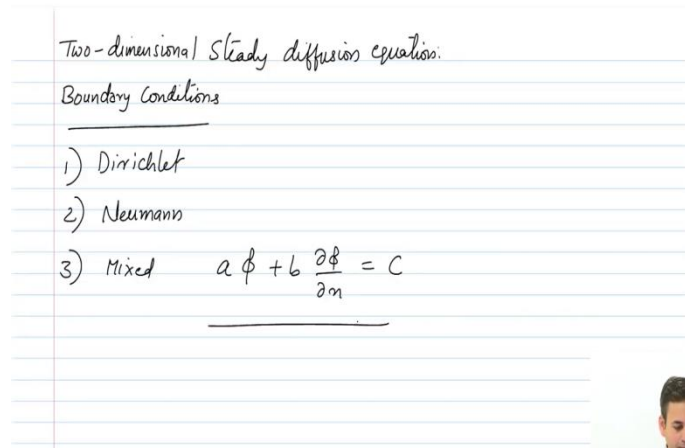


Computational Fluid Dynamics Using Finite Volume Method
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Lecture – 13
Finite Volume Method for Diffusion Equation: Discretization of 3D diffusion equation, mixed boundary conditions

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Good morning, let us get started. So, we were looking at two-dimensional Diffusion Equation and the boundary conditions right in the last lecture. So, we are looking at two-dimensional steady diffusion equation. And in that context, we are looking at the boundary conditions alright. So, we have finished discussion on Dirichlet boundary condition, and also on Neumann boundary condition right.

The only one that is remaining is the discussion on mixed boundary condition where we specify a kind of proportionate amounts or a linear combination of a Dirichlet and a Neumann right. We are going to specify $a\phi + b \frac{\partial \phi}{\partial n} = c$.

So, this will be a combination of Dirichlet and a gradient boundary conditions. We said one of the examples for having a mixed boundary condition is convection right. So, for example, if we have so I am going to just go to next page and the convection.

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3) Mixed $a\phi + b \frac{\partial \phi}{\partial n} = C$

$-(\Gamma \nabla \phi)_b \cdot i = h(\phi_\infty - \phi_b)$

$-\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b = h(\phi_\infty - \phi_b)$



So, essentially if we have a fluid that is moving at certain velocity with the temperature of the fluid being phi infinity or the scalar being phi infinity and if h being the heat transfer coefficient, then we said we can have a mixed boundary condition and if we discretize the near boundary cells as this.

So, if we have P, E, and north and south ok, and the excuse me. So, and the cell widths that is delta x delta y remain the same as before. And then we also have these distances those are δx_e between the p cell, and the east cell and δx_b between the boundary and the p cell right. So, we have these distances. So, we have δx_e , δx_b , δy_n , and δy_s ok. So, these are denoted as before delta y north and then delta y south ok. So, these are there.

Now, coming to the specification of the boundary condition what we have is if let say the temperature on the boundary is ϕ_b ok, then a convection would read the heat flux that is coming in let say if we call it q, then it will be $-(\Gamma \nabla \phi)_b \cdot i = h(\phi_\infty - \phi_b)$ that is the heat flux in the positive x direction would be equal to would be equal to what would be equal to the convection heat transfer right. So, this is , so that is what we have. So, essentially this c is a mixed boundary condition right.

So, if we look at if you write this rewrite this thing, this will be $-\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b = h(\phi_\infty - \phi_b)$

. So, we essentially have a combination of the Dirichlet and a Neumann adding up to some constant here. So, we have a ϕ plus b partial ϕ partial n equal to constant ok, so that is kind of boundary condition.

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$$-(\Gamma \nabla \phi)_b \cdot i = h(\phi_w - \phi_b)$$

$$-\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b = h(\phi_w - \phi_b)$$

$$-\Gamma_b \left(\frac{\phi_p - \phi_b}{\delta x_b} \right) = h(\phi_w - \phi_b)$$

Now, of course, we can discretize this, and rewrite this part as the following. We know that minus gamma b can we write a partial phi partial x at b in terms of P and the boundary value we can. So, that will be how much?

Student: (Refer Time: 04:11).

$-\Gamma_b \frac{\phi_p - \phi_b}{\delta x_b} = h(\phi_w - \phi_b)$. Now, the idea here is that if you discretize the p cell, what are the dependent variables you are going to get? You are going to get the dependent variables for phi east right, phi north, phi south, and if you discretize it here you would probably get in terms of phi b as well right if you discretize for this p cell.

Now, the idea is let us not have phi b in picture ok. Let us try to get rid of phi b, and let us have a dependency on phi infinity ok, and of course, on phi p right. You will have phi p which you will calculate, and then we are going to have dependency on phi infinity ok. So, we want to get rid of phi b. As a result what we want to do is we want to obtain an expression for phi b in this from this relation ok. Can we obtain a relation for phi b in terms of phi p and phi infinity? Yes, we can ok. So, that is what I am going to do.

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$$-(\Gamma \nabla \phi)_b \cdot i = h(\phi_\infty - \phi_b)$$

$$-\Gamma_b \frac{\partial \phi}{\partial x}|_b = h(\phi_\infty - \phi_b)$$

$$-\Gamma_b \left(\frac{\phi_p - \phi_b}{\delta x_b} \right) = h(\phi_\infty - \phi_b)$$

$$\phi_b \left(h + \frac{\Gamma_b}{\delta x_b} \right) = h(\phi_\infty) + \frac{\Gamma_b}{\delta x_b} \phi_p$$

$$\phi_b = \frac{h \phi_\infty + \frac{\Gamma_b}{\delta x_b} \phi_p}{h + \frac{\Gamma_b}{\delta x_b}}$$

So, that would be how much, that would be phi b times h is what I have here plus gamma b upon delta x b right that is what I have equals h times phi infinity is what I have here and then plus gamma b by delta x b times phi p. Is that algebra correct? Ok, so

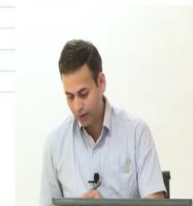
essentially we got an expression for phi b. So, $\phi_b = \frac{h \phi_\infty + \frac{\Gamma_b}{\delta x_b} \phi_p}{h + \frac{\Gamma_b}{\delta x_b}}$ b ok, so that is

what we have for phi b ok.

Now, what we said is we want to get rid of the dependency on phi b. So, we have to substitute this phi b back into where into the diffusion flux right. So, essentially I am going to substitute phi b back into the definition for diffusion flux that we have here ok, because in the discretized equation we do not want a dependency on phi b. We only wanted it in terms of phi p east north south and phi infinity ok. So, so this is the discretized expression.

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$$\begin{aligned}
 -\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b &= -\Gamma_b \left(\frac{\phi_p - \phi_b}{\delta x_b} \right) \\
 &= -\Gamma_b \left(\frac{\phi_p - \frac{h\phi_\infty + (\Gamma_b/\delta x_b)\phi_p}{h + (\Gamma_b/\delta x_b)}}{\delta x_b} \right) \\
 &= -\Gamma_b \left(\frac{h(\phi_p - \phi_\infty)}{\delta x_b (h + \Gamma_b/\delta x_b)} \right) \\
 &= \frac{(\Gamma_b/\delta x_b)h}{h + (\Gamma_b/\delta x_b)} (\phi_\infty - \phi_p)
 \end{aligned}$$



So, I am going to substitute for phi b in this ok. So, what would that read like essentially the discretization is $-\Gamma_b \frac{\partial p}{\partial x} \Big|_b = -\frac{\Gamma_b(\phi_p - \phi_b)}{\delta x_b}$

that would be your west phase flux which is nothing but. And I am going to replace phi b here with what we found from here ok, essentially in terms of phi p and phi infinity ok.

Let us do that. What would that lead to? That would be $\Gamma_b \frac{\phi_p - h\phi_\infty + (\frac{\Gamma_b}{\delta x_b})\phi_p}{h + (\frac{\Gamma_b}{\delta x_b})}$ minus that is what we have.

So, if I simplify this further, what would that be? Minus gamma b times what do we get here, what gets cancelled? Gamma b by delta x b times phi p is a positive here, and there is a minus here, so gamma v by delta x b times phi p this gets cancelled ok. So, what remains here is what? $-\Gamma_b \left(\frac{h(\phi_p - \phi_\infty)}{\delta x_b (h + \frac{\Gamma_b}{\delta x_b})} \right)$

h times.

Student: Phi p.

Phi p minus.

Student: p infinity.

. So, this denominator still remains and gets multiplied with this guy that is what we get right. So, here we can rewrite this as $-(\Gamma_b/\delta x b)h/h + (\frac{\Gamma_b}{\delta x b}) (\phi_\infty - \phi_p)$ what do we have here, we have phi p minus phi infinity ok. So, I am going to get rid of the minus sign here, then I can rewrite this as what? Phi infinity minus phi p. Is that correct?

Essentially, the west face flux $\Gamma_b \partial \phi / \partial x|_b$ we have written in terms of completely in terms of phi p the dependent variable at the cell p and in terms of phi infinity right. So, phi infinity is the free stream scalar value or the temperature value ok, correct ok. Now, let us call this coefficient that we have here as a constant ok. Let us call this has some constants.

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Handwritten derivation on a slide:

$$-\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b = k (\phi_\infty - \phi_p)$$

$$k = \frac{(\Gamma_b / \delta x b) h}{h + (\Gamma_b / \delta x b)}$$

$$\Gamma_e \Delta y \frac{\partial \phi}{\partial x} \Big|_e - \Gamma_b \frac{\partial \phi}{\partial x} \Big|_b \Delta y + \Gamma_n \Delta x \frac{\partial \phi}{\partial y} \Big|_n - \Gamma_s \Delta x \frac{\partial \phi}{\partial y} \Big|_s + (S_c + S_p \phi_p) \Delta x \Delta y = 0$$

$$a_p \phi_p = \sum_{nb = E, N, S} a_{nb} \phi_{nb} + b$$

So, this is some constant $k (\phi_\infty - \phi_p)$ This is your discretization for $-\Gamma_b \frac{\partial \phi}{\partial x} \Big|_b = k (\phi_\infty - \phi_p)$. And what is k? k is your $k = \frac{(\Gamma_b / \delta x b) h}{h + (\Gamma_b / \delta x b)}$.

Now, what do we have to do, we have to basically substitute for this expression back in the discretized flux equations right, and substitute for the other values on the east, north, and the south, and then collect the terms alright that is all we have to do. So, if we go back to the discrete equation, so the equation we have is $\Gamma_e \Delta y \frac{\partial \phi}{\partial x} \Big|_e - \Gamma_b \frac{\partial \phi}{\partial x} \Big|_b \Delta y + \Gamma_n \Delta x \frac{\partial \phi}{\partial y} \Big|_n - \Gamma_s \Delta x \frac{\partial \phi}{\partial y} \Big|_s + (S_c + S_p \phi_p) \Delta x \Delta y = 0$ that is what we have.

In which I am going to replace I am going to use linear profile assumption for all these quantities alright, for the partial phi partial x on the east partial phi partial y on the north and the south and we are going to replace this quantity minus gamma b partial phi partial x b with what we just obtained here right, we are going to write k times phi infinity minus phi p right and then collect the terms.

So, if we rearrange in the a p phi p style that would be a p phi p equals if I kind of write it in a short form. So, this would be $a_p \phi_p = \sum a_{nb} \phi_{nb} + b$ where n b goes on east north and south alright. Now, what would be the coefficients that is the question? Now, if you look at if you take a look at this one where will this contributions go, where will minus k phi p go. So, we have a minus k times phi p right this term where will minus k go, minus k go? This will go into a p right it will go into a p where will k infinity k phi infinity go.

Student: b.

It will go into the b term right, because this is known ok. So, there are two contributions one going to the right hand side, one going as a coefficient to a p. Of course, we have this multiplication of delta y that I have not put here. So, with this basically this gets multiplied with delta y right.

This is only an expression for gamma b partial phi partial x times delta y. So, essentially the coefficient that will go is the delta y minus k, minus k delta y, it will become plus right because we are sending the p term. So, the right hand side k delta y will go into a p, and k phi infinity delta y will go into b ok. So, that is the contribution.

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$$a_p \phi_p = \sum_{nb = E, N, S} a_{nb} \phi_{nb} + b$$

$$a_E = \frac{\Gamma_e \Delta y}{\delta x_e}; \quad a_N = \frac{\Gamma_n \Delta x}{\delta y_n}; \quad a_S = \frac{\Gamma_s \Delta x}{\delta y_s}$$

$$a_p = a_E + a_N + a_S - S_p \Delta x \Delta y + k \Delta y$$

$$b = k \phi_\infty \Delta y + S_c \Delta x \Delta y$$

Scarborough: if $\delta = 0$;

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

In inequality



Now, can you tell me what would be the coefficients that we have? So, what is a east a east is the same as before right nothing has changed. So, this is $a_E = \frac{\Gamma_e \Delta y}{\delta x_e}$ gamma east; $a_N = \frac{\Gamma_n \Delta x}{\delta y_n}$; $a_S = \frac{\Gamma_s \Delta x}{\delta y_s}$. What we have is a p, what would be a p? $a_p = a_e + a_n + a_s - S_p \Delta x \Delta y + k \Delta y$

Student: (Refer Time: 13:13).

Plus k times.

Student: (Refer Time: 13:15).

Phi infinity? No, phi infinity will go to the right hand side. What would go into here k times.

Student: Delta y.

Delta y right, k times delta y times phi p is we what we got here right essentially k times phi p times delta y right. So, phi p is already taken out as a coefficient for a p right. Then this is what that goes into the central term. Now, what is remaining we have b term, what would be b? $b = k \phi_\infty \Delta y + S_c \Delta x \Delta y$

Student: Delta y.

Delta y plus

Student: S c.

Now, what about Scarborough criteria? Let us say we assume the $S = 0$. If the source is 0, what is $ap > \Sigma_{anb}$, is it lesser, greater, equal?

Student: Greater.

Greater because S p times delta x delta y is 0, but what about this guy, this is still nonzero right. So, this term is there. So, as a result, it will be it will be greater ok, assuming that there is a convection happening to the right to the fluid ok. Now, what about. So, and in case the source term is not 0 then anyway it satisfies Scarborough in inequality ok, so that we anyway understand. So, the essentially it satisfies in inequality.

Now, do you see why it is actually satisfying inequality? Because mixed boundary condition has this Dirichlet component in there right that is the reason; otherwise pure Neumann boundary condition does not satisfy in inequality; it only satisfies in equals right ok. Questions till now, now clear easy ok.

Student: (Refer Time: 15:21).


Very good alright. Let us move on. Then what I want to discuss next is the extension to 3 dimensions ok, 3 dimension diffusion that is very straightforward. We will not write down the equations rather I want you to kind of think in your brains and then tell me kind of dictate, and I am going to just write it down that is the 3 dimension extension.

Then that will be done quickly, then we will look at interpolation of the diffusion coefficient right. We have this gamma that we have to calculate on the phases, up till now we have kind of postponed it we said somehow we know gamma on the phases ok. But how do we actually calculate it, and which methods are will give correct results and which methods do not that is what we are going to do after the 3 dimensions is done ok.

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In inequality


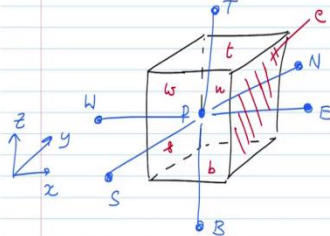
Diffusion (steady) in 3D:

$$\nabla \cdot (\Gamma \nabla \phi) + S_\phi = 0$$


So, then the next thing is diffusion or rather steady diffusion in 3 dimensions ok, steady diffusion in 3 dimensions ok. The governing equation is the same that is $\nabla \cdot (\Gamma \nabla \phi) + s_\phi = 0$

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Diffusion (steady) in 3D:

$$\nabla \cdot (\Gamma \nabla \phi) + S_\phi = 0$$
$$\nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}$$


Here your del operator now has all the three components $\nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}$ that is all we have. Of course, our domain now looks a little more complicated; because we have we are dealing with in 3 dimensions ok. Let say that is my p cell ok, let call this is my p

cell, and x is in this direction, y is in this direction, and z according to the right hand screw right hand thumb rule we have in the top direction ok.

Then what about the neighbors? So, this is the p cell. And we have one neighbor here another neighbor here, and the north, and the south neighbors, and we have of course the top and the bottom neighbors which we are not drawing all of them, rather this is your east neighbor, west neighbor, north, south, and we call this as top and bottom ok. So, we have all these neighbors.

Then we have of course the faces. What are the faces? This is which face? East face ok, so this is your east face. Similarly, you have the west face, the north face, south face, and top and bottom faces right, we have all these faces ok.

Now, what do we do we again integrate the governing equation on the control volume, invoke Gauss divergence theorem. Convert the volume integral into a surface integral, then replace the surface integral with a discrete summation right, assuming that the gradient the diffusion fluxes remain the same on the faces everywhere and the cell phase centroid value can be used to integrate ok. We all we do all that, and then we derive we kind of come for the final discrete equation.

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\Gamma_E A_e \frac{\partial \phi}{\partial x} \Big|_e - \Gamma_W A_w \frac{\partial \phi}{\partial x} \Big|_w + \Gamma_N A_n \frac{\partial \phi}{\partial y} \Big|_n - \Gamma_S A_s \frac{\partial \phi}{\partial y} \Big|_s
$$+ \Gamma_E A_t \frac{\partial \phi}{\partial z} \Big|_t - \Gamma_b A_b \frac{\partial \phi}{\partial z} \Big|_b + (S_c + S_p \phi_p) \Delta x \Delta y \Delta z = 0$$
 Below this, it states:

$$A_p = \Delta x \Delta z ;$$
 In the bottom right corner, there is a small video inset showing a man speaking at a podium."/>

That would be what? That would be $\Gamma_E A_e \frac{\partial \phi}{\partial x} \Big|_e - \Gamma_W A_w \frac{\partial \phi}{\partial x} \Big|_w + \Gamma_N A_n \frac{\partial \phi}{\partial y} \Big|_n - \Gamma_S A_s \frac{\partial \phi}{\partial y} \Big|_s + \Gamma_E A_t \frac{\partial \phi}{\partial z} \Big|_t - \Gamma_b A_b \frac{\partial \phi}{\partial z} \Big|_b + (S_c + S_p \phi_p) \Delta x \Delta y \Delta z = 0$. Of course, you are going to get

now how many terms here? 6 times, because you have six phases, so that is rather very straightforward gamma north A north partial phi partial y north minus gamma south A south partial phi partial y south plus gamma top A top partial phi partial z top.

Delta x delta y delta z which is nothing but your if I were to draw this is your delta x, this is your delta y, and the height here is the delta z right, we have all these things equals 0 right, equals 0 is what we have ok. Now, it is very simple. We do not have to write all of them, rather I want you to kind of tell me what would be A east, what is the area vector that we have now?

(Refer Slide Time: 19:43)

$$\left\{ \begin{aligned} & \Gamma_E A_e \frac{\partial \phi}{\partial x} \Big|_e - \Gamma_W A_w \frac{\partial \phi}{\partial x} \Big|_w + \Gamma_N A_n \frac{\partial \phi}{\partial y} \Big|_n - \Gamma_S A_s \frac{\partial \phi}{\partial y} \Big|_s \\ & + \Gamma_T A_t \frac{\partial \phi}{\partial z} \Big|_t - \Gamma_B A_b \frac{\partial \phi}{\partial z} \Big|_b + (\Sigma \epsilon + \Sigma_f \phi_p) \Delta x \Delta y \Delta z = 0 \end{aligned} \right\}$$

$$A_e = \Delta y \Delta z ; \quad \frac{\partial \phi}{\partial x} \Big|_e = \frac{\phi_E - \phi_P}{\Delta x_e}$$

$$A_n = \Delta x \Delta z ; \quad \frac{\partial \phi}{\partial y} \Big|_n = \frac{\phi_N - \phi_P}{\Delta y_n}$$

$$\frac{\partial \phi}{\partial z} \Big|_t = \frac{\phi_T - \phi_P}{\Delta z_t} ; \quad \frac{\partial \phi}{\partial z} \Big|_b = \frac{\phi_P - \phi_B}{\Delta z_b}$$



Student: (Refer Time: 19:50).

This is A east. What would be the area of that?

Student: (Refer Time: 19:54).

Delta y times.

Student: Delta z.

Delta z that is all ok. So, essentially we have delta y, delta z. Similarly, A west is also the same right, only thing is direction is different, it will be minus i. What would be $A_n = \Delta x \Delta z$ A north? A north is the back face right,.

Student: (Refer Time: 20:11).

it is that guy. That is how much?

Student: Delta x delta z.

Delta x times delta z ok, so that is delta x delta z. And what would be A top? That is this surface delta x times.

Student: Delta y.

Delta y ok. So, we have all these things. Then we can plug all these things back into the discrete equation for fluxes right. And what about $\frac{\partial \phi}{\partial x} \Big|_e = (\phi_E - \phi_p) / \delta x e$ would it remain the same or it would be different?

Student: Same.

e all those things right. So, essentially if I were to write partial phi sorry ok, so partial phi partial x east is phi east minus phi p upon del x e; $\frac{\partial \phi}{\partial y} \Big|_n = (\phi_N - \phi_p) / \delta y n$


And similarly we have now what is the extra which is $\frac{\partial \phi}{\partial z} \Big|_t = (\phi_T - \phi_p) / \delta z t$ that will be the extra one. And of course, we have the $\frac{\partial \phi}{\partial z} \Big|_b = (\phi_p - \phi_b) / \delta z b$ We have these expressions which you can easily do.

And essentially plug all of these back into the diffusion equation right into the diffusion equation, and then collect the terms right, you will get a linear algebraic equation ok, which is very straightforward compared to the 2D. All we get is again a p phi p equals sigma nb phi and b plus b. Where now n b goes from where?

(Refer Slide Time: 21:50)

Handwritten mathematical derivations on lined paper:

$$\Delta r = \Delta x \Delta y; \quad \frac{\partial \phi}{\partial y} \Big|_n = \frac{\phi_N - \phi_P}{\Delta y_n}$$
$$\frac{\partial \phi}{\partial z} \Big|_t = \frac{\phi_T - \phi_P}{\Delta z_t}; \quad \frac{\partial \phi}{\partial z} \Big|_b = \frac{\phi_P - \phi_B}{\Delta z_b}$$
$$a_p \phi_p = \sum_{nb=E,W,N,S,T,B} a_{nb} \phi_{nb} + b$$
$$a_p = \sum_{nb=E,W,N,S,T,B} a_{nb} - S_p \Delta x \Delta y \Delta z$$

$$b = S_c \Delta x \Delta y \Delta z$$


East, west.

Student: North, south.

North, south, and top, and bottom ok. And what would be your a p? $a_p = \sum a_{nb} - S_p \Delta x \Delta y \Delta z$

Student: a p.

a p is sigma.

Student: a.

goes from east, west, north, south, top and bottom. Anything else in a p term?

Minus S p.

Student: (Refer Time: 22:22).

. And what about b? $b = S_c \Delta x \Delta y \Delta z$ The constant of the source that is. We just have two more extra terms because of the two more faces that we have fine. So, this is rather straightforward. Now, all we have to do is we have to write these equations one for each cell, apply the boundary conditions and then we can of course use Gauss-Seidel. Can we use Gauss-Seidel for 3D or no?

Yes, we can, because Gauss-Seidel does not care right whether you are in 1D, 2D, 3D, all you have to do is go from cell to cell right. Every cell you need an equation. And as long as diagonal dominance is there Gauss-Seidel will be guaranteed to converge right. So, essentially you can of course, use Gauss-Seidel it will be slow right because if you have let say 10 cells in each direction, you have thousand cells in total. So, Gauss-Seidel will be much lower than the 1D cases you have solved, but nonetheless you can use Gauss-Seidel ok.

In the coming lectures, we will see an alternative that can be used instead of a Gauss-Seidel which will be much faster than it ok. Questions till now. So, now, we can kind of solve for structured Cartesian meshes like we can solve the diffusion equation on it in both in all the dimensions right, for a source term or all sorts of boundary conditions that can be given ok, ok. Let us move on, fine.

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$b = S_c \Delta x \Delta y \Delta z$
Interpolation of Γ_f (Diffusion Coeff. on the faces.)
Composite material
 $\Gamma(x, y, z)$
Conjugate heat transfer.
 Γ on cell centroids?
 to Γ on the faces



Then let us move on to this topic which is calculation of the diffusion coefficient on the faces that is; basically how do I calculate diffusion coefficient, that is basically interpolation of gamma f right that is your diffusion coefficient on the faces ok. The idea here is that let say if we have a composite material ok, or what you have is you have the thermal conductivity or the diffusion coefficient as a function of as a function of space.

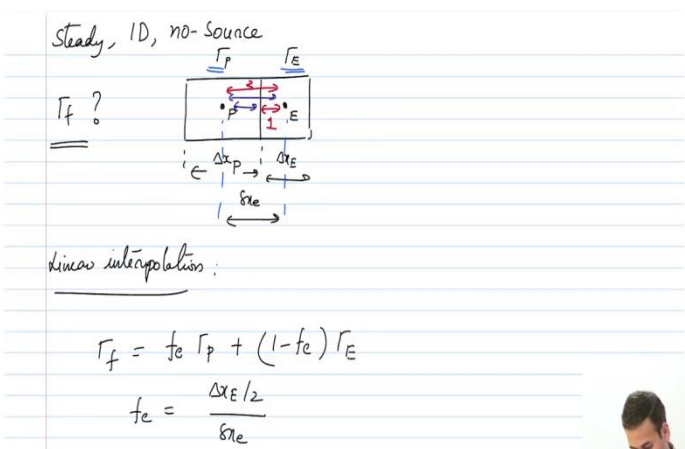
For example, gamma is a function of x, y, z, ok, that means, depending on where you are you have a different thermal conductivity. You could have a composite material in which

two slabs or multiple slabs are stitched together; in such cases how do I calculate gamma on the faces that is the question ok. So, essentially or you could think of as a conjugate heat transfer problem as well.

What is a conjugate heat transfer problem? You might have been aware of. Essentially you have a convection you have a solid and a fluid, and you have to solve for both of them right. Essentially you have a the heat is being exchanged between all these things ok, so that is the conjugate heat transfer problems. You know in all these cases you end up calculating gamma on the faces ok. And then how do we calculate it is what is the question. ah

Now, of course, what we say is that we know the gamma values on the cell centroids that is what we are starting off with ok. For example, if you have a slab, you know the what is the gamma value on the cells of these cell centroids ok. So, we know gamma on cell centroids ok, diffusion coefficient, now how do I calculate interpolate these gamma on the cell centroids to gamma on the faces right? Such then I can use it in the discrete equations fine, alright. Let us move on.

(Refer Slide Time: 26:19)



Steady, 1D, no-source

Γ_f ?



Γ_P Γ_E

Δx_P Δx_E

δx_e

linear interpolation:

$$\Gamma_f = f_e \Gamma_P + (1 - f_e) \Gamma_E$$

$$f_e = \frac{\Delta x_E / 2}{\delta x_e}$$



Let me consider a steady one-dimensional situation to simplify things and also study one-dimensional, and then there is no source term ok. Let us consider all these things. There is no source and we are looking at a steady depletion and then it is a one dimensions ok. Then I can of course, write down the discrete equation before that I want

to look at the cells ok. So, the cells are like this. Let say this is my p cell; let say the cells are not uniform the P cell is bigger than the east cell. So, I have this as my east cell, this is my P cell. As a result the delta x, I have I would like to call it as delta x p ok, this is the cell width of the p cell. And delta x capital E would be the width of the east cell ok; similarly, width of the west cell will be delta x capital W that is the cell widths. This is not uniform anymore, up till now we have used delta x for to denote the cell width for the p cell ok. Then of course, we have one more distance what was that?

Student: (Refer Time: 27:28).

Distance between the cell centroids right. This is how much? Del x e ok. This is del x e. Now, because it is said that gamma is known to you, it will be given to you right, it is a material property. So, it is known at the cell centroids. So, we know what is gamma at on the east cell, this is gamma E.

We know what is gamma on the p cell, right. The question is how do I calculate gamma f from all these things that I know ok. Ok, of course, you can use linear interpolation alright. And write gamma f as gamma on the face as some coefficient that is let us call it as f e ok, this is a some factor the linear interpolation factor f e times gamma p plus 1 minus f e times gamma east ok.

So, I have essentially f e times this gamma p plus 1 minus f e times gamma east, where f e is my ratio of the lengths that I have. And what are those lengths? Those lengths are this length to the total length right that would be f e is what I have ok, that means, I can write my f e $f_e = \left(\frac{\Delta x_e}{2}\right) / \delta x_e$ as what would be length of this guy that is denoted with 1 that is half of the cell width right. So, that is delta x by.

Student: (Refer Time: 29:03).

divided by, what will be their length of the second segment.

Student: Delta, x e.

, so that is what I have. So, this is my f e. Now, essentially I am forming a fraction of 1 to 2 right. So, that fraction times gamma p plus one minus that fraction would give me which one? It will give me a ratio of this to this right that fraction times gamma E, is that correct? I am taking the arm lengths right accordingly and I have formed a linear

interpolation right. f_e times gamma p that is on the left hand side and one minus f_e times gamma E that is on the right hand side right fine. So, this is linear interpolation, very good.

(Refer Slide Time: 29:59)

$$f_e = \frac{\Delta x_E / 2}{\Delta x_e} = \frac{1}{2}$$

f is mid-way $f_e = 0.5$
 $\Delta x_e = \Delta x_E$

$$\Gamma_f = \frac{\Gamma_P}{2} + \frac{\Gamma_E}{2}$$

$$\Gamma_f = \left(\frac{\Gamma_P + \Gamma_E}{2} \right)$$

Arithmetic Average.

Then of course, if the phase f is half way, let say if f is f is midway, then what would be if f is midway between these two, then what would that mean?

Student: (Refer Time: 30:19).

That is half that is coming because your Δx capital E equals Δx small e right. The width of the cell is same as the distance between the cell centroids right, only then if it is halfway; that means, essentially we have Δx capital E equals Δx e then what will this ratio be?

Student: (Refer Time: 30:36).

Half right, Δx E equals Δx e you have a half remaining right. So, this will be 0.5, that means, we are looking at midway interpolation. Then what will be gamma f ? Gamma P by 2 f_e is half plus this is 1 minus half that is again half this is gamma east by 2, then we get our arithmetic average right gamma P plus gamma E by 2, this is our arithmetic average of both gamma P and gamma E ok. We have not done anything great. We have pre wrote arithmetic average and a general equation for it right in terms of calculating the gamma f .

(Refer Slide Time: 31:28)

$$\Gamma_f = \left(\frac{\Gamma_p + \Gamma_E}{2} \right)$$

Arithmetic Average.

leads to incorrect results in some situations.

Alternate approach: to calculate Γ_f

Better results under all circumstances

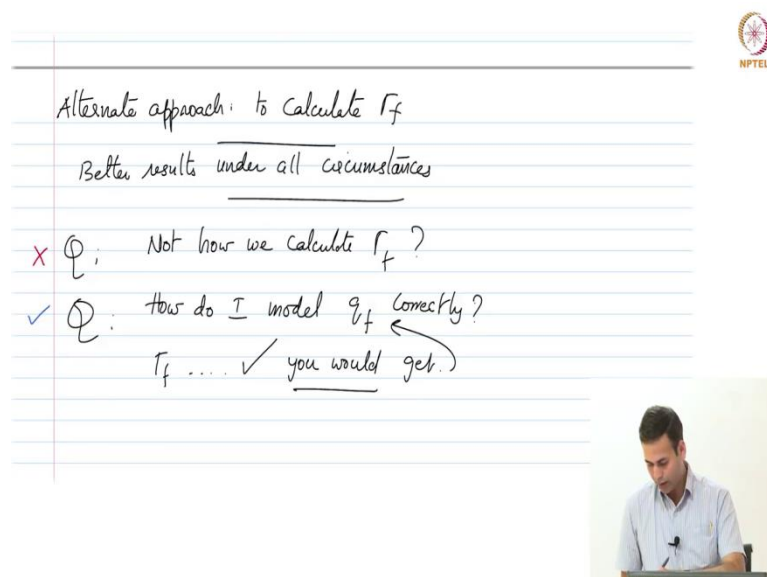


Now, of course, can I use this formula? You can. But it appears if you use a arithmetic average ok, this leads to incorrect results in some situations in some situations ok. So, in some in some of the same situations, we will not be using the arithmetic average now this is what I am kind of claiming. We have not yet proved, we will prove it in little while ok, rather we use a slightly different approach.

So, we use an alternate approach with somewhat simple like this method only to calculate gamma f ok, that will give better results under all circumstances ok. Now, I have just claimed something here ok, we have not yet proved, we will prove it in little while.

What I said is if you use arithmetic average or just linear interpolation, it may not give correct results, it will give accurate in incorrect results in some situations which we are going to see ok. Especially, if we have gamma as a function of a space, and if you have a composite material and things like that rather if you use an alternate approach, then the gamma f you would calculate with from an alternate approach would be would give you better results ok.

(Refer Slide Time: 33:13)



Alternate approach: to calculate Γ_f
Better results under all circumstances

X Q: Not how we calculate Γ_f ?

✓ Q: How do I model q_f correctly?
 Γ_f ... ✓ you would get.)

Now, this is a claim we are making which we will prove now. Before that what, what it seems is like we are actually the question we have to ask ourself is we do not want to calculate the question is not how we calculate gamma or gamma f ok. This is not the question.

The question is the correct question is actually how essentially how do I model the heat flux that is going in through the face correctly? Ok, that is the question. And if you can correctly calculate q_f , then the resulting gamma f would be the gamma f that you would need ok.

This is what you would get which is the which would give you which would give you the correct heat flux to the face ok. So, the question is how do I calculate heat flux correctly? Such that that heat flux calculation terms the gamma that whatever is kind of appearing there would be the right gamma I should use ok, so that is the question we ask ourself ok.

So, with this I am kind of going ahead and then drawing a I will redraw what we have. Essentially we have let say a composite material.

(Refer Slide Time: 34:25)

NPTEL

$$q_e = -\Gamma_e \frac{(\phi_E - \phi_P)}{\Delta x_e}$$

Heat transfer analysis
1D, no source, steady

So, this is my P cell, this is my east cell ok, this is east. This is P essentially this is of different thermal conductivity or different diffusion; and similarly this is of different thermal conductivity ok. So, essentially what we have is gamma east here and with what we have here is gamma P ok. So, these are two different materials and we have to calculate what is gamma f here that is what we have to do. And then of course, we know the distances. This distance is Δx_e and this distance is Δx_e by 2, this is Δx_P by 2 right that we already know.

Now, you have heat flux that is going this way right, this is your q , let call it q_e right that is the heat flux that is going through this. If I were to represent the temperature values or the phi values at the cell centroids, where would that be? They would be here. This should be how much? $q_e = -\frac{\Gamma_e(\phi_E - \phi_P)}{\Delta x_e}$ Phi capital E and this would be? Phi capital P right.

So, what we want to do is we want to essentially calculate the heat flux right that is q_e east would be some gamma east times phi east minus phi p right divided by Δx_e right, of course, there is a minus also there is a minus also here right. This is . Let us call that equation 1 ok.

Now, if I were to draw an equivalent let say from heat transfer analysis for a simple 1D, no source, and steady situation. If I were to draw an equivalent network here, what would that network look like between P and E? So that means, I have this is my P, I have

some resistance, then this is my face and we have some resistance, this is our capital E right. And we have q is going through this way right. We have q e is going across this one right. What would be the equivalent resistances that we get here? Resistances would be nothing but the thermal conductivity the length divided by thermal conductivity right. We are actually looking at L by K . And the L by K would correspond to, what would be the L that corresponds to here?

Student: Δ (Refer Time: 37:26).

Would be this length right, would be this length, is not it? This length. And then what will be the thermal conductivity for this one?

Student: Γ e.

Γ e. And the other length would be? This guy that is Δ x p by 2

student: (Refer Time: 37:39).

And the thermal conductivity would be Γ p ok. So, can we write? So, that means, what is the first one here this would be length is Δ x p by 2. ah

Student: By 2.

p by 2. And then this is L divided by K is how much, Γ p, this is the first one. What about here? Δ x E by 2 times a Γ e. Do you all agree that this is correct? Fine, ok. Now if I were to write an expression for q e, what would that be?

Student: (Refer Time: 38:18).

From this resistance network what would be q e?

(Refer Slide Time: 38:21)



Student: (Refer Time: 38:22).

So, these are in series right. So, it will be sum of these things, these are in series. So, what would be the potential difference?

Student: Phi (Refer Time: 38:34).

Phi P or E

Student: E.

Student: p.

P right, minus phi east is that correct?

Student: Yes.

Divided by what would be the resistances? Sum of these two, this will be $(\frac{\Delta x_p}{2\gamma_p} + \frac{\Delta x_E}{2\gamma_E})$?

That is what we have from a heat transfer analysis 1D heat transfer analysis. So, this is equation 2 ok.

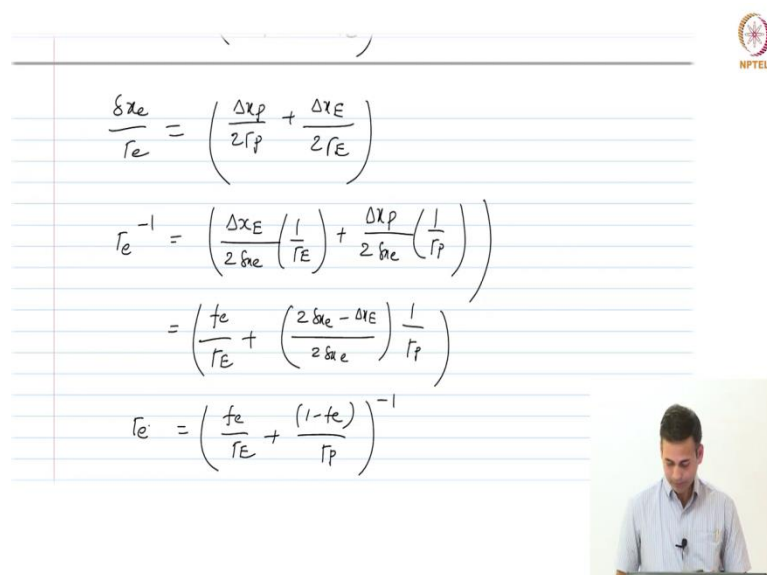
Now, what do we want? We want this is the correct heat flux that has to pass through the face q f. So, we want essentially to calculate now gamma e such that we get the same heat flux right. So, we want to equate this q e equal to this q e right. And then calculate

what would be the corresponding gamma e right, then we would get the correct heat flux passing through the interface. Agree, yes? Ok, that means, let us equate these two. So, what do I get if I equate these two?

Student: (Refer Time: 39:39).

P east minus phi p, so there is a minus here, this minus will rearrange this thing ok. Then if you bring gamma e down, we have del x e by gamma e right equals this entire thing in the denominator alright. Essentially here I have I equate this q e from equation 1 and 2, what I get here is del x e by gamma e this should be same as this quantity right, because phi east minus phi p is the same in both of them, and q e has to be the same right. Do you agree or no? Yes, ok, very good.

(Refer Slide Time: 40:20)



$$\frac{\delta x_e}{\gamma_e} = \left(\frac{\Delta x_p}{2\gamma_p} + \frac{\Delta x_E}{2\gamma_E} \right)$$

$$\gamma_e^{-1} = \left(\frac{\Delta x_E}{2\delta x_e} \left(\frac{1}{\gamma_E} \right) + \frac{\Delta x_p}{2\delta x_e} \left(\frac{1}{\gamma_p} \right) \right)$$

$$= \left(\frac{f_e}{\gamma_E} + \left(\frac{2\delta x_e - \Delta x_E}{2\delta x_e} \right) \frac{1}{\gamma_p} \right)$$

$$\gamma_e = \left(\frac{f_e}{\gamma_E} + \frac{(1-f_e)}{\gamma_p} \right)^{-1}$$

So, then that is nothing but $\frac{\delta x_e}{\gamma_e} = \left(\frac{\Delta x_p}{2\gamma_p} + \frac{\Delta x_E}{2\gamma_E} \right)$ we just equated these to equation 1 and equation 2 right. And then found what is gamma f or gamma east ok, that will give us the correct heat flux through the face ok.

Now, here I can of course, rewrite this $\gamma_e^{-1} = \left(\frac{\Delta x_E}{2\delta x_e} \left(\frac{1}{\gamma_E} \right) + \frac{\Delta x_p}{2\delta x_e} \left(\frac{1}{\gamma_p} \right) \right)$ as gamma e minus gamma e inverse right gamma e to the power minus 1 as I will bring delta x E to the down on the right hand side that would make it I am also writing the e term first and the p term next. So, I just brought delta x E on the right hand side to the denominator ok.

Now, what is Δx_P by $2\Delta x_e$? We have defined this as f_e right. This is $\left(\frac{f_e}{\Gamma_e} + \left(\frac{2\Delta x_E - \Delta x_e}{2\Delta x_e}\right) \frac{1}{\Gamma_t} f_e\right)$ upon γ_e plus Δx_P can I write Δx_P ?

(Refer Slide Time: 41:44)

The slide contains handwritten notes and a diagram. At the top right is the NPTEL logo. The main text asks: "How do I model q_f correctly?" and "you would get...". Below this is a diagram of a P-N junction. The P-region on the left has width Δx_P and potential ϕ_P . The N-region on the right has width Δx_N and potential ϕ_E . A depletion region of width Δx_e is shown in the center. Currents Γ_P and Γ_E are indicated. Below the diagram, there are two equations:
$$q_{he} = -\frac{\Gamma_e}{s} (\phi_E - \phi_P)$$
 and
$$\frac{f_e}{\Gamma_e}$$
. A video inset shows a man speaking.

So, Δx_P is what? Δx_P is this distance right ok, Δx_P is this distance. What about Δx_e is this distance right ok. Can I write Δx_P plus ok, essentially I want to calculate what is Δx_P . Can I write it as $2\Delta x_e$ minus Δx_e right? Essentially I am going to add this part and this part and then subtract of the Δx_e , can I do that to get the Δx_P ? Yes or no, ok. So, that means, I can write this as $2\Delta x_e$ right minus Δx_e upon $2\Delta x_e$, can I do this?

Student: (Refer Time: 42:36).

Right. I can do that ok. So, this is nothing but f_e by γ_e plus what would this be? 1 minus f_e by γ_p with a minus will be my γ_e minus 1 . So, this is my effective diffusion coefficient on the face in terms of something else ok.

(Refer Slide Time: 43:05)

$f_e = \frac{\Delta x_E}{2 \delta x_e}$; Interface is half-way

$f_e = \frac{1}{2}$

$\Gamma_e = \left(\frac{1}{2\Gamma_E} + \frac{1}{2\Gamma_P} \right)^{-1}$

$\Gamma_e = \left(\frac{\Gamma_P + \Gamma_E}{2\Gamma_E\Gamma_P} \right)^{-1}$

$\Gamma_e = \left(\frac{2\Gamma_E\Gamma_P}{\Gamma_P + \Gamma_E} \right)^{-1}$ Harmonic mean

Where of course, we have defined $f_e = \frac{\Delta x_e}{2\delta x_e}$. Now, let say if my interface is midway, then what would be f_e ? f_e equals?

Student: (Refer Time: 43:30).

$f_e = \frac{1}{2}$. So, can you plug in one-half into this expression for gamma e and calculate what is gamma e?

Student: (Refer Time: 43:43).

Yeah. So, plug in this thing. So, essentially what would that be that would be my $\Gamma_e = \left(\frac{1}{2\Gamma_E} + \frac{1}{2\Gamma_P} \right)^{-1}$ to the minus 1 right that would make it $\Gamma_e = \left(\frac{\Gamma_P + \Gamma_E}{2\Gamma_E\Gamma_P} \right)^{-1}$. So, what would this be $\Gamma_e = \left(\frac{2\Gamma_E\Gamma_P}{\Gamma_P + \Gamma_E} \right)$. What kind of an average is this?

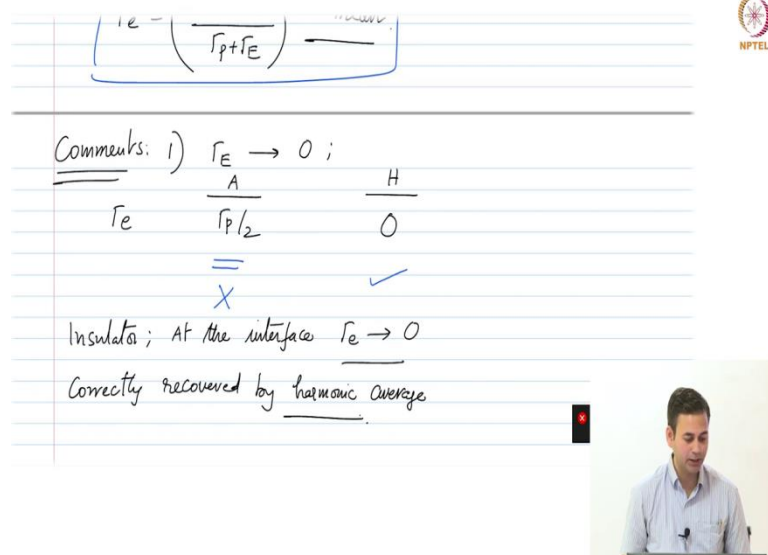
Student: Harmonic.


Harmonic average right. This is a harmonic average, not an arithmetic mean this is an harmonic mean. We got, what we got is a harmonic mean right, which is different from the arithmetic mean that we got before. We thought we will use a linear interpolation if the interface is midway alright fine.

Now, of course, we have still not proved anything ok. I will just said I claim that the this method supposedly the harmonic mean will give better results than the arithmetic mean right that is what we said. And then we said if you model the heat flux instead of calculating gamma by some-adhoc method, it gives you a better result that is all we have claimed, but we have not proved anything.

We just proved that we found another expression for gamma little east which is the harmonic mean of the two thermal conductivities that we have rather than the arithmetic mean of the thermal conductivities So, what we do next is we kind of consider specific cases and then see that whether each of these things work or not ok. So, that is what we do next.

(Refer Slide Time: 45:36)






$$\Gamma_e = \frac{A}{\frac{1}{\Gamma_p} + \frac{1}{\Gamma_E}}$$


Comments: 1) $\Gamma_E \rightarrow 0$;

Γ_e	$\frac{A}{\Gamma_p/2}$	$\frac{H}{0}$
	<u> </u>	<u> </u>
	X	✓

Insulator; At the interface $\Gamma_e \rightarrow 0$

Correctly recovered by harmonic average.





So, if I consider let say a case, so let us look at some comments. Let us consider the case where the gamma east that we have is an insulator ok. So, we have a conductor and then we have an insulator ok. So, gamma east is as a thermal conductivity that tends to 0 ok, gamma capital is 0 that means, we have two blocks and one block is conductor and the other one is insulator ok. If gamma east equal 0, then what would be the gamma little e that you would get from the arithmetic average and what would be that that you would get from the harmonic average?

Student: (Refer Time: 46:16)

Arithmetic will give you γ_p upon 2. What would be the one for harmonic average?

Student: 0.

0 right. Now, what is the what is that that you would expect if you have an insulator right, so the conductivity is 0 right, what is that that you would expect for it to behave like, should it have it at the interface, should it have a thermal conductivity or it should be 0?

Student: 0.

It should be 0 right, which is kind of given by the harmonic average. Whereas, if you had calculated from the arithmetic average, it would have half of the other average which is not correct right. So, this is not physically correct, whereas the harmonic average will give you the correct averaging in this case ok.

So, if you have an insulator, then at the interface we should have γ_e should tend to 0 that is what is correctly recovered by harmonic average ok. So, there are couple of more comments that we have to make. We will make that in the in the next lecture.