2-d Diffusion via GWS
Linear Triangles

Last quarter we spent a lot of time looking at the steady-state diffusion equation as we developed our dexterity with the GWS process. It is therefore natural that we return to it for our excursion into two dimensions. For a two-dimensional domain with both Dirchlet and Neumann boundary conditions, the governing differential equations are

$$\begin{aligned}
\mathscr{L}\big(T(x,y)\big) &= -\frac{\partial}{\partial x}\left(k\frac{\partial T(x,y)}{\partial x}\right) - \frac{\partial}{\partial y}\left(k\frac{\partial T(x,y)}{\partial y}\right) - s(x,y) = 0 \\
&\equiv -\nabla\cdot\big(k\nabla T(x,y)\big) - s(x,y) = 0 \qquad on\ \Omega\subset\Re^2 \\
l(T) &= -k\nabla T\cdot\hat{n} - q_n = 0 \qquad on\ \partial\Omega_1 \\
T(x,y)_b &= T_b \qquad on\ \partial\Omega_2
\end{aligned} \tag{1}$$

Equation (1) introduces the gradient operator $\nabla \equiv \partial/\partial x\,\hat{i} + \partial/\partial y\,\hat{j}$ and the notation $\Omega\subset\Re^2$ is read "on the region Ω contained within the two-dimensional space $\Re^2$." For a positive diffusion coefficient, the governing PDE is *elliptic*, hence a linear combination of Dirichlet, Neumann, or Robin boundary conditions must be specified all around the boundary $\partial\Omega$ of Ω. The boundary conditions meet this requirement provided that the union of $\partial\Omega_1$ and $\partial\Omega_2$ completely surround the domain Ω. By convention, the outward pointing unit normal from Ω is denoted $\hat{n}$ while $\hat{i},\hat{j}$ are the unit vectors aligned with the *x* and *y*-axes respectively. Finally, the distributed internal source is denoted $s(x,y)$, the outward-flowing fixed heat flux is denoted q_n (Neumann data) on $\partial\Omega_1$, and the fixed temperature is denoted $T(x,y)_b$ (Dirichlet data) on $\partial\Omega_2$.

As in one-dimension, we seek to generate a global approximation to our unknown solution $T(x,y)$ via

$$T(x,y)\approx T^N(x,y)=\sum_{\alpha=1}^{N}\Psi_\alpha(x,y)Q_\alpha \tag{2}$$

Assessing and measuring the error courtesy the weighted residual (weak statement)

$$WS^N=\int_\Omega \Phi_\beta(x,y)L\big(T^N(x,y)\big)d\Omega=0 \qquad 1\le\beta\le N \tag{3}$$

The error in the approximation is minimized with the Galerkin Criterion yielding

$$GWS^N=\int_\Omega \Psi_\beta(x,y)L\big(T^N(x,y)\big)d\Omega=0 \qquad 1\le\beta\le N \tag{4}$$

Doing the usual substitutions

$$GWS^N=\int_\Omega \Psi_\beta\big(-\nabla\cdot\big(k\nabla(\Psi_\alpha Q_\alpha)\big)-s\big)d\Omega=0 \qquad 1\le\alpha,\beta\le N \tag{5}$$

For multi-dimensional problem statements, integration by parts is replaced with the *Green-Gauss theorem*, resulting in

$$\begin{aligned}
GWS^N &= \int_\Omega \nabla\Psi_\beta\cdot k\nabla\Psi_\alpha\, d\Omega\, Q_\alpha - \int_\Omega \Psi_\beta s\, d\Omega - \int_{\partial\Omega}\Psi_\beta\, k\nabla Q^N d\sigma \\
&= \int_\Omega \nabla\Psi_\beta\cdot k\nabla\Psi_\alpha\, d\Omega\, Q_\alpha - \int_\Omega \Psi_\beta s\, d\Omega + \int_{\partial\Omega_1}\Psi_\beta q_n\, d\sigma - \int_{\partial\Omega_2}\Psi_\beta k\,\nabla\big(T^N\big)\cdot\hat{n}\, d\sigma
\end{aligned} \tag{6}$$

Discretizing (6)

$$GWS^h = \mathrm{S}_e\left(\int_{\Omega_e}\nabla\{N_k\}\cdot\nabla\{N_k\}^T d\Omega_e\{Q\}_e - \int_{\Omega_e}\{N_k\}\{N_k\}^T d\Omega_e\{S\}_e + \int_{\partial\Omega_1}\{N_k\}\{N_k\}^T d\sigma\{QN\}_e = \{0\}_e\right) \tag{7}$$

Unsurprisingly, this looks nearly identical to what we developed in one dimension - the only difference is the introduction of the gradient operator. Thus the elegance and ease of extending weak statement theory to higher dimensionality is verified. We can correctly guess that the resulting matrix statement will be of the form

$$[LHS]\{Q\} = \{RHS\}$$

The construction of these matrices, however, is where the challenge lies. Let's look at linear triangles. Recall from the previous lecture that the basis functions are $\{N_1(\zeta_i)\}$ where

$$\begin{aligned}\zeta_1 &= \frac{(X2Y3 - X3Y2) + (Y2 - Y3)x + (X3 - X2)y}{2A_e}\\ \zeta_2 &= \frac{(X3Y1 - X1Y3) + (Y3 - Y1)x + (X1 - X3)y}{2A_e}\\ \zeta_3 &= \frac{(X1Y2 - X2Y1) + (Y1 - Y2)x + (X2 - X1)y}{2A_e}\end{aligned} \tag{8}$$

We'll begin by tackling the [DIFF] matrix

$$\begin{aligned}[DIFF]_e &= \int_{\Omega_e}\nabla\{N_1\}\cdot k\nabla\{N_1\}^T d\Omega_e\\ &= k\,\nabla\{N_1\}\cdot\nabla\{N_1\}^T\int_{\Omega_e}d\Omega_e\end{aligned} \tag{9}$$

The gradient terms can be moved outside the integral upon recognizing that the derivatives of the linear basis functions will be constant. Let's do some vector calculus and revisit our friend the chain rule:
First, expand out the gradient operator:

$$\begin{aligned}\nabla\{N_1(\zeta_i)\} &= \frac{\partial\{N_1\}}{\partial x}\hat{i} + \frac{\partial\{N_1\}}{\partial y}\hat{j}\\ &= \frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial x}\hat{i} + \frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial y}\hat{j} \qquad 1 \le i \le 3\end{aligned} \tag{10}$$

Next, take the dot product:

$$\begin{aligned}\nabla\{N_1\}\cdot\nabla\{N_1\}^T &= \left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial x}\hat{i} + \frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial y}\hat{j}\right)\cdot\left(\frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_k}{\partial x}\hat{i} + \frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_k}{\partial y}\hat{j}\right)\\ &= \hat{i}\cdot\hat{i}\left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial x}\frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_k}{\partial x}\right) + \hat{j}\cdot\hat{j}\left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\zeta_i}{\partial y}\frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_k}{\partial y}\right)\\ &= \left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_i}{\partial x}\frac{\partial\zeta_k}{\partial x}\right) + \left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\{N_1\}^T}{\partial\zeta_k}\frac{\partial\zeta_i}{\partial y}\frac{\partial\zeta_k}{\partial y}\right)\\ &= \left(\frac{\partial\{N_1\}}{\partial\zeta_i}\frac{\partial\{N_1\}^T}{\partial\zeta_k}\right)\left(\frac{\partial\zeta_i}{\partial x_j}\frac{\partial\zeta_k}{\partial x_j}\right)_e \qquad for\begin{cases}1 \le j \le n = 2\\ 1 \le (i,k) \le n+1 = 3\end{cases}\end{aligned} \tag{11}$$

Okay, now we need to take some derivatives:

$$\frac{\partial\{N_1\}}{\partial\zeta_i} = \frac{\partial\{N_1\}}{\partial\zeta_k} = \begin{cases} \{1,0,0\}^T & for\ i = k = 1 \\ \{0,1,0\}^T & for\ i = k = 2 \\ \{0,0,1\}^T & for\ i = k = 2 \end{cases} \tag{12}$$

The next derivatives are the jacobian of the element transformation (8)

$$[J]_e = \left[\frac{\partial\zeta_i}{\partial x_j}\right]_e = \left[\frac{\partial\zeta_k}{\partial x_j}\right]_e = \begin{bmatrix} \frac{\partial\zeta_1}{\partial x} & \frac{\partial\zeta_1}{\partial y} \\ \frac{\partial\zeta_2}{\partial x} & \frac{\partial\zeta_2}{\partial y} \\ \frac{\partial\zeta_3}{\partial x} & \frac{\partial\zeta_3}{\partial y} \end{bmatrix}_e = \begin{bmatrix} \zeta_{11} & \zeta_{12} \\ \zeta_{21} & \zeta_{22} \\ \zeta_{31} & \zeta_{32} \end{bmatrix}_e = \frac{1}{2A_e}\begin{bmatrix} Y2-Y3 & X3-X2 \\ Y3-Y1 & X1-X3 \\ Y1-Y2 & X2-X1 \end{bmatrix}_e \tag{13}$$

$$for \begin{cases} 1 \le j \le n = 2 \\ 1 \le (i,k) \le n+1 = 3 \end{cases}$$

Having evaluated the derivatives, we are now ready to expand out equation (11). The term within the first parenthesis of (11) defines a 3x3 matrix with entries of either a 0 or 1 as defined by (12). For example, for i=1 and k=3:

$$\frac{\partial\{N_1\}}{\partial\zeta_1}\frac{\partial\{N_1\}^T}{\partial\zeta_3} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}\{0 \quad 0 \quad 1\} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{14}$$

Experimenting with other index pairs, we see that this term in (11) is a pointer to the i^{th} row and k^{th} column of a 3x3 matrix and as such can be represented by the *pseudo-Kronecker delta* with definition

$$\delta_{ik} \equiv \begin{cases} 1 & for\ position\ i,k \\ 0 & for\ all\ other\ matrix\ locations \end{cases}$$

With this simplification, (11) now takes the form of

$$\nabla\{N_1\}\cdot\nabla\{N_1\}^T = [\delta_{ik}]\left(\frac{\partial\zeta_i}{\partial x_j}\frac{\partial\zeta_k}{\partial x_j}\right)_e \qquad for \begin{cases} 1 \le j \le n = 2 \\ 1 \le (i,k) \le n+1 = 3 \end{cases}_e \tag{15}$$

Substituting (15) into (9) gives the explicit form of the conduction master matrix for the linear triangle as

$$[DIFF]_e = k\nabla\{N_1\}\cdot\nabla\{N_1\}^T\int_{\Omega_e} d\Omega_e = [\delta_{ik}]\left(\frac{\partial\zeta_i}{\partial x_j}\frac{\partial\zeta_k}{\partial x_j}\right)_e \int_{\Omega_e} d\Omega_e$$

$$= \frac{1}{(2A_e)^2}\begin{bmatrix} \zeta_{11}^2+\zeta_{12}^2 & \zeta_{11}\zeta_{21}+\zeta_{12}\zeta_{22} & \zeta_{11}\zeta_{31}+\zeta_{12}\zeta_{32} \\ & \zeta_{21}^2+\zeta_{22}^2 & \zeta_{21}\zeta_{31}+\zeta_{22}\zeta_{32} \\ sym & & \zeta_{31}^2+\zeta_{32}^2 \end{bmatrix}_e \int_{\Omega_e} d\Omega_e \tag{16}$$

$$= \frac{1}{4A_e}\begin{bmatrix} \zeta_{11}^2+\zeta_{12}^2 & \zeta_{11}\zeta_{21}+\zeta_{12}\zeta_{22} & \zeta_{11}\zeta_{31}+\zeta_{12}\zeta_{32} \\ & \zeta_{21}^2+\zeta_{22}^2 & \zeta_{21}\zeta_{31}+\zeta_{22}\zeta_{32} \\ sym & & \zeta_{31}^2+\zeta_{32}^2 \end{bmatrix}_e$$

The next step is to evaluate the source term in (7). Taking cue from the one-dimensional work, hopefully there is an integration formula available to make things easy. The *n*=2 generalization of the natural coordinate integration formula is

$$\int_{\Omega_e} \zeta_1^p \zeta_2^q \zeta_3^r \, d\Omega_e = 2A_e \frac{p!q!r!}{(2+p+q+r)!} \tag{17}$$

which leads to the source master matrix being

$$\int_{\Omega_e} \{N_k\}\{N_k\}^T d\Omega_e \{S\}_e = \frac{A_e}{12}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}\{S\}_e \tag{18}$$

The final step is the evaluation of the applied normal boundary flux. Assuming our triangle is shaped like

then nodes 1 and 2 define the segment on the boundary. The associated boundary length is

$$l_e = \sqrt{(X2 - X1)^2 + (Y2 - Y1)^2}$$

Thus the flux term in (7) can be evaluated, using (17), as

$$\begin{aligned} \int_{\partial\Omega_1} \{N_k\}\{N_k\}^T d\sigma \{QN\}_e &= \int_{l_e} \{N_k\}\{N_k\}^T d\bar{x} \{QN\}_e \\ &= \int_{l_e} \begin{Bmatrix} \zeta_1 \\ \zeta_2 \\ 0 \end{Bmatrix} \{\zeta_1 \quad \zeta_2 \quad 0\} d\bar{x} \{QN\}_e \\ &= \frac{l_e}{6}\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}\{QN\}_e \end{aligned} \tag{19}$$

since $\zeta_3 = 0$ on the line connecting nodes 1 and 2. Take note that the terminal form of (19) is *identical* to the 1-d source matrix for the linear element!

Homework:

1. Verify the 3,1 entry of the diffusion matrix in (16) using (15).
2. Verify the 3,1 entry of the source matrix in (18) using (17).
3. Determine the form of (19) if the flux is applied to nodes 2 and 3.