let us say central difference scheme, we of course recall that in the context of structured meshes, we wrote ϕ_e that was coming in F_e , right

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$$\sum_f D_f (\phi_1 - \phi_0)_f + (S_w)_f - F_f \phi_f + (S_C + S_P \phi_0) \Delta V_0 = 0$$

CDS : Recall $\phi_e = \frac{\phi_E + \phi_P}{2}$ Similarly $\phi_f = \frac{\phi_0 + \phi_1}{2}$
 simple average; improved

In $F_e \phi_e$, what we wrote was ϕ_e ; we have written as $(\phi_E + \phi_P)/2$ in the context of central difference scheme. Now, if I were to apply central difference scheme for unstructured non-orthogonal meshes, I can write this ϕ_f as a using a simple average as $(\phi_0 + \phi_1)/2$, right.

Now, this is ok, because although, there is a difference in the cell sizes; even if the cells are not uniform, we assume that the ϕ kind of let us say varies linearly or something. So,

this is a simple average; of course, this can be improved upon by using the gradients of phi later on, ok.

So, anyway I would make a simple average, this is basically ϕ_f equals $(\phi_0 + \phi_1)/2$; that means, I would substitute $(\phi_0 + \phi_1)/2$ into the ϕ_f value that we have here, ok. Now, what happens when we substitute this? What happens is you have $-F_f/2$ going into a 0 and then you have $-F_f/2$ going into a_1 , right.

Now, a_0 is your P cell here, right that is your 0 cell; that means, $-F_f/2$ would become plus $-F_f/2$ and it goes to the right hand side and you have a $-F_f/2$ that is remaining here, ok. So, that is what happens. Now, because the way F_f is defined, this will always be a minus here; because, F_f already contains the plus minus automatically depending on the area vector. So, as a result, we can now substitute for these values and then form the complete discrete equation for central difference scheme, when applied to convection diffusion on unstructured, non-orthogonal meshes.

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Discrete equation: $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$

$a_{nb} = D_f - \frac{F_f}{2}$; parallels to the structured mesh discretization; recall; derive!

$a_p = \sum a_{nb} - S_p \Delta V_0 + \sum F_f$

$b = S_c \Delta V_0 + \sum_{nb} (S_c)_f$ Recall $(F_e - F_w + F_n - F_s)$ what about +/- ?

Similar to Cartesian mesh case, if $F_f \geq 0$ then

So, of course, we kind of get back to our nice equation that is $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$. Now, this is where I want you to kind of draw parallels to the structured mesh discretization. So, you have to kind of recall what we have done in the structured context, in the context of convection diffusion equation.

See, how this makes sense ok; otherwise, you have to kind of go through this and kind of derive it independently after we have gone through these steps, ok. So, what would be a_{nb} ? a_{nb} is basically in the context of structured mesh, this was D_e minus F_e by 2, alright. This was so, if you go about here; again this should be D_f minus F_f by 2 right that is what we would get for the neighbors, right.

So, that is your a_{nb} ; a_{nb} would be D_f minus F_f by 2, because this will stay on the left hand side that is coefficient of phi once, alright. What about a_p ? a_p would be of course sum of $\sum a_{nb}$, sum of all these guys; but remember, that this would come with a plus. So, as a result we will have this extra term right, F_e minus F_w plus F_n minus F_s in the context of central difference scheme that same thing comes here.

But, again we do not have plus minus here, so as a result this would be summation of F_f , right. So, we would not have that plus minus thing here right, recall that was there in the context of structured meshes. So, this a_{nb} would basically we have D_f minus F_f by 2 that is the reason we are getting this, ok.

Then your b term of course, has the remaining part of the source term that is S_C times ΔV_0 plus we have the secondary gradient term as well, right. The secondary gradient term would be would remain on the left hand side as a result it will be a plus a $\sum a_{nb}$; secondary gradient for each of the face that is shared with the neighboring cells, ok.

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Discrete equation: $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$

always positive? No.. $a_{nb} = D_f - \frac{F_f}{2}$; parallels to the structured mesh discretization; recall; derive!

$a_p = \sum a_{nb} - S_p \Delta V_0 + \sum_f F_f$

$b = S_c \Delta V_0 + \sum_{nb} (S_g)_f$ Recall $(F_e - F_w + F_n - F_s)$ what about +/- ?

Similar to Cartesian mesh case, if $F_f \geq 0$ then

$a_{nb} < 0$ for $F_f > \geq D_f$

So, that is what we have. Now, similar to the Cartesian mesh case, if F_f is greater than 0 right; if this is positive, can will this coefficient be always positive? Will this be always positive? No right, this is not always positive; if F_f is positive and F_f is greater than 2 times D_f , right.

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The image shows a digital whiteboard with handwritten mathematical notes. At the top, the equation $b = S_c \Delta b_b + \sum_{n_b} (S_n)_f$ is written. To the right, there is a note: "Recall $(F_e - F_w + F_n - F_s)$ what about +/-?". Below this, it says "Similar to Cartesian mesh case, if $F_f \geq 0$ then". The main derivation shows: $a_{nb} < 0$ for $F_f > 2 D_f$, which implies $\Rightarrow \frac{F_f}{D_f} < 2$ for $a_{nb} > 0$. At the bottom, it states "Similar restriction in structured meshes also" and " $Pe_f < 2$ ".

Then essentially, this coefficient can be negative right, and we do not like negative coefficients, because if we use an iterative scheme, then this Scarborough criterion will not be satisfied and so on. So, we do not like this, that means we have to choose F_f , such that F_f/D_f should be always less than or equal to 2 right; that means, only then your a_{nb} 's will be positive, right.

That means, we are again come back to the same condition that, the cell Peclet number has to be less than 2; this is basically, we had a similar restriction in structured meshes also, right. So, the same restriction kind of comes back to us, even in the context of unstructured non-orthogonal meshes, ok. So, that, but that is how that is exactly how about you go about implementing the central difference scheme on these unstructured meshes, alright. Now, let us see, how do we implement the upwind difference scheme, ok.

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UDS: Recall

$$\phi_e = \begin{cases} \phi_P & F_e \geq 0 \\ \phi_E & F_e < 0 \end{cases} \quad \phi_f = \begin{cases} \phi_0 & F_f \geq 0 \\ \phi_1 & F_f < 0 \end{cases}$$

Upwind Differencing Scheme; Assemble the equation...

Discrete equation: $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$

$a_{nb} = D_f + \text{Max}(-F_f, 0)$ --- note --- any face that you consider in the cell

$a_p = \sum_{nb} a_{nb} - S_p \Delta V_b + \sum_{nb} F_f$ Verify!

$b = S_c \Delta V_b + \sum_{nb} (S_a)_f$ zero; u_{bar} satisfied conti.

So, the upwind difference scheme we again recall from the structured mesh case that, phi all the face ϕ_e is either ϕ_P or ϕ_E depending on the direction of the mass flow rate, right. If F_e is greater than or equal to 0, then ϕ_e equal to ϕ_P ; if F_e is less than 0, then ϕ_e equals ϕ_E , right we recall this thing.

Now, of course, the same condition applies here, only thing is that now ϕ_f is either ϕ_0 or ϕ_1 depending on the direction of the F_f . That means, if we go back to the diagram that we have drawn, which is couple of pages here, ok. So, if F_f bar is positive right, essentially you can move this arrow here. So, if this is going this way right; that means, it is in the direction of \vec{A}_f right, if that is the only way it can be positive.

Then, what will we take the phi value on the face; we would like to take it as ϕ_0 , right. If it is going this way, then we would like to take the phi comma face value equal to ϕ_1 right that is what the condition says now, ok. So, if F_f is positive, then we would take ϕ_f as ϕ_1 ; otherwise, we would take it as ϕ_0 alright, that is what we have, alright. Then of course, this is the only; this is the only thing we have to worry about right, this is your upwind differencing scheme.

So, once we have defined this thing, we can essentially assemble the equation right, assemble the equation. So, the discrete equation is basically $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$; because, we already know how to discretize and assemble all the diffusion equation and everything else right, which is basically the same as before. Now, what will be the a_{nb}

terms? This will be again if you draw a parallel to these structured mesh; what we get is a_{nb} equals, you get the D_e that is D_f plus max of $-F_f$ comma 0, ok.

Now, this will always be max of $-F_f$ comma 0, for any face that you consider in the cell or for any cell; because, this is always defined the way width direction. So, this will always have plus max of $-F_f$ comma 0, ok. So, you need to verify this; how will this come up, so you need to look at this and verify by comparison to the structured mesh case. And, a_p would have $\sum a_{nb}$ as before $-S_p$ times ΔV_0 plus we would have all this contribution.

Again, now this term would be; this term would be 0, if u bar satisfies continuity equation, alright. Now, b term as usual we will have S_c times ΔV_0 plus the secondary gradient of for each of the faces, ok. So, that is a very compact and nice equation; essentially, we got discretized the convection diffusion using the upwind difference scheme on unstructured non orthogonal meshes ok, that is very similar to the structured mesh, alright.

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what about higher-order schemes on unstructured meshes?

Structured meshes
Taylor series expansion
particular direction;
unstructured

Multi-dimensional Taylor series expansion

$$\phi_c = \phi_n + (\nabla \phi)_n \cdot \vec{\Delta r}_0 + O(\vec{\Delta r}_0 \cdot \vec{\Delta r}_0) + \dots$$

The diagram shows a diamond-shaped cell with a central node C_0 and two adjacent nodes C_1 and C_2 . A vector $\vec{\Delta r}_0$ points from C_0 to C_1 . A velocity vector \vec{u} is shown at the center, and a face normal vector \vec{A}_f is shown for the top face. A coordinate system with x and y axes is also present.

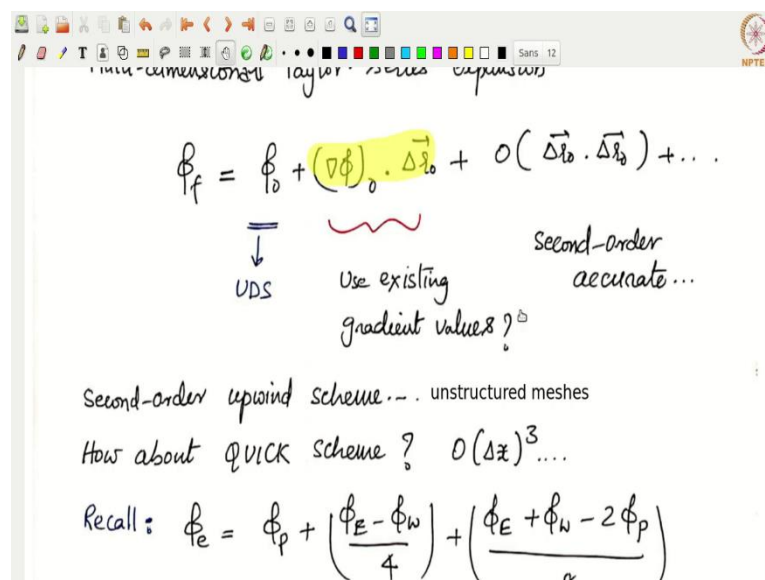
So far, so good now, the essentially we have now looked at not only about implementation issues on higher order schemes, and we have also looked at how do we go about discretizing convection diffusion on unstructured non orthogonal meshes for both the basic convection schemes; that is basically, your central difference scheme and upwind difference scheme, ok.

Now, one question that we did not answer basically is now ok, all this is fine; now how about higher order schemes. Can I extend these higher order schemes that we have learned that is basically your second order upwind scheme or the quick scheme to unstructured meshes? Yes of course we can, this is very regularly used on all the, in all the software's. So, essentially we will look at what about higher order schemes implementing higher order schemes on unstructured meshes, ok. So, again we look at the diagram here.

So, we have the C_0 cell, C_1 cell and the \vec{A}_f and we have the face, and the line joining C_0 to the face centroid we would like to call it as the vector $\vec{\Delta r}_0$ ok, bar is missing here. And then of course, we have the velocity vector that is \vec{u} , ok. So, that is what we have. Now, how about, how do we do this? Essentially, in the context of a structured meshes; what we have done is, essentially we have used the Taylor series expansion, right.

And not only the value of ϕ_P , but also the $\frac{\partial \phi}{\partial x}$ and $\frac{\partial^2 \phi}{\partial x^2}$, all these things are evaluated using central difference schemes; let us say if you want to do a quick scheme or something like that, ok. So, now, the same thing we have to do; of course, now but things are not in one direction right, because we do not have a particular direction that we can go about, because this is now essentially unstructured.

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So, we do not have a particular direction, but we know that, we can use a multi-dimensional Taylor series expansion; that is basically, to obtain the value of phi on the face, we can

expand this about the ϕ_0 , this is ϕ_0 plus $\nabla\phi_0 \cdot \overline{\Delta r_0}$ plus essentially we expand with our gradient calculation, and then we have the next term would be $\nabla^2\phi_0$ times order of Δr_0^2 , right. So, this will require you to calculate second derivative of the phi right, just like how we are done, but in multi-dimensions, alright.

So, depending on again if you only include this term, we are back to our upwind difference scheme, if you include even this term, then we are looking essentially at a second order accurate upwind scheme, because this term would evaluate itself to order Δr_0^2 , right. Now, if you of course, include this term as well, which require you to have $\nabla^2\phi$ in all the directions; then, you are essentially talking about a third order accurate upwind scheme.

Is this clear? Now, essentially we are looking at if you have only include the first term, we do not include any of these guys, then this is basically the first order of upwind scheme. If you include this, then we are essentially talking about an order Δr_0 naught square; that is basically, the second order upwind scheme. And again if you include this, term then the truncational would be order Δr_0^2 ; that means it will be a third order accurate scheme, ok.

Now, of course, we have already calculated gradients before, in the context of secondary gradients; so that means, we already know, what is $\nabla\phi$ at the cell centers, right. So, if we just include that, we can of course build a second order accurate scheme very easily right; because the $\nabla\phi$ is available at every cell, all you need to do is basically use the $\nabla\phi$ and reconstruct the value on the faces. And, again this term of course, would go into the b term right, like way the way we have described if you want to implement it. So, we can, this can be easily done, ok.

So far, so good we essentially discussed how to extend the higher order schemes or second order upwind scheme to unstructured meshes, right. So, that is what we have discussed till now, how to extend this to unstructured meshes, the second order upwind scheme. Now, how about the quick scheme, what we have to do? I do not have the second derivative is calculated already.

So, what should I do about doing, about calculating quick scheme or unstructured meshes? Because, that has that comes up with x^3 . There are multiple ways of doing this thing;

of course, you do not want to calculate the second derivative here and then include all those terms. So, as a result, there is an alternative way that is used in the literature.

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Recall: $\phi_e = \phi_p + \left(\frac{\phi_E - \phi_W}{4}\right) + \left(\frac{\phi_E + \phi_W - 2\phi_p}{8}\right)$

structured mesh
 $F_e \geq 0$

$$\Rightarrow \phi_p + \frac{1}{4}\left(\frac{\phi_E - \phi_W}{2}\right) + \frac{1}{4}(\phi_E - \phi_p)$$

e
 $W \text{ -- } P \text{ -- } E$

$$= \phi_p + \frac{1}{2}\left(\frac{\phi_E - \phi_W}{2\Delta x}\right)\left(\frac{\Delta x}{2}\right) + \frac{1}{2}\left(\frac{\phi_E - \phi_p}{\Delta x}\right)\left(\frac{\Delta x}{2}\right)$$

Generalize
 Unstructured
 Counter-part

$$= \phi_p + \frac{1}{2} \frac{\partial \phi}{\partial x} \Big|_p \left(\frac{\Delta x}{2}\right) + \frac{1}{2} \left(\frac{\partial \phi}{\partial x}\right) \Big|_e \left(\frac{\Delta x}{2}\right)$$

So, that is basically kind of generalizing the existing quick scheme on the structured meshes. So, we start off with the quick scheme that we have on the structured mesh, ok. So, recall from our structured mesh implementation, if F_e is greater than or equal to 0, then $\phi_e = \phi_p + \left(\frac{\phi_E - \phi_W}{4}\right) + \left(\frac{\phi_E - 2\phi_p + \phi_W}{8}\right)$, ok.

So, this is the original equation for quick scheme that we have already developed. This can be also rewritten as the equation here; this is basically ϕ_p plus we have ϕ_E by 4 and we have ϕ_E upon 8th. So, one-eighth I am writing it here. So, this is ϕ_E upon 8th and then minus one-eighth of ϕ_W , that is basically minus one-fourth here and plus one-eighth here. So, this would basically give you minus one-eighth that is what I have written here, and the remaining terms are ϕ_E is remaining one-fourth and ϕ_p has remaining one-fourth, ok.

So, we just modified this equation to look slightly different in terms of ϕ_p plus one-fourth of ϕ_E minus ϕ_W by 2 plus one-fourth of ϕ_E minus ϕ_p , alright. If that is the case, we can also rewrite this slightly differently by writing it like this, ϕ_p plus I would like to get the half here. So, this will be one half ϕ_E minus ϕ_W upon multiply with Δx and divide with Δx . So, we have $2\Delta x$ into $\Delta x/2$ right, in the denominator it kind of multiplies to 8 and you get back the original value here.

Similarly, here I would like to write this as one-half times $\Delta x/2$ that gives you the 4 value here and we would like to write the as ϕ_E minus ϕ_P by Δx into $\Delta x/2$, ok. So, basically this is another modification of this one by multiplying each of these terms, the second and third term with Δx and dividing with the Δx , ok. Now, what can you say about this term? This is basically, if you are at the P cell, ok.

So, we are essentially at this is our west cell; then we have the P, then we have the east right that means. If we are talking about ϕ_E minus ϕ_W by $2\Delta x$, this is basically calculating the gradient at the cell P, right. So, I can write this of course, as $\frac{\partial \phi}{\partial x}|_P$ times $\Delta x/2$ into one half plus. What about ϕ_E minus ϕ_P by Δx ? ϕ_E minus ϕ_P by Δx , this will be basically gradient evaluated at the little east right, basically at the east face right; so that means, I can write this as $\frac{\partial \phi}{\partial x}|_e$ at the east face times $\Delta x/2$.

Now, what is this $\Delta x/2$? Δx is the width of the cell right, either this one or this one; $\Delta x/2$ would be the distance between either P to the face e or between e to the E right something like that. So, essentially if you are talking about P, this would be the distance between cell centroid to the face, fine. Essentially, now we have kind of transformed this equation for quick scheme, assuming that F_e is greater than 0; you have to redo all this if it is less than 0. That will be slightly different into something else, in terms of a continuous gradients, ok.

Now, I have done this thing. Now, from here we can kind of generalize this equation, such that we can build a unstructured counterpart of this equation ok, very easily without going into the second derivatives as we saw before. So, how do I now write this? This is basically $\frac{\partial \phi}{\partial x}|_P$; in general this would be, because this is unstructured mesh, I can write this as $(\nabla \phi)_0$ evaluated at 0.

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Generalize to unstructured meshes... QUICK -- unstructured

$$\phi_f = \phi_0 + \frac{1}{2} \vec{\nabla} \phi_0 \cdot \vec{\Delta r}_0 + \frac{1}{2} \vec{\nabla} \phi_f \cdot \vec{\Delta r}_0$$

Evaluate $\vec{\nabla} \phi_0$ and $\vec{\nabla} \phi_f$ to $O(|\vec{\Delta r}_0|^2)$

then overall scheme will be $O(|\vec{\Delta r}_0|^3)$

Other higher-order scheme can be generalized to unstructured meshes....

Now if we generalize, this is basically ϕ_p would be ϕ_0 right; to obtain the value on the face this will be ϕ_0 ; plus one half times this would be what, $(\nabla\phi)_p$ evaluate cell p that is 0 dotted with, what is $\Delta x/2$? $\Delta x/2$ is nothing, but $\vec{\Delta r}_0$ right; we have just drawn this as basically, the distance between the cell centroid to the face centroid, this is delta r naught bar, ok.

So, we have generalized this formula. Plus what is the second one? This is half of partial phi partial x at east is nothing, but this is in the context of Cartesian structured meshes, this is basically the $\frac{\partial\phi}{\partial x}$. But if you were to generalize this, this is basically your $(\nabla\phi)_f$ evaluated on the face f. So, this is basically $(\nabla\phi)_f$ ok, dotted with this is again $\vec{\Delta r}_0$, ok. Now, very nicely we have got an equation here which is a generalize, generalization of the quick scheme to unstructured non orthogonal meshes, ok.

Now, only requirement of course is that, the gradients that we have computed or we will compute; these two have to be at least second order accurate right, only then this entire thing will be third order accurate, and whatever we kind of leave it here would be third order accurate, ok.

So, this is the counter part of the quick scheme for unstructured non orthogonal meshes, ok. So, only requirement is that, evaluate are the gradients at the cell centers and the faces

to at least second order accuracy, such that this entire terms here would be will be third order accurate, ok.

Now, following here similar pattern; you can of course derive other higher order scheme, such as the second order upwind scheme or Beam Warming scheme or Fromm scheme using by generalizing those equations as well into unstructured non orthogonal meshes ok, following a singular algorithm, ok.

So, that is about it. Essentially now we have covered today the unstructured mesh discretization for the convection diffusion as well as we learnt how to extent the higher order upwind schemes to the unstructured non orthogonal meshes, ok. So, I am going to stop here. Let me know if you have any questions through e mail, alright.

Thank you.