

**Introduction to Finite Volume Methods-I**  
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**Lecture - 25**  
**Finite Volume discretization of Diffusion equation-III**

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### Diffusion Equation

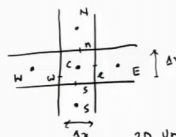
$$\rightarrow (-\nabla \cdot \nabla \phi)_e \cdot S_e + (-\nabla \cdot \nabla \phi)_w \cdot S_w + (-\nabla \cdot \nabla \phi)_n \cdot S_n + (-\nabla \cdot \nabla \phi)_s \cdot S_s = Q_c V_c$$

$a_c \phi_c + a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S = b_c$

*Algebraic eqn*

*steady, state diffusion system with source term*

$a_E = \text{Flux } F_e = -\Gamma_e D_e$	$D_e = \frac{S_e}{d_{eE}}$
$a_W = \text{Flux } F_w = -\Gamma_w D_w$	$D_w = \frac{S_w}{d_{wW}}$
$a_N = \text{Flux } F_n = -\Gamma_n D_n$	$D_n = \frac{S_n}{d_{nN}}$
$a_S = \text{Flux } F_s = -\Gamma_s D_s$	$D_s = \frac{S_s}{d_{sS}}$



2D, Unitless, Cartesian

$$a_c = \text{Flux } F_e + \text{Flux } F_w + \text{Flux } F_n + \text{Flux } F_s = -(a_E + a_W + a_N + a_S)$$

$$b_c = Q_c V_c - (\text{Flux } V_e + \text{Flux } V_w + \text{Flux } V_n + \text{Flux } V_s) = Q_c V_c$$

$\downarrow$   
0 (for present case)

So, welcome to the lectures of this Finite Volume Method. So, what will continue here where we left in the last lecture on the discretization of the diffusion system. So, if you come back or recall from your previous lecture, this is exactly where we stopped our previous calculations or the equation derivation. And what this provides? This provides the steady state diffusion equation discretized system. And just to begin with if you recall from the notation and all this that we have sort of just come back to this particular figure and we will recap this.

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## Diffusion Equation (2D)

steady-state Diffusion eqn.  

$$-\nabla \cdot (\Gamma \nabla \phi) = Q$$

(A) for cell 'c' → replicated for other interior cell.  
 (B) Boundary element → requiring special treatment

Elements → connectivity } (local indexing)  
 Faces → global indexing }  
 Nodes → discrete index }

local indexing = (i,j)  
 uniform grid spacing  
 $(\Delta x)_c = (\Delta x)_E = (\Delta x)_W$   
 $(\Delta y)_c = (\Delta y)_N = (\Delta y)_S$

$S_c$  = surface vector at face 'e'  
 $S_w, S_n, S_s$  = surface vectors at face: 'w, n, s' (respectively)

Structured (Cartesian grid)  
 discretized indexing  
 → stencil for discretization

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So, we had a 2-D uniform structured domain or Cartesian domain, that we have discretized like here which is shown here. And for this 2-D structured domain, we are interested on a particular cell sitting inside or one interior cell. And the one interior cell which would be concentrated on so, the cell that we are interested is this is the pattern of the discretization. So, this is the interior cell c and uniform grid. So, this is the delta y which is uniform, this is the delta x which is also uniform, ahead of it the element is E, behind that element W, top of that north and underneath of that is south.

So, these are the surrounding elements which are sitting alongside that particular element. And we have this uniform derivation of the distances. So, 2-D uniform Cartesian system; so, this is where we started. And the governing equation that we are discretizing is the steady state steady state diffusion system with source term. So, the that essentially our system, and the other notation that we have used so far is that this is the east face, north face, west face, south face. And once we do that we got our all the vectors.

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## Diffusion Equation

$\nabla \cdot J_D^D = Q$  ,  $J_D^D = -\Gamma \nabla \phi$   $V_c = \text{Volume of element 'c'}$

( volume integration  $\rightarrow$  surface integral  $\rightarrow$  Algebraic eqn. )

$$\sum_{f \in \text{faces}(c)} (-\Gamma \nabla \phi)_f \cdot S_f = Q_c V_c$$

$\downarrow$  expand

$$(-\Gamma \nabla \phi)_e \cdot S_e + (-\Gamma \nabla \phi)_w \cdot S_w + (-\Gamma \nabla \phi)_n \cdot S_n + (-\Gamma \nabla \phi)_s \cdot S_s = Q_c V_c$$

Uniform, Cartesian, surface vectors are normal to the respective faces

$\rightarrow S_e = (\Delta y)_e \cdot i = \|S_e\| i = S_e i$  ,  $S_w = -(\Delta y)_w \cdot i = -\|S_w\| i = -S_w i$

$S_n = (\Delta x)_n \cdot j = S_n j$  ,  $S_s = -(\Delta x)_s \cdot j = -S_s j$

East face  $J_e^D \cdot S_e = (-\Gamma \nabla \phi)_e \cdot S_e = -\Gamma_e S_e \left( \frac{\partial \phi}{\partial x} i + \frac{\partial \phi}{\partial y} j \right) \cdot i$

$$\Gamma_e, \Gamma_w, \Gamma_n, \Gamma_s$$

$$J_e^D = -\Gamma_e S_e \left( \frac{\partial \phi}{\partial x} \right)_e$$

2D element  $\rightarrow$  loops over faces (e, w, n, s)

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If you so this is how this is the system that we actually started to discretize that is our governing equations; where the diffusion flux is gamma delta phi. And after doing the algebraic calculations or the volume integration over that particular cell, we end up getting this algebraic system. Once we expand that we get a equation like this. So, it goes over all the faces surrounding that element c. So, that means, element c having 4 faces east west north south and we write down or expand that discretize equation in this fashion. Then we found out all our surface vector or surface normal vector. Since, it is a 2-D Cartesian system it was quite straight forward to estimate those.

And the way it has been estimated you can see S e was delta y i S n was delta x n j. So, it is a surface vector. So, you can assume that this is the length multiplied with the unity distance along the out of plane component. So, that is how you get all this surface vector or the vector notation of these things. Once you obtain that then for each faces; like east, west, north, south we have got this discretize system.

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### Diffusion Equation

$J_e^o = \text{Flux } T_e = \text{Flux } C_e \phi_c + \text{Flux } F_e \phi_E + \text{Flux } V_e \Rightarrow$  coefficients of  $\phi$  variation between 'c' & 'E'

**Linear variation:**

$$\left(\frac{\partial \phi}{\partial x}\right)_e = \frac{\phi_E - \phi_c}{(\delta x)_e}$$

$$\Rightarrow \text{Flux } T_e = -\Gamma_e (\delta y)_e \left(\frac{\phi_E - \phi_c}{(\delta x)_e}\right)$$

Linear variation for  $\phi$

$$\Rightarrow \Gamma_e \left(\frac{\delta y}{\delta x}\right)_e (\phi_c - \phi_E) = \text{Flux } C_e \phi_c + \text{Flux } F_e \phi_E + \text{Flux } V_e$$

$$\text{Flux } C_e = \Gamma_e D_c, \quad \boxed{\text{Flux } F_e = -\Gamma_e D_c, \quad \text{Flux } V_e = 0}$$

**West Face**

$$\text{Flux } T_w = -(\Gamma \nabla \phi)_w \cdot S_w$$

$$= -\Gamma_w S_w \left(\frac{\partial \phi}{\partial x} i + \frac{\partial \phi}{\partial y} j\right)_w \cdot (-i)$$

$$= \Gamma_w S_w \left(\frac{\partial \phi}{\partial x}\right)_w$$

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And once we get the discretize system, we assumed a this is a linear variation for phi between points C e or west. So, once we have done the linear variation, that slope will give that profile of that. From there, we have calculated each of these coefficients for the total flux definition with the linear variation. And once we obtain that, and we have defined one more parameter that D capital D for each faces these are defined as E W west, north and the definition lies here.

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### Diffusion Equation

$$\text{Flux } T_w = \Gamma_w S_w \left(\frac{\partial \phi}{\partial x}\right)_w \Rightarrow \Gamma_w S_w \frac{(\phi_c - \phi_w)}{\delta x_w} = \text{Flux } C_w \phi_c + \text{Flux } F_w \phi_w + \text{Flux } V_w$$

$$\boxed{\text{Flux } G_w = \Gamma_w D_w, \quad \text{Flux } F_w = -\Gamma_w D_w, \quad \text{Flux } V_w = 0}$$

$$D_w = \frac{(\delta y)_w}{\delta x_w} = \frac{\|S_w\|}{\|d_{cw}\|} = \frac{S_w}{d_{cw}} \quad \Bigg| \quad D_c = \frac{(\delta y)_c}{\delta x_c} = \frac{\|S_c\|}{\|d_{ce}\|} = \frac{S_c}{d_{ce}}$$

N, S  $\Rightarrow$  you can get it in similar fashion -

$$\text{Flux } T_n = \text{Flux } G_n \phi_w + \text{Flux } F_n \phi_N + \text{Flux } V_n$$

$$\text{Flux } T_s = \text{Flux } C_s \phi_c + \text{Flux } F_s \phi_S + \text{Flux } V_s$$

$$\left. \begin{aligned} \text{Flux } G_n &= \Gamma_n D_n, \quad \text{Flux } F_n = -\Gamma_n D_n, \quad \text{Flux } V_n = 0 \\ \text{Flux } C_s &= \Gamma_s D_s, \quad \text{Flux } F_s = -\Gamma_s D_s, \quad \text{Flux } V_s = 0 \end{aligned} \right\}$$

$$D_n = \frac{\|S_n\|}{\|d_{cn}\|} = \frac{(\delta x)_n}{\delta y_n} = \frac{S_n}{d_{cn}}; \quad D_s = \frac{\|S_s\|}{\|d_{cs}\|} = \frac{(\delta x)_s}{\delta y_s} = \frac{S_s}{d_{cs}}$$

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This is  $D_{west}$ , this is  $D_{east}$ , this is  $D_n$  and this is  $D_s$ . All being done, we have put all this system in this expanded equation and then finally, obtain this algebraic system algebraic equation. So, what we have done so far? We have we have considered one 2-D Cartesian grid and we have considered one interior element inside that 2-D Cartesian grid, and discretize that steady state, it stands for equation or the diffusion equation and obtain these algebraic system. Where all these coefficients are see  $\phi_C \phi_E \phi_W \phi_N \phi_S$ , they belong to the variable partening to the each cell. Like,  $\phi_C$  belongs to the element C,  $\phi_E$  represents the variable in element E,  $\phi_S$  for S element,  $\phi_N$  corresponds to n element,  $\phi_W$  corresponds to west element.

And the associated coefficients are  $a_C \phi_E \phi_W$ . And how they are obtained? If you write a E is essentially your flux  $F_e$  at that is minus  $\gamma_e D_e$ . And what is  $D_e$ ?  $D_e$  is, where  $D_e$  is  $S_e$  by  $d_{CE}$  ok. Similarly, you have a west which is flux  $F_w$  which is minus  $\gamma_w D_w$ , and  $D_w$  is  $s_w$  by distance of  $c_w$ . A N which is flux  $F_n$  which is nothing but  $\gamma_n D_n$  where  $D_n$  is  $S_n$  by  $d_{CN}$ . And finally, a S which is the south flux,  $f_s$  which is minus  $\gamma_s D_s$ ; where  $D_s$  is  $S_s$  by  $d$ . And a C which is the flux  $F_e$  flux  $c_e$  plus flux  $c_w$  plus flux  $c_n$  plus flux  $c_s$ ; which is nothing but with negative sign summation of  $a_E a_W a_N a_S$ . So, a C actually is the sum of all the individual component with the negative sign.

And the other so, in this particular equation you got all coefficients  $a_C a_E a_W a_N a_S$ . And only thing which is left over is the source term or right hand side vector term  $b_c$ . So,  $b_c$  is  $Q_c V_c$  minus all your flux  $V_e$  plus flux  $V_w$  plus flux  $V_n$  plus flux  $V_s$ . And since all this fluxes for this particular case all this terms are lead to 0 this will remain as  $Q_c V_c$  ok. So, but one can carry these terms and then finally, put the values. But this is a for the present case, these are 0. And when you do not have these fluxes, these coefficient of the fluxes are non 0, then they will contribute to this right hand side vector. So, if we write that equation in more compact form.

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## Diffusion Equation

in Compact form

$$a_c \phi_c + \sum_{f \in \text{nb}(c)} a_f \phi_f = b_c$$

$F = E, W, N, S \rightarrow$  elements  
 $f = e, w, n, s \rightarrow$  faces

$$a_f = \text{Flux}_f = -\Gamma_f D_f$$

$$a_c = \sum_{f \in \text{nb}(c)} \text{Flux}_f \quad ; \quad b_c = Q_c V_c - \sum_{f \in \text{nb}(c)} \text{Flux}_f V_f$$

Can be converted to Linear System  $\equiv \boxed{AX = b}$  form.

Notes: Discretization method  $\rightarrow$  discretized algebraic eqn. must reflect/represent the nature/characteristics of original G.E.'s

**Zero Sum Rule**  $\Rightarrow$  **Approx** linear variation of  $\phi'$  (profile of  $\phi$ )

Why not higher order profile?

Let us consider: 1D system with No source term  
 After discretization:  $\boxed{a_c \phi_c + a_E \phi_E + a_W \phi_W = 0}$

$$a_E = -\Gamma_E D_c, \quad a_W = -\Gamma_W D_c, \quad a_c = -(a_E + a_W)$$

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So, in compact form if you write that will look like an  $a_c \phi_c$  plus summation of  $a_f \phi_f$  which will go from all the faces  $a_f \phi_f$  equals to  $V_c b_c$ . And what  $a_f$  stands for?  $a_f$  stands for flux  $F_f$  which is minus  $\gamma_f D_f$  ok. So, where small  $f$  is east, west, north, south that is how they  $a_c$  is summation of small  $f$  goes from this flux  $c_f$  and  $b_c$  that would be  $Q_c V_c$  minus summation of small  $f$  flux  $V_f$ .

So, if you see this can be and capital  $F$ , essentially capital  $E$ , capital west, north, south stand for an small  $f$  is the face. So, these are the cell or elements, these are corresponding faces. So, the capital  $F$  and small  $f$  they correspond to 2 different things. So, please note that they are not same, one correspond to the cell other one to the face. Now you can once you obtain this you actually get the algebraic system like this kind of system, these are the algebraic system which can be now can be converted to linear system; that means, we can write that  $Ax$  equal to  $b$  in this form. And once you write in  $Ax$  equals to  $b$  form, you use your linear solver to get the solution.

Now, some notes or comments on this discretization; the comment is that if you have carried out proper discretization, it will basically provide you the discretize; so, the discretization method, discretization method must return or provide you back the discretize algebraic equation. So, the proper discretization method should return you back the discretized algebraic equation; which this particular equation, these must reflect or represent the characteristics of the original governing equations. The nature or

characteristics of original governing equations ok so, how would one satisfy that? This could be satisfied with the property that we have already discussed couple of lectures back, that the discretized system must possess certain properties. Through those properties only these important things must be retained.

And so, once that is done, then whatever physical system you are dealing with, theoretically the governing equations are actually the representation of my physical problem. So, the physical problem that you are dealing with which is somehow represented with series of partial differential equations, they are discretized to get the algebraic equation which should reflect or represent the characteristics ok.

Now, once we say that note, then we can move to look at some other information like, one of the thing is that sum rule or called 0 sum rule ok. So, what does it say? It says that one of the major approximations, what are the major in our discretize system? So, the approximation was or assumption whatever one can say was the assumption of linear variation of  $\phi$  or the profile. Profile of  $\phi$ ; that means, from one cell to another cell, the variation was linear. So, this is one of the major assumption or approximation that we have book so far ok.

So, this could be a question that when we assume the linear variation, why not higher order variation or higher order profile variation. So, that could be a pertinent question. To answer that we amongst the cell or the neighboring cells so, we have assume the linear variation. So, instead of that, if we assume a higher order variation how would that effect? Now to answer that let us consider one 1-D system with no source term. So, let us consider that, let us consider an 1-D system with no source term. And if you discretize this or after discretization this will be looking like a  $C \phi_C$  plus a  $E \phi_E$  plus a  $W \phi_W$  equals to 0.

So, one can see that straight way from this particular equation or the this particular equation from here. Once we said one dimensional system; that means, there is not north and south. So, these actually goes off no source term b c goes off. So, this gets you back these 3 terms in the system. So, where rest of the things will be a C is essentially a E is minus  $\gamma_e D_e$ , a W is minus  $\gamma_w D_w$ . And a C is minus a E plus a W. So, it follows all the standard equation system that we have derived so far. So, there is no variation to that. Once you write that equation you do not have any source term.

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## Diffusion Equation

There is No source term/Sink term  $\Rightarrow \phi$  is governed by diffusion only.

- Fourier's law (elliptical system/ $\phi_1$ )  $\rightarrow$  direction of decreasing  $\phi$ :

$\phi_e/\phi_w \rightarrow$  must lie between  $\phi_c$  &  $\phi_E$  /  $\phi_c$  &  $\phi_W$

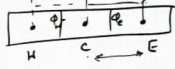
$\hookrightarrow$  guaranteed if we assume linear profile/variation.

if we assume higher order/second order profile (i.e. parabolic in nature)

$\phi_e/\phi_w >/< \phi_c/\phi_E/\phi_W$  (due to absence of  $Q$ )

$\downarrow$  unphysical phenomena  $\Rightarrow$  True for higher order ( $> 2^{\text{nd}}$  order) profiles

discretization scheme  $\rightarrow$  guarantee the physical results



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So, there is no source term; which means, in the absence of the source term, source term or you can think about sink term. So, in absence of that in absence of that sink term, the transfer of phi occurs due to one process only. So, the phi is governed by diffusion only. So, due to non-availability of source or sink term, the phi variation or the transfer of the transportation of phi is primarily governed by diffusion equation which is essentially the Fourier law, Fourier's law or rather elliptical system or elliptical equation. So, the diffusion system is governed by the Fourier's law in the direction of decreasing phi. So, the point here is that there is no source term in the system so, phi has governs by only diffusion. And the value of phi E or phi w, they must lie between the between phi C and or phi E or phi C and phi W.

So, since it is a pure diffusion process without having any source term, the surface variables would be lying between these 2 centroid values ok. But this variations is happening or this is or these variation is sort of guaranteed, guaranteed if we assume linear variation or linear profile or rather variation. Now that is what has been approximated or this is what it is assumed. And we can guaranty that so, once we look at a one dimensional system, it does guarantee that all these surface values must be lying between the centroid value in this one dimensional direction. So, what we mean to say? These are my cells, this is C, this is E, this is W. This is my phi W, this is at phi E. So, all this values will lie between this centroid values.



Now for example, if we assume higher order profile, higher order let us say second order profile, second order profile or variation, if we assume that. What would that happen? So, some sort of a parabolic profile. So, second order profile if you assume; which is sort of a for example, parabolic in nature, parabolic in nature. Once you assume some higher order profile, what that can do is that this surface values small  $\phi_e$  or small  $\phi_w$  this  $\phi_e$  or  $\phi_w$ .

This is possibly can be higher or lower than  $\phi_C$   $\phi_E$  or  $\phi_w$ . Which is absolutely possible that the because of the assumption of the higher order profiles. So, the higher order assumption can lead to that kind of situations; where the surface variable can overshoot or can undershoot from the centroid variables. And this is possibly can happen due to absence of source term or sink term. Now if these happens so, which is essentially a an physical phenomena ok. So, this is not at all justifiable or unphysical phenomena. Now this can one can immediately see through that if you assume a second order parabolic profile this can happen. Now this is also equally true for higher order. Like, greater than second order, higher order greater than equals to second order higher order profiles.

So, if you do not have any source term and if you assume higher order variation or higher order profile variation, this can lead to the unphysical phenomena which is not physical in nature; neither it is acceptable. So, the point here is that if the discretization scheme if has to be used or if it is adopted that has to guarantee the so; that means, the discretization scheme guarantee the physical results. That means, you cannot afford to get an unphysical results which is possibly happen if you assume higher order profile in this particular case.

Now, top of that this information or the importance of this profile variation which is a linear for this particular discretization will become less important as we keep on refining our mesh size; that means, as your grid spacing is getting reduced. So, that the distance between this centroid, these are getting reduced, then those linear variation will not make any significant impact on the results. And that is why in calculations we must do grid independents study, and we should carry out some grid refinement. And particularly certain problems of interest the refinement near to the boundary near to particular places become quite important.

So, we will stop here today, and we will take from here in the follow up lectures.

Thank you.