Computational Fluid Dynamics Using Finite Volume Method
Prof. Kameswararao Anupindi
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 25
Finite Volume Method for Diffusion Equation: Steady diffusion in unstructured meshes Part 2

Good morning let us get started. So, we were discussing about unsteady sorry Steady Diffusion in non orthogonal unstructured meshes right.

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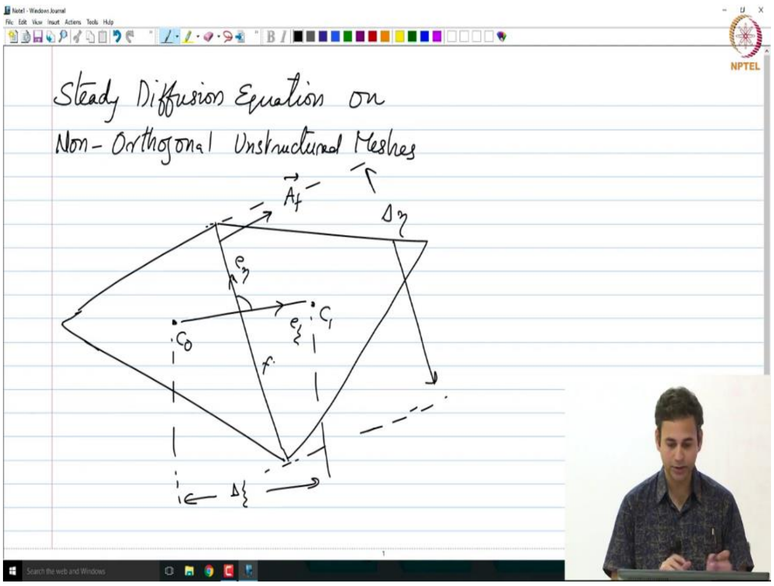

So, we kind of formulated the diffusion part of the equation right. So, we will continue with that is basically steady diffusion equation on non orthogonal unstructured meshes right. So, we have drawn a kind of a schematic for our notation for discretizing the equation right.

So, that was we have a C_0 cell and we have a C_1 cell we have the C or $\vec{\mathrm{A}}_\mathrm{f}$ and we happen to have a cell like this all right. So, this is our C_0 cell centroid this is our C_1 cell centroid right and then the line connecting them is along e_ξ which is not parallel to $\vec{\mathrm{A}}_\mathrm{f}$ ok. And then we have e_η and the angle between m is not 90 degrees right, so that is what we have.

And then we have of course, also defined delta xi as this distance. And we said with this is this would be our delta eta right the magnitude of the area vector right. That is all we have defined and then this is our face f ok. So, that is what the schematic we had and then we discretize the diffusion equation. So, diffusion equation came out to be how much? We did discretization basically gives you $(\Gamma\nabla\phi)_f \cdot \mathrm{A_f}$ sigma on all the faces plus $(S_\mathrm{C} + S_\mathrm{P}\phi_0)\Delta V_0$ equals 0 right.

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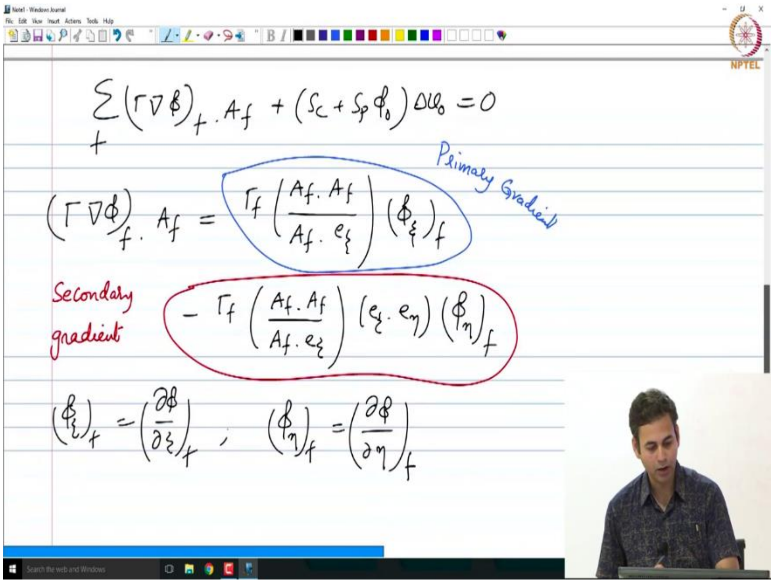

So, we said 0 cell is nothing but our p cell which is the primary focus and then we have three other neighbours which are one first cell second cell and third cell right. So, we have three more cells there fine then we formulated the value for the $(\Gamma\nabla\phi)_f \cdot \mathrm{A_f}$ right.

So, how much was that? $(\Gamma\nabla\phi)_f \cdot \mathrm{A_f}$ this came out to be a long expression right in terms of $\frac{\partial\phi}{\partial\xi}$as well as $\frac{\partial\phi}{\partial\eta}$ right. And that if you help me write it out this would be Γ_f times how much?

Student: $\mathrm{A_f}$ dot (Refer Time: 03:04).

$\mathrm{A_f}$ dot f by.

Student: (Refer Time: 03:07).

$\mathrm{A_f}$ dot e_ξ right that is what we have times?

Student: Partial phi partial (Refer Time: 03:11).

Partial phi partial?

Student: Xi.

Xi of f right and then we have what is the next term?

Student: Minus.

Minus.

Student: Gamma.

Γ_f times we have again the same metric that is A_f dot A_f by A_f dot e_ξ times e_ξ dot e_η right times $(\phi_\eta)_f$ right that is what we have. Essentially we noted that the diffusion flux right is not just ϕ_ξ rather it is a combination of a ϕ_ξ as well as ϕ_η right. These are nothing, but $(\phi_\xi)_f$ is nothing, but $\frac{\partial \phi}{\partial \xi}$ on f and $(\phi_\eta)_f$ is $\frac{\partial \phi}{\partial \eta}$ on the face f right.

So, this is a combination of two of them, which is a consequence of what? Which is a consequence of. Up till now we never got the diffusion flux to be two components right it is always only one of them would survive, what is this a consequence of?

Student: Non orthogonality.

This is a consequence of the non orthogonality of the mesh right. So, as a result we have these two terms which we would like to call it as a primary a gradient right, which is the first term.

We would like to call this as a primary gradient, which is in the direction of xi right. And then the other one we will like to call it as a secondary gradient ok. So, this is everything that is not in the direction of xi ok. So, that is what we would like to term them as.

Now, let us see how do we calculate each of these terms. So, what is the next step? Once we once we got the derivatives in on the faces what is the next step?

Student: Linear (Refer Time: 05:06).

Linear profile assumption right. So, as of now I would make a linear profile assumption only for evaluating $\frac{\partial \phi}{\partial \xi}$ only for the first term for the primary gradient. So, making a linear profile assumption. How do I write $\frac{\partial \phi}{\partial \xi}$ on the face f?

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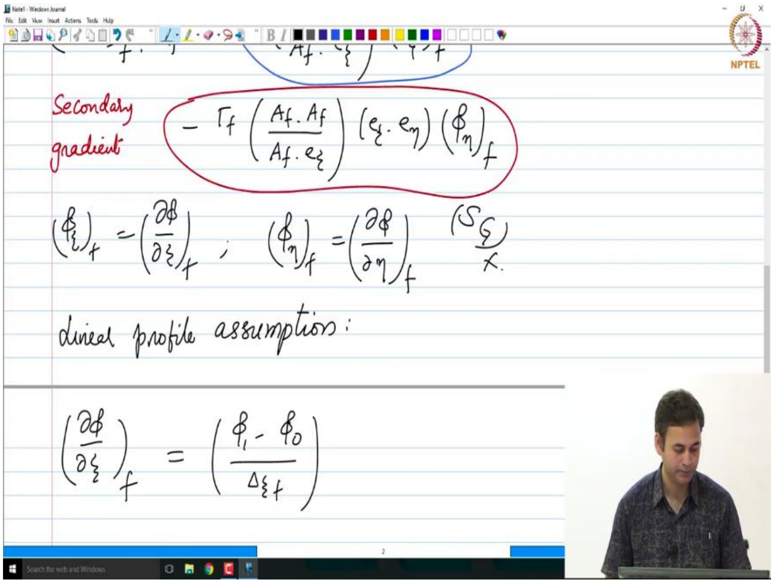

So, we are talking about this face f how do I calculate. So, we know what is ϕ_0 we know what is ϕ_1, because these are stored at the cell centroids what is $\left(\frac{\partial \phi}{\partial \xi}\right)_f$ f?

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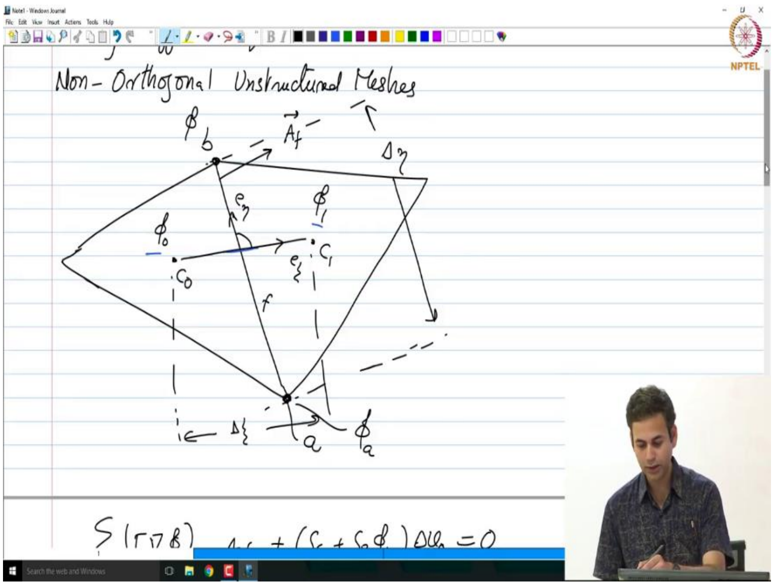

Student: (Refer Time: 05:51).

That is in this direction right, that is in the in this e_ξ direction. How much will that be?

Student: ϕ_1 (Refer Time: 05:56).

ϕ_1 minus ϕ_0 upon, what is the distance?

Student: $\Delta\xi$ (Refer Time: 06:02).

$\Delta\xi$ ok. So, I can write this as ϕ_1 minus ϕ_0 upon $\Delta\xi$ for the face f that is what we have. Note this $\Delta\xi$ sub f needs to be there because $\Delta\xi$ would be different for different faces right. Depending on the cells we are connecting to ok. Now, let us not talk anything about the secondary gradient as of now we would leave it as it is.

I would like to write this entire thing of minus Γ_f, this entire quantity as I would like to represent as some name. Let us call it a secondary gradient sub f ok. $(SG)_f$ which is basically minus this entire thing entire expression.

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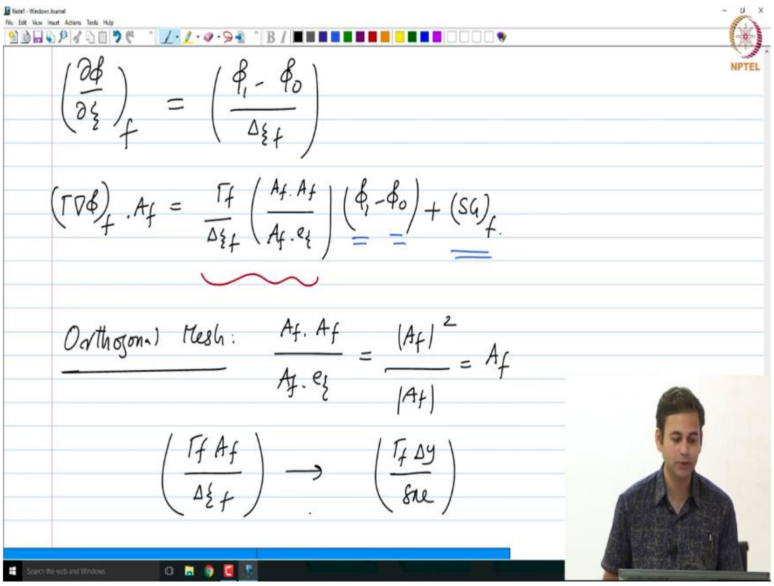

Then what would be my, then what would be the total metric $(\Gamma\nabla\phi)_f \cdot A_f$? It will be basically the primary gradient right with the derivative being replaced with the linear profile assumption right.

So, this will be Γ_f times A_f dot A_f by A_f dot e_ξ times ϕ_1 minus ϕ_0 right. And we have a $\Delta\xi_f$, I would like to write it to here as ϕ_1 minus ϕ_0 by $\Delta\xi_f$ plus we have secondary gradient of f fine. So, now, do you see what is the coefficient for your a_{nb}? What is the coefficient for your a_{nb} terms? This will be the coefficient right.

Whatever is multiplying ϕ_1 would be the coefficient for your a_{nb} right. Essentially $a_E\phi_E$ is what we have written in a Cartesian orthogonal mesh here. The neighbor a_{nb} would be this coefficient right and the same coefficient will also get added to which one?

Student: (Refer Time: 08:05).

a_0, a_P as well right, because you have ϕ_1 and ϕ_0 both of them having the same coefficient. So, the contribution for m from a_{nb} will also go to a_P and also there will be one contribution to a_{nb} also to for phi and b right. That we see of course, we are not talking anything about $(SG)_f$ as of now, fine.

So, let us say if we have an orthogonal mesh. So, if we have an orthogonal mesh what would be this quantity that we have the coefficient, what would this be? This A_f dot A_f by A_f dot e_ξ. A_f dot A_f would be how much? A_f square right this is the magnitude square divided by what would be A_f in the direction of e_ξ?

Student: (Refer Time: 08:56) A_f (Refer Time: 08:57).

That will be A_f right the magnitude. So, essentially this will be A_f magnitude. So, this will be eventually how much?

Student: A_f.

Just the magnitude A_f. So, what will be the coefficient now the for ϕ_{nb}? That will be Γ_f.

Student: A_f (Refer Time: 09:10).

A_f upon?

Student: (Refer Time: 09:13).

$\Delta\xi_f$ do you see that we have got back our orthogonal coefficient. Let us say if one of the cells are all the cells are of orthogonal in nature, then the formula that we have developed will revert back to the right expression in the context of an orthogonal mesh right.

So, this is Γ_f A_f by $\Delta\xi_f$, which this is also in line with the Cartesian values that we have developed before right. How much was the Cartesian thing? That was Γ_f Δy upon.

Student: δx_e.

δx_e right do you see that the correspondence between these two ok. So, if we have an orthogonal mesh the primary coefficients will ok.

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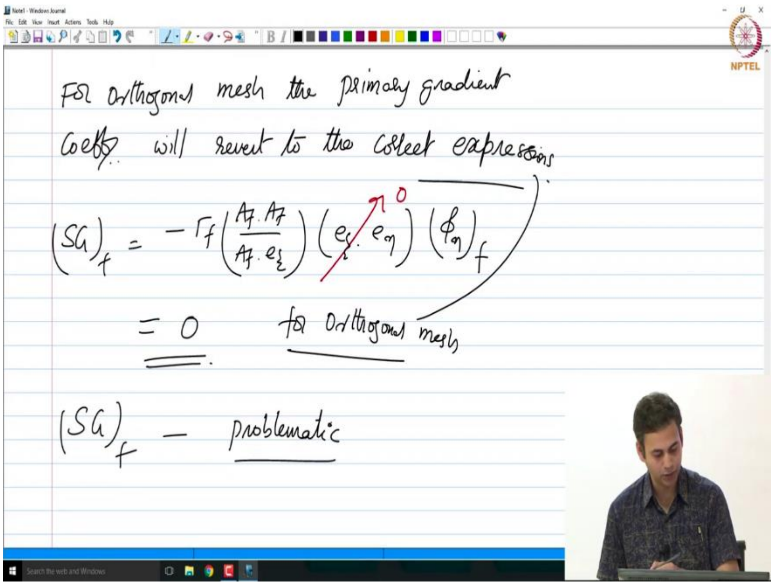

So, for orthogonal meshes the primary coefficients or the primary gradient coefficients will revert to the correct expressions right, they will revert to the correct expressions thereby the formulation will be will be the one which is for an orthogonal mesh ok. What about the secondary gradient? The secondary gradient term would.

Student: (Refer Time: 10:38).

Go to 0 ok. So, why would it go to 0 because secondary gradient term is nothing, but minus Γ_f A_f dot A_f by A_f dot e_ξ times e_ξ dot e_η times phi eta f this would go to 0 because002E

Student: e_ξ (Refer Time: 10:54).

e_ξ i dot e_η would be.

Student: 0.

0 because they are orthogonal all right. So, essentially this term goes to 0 as a result the secondary gradient term goes to 0. And we get back our orthogonal cell formulation in this particular context. Questions? Yes.

Student: (Refer Time: 11:23).

We will revert to the correct expressions essentially right expressions for an orthogonal mesh.

Student: (Refer Time: 11:29).

For an orthogonal mesh correct expressions for orthogonal meshes right. Or the formulae that are derived for orthogonal mesh would be obtained. Fine ok everybody all right with this? Ok. Now, the thing is the calculation of secondary gradient, is somewhat problematic. We say this because we do not have data in the eta direction directly available to us right.

For the primary gradient which is $\frac{\partial \phi}{\partial \xi}$ we have the cell centroid values and we could compute it directly. Whereas, for calculating $\frac{\partial \phi}{\partial \eta}$ what do we have? We can name this as let us say some a or a and b right let us call this as maybe b right that is what we are using b and this vertex as a right.

So, if we want to calculate $\frac{\partial \phi}{\partial \eta}$ we somehow have to calculate ϕ at these vertices right. We need to calculate what is ϕ at b and we need to calculate what is ϕ at a right. But this data is not directly stored right that is not what something is solved for, but how do you calculate ϕ_a and ϕ_b?

Student: Using (Refer Time: 13:03).

Using interpolation right essentially you have several cells using all the cells centroid values you can somehow calculate what is ϕ_a and ϕ_b and then use that values to calculate what is partial phi partial eta all right.

Now, it take turns out that is what we can do in the context of 2 dimensional problems. We will kind of see one by one in under what conditions we can calculate these.

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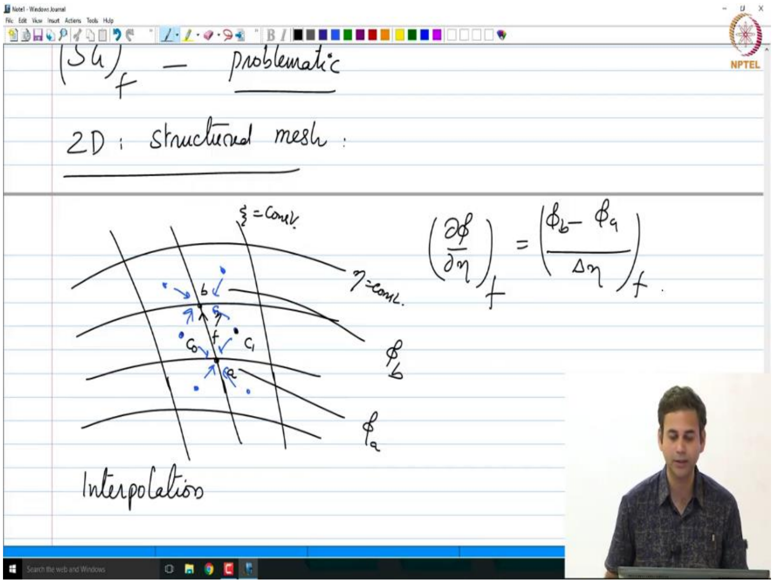

So, let us say if we have a 2 D structured mesh ok. If we have a 2 D structured mesh; that means, we are talking about a 2 dimensional curvilinear mesh right, which could be probably something like this alright.

So, essentially we are talking about a mesh like this where these are maybe some ξ equal constant and then these are η equals constant lines right these will define our cells. This is some kind of a curvilinear coordinates and these are our C_0 C_1 or east and west and so on and we are interested in calculating what is the gradient on this face in this direction right. That is our η direction right or let me write this as ξ equal constant this may not be we changes thing.

So, this is ξ equals constant let us call this as eta equals constant that is what we have and then what would be the gradient in this direction? So, we want to have we call this as b this we will call it as a right and then using these cell centroid values we can calculate the value of ϕ_b right.

Similarly using all these cell centroid values we can calculate the value of ϕ_a right essentially ϕ_b and ϕ_a can be calculated right using all the cell centroid values by using interpolation. And of course, $\frac{\partial \phi}{\partial \eta}$, on the particular face f righ which is an expression inside the secondary gradient can be calculated from ϕ_b and ϕ_a values right. Essentially as ϕ_b minus ϕ_a upon $\Delta\eta$ right on that particular face, right it can be calculated. Of course, you do not have to calculate it this way you can also calculate, what is the gradient at the cell centroids itself right.

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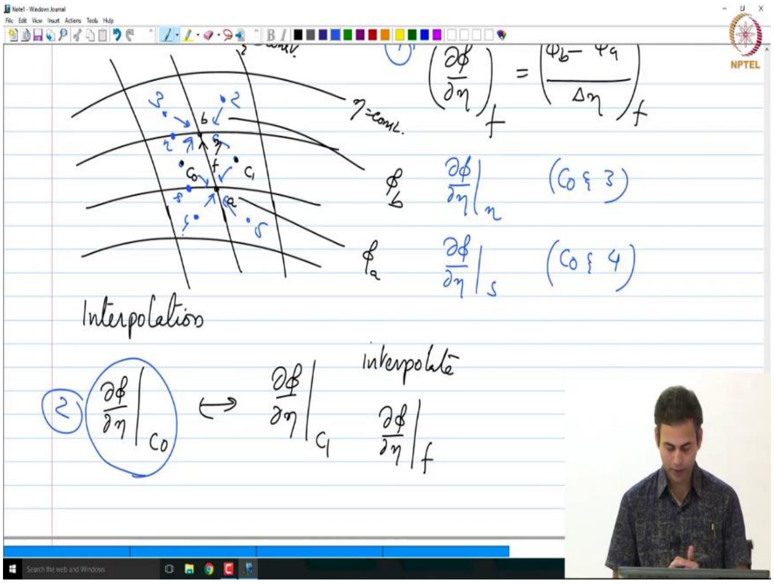

Instead of interpolating phi you can calculate what is $\frac{\partial\phi}{\partial\eta}$ at cell centroid C_0. And you can also calculate what is $\frac{\partial\phi}{\partial\eta}$ at cell centroid C_1 and then interpolate these two to obtain what is $\frac{\partial\phi}{\partial\eta}$ on the particular face f that is shared between these two cell centroids right that can also be done right.

Either you calculate the dependent variable at a and b and calculate the gradient or you directly calculate the gradient at the cell centroids and then interpolate them onto the face do you see that. Either of the methods can be used and we can certainly calculate this. Or is it possible to calculate the same way if we have an unstructured two dimensional mesh? Yes.

Student: (Refer Time: 16:49).

They should give the same answer if your interpolation are?

Student: If we use harmonic interpolation (Refer Slide Time: 16:55).

If use harmonic interpolation?

Student: For calculating the values at b a.

Ok.

Student: (Refer Time: 17:02).

They should actually give the same answer right.

Student: Harmonic interpolation for (Refer Time: 17:07).

For the second method right, then it should give the same answer right. So, these two methods either you calculate it this way or you calculate it this way, would they give the same answer that is the question. They should give the same answer right as long as your methods are correct the interpolation methods are the same, it will give you the same answer ok. Now, what will happen in the context of a 2 dimensional unstructured mesh? Can we calculate it in a similar way?

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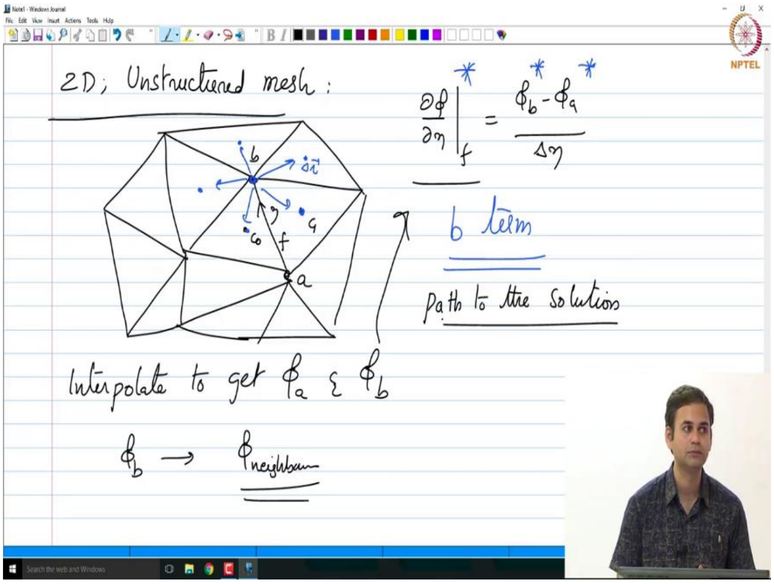

We are talking about a 2 D unstructured mesh.

Student: (Refer Time: 17:42).

So, the question is how do I calculate this quantity at the cell centroid?

Student: (Refer Time: 17:49).

All right, how do I calculate $\frac{\partial \phi}{\partial \eta}$ at C_0? how do you calculate it? you would need.

Student: (Refer Time: 17:57).

Yeah essentially you would need the north and the south values here right. So, one way is to basically calculate $\frac{\partial \phi}{\partial \eta}$, $\frac{\partial \phi}{\partial \eta}$ here and then average them right. Are you some kind of interpolation?

So, on the north face you would use a let me number these things this is 1 let us me this is 2, 3 4 and 5 ok. So, essentially you would calculate $\frac{\partial \phi}{\partial \eta}$ on the north face right which is coming from C_0 and 3 right and similarly you would calculate in the south face. So, $\frac{\partial \phi}{\partial \eta}$ on the south face you will calculate from whom? C_0 and cell 4 right, and then interpolate them right.

Essentially you got it on the phases and then you can interpolate that is one way. Of course, you can also use directly the 3 and 4 values and then calculate also right. So, it depends on the order of accuracy of the method that you are using ok. There is no single way to do this right you can also have a bigger stencil and then include more cells as well right. Any other questions?

So, there are essentially several methods we are not going into how exactly do I calculate, but given the cell values we can calculate these things right ok. That is clear, fine any more questions on this part $\frac{\partial \phi}{\partial \eta}$? No ok that is good. Then what about if we have a 2 D unstructured mesh, can we use a similar strategy to calculate the $\frac{\partial \phi}{\partial \eta}$ or not?

Student: (Refer Time: 19:41).

If we have a 2 D unstructured major means. Let us say we have a triangular cells right, which we have started off with. So, essentially we have some triangular mesh. So, can I do a similar strategy? So, we have C_0 and C_1 we call this as b. We call this as a can we of course, interpolation method has to be now generic you know such that it can interpolate for this unstructured mesh right. But somehow if let us say we know how to interpolate on this unstructured mesh can we apply a similar strategy/

Student: (Refer Time: 20:24).

Right, we can calculate what is ϕ_b, we can calculate ϕ_a and then calculate what is $\frac{\partial \phi}{\partial \eta}$ right. That is basically in this direction I can calculate $\frac{\partial \phi}{\partial \eta}$ on this particular face, from ϕ_b minus ϕ_a upon $\Delta\eta$ right. Can I do that? Essentially obtain interpolate to get ϕ_a and ϕ_b and thereafter apply this formula and then calculate what is $\frac{\partial \phi}{\partial \eta}$ all right.

Student: How do I interpolate?

How do I interpolate is the question. So, I have cell values stored at here let us say I am talking about ϕ_b then I have these cell values. I somehow have a generic 2 dimensional interpolator which will interpolate these and calculate what is ϕ_b all right.

Student: (Refer Time: 21:18).

It need not be symmetric it depends on the, whatever is the $\overrightarrow{\Delta r}$ that we have with this. And then you would have another $\overrightarrow{\Delta r}$ and so on right from there you can calculate fine.

So, in principle this can be obtained alright, then we can certainly calculate, what is $\frac{\partial \phi}{\partial \eta}$ and then move on with the calculation right. Any questions? No feels fine. What is the unknown we are trying to solve?

Student: Phi.

Phi, but what are we trying to calculate here?

Student: Gradients.

Gradients of ϕ; ϕ itself is not known right, we are trying to calculate gradients of ϕ_and then we are happy with it right we are calculating, but what is the catch here? How are we calculating gradients of ϕ, using which values?

Student: (Refer Time: 22:18) iteration.

Using previous iteration value that means these are all what?

Student: Provisional values.

Star values now these are all the provisional values. Now, when you put in a star value there will this going to the coefficient matrix on the left hand side? a. We have let us say a phi equal to b where will these terms go these contributions?

Student: (Refer Time: 22:36).

They should all go to the right hand side b right; they will all go to the b term that is what I wanted to draw your attention. So, only the coefficients that are arising out of the primary gradient will go into the coefficient matrix a_P and a neighbours. And all these guys will go into the right hand side vector right.

All the secondary gradient stuff as g sub f will all go to the right hand side ok. Now, at the time of convergence what would happen? ϕ_b would be same as ϕ_b star and your secondary gradient would be?

Student: 0.

Obtained exactly it will not be 0 it will be obtained exactly right, that is all correct, fine. Questions no? Clear ok. Let us move on then we have finished a 2 D structure, 2 D unstructured what about a 3 D structured mesh? Yes.

Student: Sir if we are writing ϕ_b as a function of that specified values of p h and (Refer Time: 23:40).

Yeah.

Student: Then we can still include that (Refer Time: 23:43)?.

So the question is cannot I put in the secondary gradient also into the coefficient matrix Right. So, the thing is you are calculating ϕ_b from phi neighbors right. So, cannot I add all of these guys into the coefficient matrix a you can do that, but what would happen, what will happen to the matrix?

Student: (Refer Time: 24:09) diagonal dominance.

Diagonal dominance it would not be banded diagonal dominance is one thing. It will not be diagonally dominant we will see why it will not be diagonally dominant what is the other one?

Student: (Refer Time: 24:21).

The bandedness is not anymore valid right. It is kind of we are in an unstructured thing, but still your coefficient matrix will have several terms right, because now up till now only the face neighbors are will enter the coefficient matrix right. For example, if you have a triangle for correspondent to three phases you will have 3 cells, but here the vertex neighbors also will enter the calculations.

Student: Sparsity (Refer Time: 24:45).

Right the sparcity of course, will be affected. And then another issue is that the diagonal dominance would also get affected, because the interpellation need not yield a kind of a diagonally dominant system we will see that. So, one of the ways you can do this is preserve your matrix structure a that is only depends on the face neighbors and then put all of these guys into the right hand side ok.

That is the strategy we are following, but nonetheless you can also do it that way the other way that is also possible. But for the purpose of this course and for the purpose of all the software that you will be using, let us say all the open source and commercial software this is how it will be treated right.

All the secondary gradients would be put into the right hand side to improve the properties of the matrix ok. The diagonal dominance and maintain the structure of the matrix ok, which is will be only connected to the face neighbors not to the vertex neighbors. Other questions? No, yeah.

Student: (Refer Time: 25:52).

Yeah. So, the question is if I want to use an implicit method right. I have an implicit method, I have to use all the current values right in that context what shall I do?

Student: We cannot do (Refer Time: 26:09).

We cannot do this what will you do if you have an implicit method for source terms?

Student: (Refer Time: 26:15).

You have an outer loop and a loop right. You have already linearized the source term right, you have $S_C + S_P\phi_P$, would you use a your S_P is anyway going there what would have used for S_C have you used the previous values/

Student: Yeah.

Right to use the current iterates values right. So, as far as the implicit method is concerned t secondary gradient terms would be still treated as previous values the current iterate values ok. We can do that it is just that these the coefficient matrix will become really dense right. And some of the properties may not be satisfied which we will see right essentially by doing this kind of a trick of dumping all the second gradients on to the right hand side we are changing what?

Student: (Refer Time: 27:05).

The path through the solution right, we are change the path to solution not the solution right. The final answer will remain the same when you achieve convergence we are only changing the path to the solution. So, we could of course do it the other way by including all of these things, but the only thing is the matrix may not be conditioned as a result we may not obtain a solution in the right way ok.

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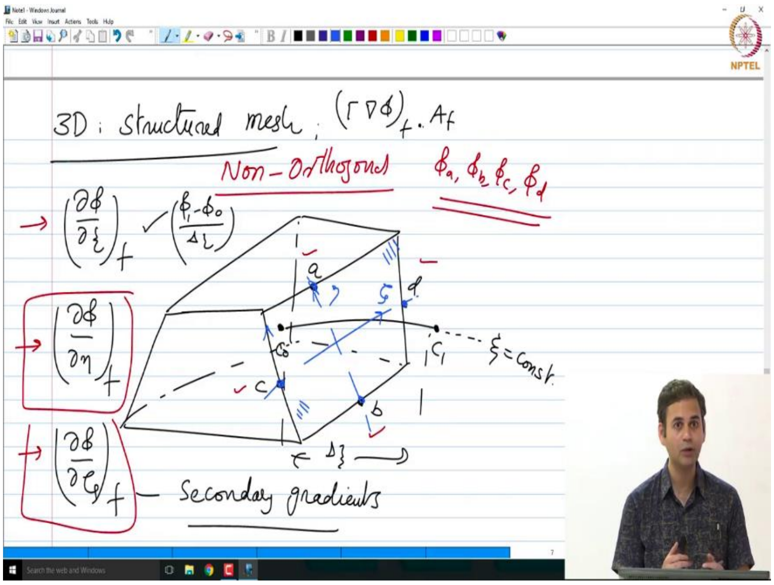

Other questions? No ok, let us move on then. So, what about we have finished 2 D structure and 2 D unstructured, what about the 3 D? Let us start off with the 3 D structured.

We have a 3 D structured to mesh. So; that means, we have some kind of a quadrilateral ok, were talking about a structured mesh. So, let me put in a some kind of a quadrilateral mesh here sorry 3 dimensional, so cuboid kind of cells all right.

So, that is what we have this is 3 dimensions and then we have of course, the cell centroid. And this is connecting the other cell centroid which is here right, and let this we call it as some xi equals constant right that is along the cell centroids right. And up till now we have only eta which is along the face right.

But now what is the face right now? This is the face right this is the face we are talking about and how many up till now we had only eta in this direction right. Now, we have two directions right on the face, which is eta along this direction and some zeta along with this direction.

So, we have essentially eta and then we have some zeta right. So, we have these two that is along the plane right on the plane we have two directions. And then normal to the plane we have xi which is connecting the cell centroids. Do you see that? Ok. So, we have xi, xi is perpendicular to the.

Student: Plane (Refer Time: 29:22).

Plane at that location, would it be always perpendicular? Need not be right fine. So; that means, up till now we had only a and b coordinates right now we will have 4 more coordinates right, we will call it as a b c d, these are the 4 vertices right, where these eta and xi needs to be calculated right.

So; that means, if we were to write a at this value $(\Gamma\nabla\phi)_f \cdot \mathrm{A_f}$ on a 3 D structured mesh right. What will be the gradients look like? You will have three terms $\left(\frac{\partial\phi}{\partial\xi}\right)_f$, $\left(\frac{\partial\phi}{\partial\eta}\right)_f$.

We will also have $\left(\frac{\partial\phi}{\partial\zeta}\right)_f$ right. In the 2 D we only had two terms in 3 D you will have these three terms, do you see that yes or no? If you go back for 2 D, we had only this is the primary direction right. We had the primary direction and then because this is not orthogonal you have these two right your e xi or e eta is nonzero. Similarly you will have e_ξ dot e_ζ also nonzero right, essentially you will get two secondary terms, do you see that?

If you just redo the entire thing what we have done for 3 D, you will see that there will be 3 gradient terms alright.

If you were to boil it down let us say to a Cartesian 3 D mesh, you essentially have these corresponding to these three you have, $\frac{\partial \phi}{\partial x}$, $\frac{\partial \phi}{\partial y}$, partial $\frac{\partial \phi}{\partial z}$, but then because A_x is only pointing in the i direction the $\frac{\partial \phi}{\partial y}$ and $\frac{\partial \phi}{\partial z}$ terms would go to 0.

Student: (Refer Time: 31:41).

Right do you have only 1, ϕ_1 minus ϕ_E minus ϕ_P by Δx surviving right? In the context of non orthogonal meshes all these three will survive right. We are talking about 3 D structured, but non orthogonal ok, fine. We are not saying how will we generate this thing, but somehow let us say we end up having a 3 D structure and non orthogonal mesh then all these things will survive right.

Student: Sir it can also be combination of orthogonal non orthogonal (Refer Time: 31:52).

It can be were talking about a particular cell right. Anyway if you have some orthogonal cells our formulation will revert to an orthogonal formulation anywhere right. So, we are developing everything for non orthogonal in the in this present context ok. We have these 3.

So, when we say secondary. So, we know how to calculate this guy right how do we do this thing? Same as before right this will be ϕ_1 minus ϕ_0 by $\Delta\xi$; that means, this is C_1 this is C_0, right. So, this distance would be your $\Delta\xi$ and then you will and these coefficients will go into the coefficient matrix right.

What about these two terms $\frac{\partial \phi}{\partial \eta}$? How can you calculate? Now you somehow have to interpolate it to the vertices a, b, c, d right these four vertices a, b, c, d right. Once you have values there you can you calculate a b ϕ_a $\frac{\partial \phi}{\partial \eta}$?

Student: (Refer Time: 32:51).

You can calculate from a and b. Similarly can you calculate $\frac{\partial \phi}{\partial \zeta}$?

Student: Yes.

You can calculate right in the values of ϕ_a, ϕ_b, ϕ_c and ϕ_d we can obtain these two secondary gradients right.

So, just like the way we have done in the context of 2 D. We can do this in the context of 3 D also ok. Fine any questions? So, these are all again starred values the existing values of phi we are using to calculate gradients on the faces two other directions other than the line connecting the cell centroids, other than the primary direction right ok. This can be done all right fine. So, so far so good we have devised different ways of calculating the secondary gradients.

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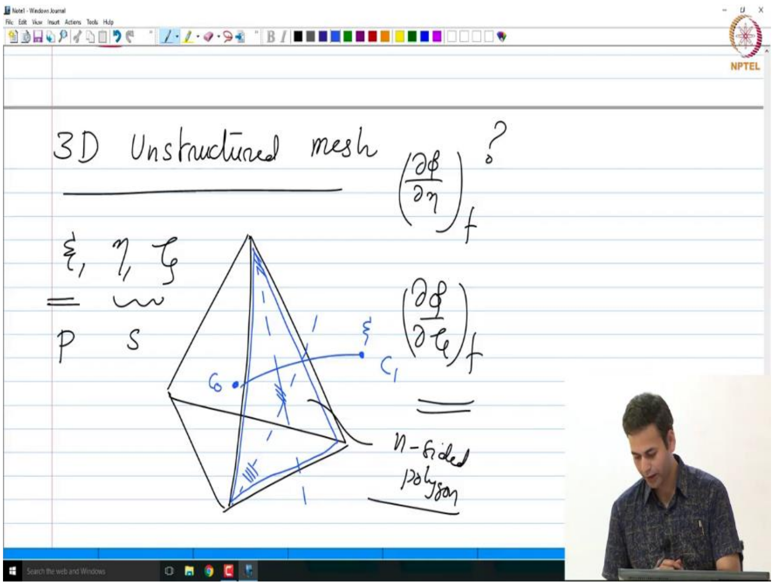

Now, what will happen if you have a 3 D unstructured mesh? If we have a 3 dimensional unstructured mesh that is of course, also non orthogonal ok. So, if we have an unstructured mesh, how does your cells look like? Let me kind of take a.

Student: Tetrahedron.

Tetrahedron so let me take out a tetrahedron, this is basically a tetrahedron. So, this is what I have. So, we have cell centroid somewhere here; let us call this as C_0 this is connecting to another cell centroid that is C_1 right that is what we have. Now, we are talking about one particular face that face happens to be this guy right. That is the face we are talking about, which I have highlighted let us say this is the face.

We are talking about right out of the tetrahedra. Now can you calculate partial phi the second gradients in this context? There will be there are three sides. So, are there can you. So, essentially what we have to do is if we call this as some xi direction right. We would end up having two different directions right, which is basically if you are calling it as ξ η and ζ this is our primary direction. These are our secondary directions right. Now, are η and ζ coming because we have assumed some kind of a structure?

Student: No.

No right that is not the case they are coming out because?

Student: (Refer Time: 35:41).

Because we have 3 axis right, we are doing a 3 D right that is why they are coming out. So, essentially we again will get these gradients which is $\frac{\partial\phi}{\partial\eta}$ on this particular face. And we will also get $\frac{\partial\phi}{\partial\zeta}$ on the particular face, which we have to calculate right. Up till now we could easily calculate them because either the eta direction is aligned with the face direction right. We could calculate what is a, b and calculate them in the context of 2 D.

Similarly, in the context of 3 D when we have a structured mesh. We could identify the face by kind of splitting it along the two sides and we said a, b, c, d there are 4 points we can interpolate and calculate. Now, we have to actually take two directions here right.

And the two directions where should they lie? They should lie in the plane of the face right on the triangular face you need to identify two directions. Do these two have to be orthogonal? No they do not have to be orthogonal there are two directions; that means, you can pick infinitely many directions right on this plane right.

There are many that are arbitrarily available can pick arbitrarily. But of course, you can also come up with one particular way of choosing them right. Essentially we want one way consistently to pick this, but we are flooded with infinite options right. We have to pick one, such that we can core it right that is you can write a program. Now, what is the another complexity that comes in here? Right.

Now I have drawn a tetrahedral, which has three sides on the face right, but in general if you have an unstructured mesh this can be an n sided polygon right. This can be an n sided polygon this face can be an n sided polygon right; that means, for that particular n sided polygon we have to pick two directions which are eta and zeta right.

Now, that we cannot have a consistent way of picking something. That means, there are infinitely many possibilities out of which we have to pick one, one set of eta and zeta. Now, we may devise something only for tetrahedral meshes. For example, you can say why not I connect this vertex with this direction and this with some other direction here can I pick this way?

Yes you can pick right, I can connect of course, you have another 3rd direction that you somehow come up with some consistency ok. So, the idea is ah, but this will not work if you have let us say a pentagonal face right or an octagonal face is not it. Let us say if we have a polyhedral cells or something like a honeycomb structure. You can have many you can have basically the face need not be it will be an un sided polygon in general right. In that context how do you choose these two different directions that is the question.

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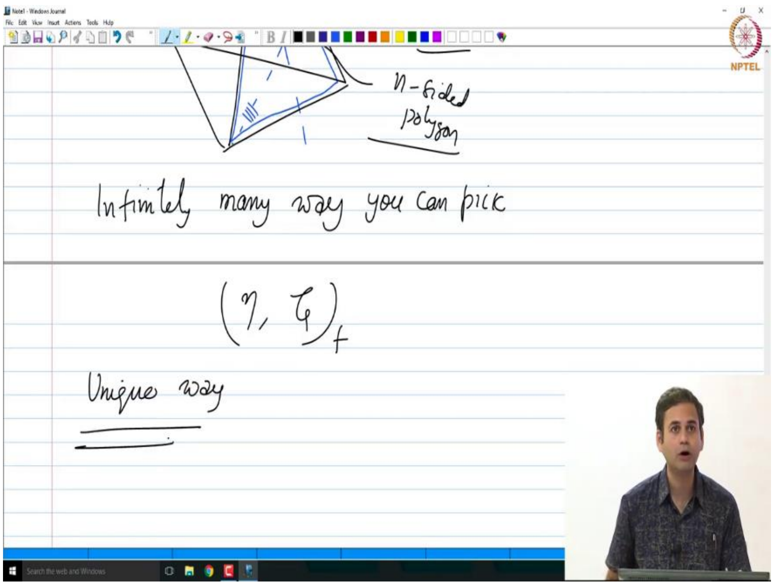

So that means, what we are convinced is that in the context of 3 D unstructured. There is a problem the problem is there are, infinitely many ways you can pick the eta and zeta right, eta and zeta can be picked in infinitely many ways.

But what we are looking for is we want to look for in a unique way by which we can implement this for all the cells. Irrespective of whether we get a tetrahedron or we get a hexahedron or a prism and so on right.

For example if you got a prism three of them have the triangles, the other one has a quadrilateral right then this would not work. So, as a result we need to have a particularly unique way of calculating the secondary gradients, such that it will work for any shape of the cell right any shape of the cell ok.

So, we will look at one particular way, which is again available in most of the commercial and the open source software in any of these C F D software that is what we will look at. But you are welcome to use any other method other than this thing ok. But as far as the course is concerned we will follow this particular method in terms of the problem solving and on and so on. Or if you end up writing a program, for calculating these things for your project ok. So, is the problem clear what we encountered? Yeah.

Student: (Refer Time: 40:12).

So in the structured case how did we choose the two directions? So, in the structured case I have a face all right, I can choose may be the midpoint of this of this line right. And then essentially I have chosen the midpoints here 1, 2, 3, 4 right. I just need to choose two different directions on this particular plane. I chose it to be passing along the center of this rectangle or quadrilateral.

Student: (Refer Time: 40:46).

Here so, essentially if it is a multisided then you cannot do it this way. So, implicitly what I have is, when I say structure we are talking about a Quadra hexahedral mesh ok. Because you would not be able to generate a tetrahedral mesh that will be structured, that is what I assumed ok.

So, were talking about a bricks kind of thing like a quadrilateral mesh hexahedral mesh. And where all the faces are quadrilaterals right then you can somehow define two different directions right, connecting the midpoints of the edges right that can be done that is what we have targeted.

But certainly whatever we develop now for the 3 D unstructures unstructured meshes, should also work for the 3 D structured meshes right. When you boil it down because you may have several tetrahedral all of a sudden you may have some prisms and these prisms might be connected to some hexahedral afterwards. Let us see if we have a kind of a mixed cell shapes right other questions is the problem clear ok.

So, there are infinitely many ways you can define this and calculate, but we will look at one particular way that way is basically is what is used prominently.

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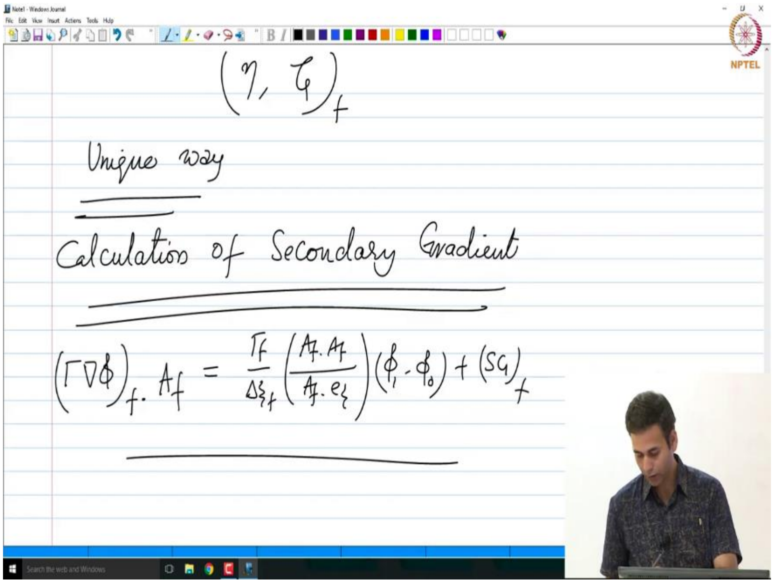

So, this is basically calculation of secondary gradient ok, calculation of secondary gradient. Now, here is where you have to be little focused. So, what is the expression we have? we have two we started off with calculating what is $(\Gamma\nabla\phi)_f$ dot A_f right. This is what we set of calculating and we have written this as Γ_f by $\Delta\xi_f$ times A_f dot A_f by A_f dot e_ξ times ϕ_1 minus ϕ_0, plus secondary gradient of f right.

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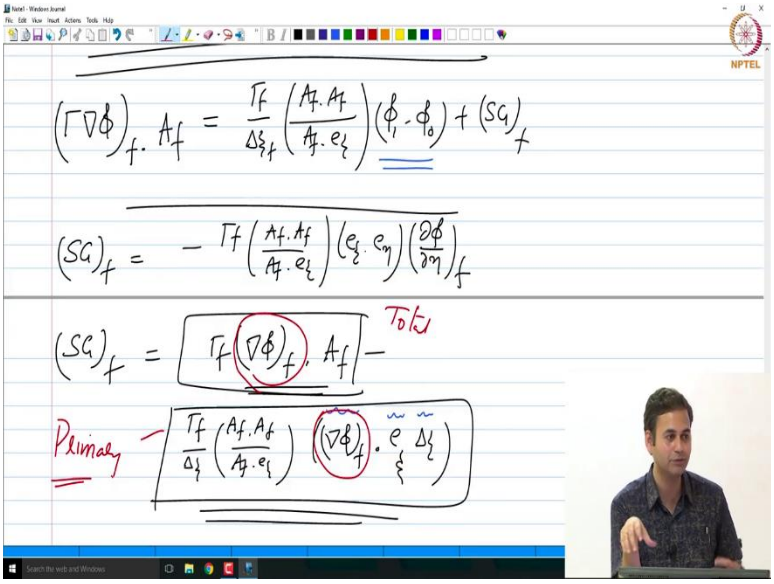

That is what we have written, is not it? That is what we have written. Now, what is the expression for secondary gradient? Secondary gradient for f is given as minus Γ_f times A_f dot A_f by A_f dot e_ξ times e_ξ dot e_η times partial phi partial eta on the face f right. This is what we got is not it. Let us say I am talking about 2 D this is what I got, if it is 3 D you would have one more term might be there. Now, the idea is to calculate the secondary gradient from the already calculated primary gradient value and the total value ok.

So, the secondary gradient value should be nothing, but the total minus the primary gradient value of course, the thing is we do not know the total gradient if we knew that the problem would have been solved right. So, now, we are looks like we are going in circles, but we will come to one point.

So, essentially calculate the secondary gradient which is the minus of this thing as the total minus the primary gradient, because the primary gradient is always uniquely defined right. The C_0 and C_1 are always uniquely defines xi is always uniquely defined. So, I can definitely calculate what is that for any cells that are given right.

So that means, this secondary gradient of f is can be written as what is Γ_f grad phi f dot A_f right, that is the total value I have all right. Minus I would subtract of the primary gradient ok. The primary gradient is how much? is this guy right? I would subtract that of; that means, minus Γ_f by $\Delta\xi_f$ A_f dot A_f by A_f dot e_ξ times grad phi f dot e_ξ times delta xi right.

Do you agree with this? So, what I have written is, I have changed a little bit here ok. Instead of writing ϕ_1 minus ϕ_0, I have replaced that with the grad phi right. I somehow know what is the gradient on the particular face. So, I know that. So, that if I take a dot product with the e_ξ direction, I would get the component of that in the direction of e_ξ multiplied with delta xi that will give me what is this difference ϕ_1 minus ϕ_0 right.

Do you see that I have replaced ϕ_1 minus ϕ_0 with grad phi f dot e_ξ right. Basically this would give me the gradient in the direction of xi that is the primary gradient times $\Delta\xi$, right that will basically ϕ_1 minus ϕ_0 ok. Now, what is the; what is the unknown in this equation? Of course, secondary gradient itself is unknown, but I have written something here what is that? That is unknown here grad phi f right.

Which I have written here this particular term here is the is the unknown; that means, you are calculating gradient of phi on the face which is shared between C_0 and C_1 somehow right. So, we are calculating the total gradient on the particular face. And then I am, I from there I can calculate what is the total gradient of the diffusion flux minus, this is what the primary right. So, this is the total this is the primary that would give me what is the secondary value. Do you see that?

Now, we have transformed the problem from the computation of secondary gradient to the computation of $\nabla\phi$ on the face f right; that means, if I can calculate what is grad phi on the particular face which is shared between C_0 and C_1, then I can calculate my secondary gradient right.

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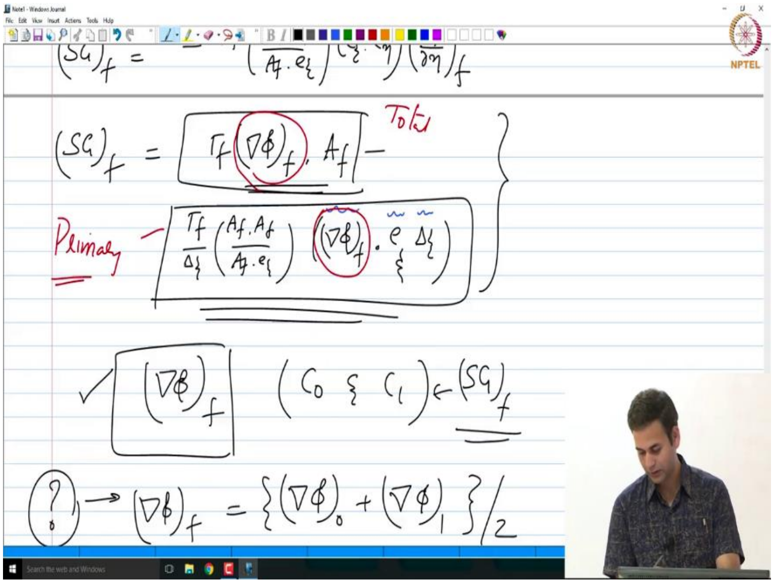

So, we have just transformed the problem of calculation of secondary gradient into calculation of gradient of phi on the particular face. Have you used any of these software the C F D software? It would ask you what is the gradient calculation scheme, right. Or some kind of how do you how should I calculate gradient? That is what it will ask you right.

This is where this is what is asking right essentially grad phi is this is what it is asking about, which scheme shall I use to calculate this and why does it have to calculate this? For use in secondary gradient. That is one reason but it is also used in many other in many other context ok which we will see in what other context you would need the ∇ϕ is.

As of now it is for the calculation of secondary gradient in case if you have a an unstructured non orthogonal mesh. Now, it is certainly a good idea to make use of this structure and calculate second gradient directly from a and b or a, b, c, d values and put it in there, but none of these software you work that way.

Because although you have a structure they will still use this secondary gradient calculations and calculate it this way calculate it this way is what they do. But in your own codes if you have a structured mesh for 3 D or if you have a 2 D structured or unstructured it is good to go with the previous methods that we have discussed ok.

But this is the generic way which will work for essentially everything right. You calculate the total and you subtract of the primary calculate the secondary gradient ok. So, this is how all of these commercial ones and the open source ones work ok. For the calculation of gradient on the particular face f. Of course, again how do I calculate the grad phi?

Usually $\nabla\phi$ can be taken as average of the cells and total values you can take grad ϕ_0 plus grad ϕ_1 by 2. That means, you calculate the gradients of phi at the cell centroids itself and store them and if you want it for the faces you would linearly interpolate and take it that is how it works.

Now, how this is calculated we will see in the coming lectures how to calculate the gradients or there is one more question for you. So, let us say we have a linear problem like the source terms are all linear ok.

We have a constant source term, gamma is also a constant. But we have we are working on a steady diffusion in 3 D with constant source and constant gamma, but our mesh that we have used is non orthogonal ok. If we have it like that what is the modification that you have to bring about or is there any modification?

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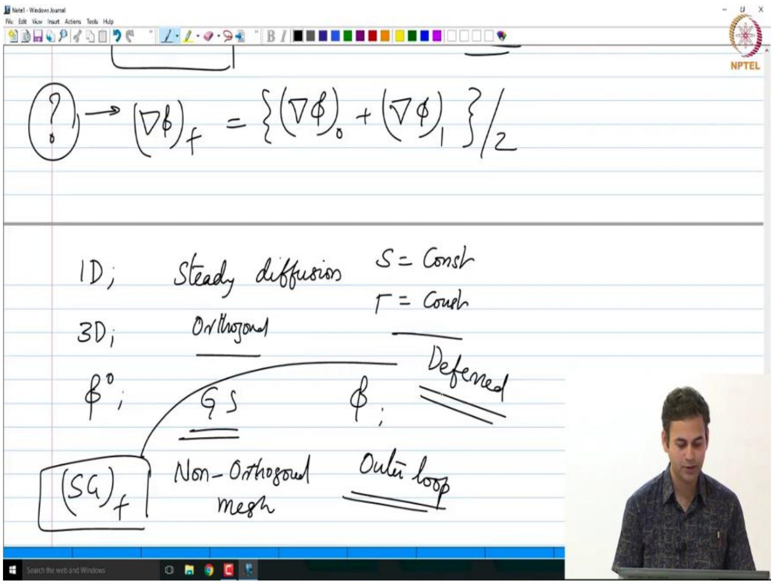

So, let us put it this way, let us talk about a 1 D problem, where you have steady diffusion ok. So, this is a steady diffusion and you have S equals constant, gamma equals constant.

And then 1 D and we are also looking at a structured mesh or rather let us talk about orthogonal mesh. How do you solve this thing? Use Gauss Seidel or something and then once Gauss Seidel or Gauss Seidel and once Gauss Seidel converges you are done right.

Because there is no non-linearity either in gamma or in s anywhere right. Now, let us say if it is a 3 D problem, but it is still orthogonal how do you solve it? You perform iterations using Gauss Seidel right.

You start off with some initial gauss ϕ_0 right, phi 0 bar and then once this ϕ_0 you perform the iterations. And once you converge phi are you done with the solution? It constant source constant gamma and you are also working on an orthogonal mesh right.

Now, what will happen if you have the same problem? 3 D steady diffusion with constant source constant gamma, but you are working on a non orthogonal mesh. Is there any change that you would see? Or you have to incorporate any other change. Would it this work this way? You have a Gauss Seidel you perform let us say 10000 iterations and you converge is that the solution that you would obtain or do you have to make any changes?

Sorry you have a non orthogonal mesh, but there is no non-linearity the source term is constant gammas are constant.

Student: (Refer Time: 52:03).

Secondary gradient. Yes, who said secondary gradient yes. So, because of secondary gradient what do I have to do? 2 loops it has to introduce a an outer loop right because the secondary gradients that I have used in the calculations are calculated with a previous value of phi right.

So, as a result I would need an outer loop right, I would this would introduce an outer loop just because my mesh is non orthogonal right. If it were not it will say if it were orthogonal, in under what conditions would you get an outer loop? If you have non-linearity either in the source terms gamma or any other non-linear terms right.

So that means, if you if you are mesh is non orthogonal even if you have a linear problem, you still have to go with a an outer loop ok. That is because of the calculation of the secondary gradient. And we have calculated secondary gradients in a in what fashion? We have calculated in a deferred fair if deferred fashion right.

We have used the previous values right, but as somebody suggested if you were to directly calculate all of these things in the coefficient matrix itself, then you do not need an outer loop right ok. Is that clear what I we just discussed? The need for an outer loop if you have deferred way of calculating the secondary gradients, ok. Think over it we will come back to this discussion later. Alright I am going to stop here I will see you guys in the next lecture.

Thank you.