Computational Fluid Dynamics and Heat Transfer
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Lecture - 23
A Finite Volume Method to solve Three-dimensional NS Equations in Complex Geometry
(Calculation of Diffusion Flux, Pressure and the Solution Algorithm)

Good morning everybody. Today, we will continue with our Finite Volume Method to solve three-dimensional Navier-Stokes equations in complex geometry. In the last lecture, we discussed about the important geometrical parameters and the procedure of calculating convective fluxes. So, today we will discuss about the diffusive fluxes.

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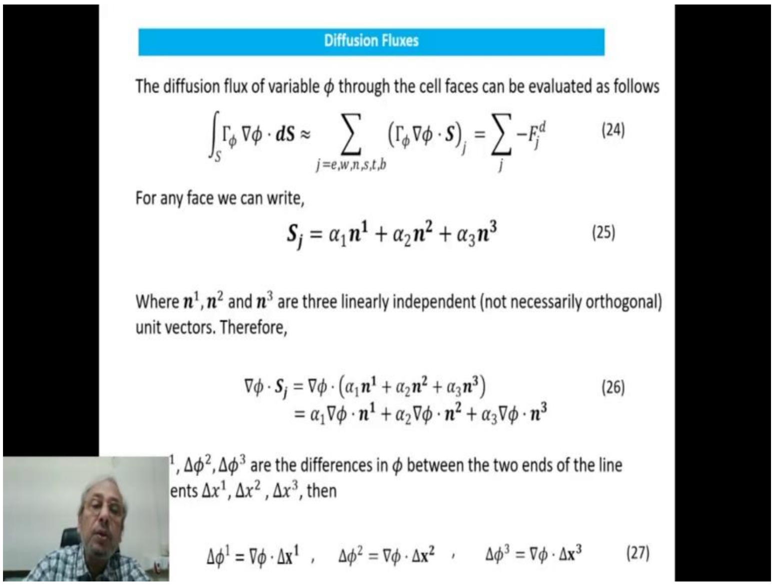

Now, diffusion flux of variable ϕ through the cell faces can be evaluated as the surface integral, this is basically diffusion coefficient $\Gamma_\phi \nabla\phi . \boldsymbol{dS}$. Now, this operation $\nabla\phi . dS$ over the confining surfaces will be summation of the again $(\Gamma_\phi \nabla\phi . S)_j$ and this is basically over the all the surfaces.

That means, over j and $j = e, w, n, s, t, b$ western face, northern face, southern face, top face and bottom face of the cell of interest of the control volume, the computational control volume of our choice and so, we can write it as finally, summation of this diffusive terms.

So, any face given by $\boldsymbol{S_j} = \alpha_1 \boldsymbol{n^1} + \alpha_2 \boldsymbol{n^2} + \alpha_3 \boldsymbol{n^3}$, where $\boldsymbol{n^1}, \boldsymbol{n^2}$ and $\boldsymbol{n^3}$ are three linearly independent unit vectors, they may be orthogonal may not be orthogonal. Now, when we operate $\nabla\phi.\boldsymbol{S_j}$ with this surface vector, we can get $\nabla\phi.(\alpha_1 \boldsymbol{n^1} + \alpha_2 \boldsymbol{n^2} + \alpha_3 \boldsymbol{n^3})$ and through this operation, we can get $\alpha_1 \nabla\phi.\boldsymbol{n^1} + \alpha_2 \nabla\phi.\boldsymbol{n^2} + \alpha_3 \nabla\phi.\boldsymbol{n^3}$.

Now, if we define $\Delta\phi^1$, $\Delta\phi^2$ and $\Delta\phi^3$ are differences of ϕ between two end points of the line segments Δx^1, Δx^2, Δx^3, then we can write $\Delta\phi^1 = \nabla\phi.\Delta\boldsymbol{x^1}$. Please note that, this $\Delta\boldsymbol{x^1}$ and this Δx^1, these are not same, this is $\Delta\boldsymbol{x^1}$ bold, and this ($\Delta\boldsymbol{x^1}$) defines a vector quantity; whereas, this (Δx^1) is the magnitude. I will come in detail in the next slides. So, $\Delta\phi^2 = \nabla\phi.\Delta\boldsymbol{x^2}$ similarly, $\Delta\phi^3 = \nabla\phi.\Delta\boldsymbol{x^3}$.

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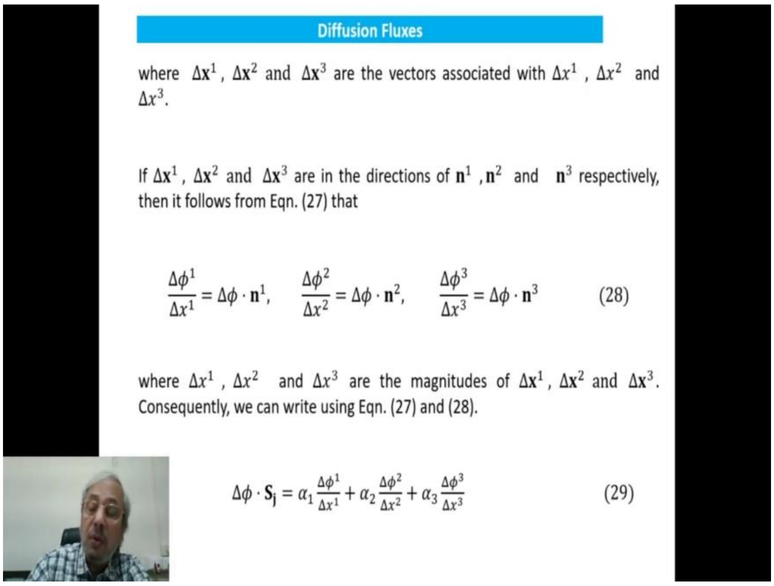

Now, as I mentioned in the last slide that this $\Delta\boldsymbol{x^1}$ when **x** is bold, $\Delta\boldsymbol{x^2}$ and $\Delta\boldsymbol{x^3}$ where all the **x**'s are bold, these are vectors associated with Δx^1, $\Delta x^2$and Δx^3. So, if $\Delta\boldsymbol{x^1}$ with **x** bold, $\Delta\boldsymbol{x^2}$ and $\Delta\boldsymbol{x^3}$ are in the directions of the unit normal vectors $\boldsymbol{n^1}, \boldsymbol{n^2}$ and $\boldsymbol{n^3}$, then from the just previous equation that means, 27. From the previous equation 27, we can see $\Delta\phi^1$, $\Delta\phi^2$ and $\Delta\phi^3$ expressions so, from there, we can write $\frac{\Delta\phi^1}{\Delta x^1} = \Delta\phi.\boldsymbol{n^1}$, $\frac{\Delta\phi^2}{\Delta x^2} = \Delta\phi.\boldsymbol{n^2}$ and $\frac{\Delta\phi^3}{\Delta x^3} = \Delta\phi.\boldsymbol{n^3}$ where Δx^1, Δx^2 and Δx^3, I have already mentioned that these are magnitudes of $\Delta\boldsymbol{x^1}$, $\Delta\boldsymbol{x^2}$ and $\Delta\boldsymbol{x^3}$ these **x**'s are bold and these are basically the vectors.

So, consequently, we can write equation 27 and 28 as so, if we look at equation 27 and 28, from both we can write

$$\Delta\phi.\boldsymbol{S_j} = \frac{\alpha_1\Delta\phi^1}{\Delta x^1} + \frac{\alpha_2\Delta\phi^2}{\Delta x^2} + \frac{\alpha_3\Delta\phi^3}{\Delta x^3}$$

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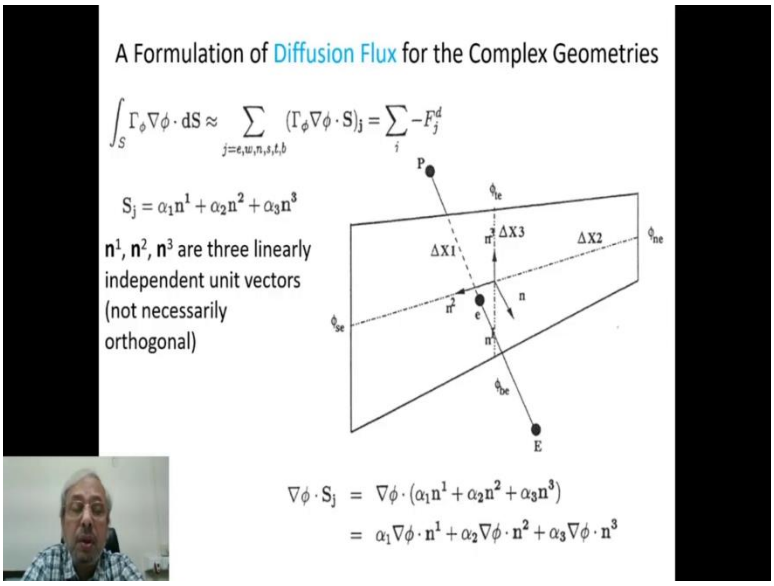

We can do a little more detailed explanation of go for detailed little more detailed explanation of what we discussed. Basically, we are performing the surface integral and this is basically diffusion coefficient $\nabla\phi$, ϕ is the quantity which can be convected or diffused, this can be for momentum equation u, v, w and for energy equation, this is temperature so, dot **dS**. So, we can we have already written this capital gamma ϕ (Γ_ϕ) $\nabla_\phi . S_j$ integration over all confining surfaces **j**, we are evaluating.

Now, since we said that $\boldsymbol{S_j} = \alpha_1\boldsymbol{n^1} + \alpha_2\boldsymbol{n^2} + \alpha_3\boldsymbol{n^3}$ and n^1, n^2 and n^3 are three linearly independent unit vectors not necessarily orthogonal. So, and this is the interface between cell P and cell E. So, basically, I mean eastern face. So, $\nabla\phi.\boldsymbol{S_j} = \nabla\phi.(\alpha_1 n^1 + \alpha_2 n^2 + \alpha_3 n^3) = \alpha_1\nabla\phi.\boldsymbol{n^1} + \alpha_2\nabla\phi.\boldsymbol{n^2} + \alpha_3\nabla\phi.\boldsymbol{n^3}$.

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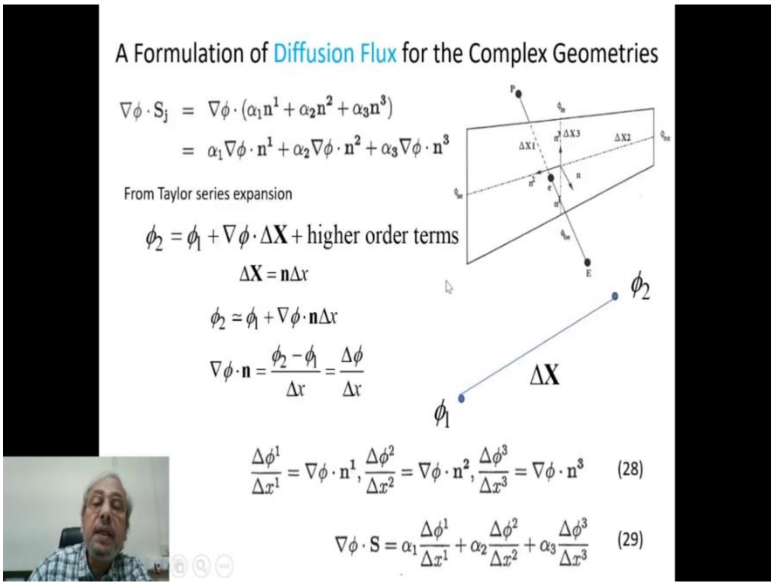

And then, as we were saying that basically this, at two different points, we have different ϕ, then the gradient of this ϕ we can write as basically, $\phi_2 = \phi_1 + \nabla\phi.\boldsymbol{n}\boldsymbol{\Delta X}$ this $\boldsymbol{\Delta X}$ is vector and this can be written as $\boldsymbol{n}\Delta x$ and this (Δx) is scalar. So, basically $\nabla\phi.\boldsymbol{n} = \phi\_1 - \phi\_2)/\Delta x = \Delta\phi/\Delta x$. Following that $\frac{\Delta\phi^1}{\Delta x^1} = \nabla\phi.n^1$, $\frac{\Delta\phi^2}{\Delta x^2} = \nabla\phi.n^2$, $\frac{\Delta\phi^3}{\Delta x^3} = \nabla\phi.n^3$.

So, $\nabla\phi.S$ that is what I mean slide before, we defined $\nabla\phi.S = \alpha_1\frac{\Delta\phi^1}{\Delta x^1} + \alpha_2\frac{\Delta\phi^2}{\Delta x^2} + \alpha_3\frac{\Delta\phi^3}{\Delta x^3}$. These are the special explanations we tried to give of the from this slide where we have already equation 29, we have already derived it that $\nabla\phi.S = \alpha_1\frac{\Delta\phi^1}{\Delta x^1} + \alpha_2\frac{\Delta\phi^2}{\Delta x^2} + \alpha_3\frac{\Delta\phi^3}{\Delta x^3}$.

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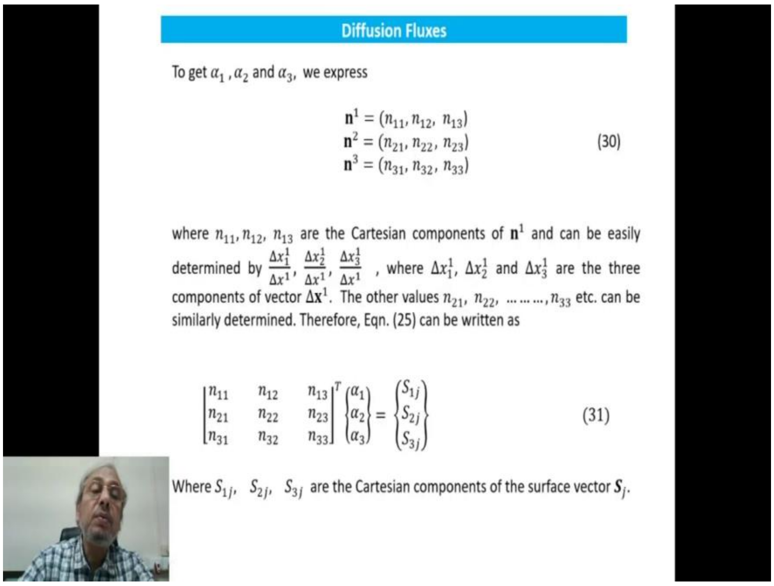

Now, we have to calculate α_1, α_2, α_3. Now, $\boldsymbol{n}^1$, this unit normal vector can be written as n_{11}, n_{12}, n_{13} where n_{11}, n_{12} and n_{13} are the Cartesian components of $\boldsymbol{n}^1$and can be easily determined by $\frac{\Delta x_1^1}{\Delta x^1}, \frac{\Delta x_2^1}{\Delta x^1}, \frac{\Delta x_3^1}{\Delta x^1}$; where delta Δx_1^1, Δx_2^1 and Δx_3^1 are three components of the vector $\Delta \boldsymbol{x}^1$.

So,$\Delta \boldsymbol{x}^1$ is a vector quantity, its magnitude is basically these Δx_1^1, Δx_2^1 and Δx_3^1 are three components of the vector from where we can get n_{11}, n_{12}, n_{13} which are basically then Cartesian components of unit normal vector $\boldsymbol{n}^1$.

Similar way, n_{21}, n_{22}, n_{23} are Cartesian component of unit normal vector $\boldsymbol{n}^2$ and n_{31}, n_{32}, n_{33} are the Cartesian components of unit normal vector $\boldsymbol{n}^3$. Then, we can write $n_{11}, n_{12}, n_{13}, n_{21}, n_{22}, n_{23}, n_{31}, n_{32}, n_{33}$ transpose into α_1, α_2, α_3 comes from equation 29 equal to S_{1j}, S_{2j}, S_{3j}.

$$\begin{bmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{bmatrix} \begin{Bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{Bmatrix} = \begin{Bmatrix} S_{1j} \\ S_{2j} \\ S_{3j} \end{Bmatrix}$$

S_{1j}, S_{2j}, S_{3j} are the Cartesian components of surface vector $\boldsymbol{S}_j$. From equation 31, it is possible to calculate α_1, α_2, α_3 by applying Cramer's rule. So, will we do that.

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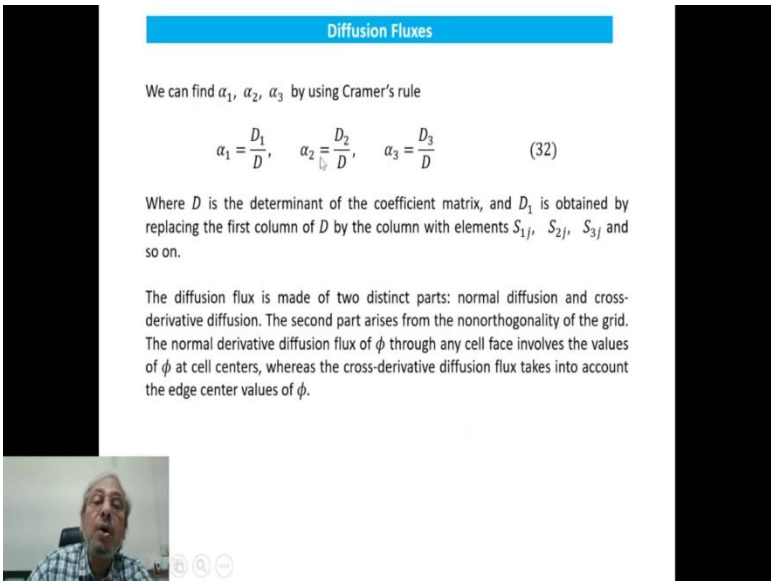

We can find α_1, α_2, α_3 by using Cramer's rule where $\alpha_1 = \frac{D_1}{D}$, $\alpha_2 = \frac{D_2}{D}$, $\alpha_3 = \frac{D_3}{D}$. D is the determinant of the coefficient's matrix. If we look at equation 31 so, basically coefficient matrix determinant is D and D_1 is obtained by replacing the first column of D by the column with the elements S_{1j}, S_{2j} and S_{3j}.

So, basically first column will be replaced by these (S_{1j}, S_{2j} and S_{3j}) quantities, then we will get D_1, second column is replaced by these (S_{1j}, S_{2j} and S_{3j}) quantities, we will get D_2 and third column is replaced by these (S_{1j}, S_{2j} and S_{3j}), then we will get D_3 and dividing by D, we will be able to find out α_1, α_2, α_3.

The diffusion flux is made of two distinct parts: normal diffusion and cross derivative diffusion. The second part arises from nonorthogonality of the grid. The normal derivative diffusion flux of phi through any cell face involves the values of phi at the cell centres, whereas cross-derivatives and cross derivative diffusion flux takes into account edge center values.

If you recall that every side, we defined edges and also edge centers of every side of a cell, cell center, then cell faces, face center and then every face has edges, edge center. These are the geometrical parameters we have to make use of.

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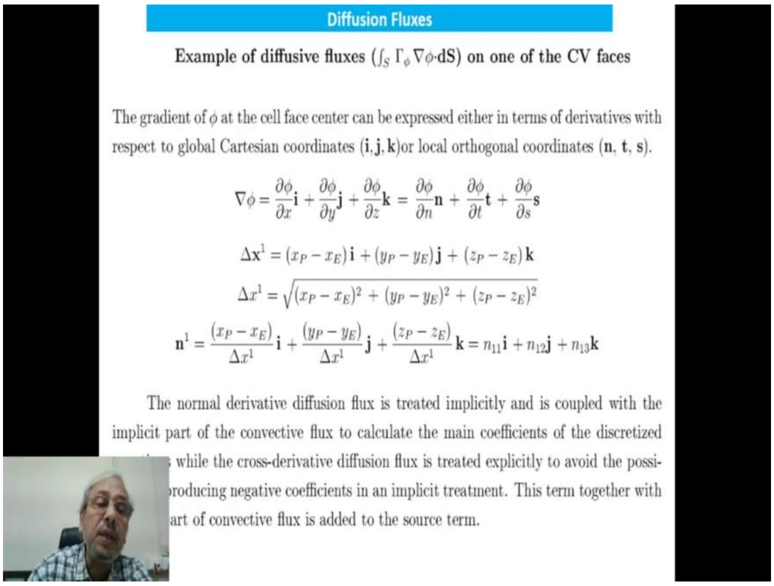

Now, let us examine the; let us examine the diffusive fluxes on one of the control volume faces. The gradient of phi at the cell face center can be expressed either in terms of derivatives with respect to global Cartesian coordinates that is (i, j, k) or local orthogonal coordinates (n, t, s). So, $\nabla\phi$ can be written as

$$\nabla\phi = \frac{\partial\phi}{\partial x}\boldsymbol{i} + \frac{\partial\phi}{\partial y}\boldsymbol{j} + \frac{\partial\phi}{\partial z}\boldsymbol{k} = \frac{\partial\phi}{\partial n}\boldsymbol{n} + \frac{\partial\phi}{\partial t}\boldsymbol{t} + \frac{\partial\phi}{\partial s}\boldsymbol{s}$$

Now, this vector $\Delta\boldsymbol{x}^1$, then will be given by $\Delta\boldsymbol{x}^1 = (x_P - x_E)\boldsymbol{i} + (y_P - y_E)\boldsymbol{j} + (z_P - z_E)\boldsymbol{k}$, these x_E, y_E and z_E are defined at the center of the eastern neighbouring cell and x_P, y_P, z_P these are defined at cell of interest. That means, P cell and then, the magnitude of this $\Delta\boldsymbol{x}^1$ is given by $\Delta x^1 = \sqrt{(x_P - x_E)^2 + (y_P - y_E)^2 + (z_P - z_E)^2}$ and the unit normal vector can be given as $\boldsymbol{n}^1 = \frac{(x_P - x_E)}{\Delta x^1}\boldsymbol{i} + \frac{(y_P - y_E)}{\Delta x^1}\boldsymbol{j} + \frac{(z_P - z_E)}{\Delta x^1}\boldsymbol{k}$ which can also be called as $n_{11}\boldsymbol{i} + n_{12}\boldsymbol{j} + n_{13}\boldsymbol{k}$. So, unit normal vector in the previous slide, if you recall, we represented by n_{11}, n_{12}, n_{13}. So, this is how unit normal vector is basically $n_{11}\boldsymbol{i}, n_{12}\boldsymbol{j},\ n_{13}\boldsymbol{k}$.

The normal derivative diffusion flux is treated implicitly and is coupled with the implicit part of the convective flux to calculate the main coefficients of the discretized equations while the cross-derivative diffusion flux is treated explicitly to avoid the possibility of producing negative coefficients in an implicit treatment. This term together with explicit part of convective flux is added to the source term.

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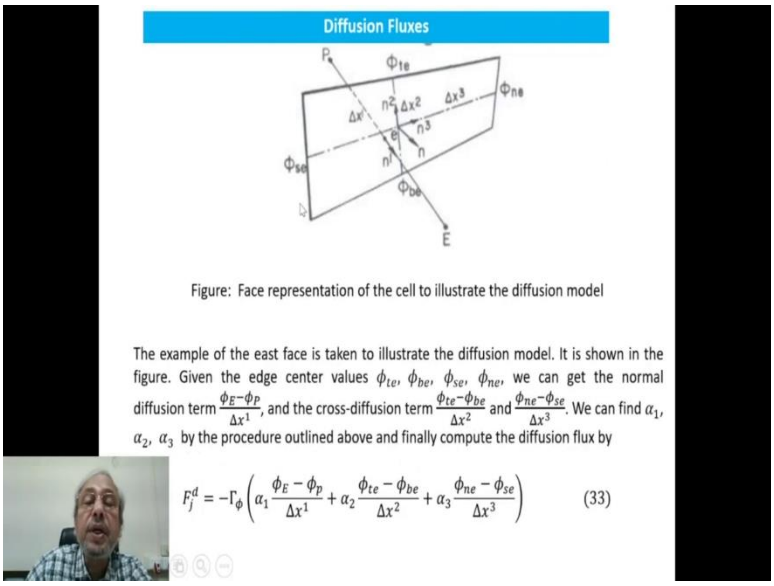

Progress further, with the example of again the eastern cell face and we can see that this is the edge of the cell and this is basically center te and this is the edge of the cell center be and ϕ has been defined here ϕ_{be}. The example of east face taken to illustrate the diffusion model. It is shown in the figure.

Given the edge center values as I said and ϕ defined there, ϕ_{te}, ϕ_{be}, ϕ_{se} and ϕ_{ne}. We can get the normal diffusion term as ϕ_E minus ϕ_P divided by Δx^1, this is the distance magnitude of the distance between the cell center of a P cell which is identified by P and cell center of E cell which is identified by capital E. So, $\frac{\phi_E-\phi_P}{\Delta x^1}$ this is separated by a distance magnitude of which is Δx^1.

And the cross-diffusion terms basically $\frac{\phi_{te}-\phi_{be}}{\Delta x^2}$, $\frac{\phi_{ne}-\phi_{se}}{\Delta x^3}$. So, we can find α_1, α_2, α_3 by the procedure, we have already mentioned it earlier that applying Cramer's rule, by applying Cramer's rule D_1 by D is α_1, D_2 by D is α_2 and D_3 by D is α_3.

By the procedure as I said, outlined earlier, we can calculate α_1, α_2, α_3 and then, we can write that diffusion flux is

$$F_j^d = -\Gamma_\phi \left(\alpha_1 \left(\frac{\phi_E - \phi_P}{\Delta x^1}\right) + \alpha_2 \, \frac{\phi_{te} - \phi_{be}}{\Delta x^2} + \alpha_3 \, \frac{\phi_{ne} - \phi_{se}}{\Delta x^3}\right)$$

These (2nd and 3rd term) are the diffusion fluxes in the cross normal directions and this is the (1st term) basically normal diffusion flux equation 33.

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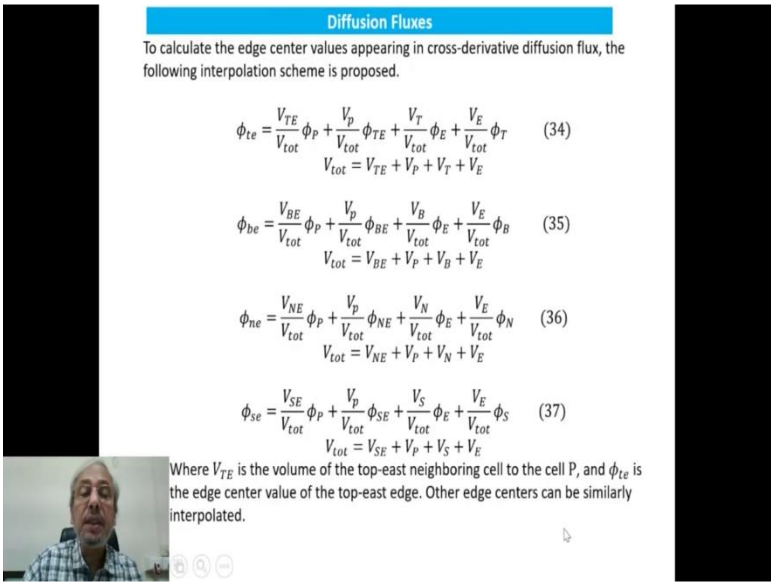

Now, this here, when we calculate ϕ_E and ϕ_P are defined by, but quantities like ϕ_{te}, ϕ_{be}, ϕ_{se} and ϕ_{ne} are not defined because these are edge centers and I mean center of the face it is it can be defined, center of the cell it is defined, but at this center of the edges, how it is to be calculated.

We will see in this calculation for example, ϕ_{te}, in this calculation, cell of interest that means, P, eastern cell E, this is interface so, eastern cell, entire eastern cell, cell of interest P and the cell which is at the top of P cell that cell and cell which is at the top of E cell that cell. So, these four cells will be involved in basically defining ϕ_{te}.

So, ϕ_{te}

$$\phi_{te} = \frac{V_{TE}}{V_{tol}}\phi_P + \frac{V_P}{V_{tol}}\phi_{TE} + \frac{V_T}{V_{tol}}\phi_E + \frac{V_E}{V_{tol}}\phi_T$$

So, what is ϕ_{te}? Basically, ϕ_{te} is a volume of the top eastern neighbor cell of P so, that means, the again let me say this will be P cell, where P is a cell center, this is E cell where E is the cell center. Above P cell, there is a cell, center of which is given by uppercase T and above this eastern cell there is a cell, center of which is given by uppercase TE, it is basically eastern neighbor of the top cell which is just above P cell.

$$\phi_{te} = \frac{V_{TE}}{V_{tol}} \phi_P + \frac{V_P}{V_{tol}} \phi_{TE} + \frac{V_T}{V_{tol}} \phi_E + \frac{V_E}{V_{tol}} \phi_T$$

So, this is V TE, V P, V T, V E cell volumes. This is cell of interest P its volume, then this is cell which is basically eastern neighbor of the top cell over P-th cell and this is volume of top cell, this is volume of eastern cell and V total is volume of that cell which is basically eastern neighbor of the top cell V TE, V P cell of interest, V T top cell over P-th cell and V E eastern neighbor of cell P.

So, this is how ϕ_{te} is calculated involving four neighbouring cells; four neighbouring cells that means, cell of interest P, cell above it T, eastern neighbor E and basically the corner at this on the above P, the cell is T and its eastern neighbor that means, cell which is just at the top of eastern cell that is te. So, you are involving four cells to define ϕ_{te}.

Similarly, ϕ_{be} we will involve bottom cell, here the ϕ_{te} involved top cell and top eastern neighbor. Similarly, when we define phi be, it will involve P-th cell, its bottom cell, eastern neighbor and the bottom cell of the eastern neighbor and then, this will be defined through interpolation.

Similarly, a ϕ_{ne} will involve four neighboring cells, ϕ_{se} will also involve four neighboring cells and these are to be defined. So, basically that is how these quantities ϕ_{te}, ϕ_{be}, ϕ_{ne}, ϕ_{se} are calculated so; so that we can find out from equation 33, the cross diffusion and normal diffusion will be given by ϕ_E minus ϕ_P by Δx^1.

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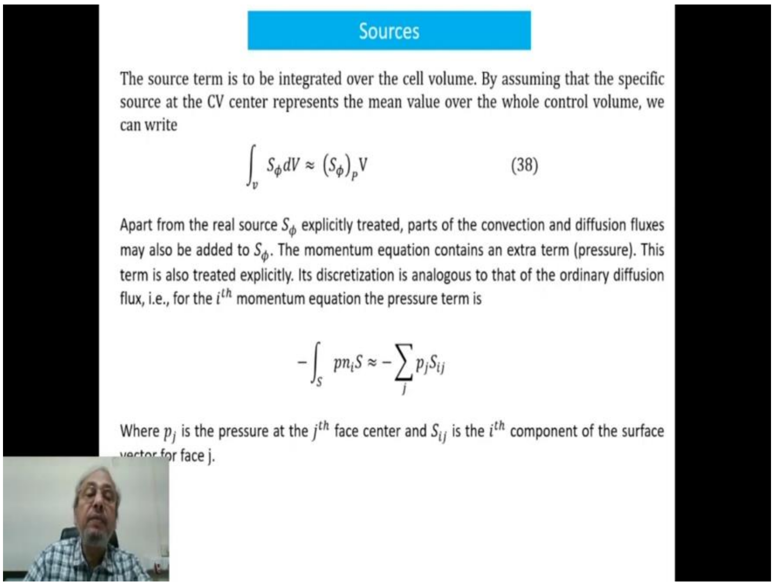

Having done that we can go for all other cell faces and calculate the complete diffusion from the cell of interest P. Then, we consider source term, this is to be integrated over the cell volume. By assuming the specific source at the control volume center, then we can write that volume integral of S_ϕdV is S_ϕ defined at point P into the cell volume.

So, apart from S_ϕ explicitly treated, parts of the convection and diffusion fluxes may also be added to this term. Momentum equation contains the very important term which is pressure. Now, this term is also treated explicitly. Its discretization is analogous to that of the ordinary diffusion flux that is for i^{th} momentum equation pressure term can be written as pn_iS integrated over S surface.

And then, on all the confining surfaces we can write summation of p_jS_{ij} minus summation of p_j S_{ij}. p_j is a pressure at the jth cell center and S_{ij} is the i^{th} component of the surface vector for the face j. This is relatively easy to handle.

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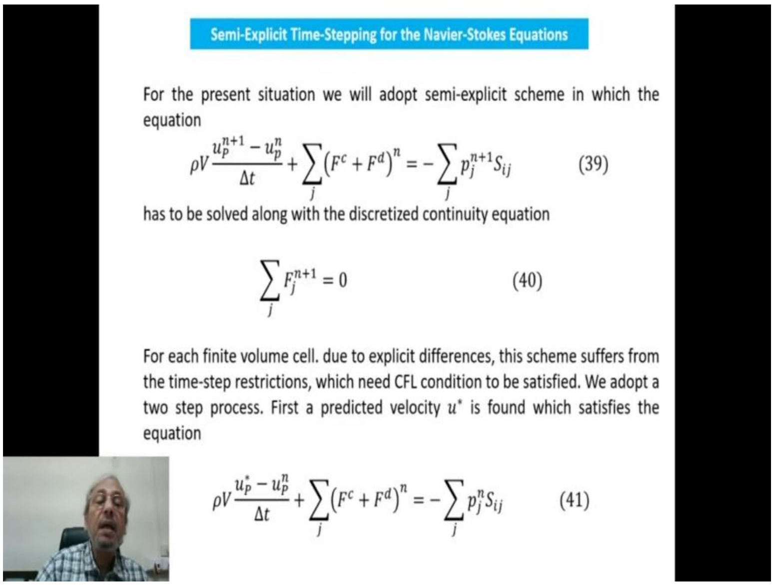

Now, having done that, we have evaluated if you look into the Navier-Stokes equations, now we have evaluated these convective diffusive fluxes at the time level n that means, at the current time level in all the cells, we have calculated the pressure terms, but pressure terms also we have used n^{th} level pressure, but ideally, it should have been $n+1^{th}$ level pressure.

And then, we have done mass lumping here rho into volume and this is $\frac{u_P^{n+1}-u_P^n}{\Delta t}$ and this u a can be; u can be, v can be, w then accordingly, p has to be adjusted and these are the momentum equations in three directions. This has to be solved along with the discretized continuity equation, continuity equation has to be this.

But at the movement, we do not have also value of F_j over all this confining surfaces at n $n+1^{th}$ level, we know at n^{th} level. So, at each finite volume cell, due to explicit differences, this scheme suffers from, of course, the time step restriction etcetera, we have to follow from CFL condition.

Now, first what we do? Since all pressure at n^{th} level is available, convection diffusion contribution at n^{th} level is available, we advance it explicitly through this equation, but we cannot write $n+1^{th}$ here because we are advancing through a time step Δt, but this velocity whether it is u velocity, v velocity or w velocity, these has not satisfied continuity equation as yet.

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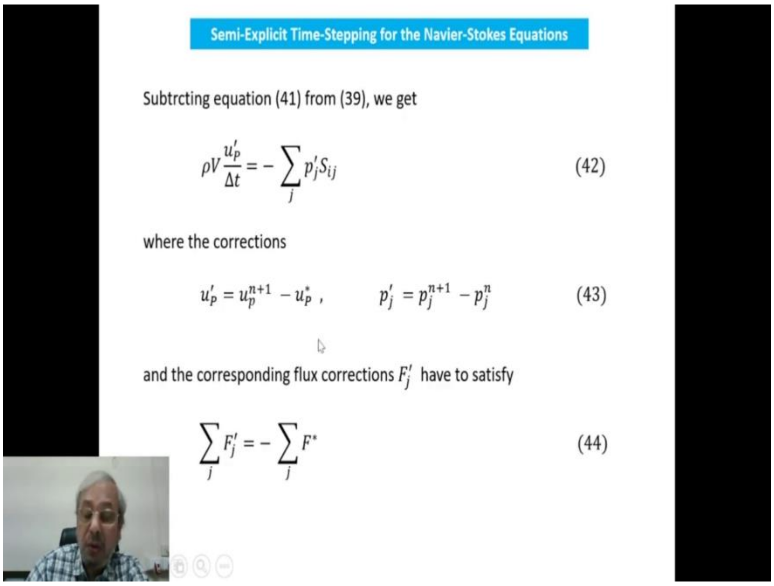

So, we this is basically the equation that we are using to calculate provisionally advanced velocity quantities and difference between these two equations basically, you can see, we can write in symbolic form that means, ρ into V, volume this V is volume into difference between velocity at $n+1^{th}$ level and the star quantity which is $\frac{u'_P}{\Delta t}$.

$$\frac{\rho V u'_P}{\Delta t} = -\sum_j p'_j Sij \qquad (42)$$

So, we are calling just you know, we are calling it as u'_P, we could have called it u_P correction as we have done in simple and math algorithm, but here just you know meaning is same, this prime has been used. $-\sum_j p'_j Sij$, again it is same, p'_j means $p_j^{n+1} - p_j^n$. So, this difference in pressure is p'_j summation over all surfaces where the corrections are so exactly what I said we can call it velocity correction, we can call this as pressure correction.

So,

$$u'_P = u_P^{n+1} - u_P^*$$

$$p'_j = p_j^{n+1} - p_j^n$$

and the corresponding flux corrections. So obviously, since velocity is being corrected so, flux also, the mass flux required to be corrected, requires to be corrected and then, this is basically

$$\sum_j F_j' = -\sum_j F^*$$

So, this mass flux, if we calculate using correction term (left side term), this is mass flux correction and if we calculate using provisional velocity u^* , this is F^* (right side term).

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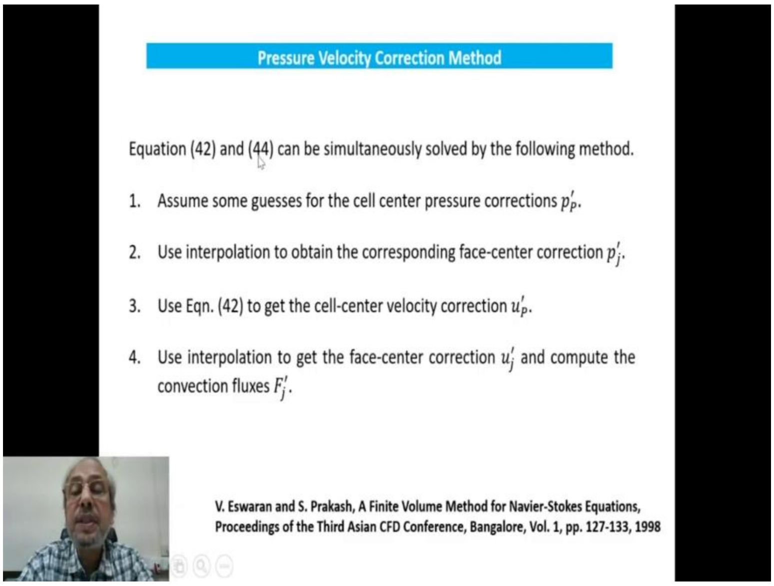

So, equation 42 and 44 can be simultaneously solved by the following way, this is as usual the pressure velocity iteration which we already know from MAC algorithm and simple algorithm. Assume some guesses for the cell center pressure corrections p_P'. Use interpolations to obtain the corresponding face center correction pressure correction p_j'.

Use equation 42 that means, this equation to get cell center velocity corrections. Use interpolation to get then face center velocity; face center flux correction and compute the convection flux correction rather F_j'.

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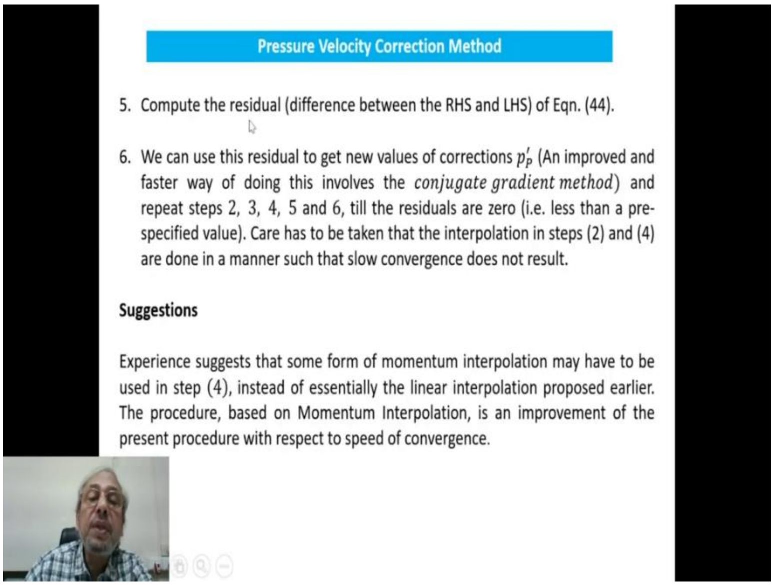

Compute the residual that is basically difference between in equation 44, these two equations, left left-hand side, when there will be no velocity correction obviously, the stared quantities have reached $n + 1^{th}$ quantity. So, basically that is what we have written compute the residual difference between RHS and LHS. So, there will be no difference when you know the velocities have evolved to the velocity at a level $n + 1$.

We can use this residual to get new values of the corrections p'_P an improved and faster way of doing this involves maybe you can use conjugate gradient method and repeat step 2, 3, 4 and 6 till residuals are zero that that is less than a pre-specified value. Care has to be taken that interpolation in steps 2 and 4 are done in a manner such that slow convergence does not result.

Experience suggest that some form of momentum interpolation may have to be used in step 4 that means, a here, instead of essentially the linear interpolation proposed earlier. The procedure based on momentum interpolation is an improvement of the present procedure with respect to speed of convergence.

So, basically what we can say that in this process, calculation of diffusion flux, calculation of convection flux, calculation of the contribution from the pressure these are different than what we discussed about MAC and simple algorithm. In arbitrary geometry, arbitrary control volume very special procedures we have outlined.

But having outlined that we can define this equation as a projection equation that means, at the next time step, u_P^{n+1} has to evolve, but since we are not using pressure at $n+1^{th}$ level, we are getting velocities which we are calling as provisional velocity and this is identified by the star mark.

And then, difference between these two equations will give us a relationship 39 and 41, velocity correction and pressure correction. So, pressure has to be corrected so that p^n evolves as p^{n+1} and velocity has to be corrected so that u_P^* becomes u_P^{n+1} and then, we have progress from nth level to a level $n+1$.

And if this is basically, we have to find out the velocities in a steady flow problem, we have to progress in the time direction till we get same values for two consecutive time steps. It is; if it is unsteady, you know flow is inherently unsteady, then we will have to reach a dynamically steady state condition.

So, with this, we will finish this lecture today. In the next lecture, we can probably discuss about obtaining faster convergence and few other concepts of relevance.

Thank you very much, thank you.