

Computational Fluid Dynamics Using Finite Volume Method
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Lecture - 26
Finite Volume Method for Diffusion Equation: Steady diffusion in unstructured meshes Part 3

Good morning, let us get started. So, we were continue our discussion on Steady diffusion discretization for unstructured non-orthogonal meshes ok.

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Steady Diffusion on non-Orthogonal meshes

$$\sum_f (\Gamma \nabla \phi)_f \cdot A_f + (S_C + S_P \phi_0) \Delta V_0 = 0$$

$$(\Gamma \nabla \phi)_f \cdot A_f = (\dots) (\phi_\xi)_f + (\dots) (\phi_\eta)_f$$

Primary \rightarrow $(\dots) (\phi_\xi)_f$

Secondary \rightarrow $(\dots) (\phi_\eta)_f$

So, this is steady diffusion on unstructured non-orthogonal meshes ok, fine. So, what the equation that we have kind of derived is basically $\sum_f (\Gamma \nabla \phi)_f \cdot A_f$ plus $(S_C + S_P \phi_0) \Delta V_0$ equals 0 right that is the equation we have.

And we are working with the diffusion flux term. And the diffusion flux term we have seen that we can write this as $(\Gamma \nabla \phi)_f \cdot A_f$ as some quantity right some quantity times $(\phi_\xi)_f$ right that is the gradient in the xi direction plus some other quantity times $(\phi_\eta)_f$ right, these specific quantities we have derived in the previous lectures right. So, we have done that decomposed this into the xi direction and eta direction.

And then what we said is of course, the derivative in the xi direction can be written in terms of the cell values right using a linear profile assumption $(\phi_\xi)_f$ can be written as ϕ_1

minus ϕ_0 upon $\Delta\xi$ right that is what we have said. And we called this first term which is multiplying $(\phi_\xi)_f$ as the primary gradient right.

So, this we said as the primary gradient. And the second term we said this is the or secondary gradient ok. Now, we devoted a considerable amount of time in understanding how to calculate the secondary gradient itself right. So, this term itself.

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Handwritten equations on a whiteboard:

$$\underline{(SG)}_f = - \Gamma_f \frac{A_f \cdot A_f}{A_f \cdot e_\xi} (e_\xi \cdot e_n) (\phi_n)_f$$

3D, Unstructured mesh

$$= \Gamma_f (\nabla \phi)_f \cdot A_f -$$

Total gradient on the face

Primary value $\left\{ \frac{\Gamma_f}{\Delta \xi_f} \frac{A_f \cdot A_f}{A_f \cdot e_\xi} (\nabla \phi)_f \cdot e_\xi \Delta \xi \right\}$

$(SG)_f \longrightarrow$ calc. of $(\nabla \phi)_f$

Now, the secondary gradient term we denoted using SG sub f this we said actually will come out to be minus $\Gamma_f A_f$ dot A_f by A_f dot e_ξ right that is what we have and times e_ξ dot e_n times $(\phi_n)_f$ right.

This is the coefficient that we will have for the secondary gradient. And we said calculating this would be straightforward if you have a any 2D mesh whether it is structured or unstructured, or if you have a 3-dimensional structured mesh right. Whereas, if you have a 3-dimensional unstructured mesh, then selecting the two directions on the plane right which is eta and zeta may not be unique, as a result we may not be able to find it in one particular wave for all the cells right.

So, we said ok, then a one good way to calculate this is basically somehow we can calculate the total face gradient, and then subtract of the component of the xi direction from this total gradient right that is what we kind of wrote this.

So, if we have a let say in general a 3-dimensional unstructured mesh, then we said the secondary gradient can be calculated using $\Gamma_f (\nabla\phi)_f \cdot A_f$. So, this is the total transport of ϕ right through the face f . And we said this minus the gradient in the primary direction right, so that would give you what is the gradient, what is whatever is the transport in the secondary direction ok.

So, this minus the gradient in the primary direction would be $\Gamma_f \text{ upon } (\phi_{\xi})_f A_f \text{ dot } A_f \text{ upon } A_f \text{ dot } e_{\xi}$ times we said $(\nabla\phi)_f$ is what we would calculate on the face. Then if we were to subtract of the gradient in the primary direction this would the e_{ξ} right that will give you the value times $\Delta\xi$ right, that is your term.

So, this is your primary value. And this term is your total gradient on the face right ok. So, essentially the total minus the xi direction we will give you the entire secondary gradient term that is this term right that is what we said.

Of course, now we said we do not know the phi value itself that is the unknown, but we are now talking about calculating the value of gradient of ϕ right so which needs to be somehow computed on the face. So, now, the calculation of secondary gradient is reduced to the problem of calculation of gradient of ϕ on the faces right. If we can somehow calculate the gradient of the ϕ on the faces, then we can calculate the secondary gradient term right.

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$(\nabla\phi)$ can be assumed to be constant in any cell

$$(\nabla\phi)_f = \frac{1}{2} ((\nabla\phi)_o + (\nabla\phi)_i)$$

✓ $(\nabla\phi)$ at cell centers -

$(\nabla\phi)$ -

The diagram shows a 3D cell with a face f and a primary direction ξ . The cell center is labeled o and the face center is labeled i . A vector $(\nabla\phi)$ is shown pointing from the cell center towards the face.

Again we say that using an approximation if we have if the gradient of phi can be assumed to be constant in a cell, if it can be assumed to be constant in any cell, then the gradient on the face can be written as an arithmetic mean of the gradients on the of the cell values ok, because grad phi itself will be a constant or the entire cell right. Then the average of these two would give you the gradient on the faces ok, that means, we have to somehow calculate this gradient at cell centers right.

So, essentially for all the cells we have to somehow calculate this gradient ok. This we will see little later how to calculate this we will address it little later. As of now if there is a method by which we can calculate the gradients at the cell centers, we can calculate the gradients at the faces which further can be used in calculating the secondary gradients. Yes.

Students: Why (Refer Time: 06:52)?

Why arithmetic means. So, essentially you have you have two cells, and the gradient is assumed to be constant over these entire cells. So, then the face value could be taken as the arithmetic mean of these two.

Students: (Refer Time: 07:12).

So, we are assuming that this $\nabla\phi$ remains a constant over the entire cell.

Students: (Refer Time: 07:21).

Yes. So, this distance.

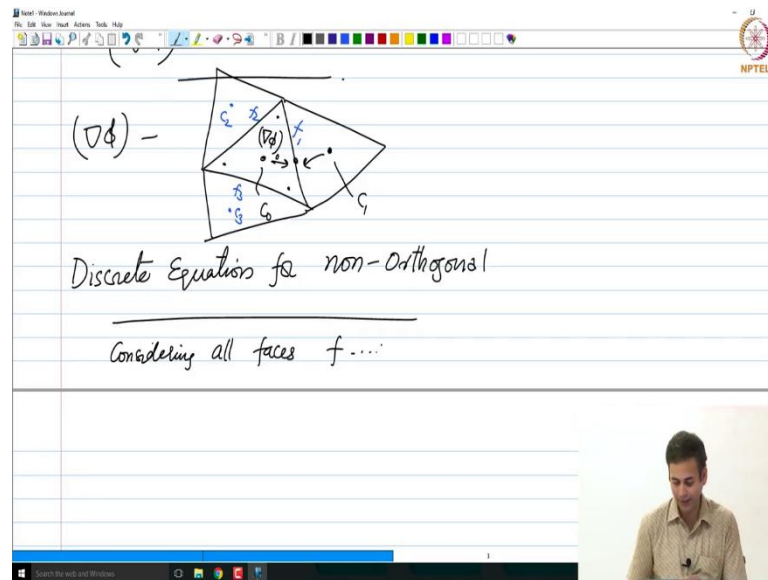
Students: (Refer Time: 07:26).

So, even if it is not equal what is $\nabla\phi$? $\nabla\phi$ is assumed to be constant over the entire cell, but I am assuming that it is constant. So, whatever is the distance it does not make a difference right. So, for example, even if I have a if there is a variation of grad phi inside, then there will be a an effect of the distance right I am assuming that grad phi is constant over the entire cell. So, wherever I go whether I come here I go here wherever I go it will be the same value that is what I am assuming right.

Grad phi is a constant for the entire cell as a result I can take an average right. Now, if it is not constant then of course, you have to take a kind of a linearly interpreted value ok.

Other questions, is it clear the concept of coming to the concept of gradient of calculations gradient of phi from the motivation of the secondary gradients right? Ok, fine ok. Then let us move on all right. So, we have all these values. Then let us write to try to write a discrete equation which will be for a non-orthogonal meshes ok.

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So, let us assemble all these things and write the discrete equation for non-orthogonal meshes ok. So, just like before up till now we have been talking about let say one face f here right, but actually you would have several faces and several cells right.

You will have another cell here, another cell here, as a result you will have this could be f 1, this could be f 2 and f 3 you would have cell C_2 , and C_3 and so on right, you will have several cells and several faces. So, you have to do a summation of the gamma grad phi's right, so that has to be done. So, that we have to do it, because we have only dealt with one particular face between C_0 and C_1 ok.

Then if we write similar equations for each of the faces and then kind of assemble them. So, considering all faces f for the cell, and then assembling them we would write the equation the discrete equation for the cell C_0 right. And we would like to put it in the standard form that is our $a_p \phi_0 = \sum a_{nb} \phi_{nb} + b$ ok.

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Considering all faces $f \dots$

$$a_p \phi_0 = \sum_{nb} a_{nb} \phi_{nb} + b$$

$$a_{nb} = \left(\begin{array}{cc} \Gamma_f & A_f \cdot A_f \\ \Delta \xi_f & A_f \cdot e_\xi \end{array} \right)_{nb=1,2,\dots,M}$$

$$a_p = \sum_{nb} a_{nb} - S_p \Delta b$$

$$b = \sum_c S_c \Delta b + \sum_{nb} (S_G)_f$$

Similar in structure to an orthogonal sys.

Where a_{nb} 's are the coefficients for the neighboring cell values. So, those will be given as a_{nb} would be what? Would be coming from your primary gradient right.

(Refer Slide Time: 10:32)

Primary

Secondary

$$\Gamma_f \phi_f \cdot A_f = \left(\begin{array}{c} \text{Primary} \\ \text{Secondary} \end{array} \right) (\phi_i)_f + \left(\begin{array}{c} \phi_i - \phi_0 \\ \Delta \xi \end{array} \right)$$

$$b = \left(\begin{array}{cc} \Gamma_f & A_f \cdot A_f \\ \Delta \xi_f & A_f \cdot e_\xi \end{array} \right) (\phi_i - \phi_0)$$

$$(S_G)_f = - \Gamma_f \frac{A_f \cdot A_f}{A_f \cdot e_\xi} (e_\xi \cdot e_n) (\phi_m)_f$$

3D, Unstructured mesh

Total gradient on the

So, whatever was this primary gradient how much was this? This was Γ_f upon, so this entire term right, we wrote it as Γ_f by $(\phi_\xi)_f$ A_f dot A_f by A_f dot e_ξ times ϕ_1 minus ϕ_0 right. This is what we have written.

That means, what is the coefficient here this entire term in the parentheses is the coefficient that is going into a_{nb} right that is for as the coefficient of ϕ_1 a 1 and then this will also going into a_p as a coefficient of ϕ_0 , but a p terms would go to the right hand side right. So, what would be your a_{nb} now? a_{nb} is just this term right, and is what we have to write.

So, that means, a_{nb} would be Γ_f upon $\Delta \xi_f A_f \cdot A_f$ upon $A_f \cdot e_\xi$. Where f is for the face when you consider C_0 and the neighboring cell right, and the neighboring cells are 1, 2 all the way to let say if we have M neighbors, then this would be the face f between C_0 and that neighbor right. C_0 and C_1 could be the face f between C_0 and C_2 could be f_2 and so on right. So, we have several of these that is your a_{nb} .

We do not have any contribution from incoming from the secondary gradient right into the a_p , because we said the all the contributions coming from the secondary gradient would go into b term ok. This will going to b as a result we do not have anything there ok. Then what else will what else will be expressions for a_p ?

Student: Summation a_{nb} .

Summation a_{nb} because $\sum a_{nb}$ all the neighbors what else will go into a_p .

Student: Plus.

Minus $S_p \Delta V_0$ right that is what will go into a_p . What will be the contributions for b ?

Students: Secondary gradient.

Secondary gradient ok. Before that we have the.

Student: S_C .

Source term also, so $S_C \Delta V_0$. And then we have how many secondary gradients only one neighbors right. So, essentially it would be summation of all the secondary gradients for all the faces right. So, that could be plus $\sum_{nb} (SG)_f$ right. Would it be plus or minus?

Students: Plus.

It should be plus right, because there is the secondary gradient we have denoted it as plus the minus entire thing we denoted it as plus and it remains on the left hand side right as a

result this is plus fine. Anything else or is it all? So, the primary gradient went into a_0 a_{nb} 's and a_p secondary gradient went into b and the source terms, that is alright, there is nothing left over ok. So, all these things are there.

That means if we look at it the equation as such is very similar to the orthogonal system of equations right. Even if we had an orthogonal system we had $a_p \phi_p = \sum a_{nb} \phi_{nb}$ right. So, this is similar to similar in structure to an orthogonal system right ok. What about the you know the Scarborough criteria or the summation properties?

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nb

$$b = \sum_{nb} \Delta b_b + \sum_{f} (S_u)_f$$

Similar in structure to an orthogonal sys.

In the absence of source term $\bar{S} = 0$

$$a_p = \sum a_{nb} \quad \text{Scarborough}$$

Boundedness

So, let say we do not have source terms. In the absence of source term; that means, your entire \bar{S} equals 0, what is your a_p ? Is a p summation of $\sum a_{nb}$ or no? Yes, it is a_p is summation of $\sum a_{nb}$. So, Scarborough is satisfied in.

Students: Inequality.

Inequality ok. Equality is satisfied. What about boundedness?

Students: Boundedness.

Boundedness, that means, you have source equals 0 right. So, essentially source is 0. So, this term is 0, this term is 0, then $a_p \phi_0 = \sum a_{nb} \phi_{nb}$ plus is b 0 now?

Students: (Refer Time: 15:12) secondary gradient, secondary gradient.

b is not 0; b has secondary gradient right. So, that means, ϕ_P or ϕ_0 is not just $\sum a_{nb}\phi_{nb}$ right which was the case in the context of orthogonal meshes right.

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In the absence of source term $\bar{S} = 0$

$$a_p = \sum a_{nb} \quad \text{-- Scarborough}$$

Boundedness $\phi_0 = \frac{\sum a_{nb}\phi_{nb} + b}{a_p}$ $\neq 0$ (SG)_f

- Boundedness is not assured
- (SG)_f will produce oscillations in ϕ

So, here our equation is ϕ_0 equals $\sum a_{nb}\phi_{nb} + b$ upon a_p right. This is still not equal to 0 because of secondary gradients right. As a result, is it bounded?

Students: No.

No, it is not; boundedness is not guaranteed right. Now, what about SG? SG, what terms would go into secondary gradient? Some coefficient right times what is the derivative that is multiplying these coefficient, $\frac{\partial \phi}{\partial \eta}$. Now, how do you calculate $\frac{\partial \phi}{\partial \eta}$?

Students: Previous value.

Previous values, but those are also neighbors of these cells right, but they may not be the face neighbors, they could be the.

Students: Vertex neighbors.

Vertex neighbors, we are sharing the same vertex. So, as a result, SG will also have values from ϕ right coming into play. And these ϕ neighbors will actually contribute to the secondary gradient as well right. So, in some sense we can think of the boundedness as not

just by the face neighbors, but also with the cell vertex neighbors as well might be there right.

But the thing is it is still not a it may not be bounded because it is not the property of σ_{nb} by a_p equal to 1 is not satisfied for those coefficients right. As a result boundedness is not guaranteed, is not assured right, because ϕ_0 is not just σ_{nb} by a_p times ϕ_{nb} plus you have this b term which has the secondary gradients, as a result boundedness is not assured.

And we will see a little later that the computation of calculations of the secondary gradients will produce oscillations ok, oscillations in ϕ values ok. Essentially in the calculation of ϕ when you use the secondary gradients, it will produce some oscillations. As a result the boundedness is not guaranteed ok, this we will see a little later. So, that means, if you have a non-orthogonal mesh, that means, boundedness is not assured right you can still have slightly higher values than your neighbors right.

Now, how do you get rid of this thing? I mean how do you make sure that boundedness will always happen depending on the mesh you use right? If we have a good mesh as close are possible to an orthogonal mesh, then you would have this boundedness criteria satisfied right; otherwise, you will still introduce some error in the solution ok. There are several ways you can get rid of this problem by having limiters and things like that, we will see that little later in the course ok. Yes, questions.

Students: So, like (Refer Time: 18:22) steady state because then the solution will be boundedness (Refer Time: 18:26).

In the context of yes, if you have a steady state solution it has to be bounded that is what it should happen if you have a very good mesh right. But in this context, if you have if the mesh is has these problem with secondary gradients, then it need not be bounded right that is what the essentially that is the problem with non-orthogonal meshes. The non-orthogonality will come into play as a numerical artifact right. So, you still get a steady state solution, it is just that it may it will not be bounded.

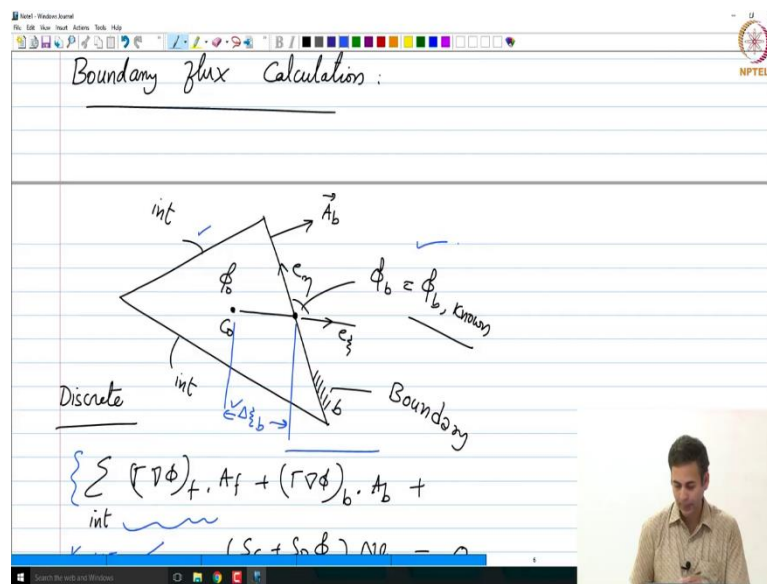
Students: (Refer Time: 18:57) incorrect.

It is actually incorrect because it is not bounded, but you will still get a steady state solution for that right, only way you can improve you say that through having a better mesh quality ok. Other questions? So, that means, if you emphasizes on the need for a good mesh to start with right.

The same thing if we had an orthogonal mesh let say Cartesian mesh or something, then you would have got like a beautiful result with satisfies the physics right ok. Other questions? Ok, so in this context, we have boundedness is not guaranteed, but this Scarborough is satisfied right that is kind of there fine ok.

Then one more thing that remains is basically looking at the boundary conditions in the context of non orthogonal meshes ok. Up till now we have talked about any interior cell right. Now, how do we do this for a boundary cell ok? So, let us look at extension of this to discretizing boundary fluxes.

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So, that is boundary flux calculation that means, we are looking at a particular cell that has one face as a on the boundary right, it could be one of the Dirichlet boundary conditions or any other boundary conditions that we have seen ok.

So, I would draw here again a particular typical cell. So, typical cell is let us say this way and this is my cell centroid, the area vector is here we call it \vec{A}_b which is again pointing

away from the cell outwards from the cell, and this is our C_0 cell right, and the face centroid is somewhere here ok.

And the line connecting the cell centroid to the face centroid now defines the direction e_ξ right. If it were interior, the line connecting the C_0 to C_1 defined our e_ξ ; now we do not have an i bar right, because this is a boundary right and these are the interior faces ok.

What about e_η , e_η would be tangential to the face as before, so that means, this is my e_η . And now again, \vec{A}_b is not need not necessarily be parallel to e_ξ right; the line connecting the cell centroid to the face centroid, need not be parallel to the \vec{A}_b that is where we have a non-orthogonal mesh, yes question.

Students: (Refer Time: 21:48) eta.

Sorry, it should be eta fine, good ok, anything else ok. So, this is e_η we have e_ξ , and this is need not be 90 degrees ok, alright.

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The diagram shows a triangular cell with a cell centroid G_0 and a face centroid. A line connects G_0 to the face centroid, defining the direction e_ξ . A vector \vec{A}_b is shown normal to the boundary face. The face is labeled 'Boundary' and the interior is labeled 'int'. The face area is A_b and the cell area is ΔV_b . The diagram also shows the unit vectors e_η and e_ξ at the face centroid.

Below the diagram, the discrete equation is written as:

$$\sum_{\text{int}} (\Gamma \nabla \phi)_f \cdot A_f + (\Gamma \nabla \phi)_b \cdot A_b + \text{Knows } \checkmark (S_c + S_p \phi_0) \Delta V_b = 0$$

The boundary term is further expanded as:

$$(\Gamma \nabla \phi)_b \cdot A_b \Rightarrow \Gamma_b \frac{A_b \cdot A_b}{A_b \cdot e_\xi} (\phi_\xi)_b$$

So that means, the discrete equation that we have can be written as sigma $(\Gamma \nabla \phi)_f$ dot A_f ok, this is over all the interior faces, I would like to call it as interior ok. So, essentially I am separating the diffusion flux for the interior faces that is for let us say, this face and this face; and for the boundary face separately that means, plus I would have $(\Gamma \nabla \phi)_b \cdot A_b$.

Let us call this face as b ok, this is my face b ; so the diffusion flux is now written out separately that means, this summation the first one only goes around how many faces here?

Students: 2.

2 faces. So, plus we have $S_C + S_P \phi_0$ times ΔV_0 equals 0 right that is our discrete equation for a boundary cell. Now, do we know how to calculate the first term here for all the interior faces, we know right that is what we have been discussing till now. So, this is already know how to discretize this thing, know this thing, fine.

So, only thing we have to discuss is the boundary term, $(\Gamma \nabla \phi)_b \cdot A_b$ right. Now, this will be very similar to what we have done in the context of an interior face, but with very few subtle changes here and there which we will see that means, we have to now discuss how do I calculate, $(\Gamma \nabla \phi)_b \cdot A_b$, ok.

So, again this can be written in terms of two gradients right; one is along ϕ_ξ and one is along ϕ_η , just like what we have done for any interior cell right. So, the same steps follow right, we have done whatever we have done for the interior face can be done for the boundary face right; only thing is that instead of A_f , you have now A_b ok. And of course, how do you define the distance here, what is $\Delta \xi$; would be the distance between the face centroid and the?

Students: Cell centroid.

Cell centroid, this is like your Δx by 2; if you had a you know Cartesian mesh right, so this is basically $(\phi_\xi)_b$ which will connect the cell centroid to the face centroid fine, alright.

Then I can again decompose this into two components one is along ϕ_ξ , other one is along ϕ_η ; and I can write the same thing that would be $\Gamma_b A_b \text{ dot } A_b$ by $A_b \text{ dot } e_\xi$ right that is the first term I have; times ϕ_ξ on the face b right that is the first term primary gradient I would get, minus I would get $(\Gamma \nabla \phi)_b \cdot A_b$ upon $A_b \text{ dot } e_\xi$ times $e_\xi \text{ dot } e_\eta$, ok.

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Secondary gradient:
$$-\Gamma_b \frac{A_b \cdot A_b}{A_b \cdot e_\xi} (e_\xi \cdot e_\eta) (\phi_\eta)_b$$

$$(\phi_\xi)_b = \left(\frac{\partial \phi}{\partial \xi} \right)_b = \left(\frac{\phi_b - \phi_0}{\Delta \xi_b} \right)$$

Primary gradient:
$$\left(\frac{\Gamma_b \cdot A_b \cdot A_b}{\Delta \xi_b \cdot A_b \cdot e_\xi} \right) (\phi_b - \phi_0)$$

2D, stru (or) Unsk. ✓ a_b
 3D stru ✓ (a_p, b)
 3D unsk... →

Times $(\phi_\eta)_b$ right, those are the two components we would get if you follow the same process we have done for the interior face ok, with only changes being you would use A_b instead of A_f right for a boundary face, fine ok. Then what about the first term, how do we calculate $(\phi_\xi)_b$, because we have a boundary face just like the structured or the Cartesian meshes, we would also somehow store a value of this on the face right, we would also store a value irrespective of the boundary condition.

The boundary condition can be a Dirichlet, Neumann or a mixed, but we will still show store a value of ϕ on the face right, you remember. If it were Dirichlet of course, ϕ_b would be known; if it were not Dirichlet, we would somehow calculate it right by the balance of the fluxes.

So, ϕ_b on the face will be stored and it will be updated, and we also know what is ϕ_0 at the cell centroid C_0 , right. Now, how do I calculate $\frac{\partial \phi}{\partial \xi}$ on the for the boundary face?

Students: ϕ_b .

ϕ_b minus.

Students: Phi.

ϕ_0 , upon?

Students: $\Delta\xi$.

$\Delta\xi$.

Students: b.

b ok, fine. So, we have this thing that means, what about the primary gradient term; if I write it here, this would be Γ_b by $\Delta\xi_b$ A_b dot A_b by A_b dot e_ξ times ϕ_b minus ϕ_0 right that is what we have, is not it that is the primary gradient, ok. What about the secondary gradient, now how do we calculate this guy; this is our secondary gradient.

Essentially, we are burdened with the same problem as we had with the interior faces right that means again if it is a structure, if it is a 2D mesh, we can ask or somehow calculate $(\phi_\eta)_b$ along the tangent; if it is a 3D structure, again we can somehow calculate it; but if it is 3D unstructured, then we have to go to this business of calculating the total value minus subtracting the primary gradient ok. So, we will do all that so that means, calculation of secondary gradient for boundary is also the same thing.

So, if it is 2D structured or unstructured, this can be calculated using interpolation; if it is 3D structured, also this can be calculated; but if it is 3D unstructured, then we do not have a unique way of defining the two secondary directions, as a result we will resort to calculating the total minus the primary that is going to give us the secondary ok, so we will resolve to a new different method. Now that means, I can rewrite the secondary gradient as what, if I were to write this as $(SG)_b$.

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$$(S_q)_b = \Gamma_b (\nabla \phi)_b \cdot A_b - \frac{\Gamma_b}{\Delta \xi_b} \frac{A_b \cdot A_b}{A_b \cdot e_\xi} (\nabla \phi)_b \cdot e_\xi \Delta \xi_b$$

Assumption $(\nabla \phi)_b \approx (\nabla \phi)_0$

$$= \Gamma_b (\nabla \phi)_0 \cdot A_b - \frac{\Gamma_b}{\Delta \xi_b} \frac{A_b \cdot A_b}{A_b \cdot e_\xi} (\nabla \phi)_0 \cdot e_\xi \Delta \xi_b$$

$(\nabla \phi)_0 \cdot e_\xi \Delta \xi_b = (S_q)_b$

Dirichlet BC: $\phi_b = \phi_b \text{ known}$

Discrete Equations

This can be written as, the total transport of phi through the boundary face that will be how much $(\Gamma \nabla \phi)_b \cdot A_b$ right that is the total transport of phi through the boundary face minus what would be the one going through the primary direction that will be Γ_b upon $\Delta \xi_b$ A_b dot A_b upon A_b dot e_ξ $(\nabla \phi)_b$ dot e_ξ times?

Student: Delta.

$\Delta \xi_b$ ok, we can again calculate it this way fine. Now, I do not have gradient of phi on the face, boundary face to calculate as a linear interpolation of the two cells right. So, I would make an assumption here and I would say that the gradient of phi on the boundary face would be just equal to gradient of phi of the cell C_0 ok, because I do not have a gradient on the other side; I do not have see one cell right, because that is a boundary face, so I would make this assumption and approximation.

Then I can rewrite this as, $\Gamma_b \text{ grad } \phi_0 \text{ dot } A_b$ minus Γ_b by $\Delta \xi_b$ A_b dot A_b upon A_b dot e_ξ $\nabla \phi_0$ dot e_ξ $\Delta \xi_b$, ok. $\nabla \phi_0$ is already calculated right, somehow through some gradient calculation method fine, so far so good. This is very much same as the how we dealt with the interior faces, any interior face ok.

Now, let us look at a specific boundary condition, so this is how we discretize the boundary fluxes. Now, let us look at a specific boundary condition, let us call it as the Dirichlet

boundary condition that means, we are talking about Dirichlet boundary condition. What is a Dirichlet boundary condition in this context, what is specified?

Students: Phi b.

Phi b would be known, this means ϕ_b is ϕ_b known right, this will be known ok. If this is known, let us look at what will happen to the primary gradient term. So, we come back here this is the coefficient right, what will be the contribution of the primary gradient, where all the primary gradient terms go, ok. ϕ_b is known right, this is known, this is not an unknown anymore; ϕ_0 is it unknown or known?

Students: Unknown.

Unknown right, this is unknown. So, what will be what will be the contribution of primary gradient to what terms?

Students: a p.

a_p , because there is a ϕ_0 term; so there will be a contribution to a_p which is about this value, this value what do you usually call a_b right, a_b is what we call this is a_b ; a_b contributes to a_p , what else will be there to?

Students: b term.

b term, right.

Students: b term.

What will be the b term?

Students: a_b .

a_b times phi b known would go to b.

Students: b term.

Right, because this is known now, this is a Dirichlet boundary condition. Everybody with that yes that means, this is contributing to two terms that is a_p and b right, to both of them.

What about the other term that is the secondary gradient, where will this guy go; $(SG)_b$, secondary gradient on the boundary, where will this term go?

Students: b.

Goes to the b always as it is fine, so that means we can now ready to write the discrete equation that means, if you have a Dirichlet boundary condition, we know what is ϕ_b is ϕ_b known right, this is a known value. Then we are ready to write the discrete equation ok, so what would be the discrete equation it would be we want it to come.

(Refer Slide Time: 33:01)

Discrete Equation

$$a_p \phi_0 = \sum a_{nb} \phi_{nb} + b$$

$$a_{nb} = \begin{pmatrix} \Gamma_f & A_f \cdot A_f \\ \Delta \xi_f & A_f \cdot e_\xi \end{pmatrix}_{nb=1, 2, \dots, M-1} \quad \text{int. faces}$$

$$a_p = \sum_{nb=1, 2, \dots, M-1} a_{nb} + a_b - S_p(\Delta \phi_0)$$

$$b = S_c(\Delta \phi_0) + \sum_{nb \text{ int}} (SG)_f + a_b \phi_{b, \text{known}} + (SG)_b$$

And fit in the same form that is $a_p \phi_0 = \sum a_{nb} \phi_{nb} + b$ right, we always wanted to come and fit in the standard form. Now, what will be a_{nb} ; a_{nb} would be same as before right. So, this would be Γ_f by $\Delta \xi_f$ A_f dot A_f by A_f dot e_ξ for all the neighbors.

But what are all these neighbors now, these are only the interior faces so that means, 1, 2 all the way to M minus 1 if you have one boundary face; if you have two boundary faces, it will be different right. If you have a corner cell, where there are two boundary faces, you have to say M minus 2 and then include those boundary effects ok, fine. Let us say we are talking about now one cell here, what about a_p ? So, these are the interior faces only, what about a_p term, a_p would be?

Students: Summation.

Summation of?

Students : a_{nb} .

a_{nb} where, n b goes from 1, 2 all the way to M minus 1.

Plus.

Students: a_b .

a_b ok, this goes to if you have one boundary face, this will go to a_b ; what else?

Students: S_p .

Minus.

Students: S_p .

S_p .

ΔV_0 that is all right, that is all will be there ok. What about the b term?

b term would have.

Students: Gamma (Refer Time: 34:43).

S_c times.

Students: ΔV_0 .

S_c times ΔV_0 source term, what else?

Students: Secondary gradient.

Secondary gradient coming from interior faces right as before that means, σ_{nb} , $(SG)_f$, where nb are the interior faces again; let us call it as nb interior what else?

Students: $a_b \phi_b$.

$a_b \phi_b$ that is plus or minus?

Students: Plus.

Plus.

Students: Plus.

This is $a_b \phi_b$ anything else; what about the secondary gradient for the boundary face, would that be there?

Students: Yes.

That should all with that will be here.

Students: Yes.

That means plus S G boundary alright; if you have one boundary face or sigma $(SG)_b$ if we have multiple boundary faces fine, is that ok.

(Refer Slide Time: 35:46)

The image shows a digital whiteboard interface. At the top, there is a toolbar with various drawing tools. The main area contains the following handwritten text:

$$+ (S_G)_b$$
$$a_b = \left(\frac{\Gamma_b}{\Delta \xi_b} \quad \frac{A_b \cdot A_b}{A_b \cdot e_\xi} \right)$$

Below the whiteboard, there is a small video inset showing a person in a light-colored shirt.

Of course, I did not write what is a_b , a_b itself is similar to the a_{nb} ; a_b would be Γ_b by $\Delta \xi_b$ A_b dot A_b by A_b dot e_ξ , right that is your a_b fine, is that ok; everybody any questions on this?

Students: Sir.

Yeah.

Students: Sir, in boundary calculation $(SG)_b$ for the we do the previous equation that we cause (Refer Time: 36:12) so gamma grad phi where have to calculate?

Gamma grad phi.

Students: For the boundary calculation.

Essential this has to be calculated $(\Gamma \nabla \phi)_b \cdot A_b$.

Students: So that means, we use the previous attrition (Refer Time: 36:26).

Yes, we use the previous attrition $\nabla \phi$ would be the $\nabla \phi$, you would use the previous attrition values so ϕ and calculate the gradient right. But the assumption we are making here is that $\nabla \phi_b$ would be equal to $\nabla \phi_0$ that is what I am making here, we will again discuss this thing the efficacy of this approximation right, we will we will discuss a little later; fine, is that clear.

As of now, we are we somehow through some method know the value of the gradients of the ϕ ok, which we can use here that is the; that is the idea here. Questions, other questions? No, fine, clear. So, we have looked in Dirichlet boundary condition, then let us look at the boundedness properties ok.

(Refer Slide Time: 37:16)

In the absence of $S = 0$

$$a_p > \sum a_{nb}$$

Satisfies Scarborough's inequality

Boundedness

ϕ_0 is not assumed to be bounded by cell neighbour values.

The what about so in the absence of source terms S equal to 0, what will be a_p , relation between a_p and $\sum a_{nb}$; a_p equals $\sum a_{nb}$ or is it greater. What are the neighbors here?

What, what constituted as neighbors, only the interior right, not the boundary right. When you write the equation, you do not have the coefficient coming from the ϕ_b in the matrix, because that guy went to the right hand side.

So, what is a_p , is it equal to $\sum a_{nb}$? No, it is greater than $\sum a_{nb}$ by an amount of a_b . This is same as nothing new right, this is same as the Dirichlet boundary condition for structured Cartesian meshes that we have seen before, so that means, a_p is greater than $\sum a_{nb}$; so this satisfies your Scarborough in.

Students: Inequality.

Inequality, ok. So, this satisfies Scarborough in inequality fine, very good. What about boundedness? So, S equal to 0, S equal to 0 is your $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$ is b , S is 0; so this guy goes to 0, is b 0 ok. We can leave this guy, but this guy is still contributes to the boundedness right.

Students: (Refer Time: 38:50).

Because a b is included in the calculation of a_p and also this one, so we can think of this as if it is bounded it can be bounded by the face value as well as by the cell neighbor values, but what is the other one that is preventing us from having boundedness.

Students: Secondary gradients.

Secondary gradients of the faces interior faces and the boundary face ok, as a result ϕ_0 is not assured to be bounded by cell neighbor values fine, alright that means, we have done discretization.

(Refer Slide Time: 39:42)

values.

Extend this to 1) Unsteady } Extend

2) Γ_f interpolation }

3) Source term linearization } the concepts

4) Under-relaxation }

5) stability analysis .

6) Neumann BC } Check!

7) Mixed BC }

Then you can of course extend this concept to if you have unsteady diffusion right on non-orthogonal meshes, can you extend this concept? Ultimately, the equation we are working with is $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$ right. Can you extend this concept to unsteady right? All the explicit implicit and Crank-Nicolson methods ok, it can be done. [vocalized noise]

What about Γ_f interpolation, can that be performed in this case using a harmonic mean right? You have to find the distances, and calculate what is Γ_f interpolation ok. I am writing all this, because I am not doing all this right. All this would be your work for you have to do it ok, verify later on ok. What else, this is the most exciting part right Γ_f interpolation. What else?

Students: Source term.

Source term linearization ok. So, source term linearization can also be will remain the same as before. What about under relaxation right? Can you perform under relaxation for these cases?

Students: Yes.

Yes. So, under relaxation can also be performed on this for non-orthogonal meshes right. So, you can verify that all these things can be done ok. This is for you to verify or extend to all these different scenarios ok. We have now left over one more thing what is that?

Students: (Refer Time: 41:33).

Sorry.

Students: Stability analysis.

Stability analysis of course you can also do. What else?

Students: (Refer Time: 41:38).

That is right stability analysis ok, but stability analysis would not be very different right; it probably would not be it probably not very easy to do because you have now unstructured meshes right. We just discussed that if you have a uniform 1D structured mesh, it can be done easily right.

So, this is probably not very easy to do, but of course you are well come to check and see where you get stuck or something. What else? I have only done it for a Dirichlet boundary condition right. We have two other boundary conditions. What are those?

Students: Neumann.

Neumann boundary condition, and mixed boundary condition ok. So, you will extend the concept to include these two boundary conditions also for non-orthogonal unstructured meshes ok. Now, I would not leave you alone like that.

So, what will happen in the context of Neumann boundary condition? Let us go back and see. Let us say if you have a homogeneous Neumann condition, what will be the condition that is specified. What will be specified if you have a Neumann homogeneous Neumann?

Students: $\nabla\phi$.

$\nabla\phi$ will be specified right. $\nabla\phi$ will be specified in which direction?

Students: Xi direction.

In the xi direction. So, what will happen to the primary gradients? Primary gradients is what is the term that goes away right. What about the secondary gradients would that remain?

Student: Still.

That will still remain right. So, that will still remain, that is how you would implement right. Now, how do you do for mixed boundary conditions?

Students: Sir.

Yeah.

Students: (Refer Time: 43:15), what flux will be known in primary direction (Refer Time: 43:20).

Why flux will be known we are assuming that that is what is given to us. Usually, if we have a face it would be given in the direction of the normal to the face right that is kind of a if you have let us say insulation or something, the flux going in that direction would be 0 right, in the direction of a b would be 0 right that is minus $k dt d x_i$ would be equal to 0 right.

But it need not be known in the same direction right. If it is not known, what would you do? If it is given in a let say in general you would be given what would you do in that context?

Students: (Refer Time: 43:54) take component.

Take components and then work with this. What about mixed boundary conditions? That is a if you have convection happening on the particular phase, how would you implement it now? You remember the concept how we have done what did we do? You get rid of phi b from the equations right.

You have to go to ϕ_0 an phi stream phi infinity and then work with the equations fine ok. So, all of these is for you to check and verify an extent ok, alright. Questions still now?

Students: Neumann boundary condition.

Neumann boundary condition ok.

Students: We know the primary gradient.

We know the primary gradient ok.

Students: Secondary gradient (Refer Time: 44:45).

Right.

Students: What about the eta direction?

So, you have to calculate the total and then subtract of the xi direction right. So, how do I deal with secondary gradient? Essentially the question is if I have a Neumann boundary condition, how do I deal with it $(SG)_b$ term right?

(Refer Slide Time: 44:55)

The image shows a whiteboard with handwritten notes. The notes are organized into two groups. The first group, labeled 'the concepts', includes: 3) Source term linearization, 4) Under-relaxation, and 5) stability analysis. The second group, labeled 'Check!', includes: 6) Neumann BC and 7) Mixed BC. Below these lists are three circled terms: $(SG)_b$, \vec{q} , and $(\nabla\phi)$. The whiteboard also features a toolbar at the top and an NPTEL logo in the top right corner. A small video inset of a man is visible in the bottom right corner of the whiteboard frame.

You would calculate what is $\nabla\phi_0$ for the cell right, and you can also calculate the primary gradient right that is $\phi_{xi b}$ right. Now, that is not the same as what is given right. What is given to you is in the direction normal to the face right, so that you have to check and perform right. But $(SG)_b$ would still remain right, unless that boundary cell is orthogonal. How do you calculate secondary gradient of b?

Students: Primary.

Primary the total minus the primary right that will that concept be the same thing here. Yes.

Students: Sir, suppose we have a domain as a plane (Refer Time: 45:43).

Hm.

Students: So, in that case, suppose the domain is divided into unstructured (Refer Time: 45:50).

Hm.

Students: So, that plane will be having mili cells whose boundary from the plane.

Hm.

Students: then a cell is unstructured. So, each cell will be a different, different direction.

Yes.

Students: So, in that case, the fluxes that would be allows a minus n (Refer Time: 46:07).

Hm.

Students: But easily as difference (Refer Time: 46:07).

True. That is true it depends on the cell. It, it varies from face to face, but your boundary condition is already known to you how the flux is in what direction the flux is right. You are applying some \vec{q} , now this \vec{q} is known to you right. It has a certain i, j, k components.

From there you have to take a dot product with your particular face direction \vec{A}_b and then calculate. So, it is not that your primary gradient would always be 0 right, so that is that is possible. So, that is where you have to look at and see how this comes up right.

Students: (Refer Time: 46:43), but not in the direction of xi.

May not be in the direction of xi right \vec{q} is perpendicular to the is along the normal to the face, but it is need not be in the direction of xi because xi is defined by how your cell is positioned right.

If the line connecting the cell centroid to the face centroid is along the direction of xi, along the direction of a b, then you do not have an issue, but otherwise you will get the secondary gradient and all these things right. Otherwise it will be like if you have an orthogonal cell, your secondary gradient will go to 0 right automatically $e_\xi \cdot d n$ will go to 0 and you do not do anything there fine.

Other questions? Ok. So then that kind of finishes the discussion on diffusion equation per say on unstructured non-orthogonal meshes as well ok. We have one more concept which we have not covered that is calculation of the gradient right that is what we have introduced. So, we have this small topic on the calculation of gradients for the dependent variable that is how do I calculate $\nabla\phi$.

There are several methods available we will look at couple of methods in this particular course and see how $\nabla\phi$ can be calculated ok. So, that is gradient calculation will be our next topic that we discuss, then that finishes our chapter on diffusion ok. After this we will move on to the convection chapter fine, so alright. So, in the next lecture we will look at calculation of gradient for the dependent variables ok.

Thank you. See you guys in the next lecture.