Computational Fluid Dynamics and Heat Transfer
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Lecture - 22
A Finite Volume Method to solve Three-dimensional NS Equations in Complex Geometry

Good morning everybody, today we will start a new topic on Finite Volume Method to solve Three-dimensional Navier Stocks Equations in Complex Geometry.

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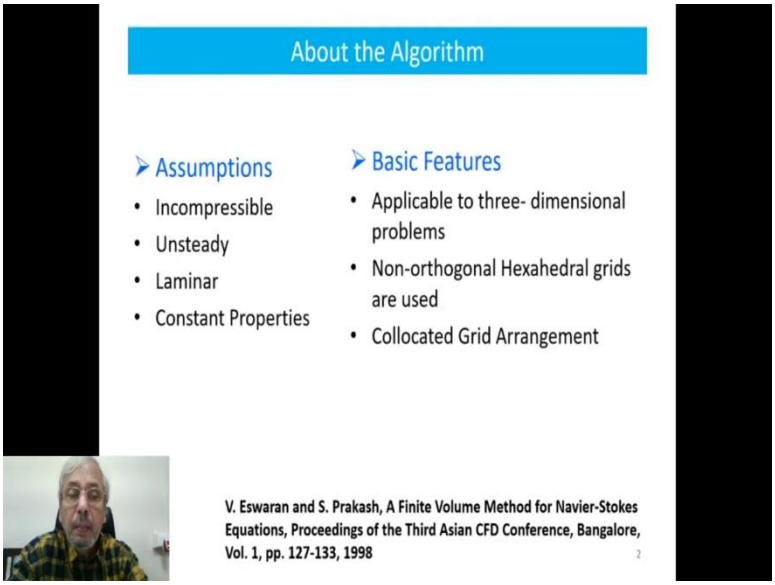

Here the assumptions are the following flow is incompressible, it is unsteady flow, laminar. Of course, laminar assumption per say it has been mentioned, but even if the flow is turbulent, we can use the same algorithm through appropriate turbulent flow models; to appreciate turbulence models and there are ways to handle the issues of turbulence, but same algorithm can be enhanced.

But, right now maybe you know for the purpose of it we can say that flow is laminar and constant properties all the properties are constant. Basic features this is applicable to three-dimensional problems. And the grid is such that elements are all non-orthogonal hexahedral, basically in order to mesh a geometry the body fitted coordinate is used and the grid meshes are such that it fits in the geometry appropriately.

While doing so the individual elements those are hexahedral with different sizes and different orientations and here, we will use collocated grid arrangement. That means, all the dependent variables $u\ v\ w\ p$ and temperature (T) will be defined at the same location at the center of the cell.

A basic version of this algorithm was presented by professor Eswaran and Doctor Satya Prakash in a conference at Bangalore and this version was developed by professor Eswaran and Doctor Satya Prakash completely indigenously in 1998. Later on, some work was done and work is still going on for further improvement. I will mention about those aspects at the end of the lecture.

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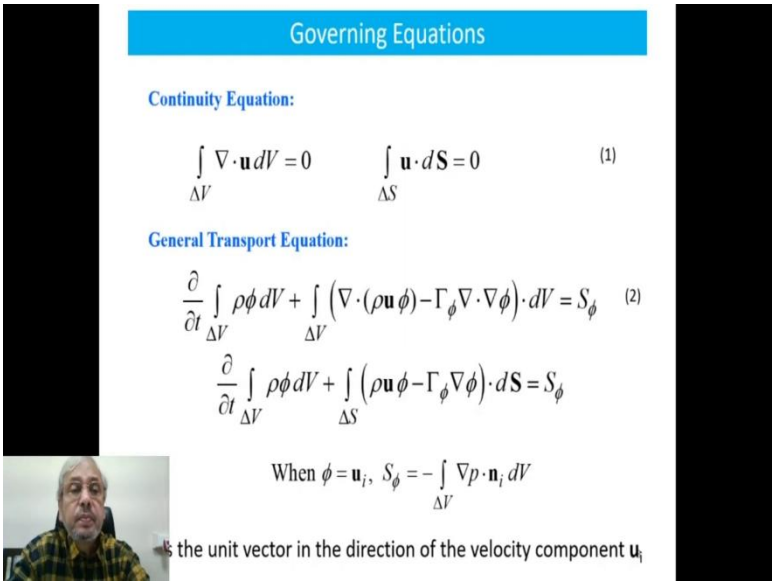

Now, governing equations are obviously first equation comes Continuity equation, that is divergence of velocity vector in a flow field is zero and in a in an element of course, it is zero and we have the written volume integral of divergence of velocity vector over the control volume of interest equal to zero.

Then we have converted that volume integral into surface integral. Now, general transport equation this equation 2 (Refer Slide Time: 03:47) is basically Navier Stokes equations in

three-dimensions and it can be representative equation for the scalar transport. That means, for temperature or for energy transport as well.

And we have written the generalized form as you can see this is basically $\frac{\partial}{\partial t}\int_{\Delta V}\rho\phi dV + \int_{\Delta V}\left(\nabla.(\rho\mathbf{u}\phi) - \Gamma_\phi\nabla.\nabla\phi\right).dV = S_\phi$.

Basically, this will produce something like $\nabla^2\phi$ type of terms, together with diffusion coefficient it is basically the diffusion either momentum diffusion or energy diffusion and it is integrated over the volume of interest and this is the source term.

So, this is the generalized way of writing this, here we combined the convection and diffusion part so together and evaluate this volume integral through the surface integral basically the confining surfaces. And we apply the mass lumping here. So, basically this $\frac{\partial}{\partial t}\int_{\Delta V}\rho\phi dV$ is basically mass and into ϕ, it is $\frac{\partial}{\partial t}$ of that quantity.

And this source term as you can see in the Navier Stocks equations x y and z direction or you know 3 perpendicular directions it is ∇p dot n dV. So, pressure gradient forms the source term similarly we will have to write corresponding source term in the energy equation when we reuse this equation as the energy equation. So, $\mathbf{n_i}$ is the unit vector in the direction of the velocity component $\mathbf{u_i}$.

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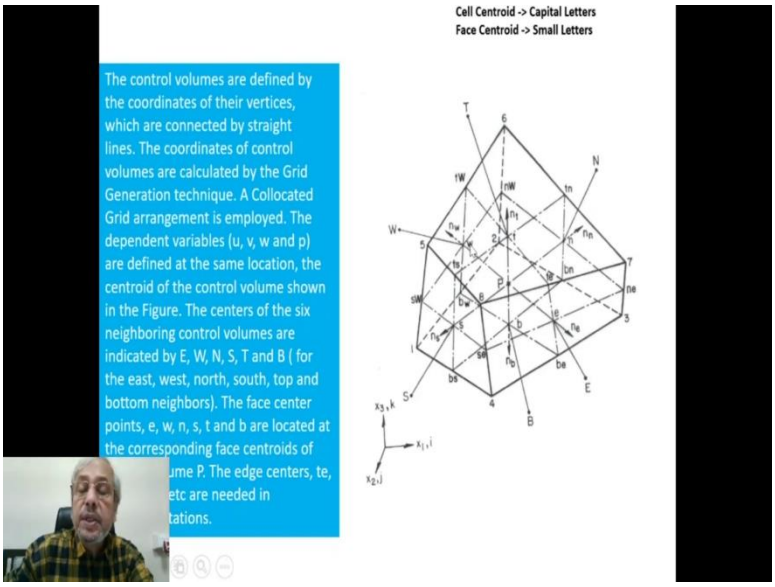

Now, the control volumes I have already mentioned are defined by the coordinates of their vertices, you can see 1, 2, 3, 4 then 5, 6, 7, 8 coordinate of their vertices which are connected by straight lines. So, as you can see 1 2, 2 3, 3 4, 4 1 similarly 5 6, 6 7, 7 8, 8 5 these are connected through straight lines.

The coordinates of control volumes are calculated by the grid generation technique a collocated grid arrangement is employed. The dependent variables u, v, w and p are defined at the same location the centroid of the control volume shown in the figure. The centers of the six neighboring control volumes, so center of this control volume is p and centers of the neighboring control volumes.

If you imagine another control volume on the eastern face center of that control volume is e upper case E. Similarly, if there is another control volume just on the western side of it center of that control volume is given by upper case W. Similarly upper-case N, upper case S, upper case T and upper-case B, so for the east, west, north, south, top and bottom neighbors neighboring control volumes.

The face center points here we can see that face center point of eastern face is given by lower case e and the western face also it is given by lower case w, similarly lower-case n, lower case s, lower case t and lower-case b are located at the corresponding face centroids of the control volume of b.

The edge centers like if we if you consider this as one edge or this side as one edge, so they are also the center of the edges are called as ah. For example, here it is te and this center is given by be, similarly this center of the edge is given by ne.

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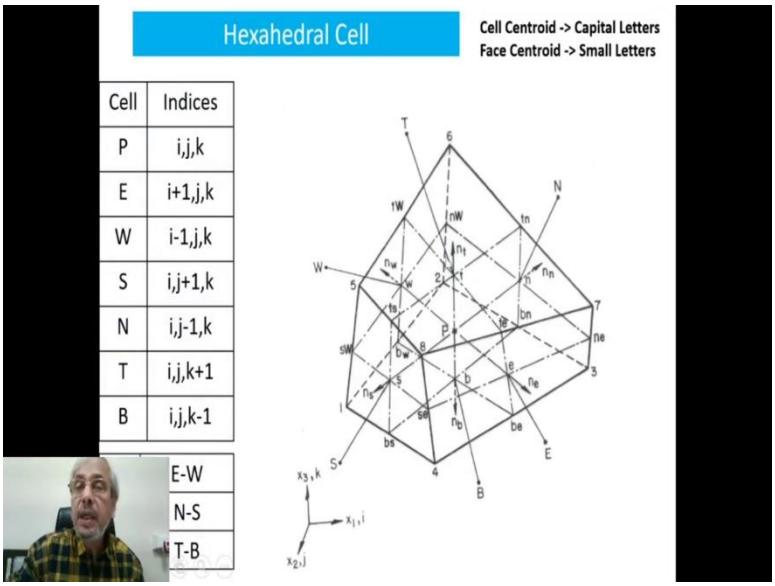

And so when we go for i, j, k indices then this is the cell of interest we are calling P cell, so the indices are i, j, k . So, i, j, k cell is basically the P cell. Similarly eastern neighbor cell, cell which will located at the eastern neighbor it will be identified as $i + 1, j, k$, western neighbor that cell is identified as $i - 1, j, k$, Southern neighbor will be identified as $i, j + 1, k$; j is basically as you can see j is in this direction and this is increasing j direction.

So, $i, j + 1, k$; Northern neighbor $i, j - 1, k$;, Top neighbor is $i, j, k + 1$ and Bottom neighbor is $i, j, k - 1$ and East West direction variation is the variation in i. As you can see that eastern side i is increasing $i + 1$ $i + 2$ and western side i is decreasing you know $i - 1$ $i - 2$ etcetera.

Similarly, j is in North South direction, so j is increasing in southern direction $j + 1$

$j + 2$ etcetera j will decrease in northern direction $j - 1$ $j - 2$ etcetera and k is in top and bottom direction. So, basically $k + 1$ $k + 2$ is in the you know top direction and the bottom direction it will be $k - 1$ $k - 2$ etcetera.

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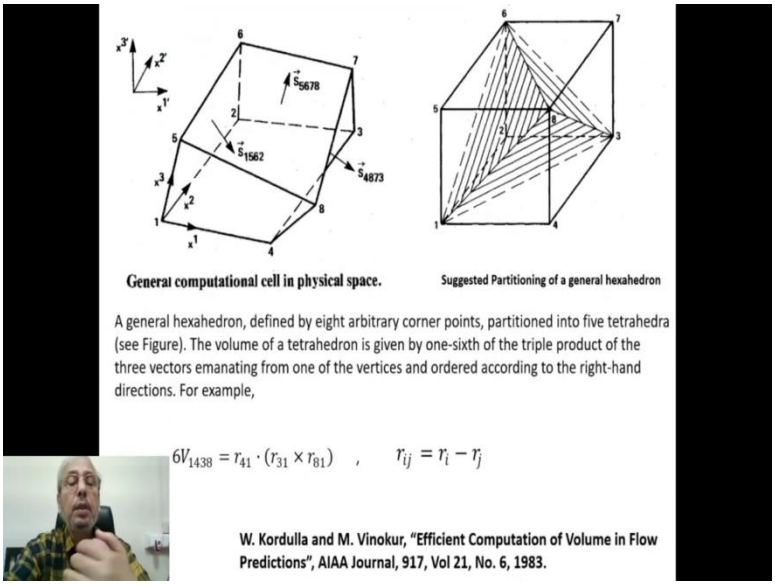

So, that is basically the grid topology. Now, we will discuss how to calculate the volume of hexahedral and the volume of tetrahedrons, this is a very important aspect and this topic was discussed in detail in a very well known well referred paper of Kordulla and Vinokur which was published in AIAA Journal in 1983.

Now, let us consider a general hexahedron defined by 8 arbitrary corner points like you know 1, 2, 3, 4, 5, 6, 7, 8. Now, this hexahedron can be divided into five tetrahedrons right, five tetrahedral and we can calculate volume of each tetrahedron. Like you know here we can divide it in such a way that we can get the following tetrahedral 1 is given by 1, 4, 3, 8, another is given by 1, 6, 5, 8 another is given by 3, 6, 7, 8.

It is clear one is given by 1, 4, 3, 8 another is given by 1, 6, 5, 8 another is given by 3, 6, 7, 8. So, these 3 plus 2 more those 2 more are 1, 6, 3, 8; 1, 6, 3, 8 is one; another is 1, 6, 3, 2 so these are the five hexahedrons. And we know how to calculate volume of such hexahedrons like you know that is written here also, it is given by one-sixth of the triple product of the three vectors emanating from one of the vertices and ordered according to the right-hand directions.

For example, how to calculate volume of tetrahedron given by 1, 4, 3, 8? And it is then according to what we have written it is triple product that means and triple product of the vectors emanating from one of the vertices. So, from 1 the basically the vectors are then

we can say 4 1, 3 1 and 8 1. So, triple product of r_{41} r_{31} and r_{81} divided by 6 is the volume of the tetrahedron 1438.

So, it is given by one sixth of the triple product of the three vectors emanating from one of the vertices and the vectors are defined as $r_{ij} = r_i - r_j$. So, we can write then 6 times volume of 1438 equal to r_{41} multiplied by r_{31} into r_{81}. So, this way if we can calculate individually the volumes of 5 tetrahedral, then we will get the total volume of the hexahedron.

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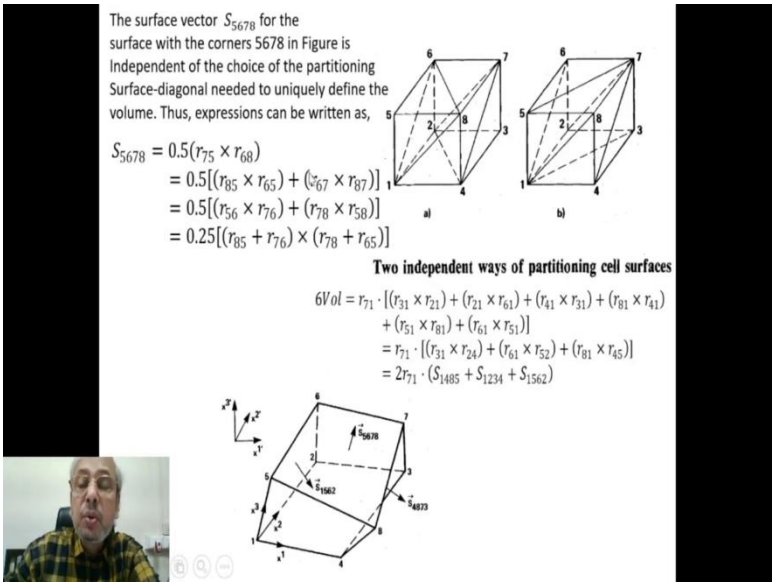

Now, following these two more short discussions, but as I said this Kordulla's paper is very important paper and many of you may be interested in that I have given the reference please try to have a look at the paper and read the paper if possible. The surface vector S_{5678}, whether you calculate here S_{5678} or S_{5678}? In figure is independent of the choice of the partitioning surface diagonal. See once we have partitioned it this way the 6 8 is the surface diagonal at another instant, we have partitioned it this way 5 7 is considered as the surface diagonal.

So, basically independent of the choice of the partitioning surface diagonal needed to uniquely define the volume, thus expressions can be written as so S_{5678} we have given the expressions like you know 0.5 into r_{75} into r_{68} and there are all these options are possible.

And these are independent of dividing the surface by the diagonal whether this diagonal or this diagonal we can get these expressions and they mean basically is 5678. So finally, what is very important for us that for some such you know arbitrary hexahedral, how to calculate it is volume and we have written that you can bring 6 to right hand side that then volume will be $r_{71}/3$; 71 means this diagonal which connects point 1 and 7 r_{71} into surface area 1, 4, 8, 5 this surface 1, 4, 8, 5 plus surface area 1, 2, 3, 4.

That means, this surface base with respect to this particular hexahedral and plus 1, 5, 6, 2 that means this surface. So, basically this diagonal emanating from 1 and three surfaces that are also emanating from or connected with 1. So, one surface is 1, 4, 8, 5 another surface is 1, 2, 3, 4 and another surface is 1, 5, 6, 2.

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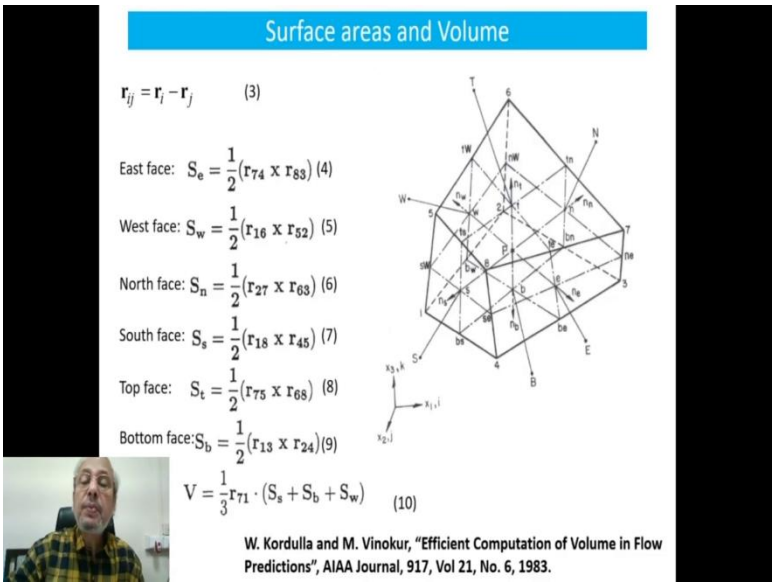

So, having known this if we come back to our hexahedral that we have already defined we can calculate different surface areas like you know eastern surface, western surface, northern surface, southern surface, top surface and bottom surface.

So, these expressions have been given I have been given this surface area of eastern face is given by $\frac{1}{2}(r_{74} \times r_{83})$. Similarly surface area of western surface is given by $\frac{1}{2}(r_{16} \times r_{52})$. Northern face this is the northern face given by $\frac{1}{2}(r_{27} \times r_{63})$. Southern face is given by half surface area is given by $\frac{1}{2}(r_{18} \times r_{45})$.

Similarly, Top surface St is given by $\frac{1}{2}(r_{75} \times r_{68})$ and the Bottom surface is given by $\frac{1}{2}(r_{13} \times r_{24})$ and then just following our previous slide the volume occupied by this particular arbitrary control volume is one third of r_{71} exactly what we did in the earlier slide r_{71} multiplied by surface area of the southern surface. That means, 1, 4, 8, 5 plus surface area of the bottom surface that means 1, 2, 3, 4 plus surface area of the western surface that means 1, 2, 6, 5. So, this is how we will calculate the geometrical parameters, we will see these are extremely important and we will need this at every step of our calculation.

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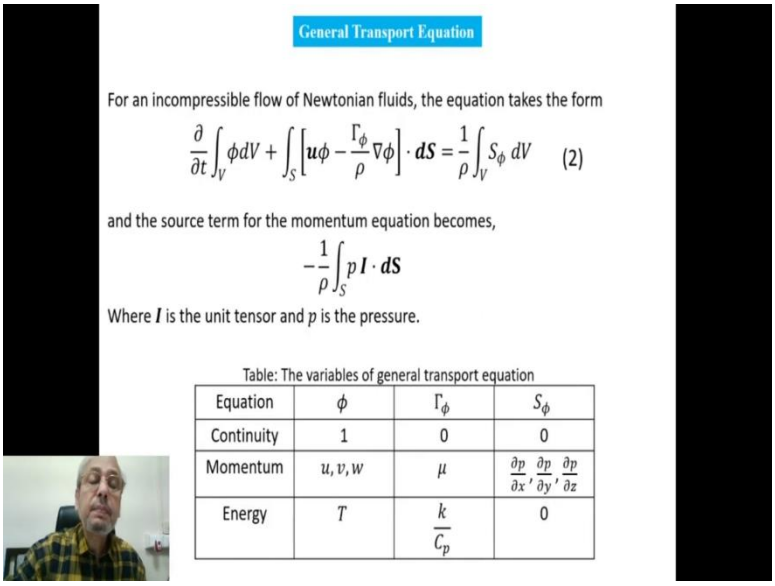

Now for an incompressible flow of Newtonian fluid already we have written this, the general form of governing equation we can write $\frac{\partial}{\partial t}\int_V \phi dV + \int \left[\boldsymbol{u}\phi - \frac{\Gamma_\phi}{\rho}\nabla\phi\right].\boldsymbol{dS} = \frac{1}{\rho}\int_V S_\phi dV$. So, uppercase u, u ϕ minus Γ_ϕ this is the coefficient of transport, momentum transport or thermal transport. In the case of Navier Stokes equations, it (Γ_ϕ) is coefficient of viscosity by rho into grad phi dot dS surface vector equal to 1 by ρ this is the source term integrated over the volume S_ϕ. And the source term for when we are considering this as momentum equation then source term will be the pressure term.

So, this is 1 by ρ surface integral of p into I, I is unit tensor it will be given by 1 0 0 0 1 0 0 0 1 dot dS. Now, the variables so this is we are calling this as general transport equation, because the same equation can be used for continuity momentum and basically energy.

When we consider continuity equation then basically ϕ will be 1 and this term and these two terms will be 0, in order to make them 0 that you know Γ_ϕ phi is 0, S_ϕ is 0.

When it is momentum equation this ϕ will be u, v and w and Γ_ϕ will be μ coefficient of viscosity and S_ϕ will be $\frac{\partial p}{\partial x}$ x momentum equation, $\frac{\partial p}{\partial y}$ for y momentum equation and $\frac{\partial p}{\partial z}$ for z momentum equation. And for the energy equation ϕ will be T and basically this Γ_ϕ will be k/C_p because ρ is already there ok, this term has to be k/C_p.

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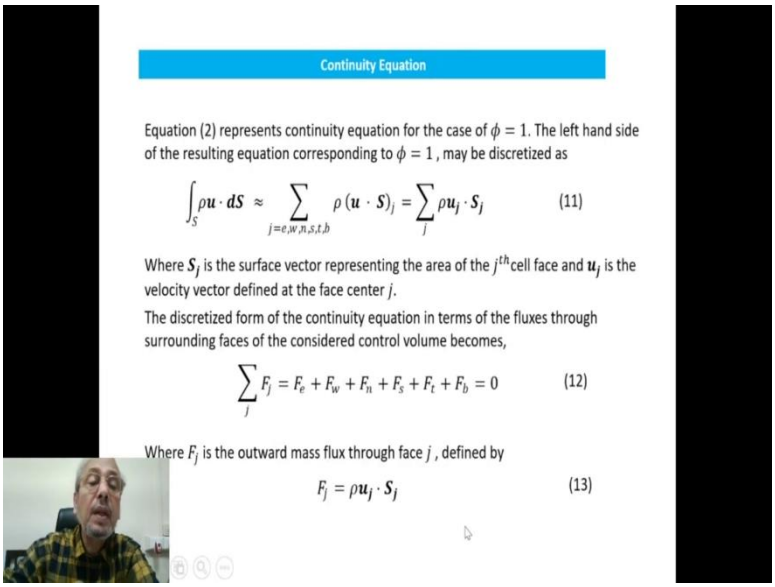

Now, again let us you know refer to the general equation 2 and try to get the expression for Continuity Equation. So, in order to get the expression for continuity equation we have to substitute ϕ equal to 1 and we have also seen that source S_ϕ will be 0 and the coefficient of diffusivity that means Γ_ϕ will be also 0.

So, only the first term well be there which will contribute as surface integral of $\rho \mathbf{u}. S_j$ and that means in this case it is basically summation of $\rho \mathbf{u}. S_j$ surface; whereas, j means eastern, western, northern, southern top and bottom surfaces. So, it is $\sum_j \rho \mathbf{u_j}. s_j$.

Now, $\boldsymbol{S_j}$ is the surface vector representing the area of the i^{th} cell face and u_j is the velocity vector defined at the cell center of j or j surface. The discretized form of continuity equation in terms of the fluxes through surrounding surfaces of the control volume, then will be summation of F_j, which means $F_e + F_w + F_n + F_s + F_t + F_b$.

And this summation obviously there will be no mass accumulation or no mass deficiency will be 0. So, where F_j is the outward mass flux through face j, defined by F_j equal to $\mathbf{u_j}.S_j$ and this **u** is vector. So, all the components of the velocity and $\boldsymbol{S_j}$ is the surface vector, vector representing all the surfaces each one of the surfaces.

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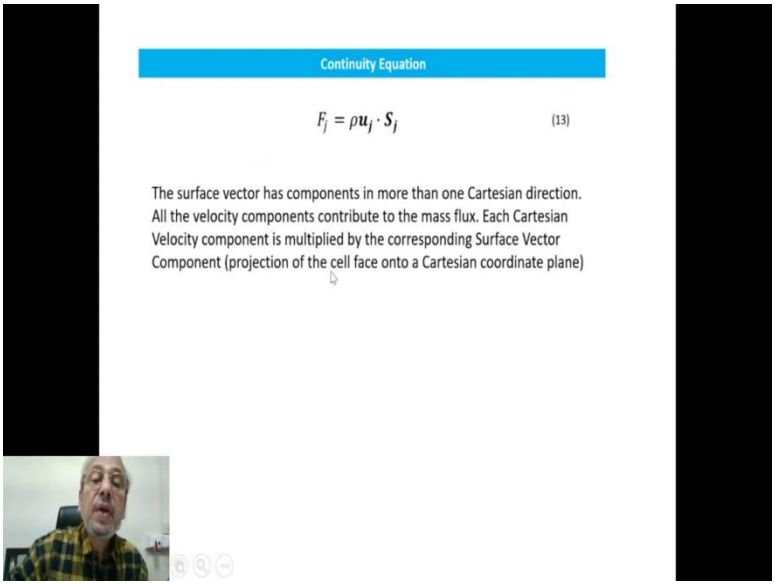

So, we can write $F_j = \rho u_j.S_j$ and we can further explain it that the surface vector has components in more than one Cartesian direction, all the velocity components contribute to the mass flux. So, each Cartesian velocity component is multiplied by the corresponding surface vector component.

So, each surface vector will have components in three Cartesian directions and we have three Cartesian velocity components. So, that is why each Cartesian velocity component is multiplied by the corresponding surface vector component projection of the cell face onto Cartesian coordinate planes and then we evaluate this. This way we evaluate $F_j = \rho u_j.S_j$.

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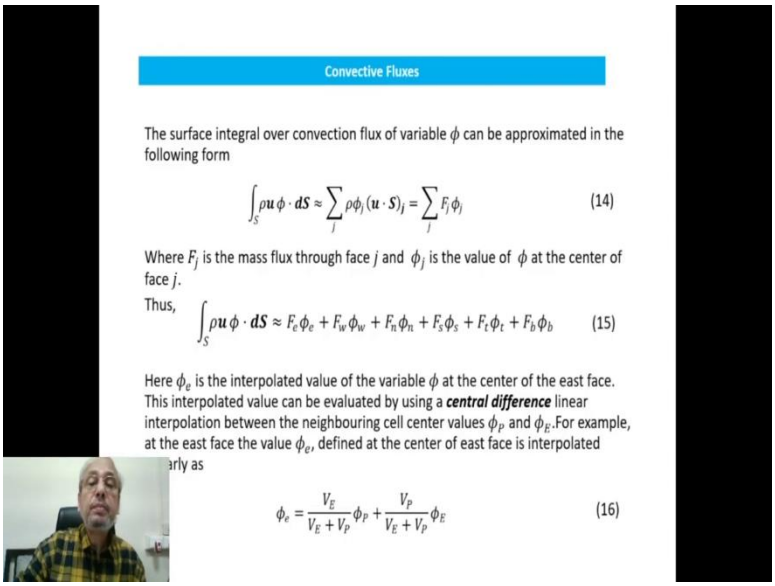

Now, we go to the convective fluxes now surface integral over convection flux of variable ϕ can be approximated in the form that this is also through all the confining surfaces. So, integral over the surfaces $\rho u\phi.dS$ $(\int_s \rho u\phi.dS)$. So that means summation over j , $\rho\phi_j(u.S)_j$, which again if we plug in our F definition we will get $\sum_j F_j\phi_j$.

Where F_j is the mass flux through face j and ϕ_j is the value of ϕ at the center of the cell, this ϕ can be any quantity that can be convected. So, it can be 3 velocity components u, v, w it can be temperature. So, this is how we define$\sum F_j\phi_j$. So, $(\int_s \rho u\phi.dS)$. we can write this now then $F_e\phi_e + F_w\phi_w + F_n\phi_n + F_s\phi_s + F_t\phi_t + F_b\phi_b$ all are summations.

Here for example, ϕ_e is the interpolated value, see e is the midpoint of the eastern small e is the midpoint of the eastern cell face. So, ϕ_e is the interpolated value of the variable phi at the center of the face. This interpolated value can be evaluated very simply by taking a central difference, which is basically linear interpolation between the neighboring cell center values.

That means, the cell of interest we have already defined is P and at the center ϕ is ϕ_P and eastern neighbor at the center ϕ is defined as ϕ_E. For example, at the east face that means ϕ_e defined as the center of east face and this will be interpolated using the values of the ϕ defined at the cell P and ϕ defined at the cell E eastern neighbor.

So ϕ_e this is linear interpolation but central reference we can see so V_E volume of eastern neighbor divided by volume of eastern cell plus volume of the cell of interest P into ϕ_P plus volume of P cell of interest divided by total volume. That means, volume of E and volume of P into ϕ whether ϕ_E is defined at the center of volume E and ϕ_P is defined at the center of volume P. So, this way we can do the basically taking either side of the cell face and do the linear interpolation following a central difference philosophy.

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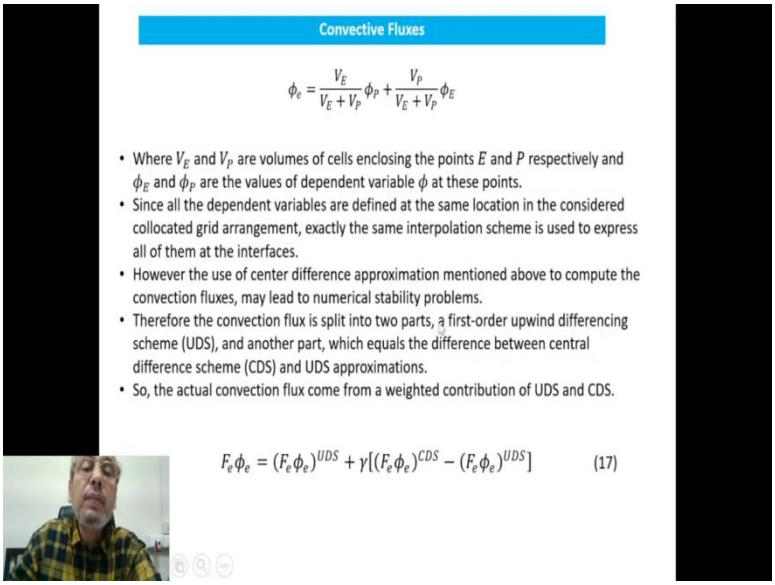

So, ϕ_e equal to V_E we have written it again divided by V_E plus V_P multiplied by ϕ_P plus V_P divided by V_E plus V_P multiplied by ϕ_E. Where V_E and V_P are volumes of cells enclosing the points E and P respectively and ϕ_E and ϕ_P are the values of independent variable ϕ at these points that is what we are explaining.

$$\phi_e = \frac{V_E}{V_E + V_P}\phi_P + \frac{V_P}{V_E + V_P}\phi_E$$

So, basically the eastern neighbor volume of that cell is V E and ϕ_E is defined at it is center cell of interest volume is V P and ϕ_P is defined at it is center. And this is way at the eastern cell face center we define through the interpolation.

Since all the dependent variables are defined and the same location in the collocated grid arrangement, exactly same expression or same interpolation scheme will be used to

express all other dependent variables, that means u velocity, v velocity, w velocity p all the quantities will be interpolated can be interpolated following this philosophy.

However, the use of central difference a center difference approximation mentioned above to compute the convection fluxes, may lead to numerical stability problems, that we have seen earlier also that central difference sometimes for high velocity flows I mean can give stability problem.

Therefore, the convection flux is split into two parts, a first-order upwind differencing upwind difference scheme we are calling it UDS, and another part which equals the difference between central difference and upwind difference approximation.

So, upwind difference scheme plus difference between central difference and upwind difference so; that means, $F_e\phi_e = (F_e\phi_e)^{UDS} + \gamma[(F_e\phi_e)^{CDS} - (F_e\phi_e)^{UDS}]$ means in the differentiation we will involve the upstream point, depending on the direction of the velocity.

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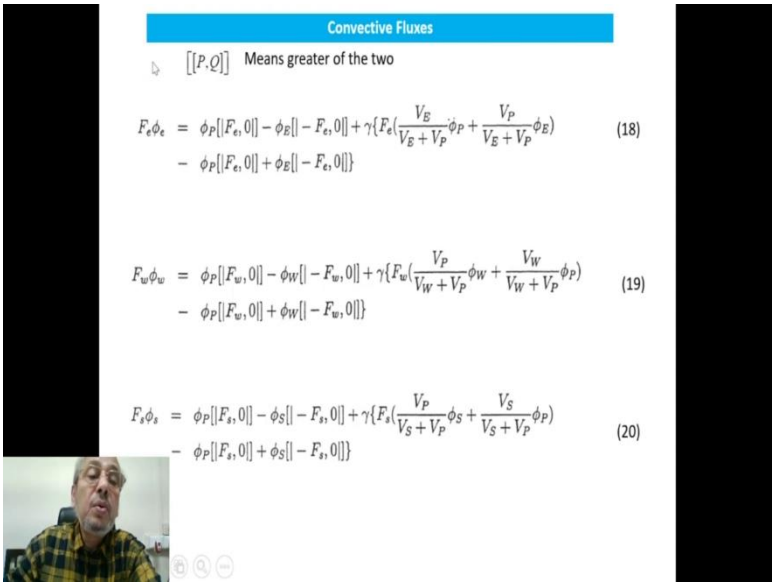

So, now from this philosophy $F_e\phi_e$ what we have written here, if we want to write it in computational algorithm then we have to write ϕ_P within this bracket F_e comma 0 minus ϕ_e within this double racket minus F_e comma 0 plus gamma, gamma is a fraction and multiplied by the central difference minus we are calling this upwind difference.

$$F_e\phi_e = \phi_P[|F_e, 0|] - \phi_E[|-F_e, 0|] + \gamma\left\{F_e\left(\frac{V_P}{V_E + V_P}\phi_P + \frac{V_P}{V_E + V_P}\phi_E\right) - \phi_P[|F_E, 0|] + \phi_E[|-F_e, 0|]\right\}$$

Now, if you look at it typically this will involve up stream point depending on the direction of the velocity and that is why this special symbol has been used, which is double bracket. And this double bracket means if we write the P, Q inside a double bracket which will mean greater of the two, right. So, velocity can be negative in that case you know this will be minus F_e will be greater of the two so and if it is positive then obviously it will be greater of the two.

So, this will eventually decide the depending on direction of velocity will involve the upstream point ϕ_P of ϕ_E and this is the central difference. So, you can see this symbol double bracket has substituted when we define this you know, if you recall that involvement of upstream points through the modulus sign in several schemes, we have done so far, we have done that so and it is just equivalent to that.

Now $F_w\ \phi_w$ following the same philosophy this is basically central difference and this is sorry this is basically upwind difference and this is basically a factor multiplied by central difference minus upwind difference. Same here this is upwind difference this is a factor multiplied by curly bracket is getting closed here inside we have central difference minus upwind difference.

So, this is you know flux at eastern surface, convective fluxes western surface, convective fluxes southern surface in the same way just you have to follow the expressions and look at how we have applied upwind differencing by involving up stream point $F_n\phi_n$, $F_t\phi_t$ and $F_b\phi_b$ bottom surface, top surface, northern surface and everywhere basically we have taken UDS plus central difference minus UDS minus upwind difference scheme. So, this is how we can compute the convective fluxes.

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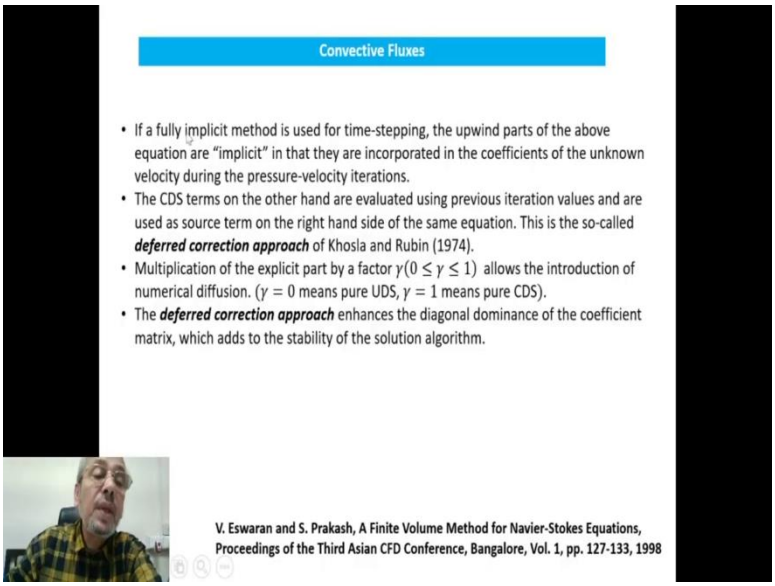

If a fully implicit method is used for time stepping the upwind parts of the above equation are implicit and they are incorporated in the coefficients of the unknown velocity during pressure velocity iteration. This I will explain again while doing the pressure-velocity iterations. The central difference terms on the other hand are evaluated using previous iteration values and are used as source term on the right-hand side of the same equation.

This is the so-called deferred correction approach. If you recall our first preliminary few lectures when we introduced finite difference, finite volume methods we refer to the scheme very well-known scheme Khosla and Rubins scheme is called deferred flux correction approach. Professor Prem Khosla and professor Stanley Rubin, they formulated it. Multiplication of the explicit part I have already mentioned.

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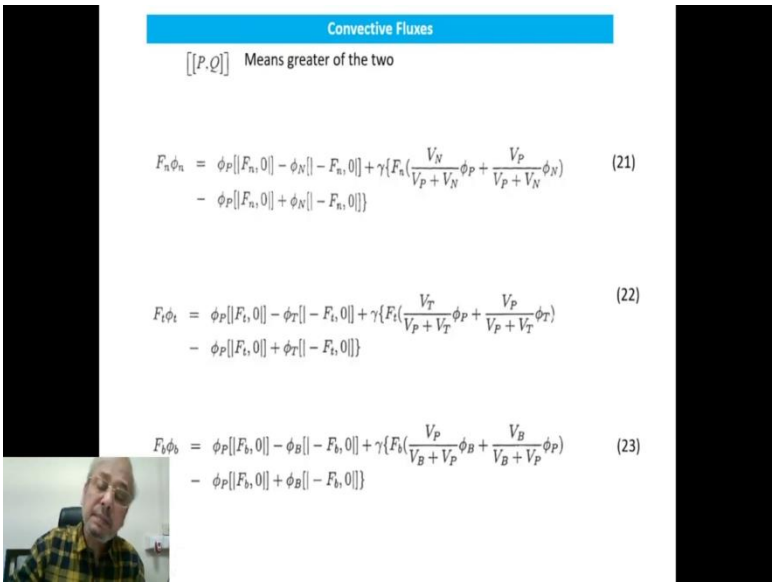

This is a; this γ is a factor which is basically a fraction. So, this factor γ which lies between 0 and 1 allows the introduction of numerical diffusion. If γ equal to 0 this means pure upwind differencing if γ equal to 1 means pure central differencing. So, here basically we have to since you know if you compare it with the schemes, we used for simply learn math, there also we used something like alpha which varied between 0 and 1.

But there when it was tilting towards 0 it was getting closer to central difference when it was you know tilting towards 1 it was shifting towards upwind difference here it is just little different. When γ is 0 it is upwind difference pure first order upwind and γ equal to 1 is pure central difference second order central difference. So, for higher accuracy we can go for gamma which is on the side of 1.

The differed correction approach enhances the diagonal dominance of the coefficient matrix, when we will arrange this, you know pressure iteration matrix we will again discuss it. But it is better to mention here now that differed correction approach enhances the diagonal dominance of the coefficient matrix, which adds to stability of the solution algorithm.

So, we have discussed today about the discretization of the continuity equation following finite volume approach on arbitrary shaped hexahedral and also, we have discussed about calculation of convective fluxes. In the next class we will take a diffusive flux and setting

up the pressure velocity correction scheme and we will discuss about the complete solution algorithm.

Thank you very much, thank you.