Lecture No. 12

<u>Solution of C-D Equation</u>

FE in space, FE in time, 1-D form of the equation:

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) \quad a \le x \le b$$

We'll assume that

$D = D(x) =$ spatially varying

$V = V(x) =$ spatially varying

Note that the form: $\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}$ is only valid if $D =$ constant. When $D = D(x)$ is variable in space, it must be embedded into the derivative since the term represents the gradient of flux.

- b.c's

$u(x,t)|_{\Gamma_e} = \bar{u}(x,t)|_{\Gamma_e}$ essential b.c.

$D\left.\frac{\partial u(x,t)}{\partial x}\right|_{\Gamma_N} = \bar{q}(x,t)|_{\Gamma_N}$ natural b.c.

Fundamental Weak Weighted Residual Form

$$\int_a^b \left[\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} - \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)\right]\delta u dx + \left[\left(-\bar{q} + D\frac{\partial u}{\partial x}\right)\delta u\right]_{\Gamma_N} = 0$$

Symmetrical Weak Weighted Residual Form

Integrating the diffusion term by parts leads to:

$$\int_a^b \left(\frac{\partial u}{\partial t}\delta u + V\frac{\partial u}{\partial x}\delta u + D\frac{\partial u}{\partial x}\frac{\partial(\delta u)}{\partial x}\right)dx - \left[D\frac{\partial u}{\partial x}\delta u\right]_{\Gamma} - \bar{q}\delta u|_{\Gamma_N} + D\frac{\partial u}{\partial x}\delta u|_{\Gamma_N} = 0$$

$$\int_a^b \left(\frac{\partial u}{\partial t}\delta u + V\frac{\partial u}{\partial x}\delta u + D\frac{\partial u}{\partial x}\frac{\partial(\delta u)}{\partial x}\right)dx - \left[D\frac{\partial u}{\partial x}\delta u\right]_{\Gamma_e} - \left[D\frac{\partial u}{\partial x}\delta u\right]_{\Gamma_N}$$

$$-\bar{q}\delta u|_{\Gamma_N} + D\frac{\partial u}{\partial x}\delta u|_{\Gamma_N} = 0$$

$$\Rightarrow$$

$$\int_a^b \left[\frac{\partial u}{\partial t}\delta u + V\frac{\partial u}{\partial x}\delta u + D\frac{\partial u}{\partial x}\frac{\partial(\delta u)}{\partial x}\right]dx - \bar{q}\delta u|_{\Gamma_N} = 0$$

- This requires at least C^o functional continuity for u. Thus we must use Lagrange interpolation.
- Let's approximate <u>over each element n</u> and zero everywhere else:

$$u \cong \sum_{n=1}^{\#el} \hat{u}^{(n)} = \sum_{n=1}^{\#el} \underline{\phi}^{(n)} \underline{u}^{(n)} = \sum_{n=1}^{\#el} \left[\phi_1^{(n)} \phi_2^{(n)} \cdots \right] \begin{bmatrix} u_1^{(n)} \\ u_1^{(n)} \\ \vdots \end{bmatrix}$$

where

$\underline{\phi}^{(n)}$ is a vector containing the interpolating polynomials

$\underline{\bar{u}}^{(n)}$ is a vector containing the elemental unknowns

- At this point we can represent <u>any</u> order <u>Lagrange</u> interpolation.
- Since we've selected Galerkin:

$$\delta u \cong \sum_{n=1}^{\#el} \delta \hat{u}^{(n)} = \sum_{n=1}^{\#el} \underline{\phi}^{(n)} \delta \underline{u}^{(n)}$$

$\delta \underline{u}^{(n)}$ is an elemental vector containing arbitrary values

- Furthermore let's approximate $V(x)$ in the same way as u for element n:

$$V \cong \sum_{n=1}^{\#el} \hat{V}^{(n)} = \sum^{\#el} \underline{\phi}^{(n)} \underline{V}^{(n)}$$

where $\hat{V}^{(n)}$ is an elemental vector containing nodal <u>known</u> values of velocity. Note that it is not necessary to select the same interpolation for $\underline{V}$ as for u. Lower or higher interpolation could be selected. This is <u>our approximation</u> for V. For example we could have had used L_2 interpolation (constant values of V over the element).

- Let's approximate $D(x)$ as constant over each element.

$$D \cong \sum_{n=1}^{\#el} D^{(n)}$$

Thus D will vary from element to element but will be constant over a given element (histogram).

Each function $\underline{\phi}^{(n)} \equiv 0$ outside of element n.

Substituting into our symmetrical weak weighted residual form:

$$\int_b^a \frac{\partial}{\partial t}\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\underline{u}\right)\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)$$

$$+\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\underline{V}^{(n)}\right)\frac{\partial}{\partial x}\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\underline{u}^{(n)}\right)\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)$$

$$+ D^{(n)}\frac{\partial}{\partial x}\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\,\underline{u}^{(n)}\right)\frac{\partial}{\partial x}\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)\Bigg]dx - \left[\bar{q}\sum_{n=1}^{\#el}\left(\underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)\right]_{\Gamma_N}$$

$$= 0$$

1. Since the interpolating functions $\underline{\phi}^{(n)}$ are defined as non-zero only over the element *n*.

$$\frac{\partial}{\partial t}\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\underline{u}^{(n)}\right)\left(\sum_{n=1}^{\#el} \underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right) = \sum_{n=1}^{\#el}\left[\frac{\partial}{\partial t}\left(\underline{\phi}^{(n)}\underline{u}^{(n)}\right)\left(\underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)\right]$$

2. Again since the components of $\underline{\phi}^{(n)}$ equal zero over all elements except *n*, we can sum over the integral of each element domain.

$$\int_b^a \sum_{n=1}^{\#el}\frac{\partial}{\partial t}\left(\underline{\phi}^{(n)}\underline{u}^{(n)}\right)\left(\underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)dx = \sum_{n=1}^{\#el}\int_{\Omega^{(n)}}^{\#el}\frac{\partial}{\partial t}\left(\underline{\phi}^{(n)}\underline{u}^{(n)}\right)\left(\underline{\phi}^{(n)}\delta\underline{u}^{(n)}\right)dx$$

Thus we can write:

$$\sum_{n=1}^{\#el}\left\{\int_{\Omega^{(n)}}\left[\frac{\partial}{\partial t}\left(\underline{\phi}\,\underline{u}^{(n)}\right)\left(\underline{\phi}\,\delta\underline{u}^{(n)}\right)+\left(\underline{\phi}\,\underline{V}^{(n)}\right)\frac{\partial}{\partial x}\left(\underline{\phi}\,\underline{u}^{(n)}\right)\left(\underline{\phi}\,\delta\underline{u}^{(n)}\right)\right.\right.$$

$$\left.\left.+\,D^{(n)}\frac{\partial}{\partial x}\left(\underline{\phi}\,\underline{u}^{(n)}\right)\frac{\partial}{\partial x}\left(\underline{\phi}\,\delta\underline{u}^{(n)}\right)\right]dx-\left[\bar{q}\left(\underline{\phi}\,\delta\underline{u}^{(n)}\right)\right]_{\Gamma_N}\right\}=0$$

- This is the usual form with which we go from the weighted residual formulation to the FE formulation (i.e. from the weighted residual form we go directly to this form upon substitution).
- Note that we can drop the (n) superscript from the interpolating functions vector $\underline{\phi}^{(n)}$ since these functions are identical over each element domain $\Omega^{(n)}$ (in local coordinates).
- The coefficients $\underline{u}^{(n)}$ are time varying but not spatially varying. The functions $\underline{\phi}$ are spatially but not time varying. Hence:

$$\sum_{n=1}^{\#el}\left\{\int_{\Omega^{(n)}}\left[\underline{\phi}\underline{u}_{,t}^{(n)}\underline{\phi}\delta\underline{u}^{(n)}+\underline{\phi}\underline{V}^{(n)}\underline{\phi}_{,x}\underline{u}^{(n)}\underline{\phi}\delta\underline{u}^{(n)}+D^{(n)}\underline{\phi}_{,x}\underline{u}^{(n)}\underline{\phi}_{,x}\delta\underline{u}^{(n)}\right]dx\right.$$

$$\left.-\left[\bar{q}\underline{\phi}\delta\underline{u}^{(n)}\right]_{\Gamma_N}\right\}=0$$

Let's further re-arrange things:

$$\underline{\phi}\underline{u}_{,t}^{(n)}\underline{\phi}^{(n)}\delta\underline{u}^{(n)}=\underline{\phi}\delta\underline{u}^{(n)}\underline{\phi}\underline{u}_{,t}^{(n)}=\delta\underline{u}^{(n)^T}\underline{\phi}^T\underline{\phi}\underline{u}_{,t}^{(n)}$$

Re-arranging the other terms in a similar manner we have:

$$\sum_{n=1}^{\#el}\left\{\int_{\Omega^{(n)}}\left[\delta\underline{u}^{(n)^T}\underline{\phi}^T\underline{\phi}\underline{u}_{,t}^{(n)}+\delta\underline{u}^{(n)^T}\underline{\phi}^T\underline{\phi}\underline{V}^{(n)}\underline{\phi}_{,x}\underline{u}^{(n)}+D^{(n)}\delta\underline{u}^{(n)^T}\underline{\phi}_{,x}^T\underline{\phi}_{,x}\underline{u}^{(n)}\right]dx\right.$$

$$\left.-\left[\bar{q}\delta\underline{u}^{(n)}\underline{\phi}^T\right]_{\Gamma_N}\right\}=0$$

Factoring out $\delta \underline{u}^{(n)^T}$ and grouping integrations:

$$\sum_{n=1}^{\#el} \delta \underline{u}^{(n)^T} \left\{ \left[\int_{\Omega^{(n)}} \underline{\phi}^T \underline{\phi} dx \right] \underline{u}_{,t}^{(n)} + \left[\int_{\Omega^{(n)}} \underline{\phi}^T \underline{\phi} \underline{V}^{(n)} \underline{\phi}_{,x} dx \right] \underline{u}^{(n)} + \left[D^{(n)} \int_{\Omega^{(n)}} \underline{\phi}_{,x}^T \underline{\phi}_{,x} dx \right] \underline{u}^{(n)} - \left[\bar{q} \underline{\phi}^T \right]_{\Gamma_N} \right\} = 0$$

Let:

$\underline{M}^{(n)} = \left[\int_{\Omega^{(n)}} \underline{\phi}^T \underline{\phi} dx\right]$ = elemental mass or geometric matrix

$\underline{A}^{(n)} = \left[\int_{\Omega^{(n)}} \underline{\phi}^T \underline{\phi} \underline{V}^{(n)} \underline{\phi}_{,x} dx\right]$ = elemental convection matrix

$\underline{B}^{(n)} = \left[D^{(n)} \int_{\Omega^{(n)}} \underline{\phi}_{,x}^T \underline{\phi}_{,x} dx\right]$ = elemental diffusion matrix

$\underline{P}^{(n)} = \left[\bar{q} \underline{\phi}^T\right]_{\Gamma_N}$ = normal flux load vector

Hence:

$$\sum_{n=1}^{\#el} \delta \underline{u}^{(n)T} \left\{\underline{M}^{(n)} \underline{u}_{,t}^{(n)} + \left(\underline{A}^{(n)} + \underline{B}^{(n)}\right) \underline{u}^{(n)} - \underline{P}^{(n)}\right\} = 0$$

Summing over all elements and taking into account the required functional continuity constraints leads to a global system of equations:

$$\delta \underline{u}^T \left\{\underline{M u}_{,t} + \left(\underline{A} + \underline{B}\right) \underline{u} - \underline{P}\right\} = 0$$

$\underline{M}$ = global mass matrix (assembled from local mass matrices)

$\underline{A}$ = global convection matrix

$\underline{B}$ = global diffusion matrix

$\underline{P}$ = global normal flux load vector

Recall that $\delta \underline{u}^T$ was a vector consisting of an arbitrary set of coefficients δu_i. Therefore in order to allow this equation to be valid for any arbitrary vector $\delta \underline{u}$ we must have:

$$\underline{M} \underline{u}_{,t} + \left(\underline{A} + \underline{B}\right)\underline{u} - \underline{P} = 0$$

$$\Rightarrow$$

$$\underline{M} \underline{u}_{,t} + \left(\underline{A} + \underline{B}\right)\underline{u} = \underline{P}$$

- All the global matrices are formed from the local matrices.

Development of Elemental Matrices

The equations for the elemental matrices as they now stand are valid for any order Lagrange interpolation. We also note that:

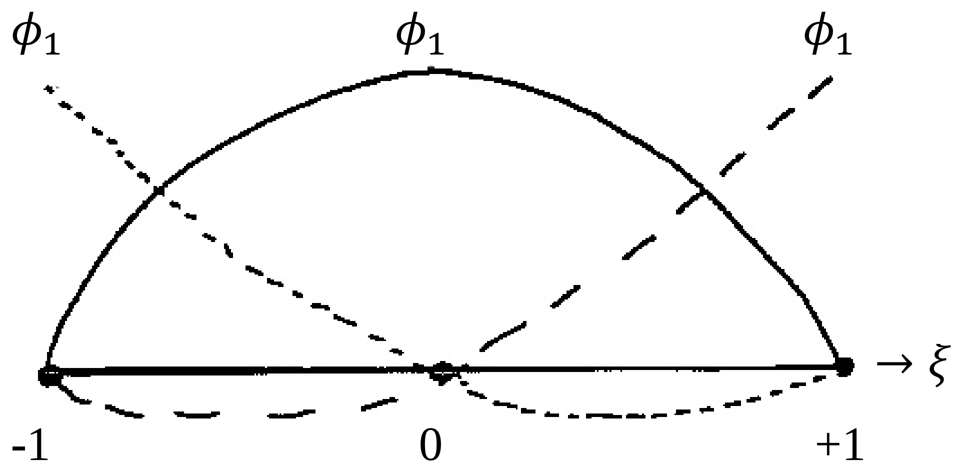
1. The equations require C_o continuity. This satisfied the minimum necessary requirements.
2. We have assumed that *u* and *V* vary with the same type and degree interpolating functions. This is not necessary (it's problem dependent).
3. We could also have formulated the problem using Hermite's.

Let's use 2nd order Lagrange functions (quadratic)

Element has 3 nodes:

3 elemental interpolating functions

3 unknown coefficients per element. These coefficients equal the dependent variable at the nodes.



$u_1^{(n)}$ $\quad$ $u_2^{(n)}$ $\quad$ $u_3^{(n)}$ for element n

Hence:

$$\underline{u}^{(n)} = \begin{bmatrix} u_1^{(n)} \\ u_2^{(n)} \\ u_3^{(n)} \end{bmatrix} \quad \text{and} \quad \underline{\phi} = [\phi_1 \quad \phi_2 \quad \phi_3]$$

where

$$\phi_1 = \frac{\xi(\xi - 1)}{2}$$

$$\phi_2 = (1 - \xi^2)$$

$$\phi_3 = \frac{\xi(1 + \xi)}{2}$$

Recall that the transformation from global to local coordinates was:

$$\xi = -1 + 2\left(x - x_j\right)/\left(x_{j+1} - x_j\right)$$

vice-versa we have:

$$x = x_j + \left(x_{j+1} - x_j\right)(\xi + 1)/2 = x_j + \frac{L_n}{2}(\xi + 1)$$

where L_n = length of element *n*.

<u>Let's evaluate the elemental matrix</u> $\underline{M}^{(n)}$

$$\underline{M}^{(n)} = \int_{\Omega^e} \underline{\phi}^T \underline{\phi} dx$$

However we wish to work in local coordinates and therefore we transform to the ξ coordinate system

- $dx = \frac{L_n}{2} d\xi$
- limits for each element become $-1 \leq \xi \leq +1$

Hence we may evaluate $\underline{M}^{(n)}$ as:

$$\underline{M}^{(n)} = \frac{L_n}{2} \int_{-1}^{+1} \underline{\phi}^T \underline{\phi} d\xi$$

$$= \frac{L_n}{2} \int_{-1}^{+1} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} [\phi_1 \quad \phi_2 \quad \phi_3] d\xi$$

$$= \frac{L_n}{2} \int_{-1}^{+1} \begin{bmatrix} \phi_1^2 & \phi_1\phi_2 & \phi_1\phi_3 \\ \phi_2\phi_1 & \phi_2^2 & \phi_2\phi_3 \\ \phi_3\phi_1 & \phi_3\phi_2 & \phi_3^2 \end{bmatrix}$$

$$\underline{M}^{(n)} = \frac{L_n}{2} \int_{-1}^{+1} \begin{bmatrix} \frac{\xi^2(\xi-1)^2}{4} & \frac{\xi(\xi-1)(1-\xi^2)}{2} & \frac{\xi^2(\xi-1)(\xi+1)}{4} \\ \frac{\xi(1-\xi^2)(\xi-1)}{2} & (1-\xi^2)^2 & \frac{\xi(\xi+1)(1-\xi^2)}{2} \\ \frac{\xi^2(1+\xi)(\xi-1)}{4} & \frac{\xi(\xi+1)(1-\xi^2)}{2} & \frac{\xi^2(1+\xi)^2}{4} \end{bmatrix} d\xi$$

- Note that the matrix is symmetrical

Evaluating the integrals and evaluating the integration limits:

$$\underline{M}^{(n)} = \frac{L_n}{30} \begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}$$

Therefore for quadratic interpolation, each elemental matrix is given by the given expression and only L_n need be computed from element to element.

Evaluate elemental convection matrix $\underline{A}^{(n)}$

$$\underline{A}^{(n)} = \int_{\Omega_e^{(n)}} \underline{\phi}^T \underline{\phi} \underline{V}^{(n)} \underline{\phi}_{,x} dx$$

For local coordinates:

$$dx = \frac{L_n}{2} d\xi$$

$$\underline{\phi}_{,x} = \frac{d\underline{\phi}}{d\xi}\frac{d\xi}{dx} = \frac{2}{L_n}\underline{\phi}_{,\xi}$$

limits of integration

$$\int_{\Omega_e^{(n)}} \rightarrow \int_{-1}^{+1}$$

Furthermore we note that:

$$\underline{\phi}_{,\xi} = [\phi_{1,\xi} \quad \phi_{2,\xi} \quad \phi_{3,\xi}]$$

$$\phi_{1,\xi} = \frac{1}{2}(2\xi - 1); \quad \phi_{2,\xi} = -2\xi; \quad \phi_{3,\xi} = \frac{1}{2}(2\xi + 1)$$

Thus:

$$\underline{A}^{(n)} = \int_{-1}^{+1} \underline{\phi}^T \underline{\phi}\underline{V}^{(n)} \underline{\phi}_{,\xi} \; \frac{2}{L_n} \cdot \frac{L_n}{2} d\xi$$

$$= \int_{-1}^{+1} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} \begin{bmatrix} \phi_1 & \phi_2 & \phi_3 \end{bmatrix} \begin{bmatrix} V_1^{(n)} \\ V_2^{(n)} \\ V_3^{(n)} \end{bmatrix} \begin{bmatrix} \phi_{1,\xi} & \phi_{2,\xi} & \phi_{3,\xi} \end{bmatrix} d\xi$$

Taking the product of these

$$\underline{A}^{(n)} = \begin{bmatrix} -0.3333V_1^{(n)} - 0.2000V_2^{(n)} + 0.03333V_3^{(n)} & 0.4000V_1^{(n)} + 0.2666V_3^{(n)} & -0.06667V_1^{(n)} - 0.06667V_2^{(n)} - 0.16667V_1^{(n)} \\ -0.2000V_1^{(n)} - 0.5333V_2^{(n)} + 0.06667V_3^{(n)} & 0.26666V_1^{(n)} - 0.2666V_3^{(n)} & -0.06667V_1^{(n)} + 0.53333V_2^{(n)} + 0.2000V_3^{(n)} \\ +0.03333V_1^{(n)} + 0.06667V_2^{(n)} + 0.13333V_3^{(n)} & -0.2666V_1^{(n)} - 0.4000V_3^{(n)} & 0.10000V_1^{(n)} + 0.26667V_2^{(n)} + 0.13333V_3^{(n)} \end{bmatrix}$$

- The elemental convection matrix depends <u>only</u> on the elemental nodal velocities. $\underline{A}^{(n)}$ therefore varies from element to element if $V^{(n)}$ varies. We must reevaluate the elemental matrix for each element in the above form.

- Note that this matrix is not symmetric. This is not expected since the convection part of the operator is not self adjoint.
- Other matrices are treated similarly.
- In general the elemental coefficient matrices depend on geometrical properties of the element and its prescribed material properties (e.g. in this case the nodal velocities and elemental diffusion values).

Notes

1. Natural b.c. treatment such that the normal flux includes both a diffusive and convective component. Recall that the natural b.c. previously developed only included the diffusive flux component. However we can transform our operator to a symmetrical point such that the natural b.c. includes both a diffusive and convective flux.

- Consider $u_{,t} + Vu_{,x} = \left(Du_{,x}\right)_{,x}$

  We note that from the 1-D continuity equation that $V_{,x} = 0$. Hence:

$$(Vu)_{,x} = V_{,x}u + Vu_{,x} = Vu_{,x}$$

  Therefore we can substitute $Vu_{,x}$ and thus the C-D equation can be written as:

$$u_{,t} + (Vu)_{,x} = \left(Du_{,x}\right)_{,x}$$

- Let's perform a halfway integration from

  $\langle L(u), \delta u\rangle = \langle L^*(\delta u), u\rangle$ + boundary terms

$$\int_{\Omega} \left(u_{,t} + (Vu)_{,x} - \left(Du_{,x}\right)_{,x}\right) \delta u d\Omega$$

$$= \int_{\Omega} \left(u_{,t}\delta u - Vu(\delta u)_{,x} + Du_{,x}(\delta u)_{,x}\right) d\Omega + \left[-Du_{,x} + Vu\right] \delta u|_{\Gamma}$$

- The essential boundary is represented by u.
- The natural boundary is represented by $\left(-Du_{,x} + Vu\right)$.
- Since we have integrated both the diffusive and the convective terms in the first part of the integration by parts procedure, we now have a *different* natural b.c. This is associated with the non-self-adjoint nature of the operator.

$$\bar{q} = Vu + \bar{q}^D$$

  where

  $\bar{q}^D$ = diffusive flux $= -D \dfrac{\partial u}{\partial x}$

  Vu = convective flux

2. 2-D C-D equation:

$$u_{,t} + V_x u_{,x} + V_y u_{,y} = \left(D_{xx} u_{,x} + D_{xy} u_{,y}\right)_{,x} + \left(D_{xy} u_{,x} + D_{yy} u_{,y}\right)_{,y}$$

Thus diffusion (or dispersion) coefficients now form a 2x2 tensor. Again the convective terms may be rewritten as:

$$(V_x u)_{,x} + \left(V_y u\right)_{,y} = V_x u_{,x} + V_y u_{,y} + u\left(V_{x,x} + V_{y,y}\right)$$

However from continuity

$$V_{x,x} + V_{y,y} = 0$$

Thus:

$$u_{,t} + (V_x u)_{,x} + \left(V_y u\right)_{,y} = \left(D_{xx} u_{,x} + D_{xy} u_{,y}\right)_{,x} + \left(D_{xy} u_{,x} + D_{yy} u_{,y}\right)_{,y}$$

- The essential b.c. will be $u|_{\Gamma_e} = \bar{u}|_{\Gamma_e}$
- The natural b.c. will be $q|_{\Gamma_N} = \bar{q}|_{\Gamma_N}$

where $q_n = \alpha_{nx} q_x + \alpha_{ny} q_y$

- It is noted that q_n can represent 2 different natural b.c.'s:

  (i) $q_x = V_x u + q_x^D$

  $q_y = V_y u + q_y^D$

  where

$$q_x^D = -D_{xx}\frac{\partial u}{\partial x}$$

$$q_y^D = -D_{yy}\frac{\partial u}{\partial y}$$

  In this case q_x and q_y include both convective and diffusive flux.

  (ii) $q_x = q_x^D$

  $q_y = q_y^D$

  In this case normal flux only represents diffusive flux.