University of Bath
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Systems Modelling & Simulation Coursework 1

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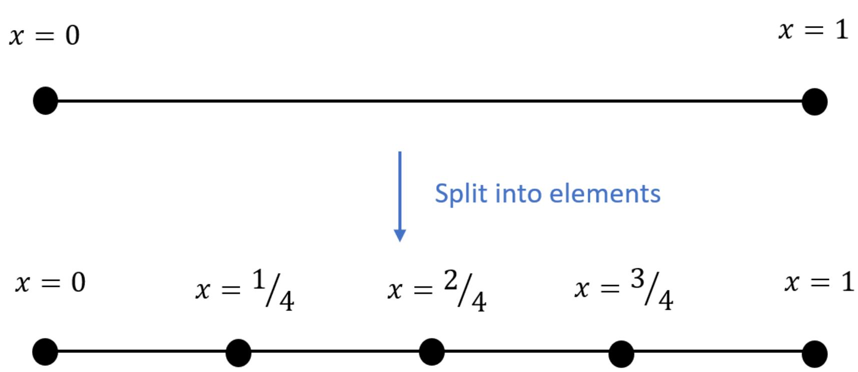
1.1 Quation 1a

1.1.1 Derivation of Diffusion Element Matrix

Here we will derive the 2-by-2 element matrix for a diffusion operator for an arbitrary element e_n between the points x_0 x_1. The derivation will start from the weak form version of the diffusion integral, after performing integration by parts. This is given by equation 1 in the domain $x = 0$ to $x = 1$.

$$\int_0^1 D\frac{\partial c}{\partial x}\frac{\partial v}{\partial x}dx = \int_0^1 vf\,dx + \left[vD\frac{\partial c}{\partial x}\right]_0^1 \tag{1}$$

We have the domain from $x = 0$ to $x = 1$ which we can split into ne number of elements. This is shown pictorially below for the case $ne = 4$.



We can now say the integral from $x = 0$ to $x = 1$ is equivalent to the sum of the integral of the individual elements, for the $ne = 4$ case:

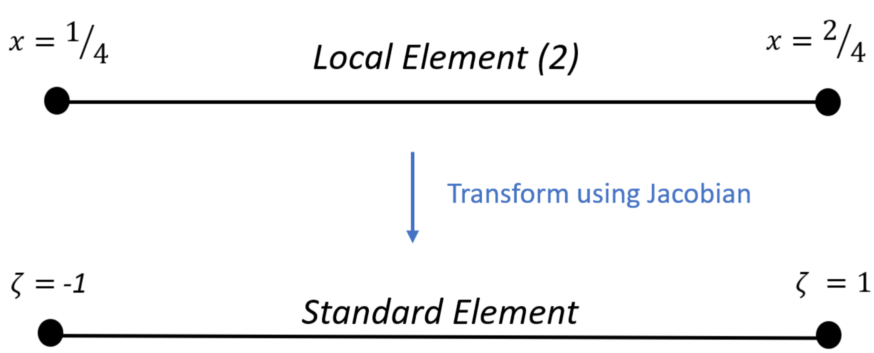
$$\int_0^1 dx = \int_0^{\frac{1}{4}} dx + \int_{\frac{1}{4}}^{\frac{2}{4}} dx + \int_{\frac{2}{4}}^{\frac{3}{4}} dx + \int_{\frac{3}{4}}^{1} dx \tag{2}$$

To integrate an individual element we will use linear Lagrange nodal basis function 3 to represent c and x, the functions are shown below. The test function v is set to be equal to the basis function ψ.

$$c = c_0\psi_0(\zeta) + c_1\psi_1(\zeta) \tag{3a}$$
$$x = x_0\psi_0(\zeta) + x_1\psi_1(\zeta) \tag{3b}$$
$$v = \psi_0, \psi_1 \tag{3c}$$
$$\text{where,} \tag{3d}$$
$$\psi_0 = \frac{1-\zeta}{2} \quad , \quad \psi_1 = \frac{1+\zeta}{2} \tag{3e}$$
$$\text{and,} \tag{3f}$$
$$\zeta = 2\left(\frac{x - x_0}{x_1 - x_0}\right) - 1 \tag{3g}$$

for x in that element between x_0 and x_1.
We need to map the local element to a standard element as shown below. The Jacobian transform J is used to map from the x to the ζ coordinate system.

$$J = \left|\frac{dx}{d\zeta}\right| \tag{4}$$



Starting with the left hand side of equation 1 transforming with the Jacobian to a standard using $dx = Jd\zeta$ we get:

$$\int_{x_0}^{x_1} D\frac{\partial c}{\partial x}\frac{\partial v}{\partial x}dx = \int_{-1}^{1} D\frac{\partial c}{\partial x}\frac{\partial v}{\partial x}Jd\zeta \tag{5}$$

We need to evaluate the derivatives $\frac{\partial c}{\partial x}$ and $\frac{\partial v}{\partial x}$ which we can obtain by applying the chain rule to the definitions of c and v given by equations eq:LagrangeC and eq:LagrangeV. This gives the results

$$\frac{dc}{dx} = c_0\frac{d\psi_0}{d\zeta}\frac{d\zeta}{dx} + c_1\frac{d\psi_1}{d\zeta}\frac{d\zeta}{dx} = c_n\frac{d\psi_n}{d\zeta}\frac{d\zeta}{dx} \quad \text{for } n = 0, 1 \tag{6a}$$
$$\frac{dv}{dx} = \frac{d\psi_m}{d\zeta}\frac{d\zeta}{dx} \quad \text{for } m = 0, 1 \tag{6b}$$

We can now rewrite equation 7 as the following, recognising c is independent of x and therefore ζ.

$$c_n \int_{-1}^{1} D \frac{d\psi_n}{d\zeta} \frac{d\zeta}{dx} \frac{d\psi_m}{d\zeta} \frac{d\zeta}{dx} J d\zeta \tag{7}$$

Knowing that $\frac{d\zeta}{dx} = J^{-1}$ (for $x_1 > x_0$) from equation 4 and that for a given element J is constant, we can rewrite equation 7 as

$$c_n J^{-1} \int_{-1}^{1} D \frac{d\psi_n}{d\zeta} \frac{d\psi_m}{d\zeta} d\zeta \qquad \text{for} n = 0, 1 \& m = 0, 1 \tag{8}$$

From 8 we have two equations, one for each node, which when written in full, is clearly suitable for matrix representation.

$$J^{-1} \left[c_0 \int_{-1}^{1} D \frac{d\psi_0}{d\zeta} \frac{d\psi_0}{d\zeta} d\zeta + c_1 \int_{-1}^{1} D \frac{d\psi_1}{d\zeta} \frac{d\psi_0}{d\zeta} d\zeta) \right] \tag{9a}$$

$$J^{-1} \left[c_0 \int_{-1}^{1} D \frac{d\psi_1}{d\zeta} \frac{d\psi_0}{d\zeta} d\zeta + c_1 \int_{-1}^{1} D \frac{d\psi_1}{d\zeta} \frac{d\psi_1}{d\zeta} d\zeta) \right] \tag{9b}$$

The matrix representation is as follows where I_{nm} represents the individual integrals in the above equations 9a and 9b.

$$J^{-1} \begin{bmatrix} Int_{00} & Int_{01} \\ Int_{10} & Int_{11} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} \tag{10}$$

We now need to evaluate each Int_{nm} term individually. In order to evaluate the integrals we need to calculate the derivatives of ψ_0 and ψ_1 with respect to ζ using the definition of the basis function given by equation 3e. The results is as follows.

$$\frac{d\psi_0}{d\zeta} = \frac{d}{d\zeta} (\frac{1 - \zeta}{2}) = -\frac{1}{2} \tag{11a}$$

$$\frac{d\psi_1}{d\zeta} = \frac{d}{d\zeta} (\frac{1 + \zeta}{2}) = \frac{1}{2} \tag{11b}$$

$\underline{Int_{00}}$

$$\begin{aligned}
Int_{00} &= \int_{-1}^{1} D \frac{d\psi_0}{d\zeta} \frac{d\psi_0}{d\zeta} d\zeta \\
&= \int_{-1}^{1} D.(-\frac{1}{2}).(-\frac{1}{2}) d\zeta \\
&= \left[\frac{D}{4}\zeta\right]_{-1}^{1} \\
&= \left[(\frac{D}{4}.1) - (\frac{D}{4}. - 1)\right] \\
&= \frac{D}{2}
\end{aligned} \tag{12}$$

<u>Int_{01}</u>

$$\begin{aligned}
Int_{01} &= \int_{-1}^{1} D \frac{d\psi_0}{d\zeta} \frac{d\psi_1}{d\zeta} d\zeta \\
&= \int_{-1}^{1} D.(-\frac{1}{2}).(\frac{1}{2}) d\zeta \\
&= \left[-\frac{D}{4}\zeta\right]_{-1}^{1} \\
&= \left[(-\frac{D}{4}.1) - (-\frac{D}{4}. - 1)\right] \\
&= -\frac{D}{2}
\end{aligned} \tag{13}$$

<u>Int_{10}</u>

$$\begin{aligned}
Int_{01} &= \int_{-1}^{1} D \frac{d\psi_1}{d\zeta} \frac{d\psi_0}{d\zeta} d\zeta \\
&= \int_{-1}^{1} D.(\frac{1}{2}).(-\frac{1}{2}) d\zeta \\
&= \left[-\frac{D}{4}\zeta\right]_{-1}^{1} \\
&= \left[(-\frac{D}{4}.1) - (-\frac{D}{4}. - 1)\right] \\
&= -\frac{D}{2}
\end{aligned} \tag{14}$$

$\underline{Int_{11}}$

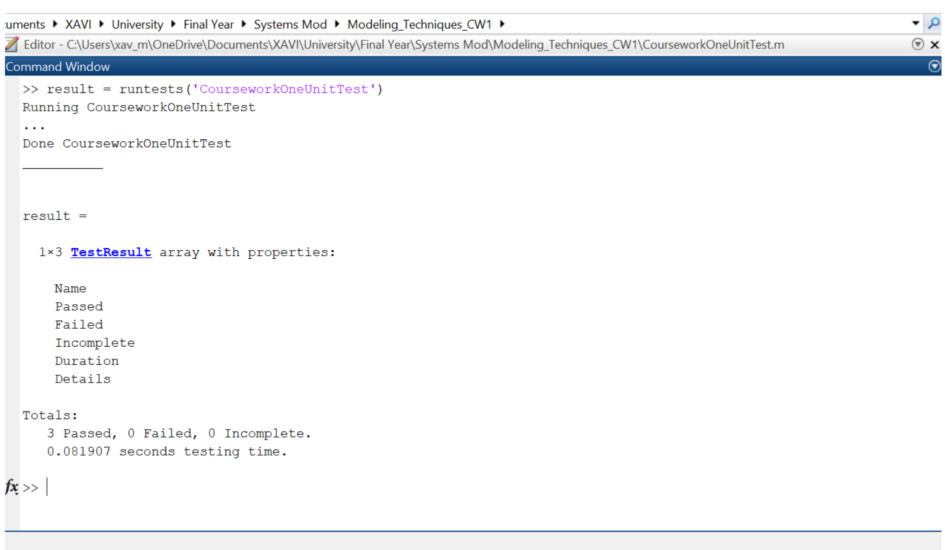
$$\begin{aligned} Int_{11} &= \int_{-1}^{1} D \frac{d\psi_1}{d\zeta} \frac{d\psi_1}{d\zeta} d\zeta \\ &= \int_{-1}^{1} D.(\frac{1}{2}).(\frac{1}{2}) d\zeta \\ &= \left[\frac{D}{4} \zeta \right]_{-1}^{1} \\ &= \left[(\frac{D}{4}.1) - (\frac{D}{4}. - 1) \right] \\ &= \frac{D}{2} \end{aligned} \tag{15}$$

We can now assemble our local element matrix (not including the c term matrix). This is the form used in the code for LaplaceElemMatrix.m function. Where J and D are scalars (we have assumed D to be constant).

$$J^{-1} D \begin{bmatrix} 0.5 & -0.5 \\ -0.5 & 0.5 \end{bmatrix} \tag{16}$$

1.1.2 Passes Unit Tests

Figure **??** shows the function LaplaceElemMatrix.m passes the unit tests defined in CourseworkOneUnitTest.m with no errors.



1.2 Question 1b

1.2.1 Derivation of Reaction Element Matrix

We need to calculate the local element matrix for the diffusion term. This is found by evaluating equation 17 term from equation XXXX(Overall equation).

$$\int_{x_0}^{x_1} \lambda cv dx \tag{17}$$

As in part a we will apply the Jacobi to map to the ζ domain. This gives us equation **??**.

$$\int_{-1}^{1} \lambda cv J d\zeta \tag{18}$$

We will again use the basis function for c defined by equation 3a and the Galerkin assumption to set the weighting to be the same as that of the basis function for optimal convergance as per equation 3c. We can then write equation 18 as a set of two equations similar to equations 9a and 9b, assuming λ to be independent of x we get the following result. These equations can also be written in the form of a matrix as shown by equation 20.

$$J\lambda \left[c_0 \int_{-1}^{1} \psi_0 \psi_0 d\zeta + c_1 \int_{-1}^{1} \psi_1 \psi_0 d\zeta) \right] \tag{19a}$$

$$J\lambda \left[c_0 \int_{-1}^{1} \psi_0 \psi_1 d\zeta + c_1 \int_{-1}^{1} \psi_1 \psi_1 d\zeta) \right] \tag{19b}$$

$$J\lambda \begin{bmatrix} Int_{00} & Int_{01} \\ Int_{10} & Int_{11} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} \tag{20}$$

We shall now evaluate the Int_{nm} integrals to derive the matrix.
$\underline{Int_{00}}$

$$\begin{aligned} Int_{00} &= \int_{-1}^{1} \psi_0 \psi_0 \, d\zeta \\ &= \int_{-1}^{1} \left(\frac{1-\zeta}{2}\right)^2 d\zeta \\ &= \left[\frac{1}{3} \left(\frac{1-\zeta}{2}\right)^3 (-2) \right]_{-1}^{1} \\ &= \frac{2}{3} \end{aligned} \tag{21}$$

$\underline{Int_{01} = Int_{10}}$

$$\begin{aligned}
Int_{00} &= \int_{-1}^{1} \psi_0 \psi_1 \; d\zeta \\
&= \int_{-1}^{1} \Big(\frac{1-\zeta}{2}\Big)\Big(\frac{1+\zeta}{2}\Big) d\zeta \\
&= \Big[\frac{\zeta}{4} - \frac{\zeta^3}{12}\Big]_{-1}^{1} \\
&= \Big[\frac{1}{6} - \Big(-\frac{1}{4} + \frac{1}{12}\Big)\Big]_{-1}^{1} \\
&= \frac{1}{3}
\end{aligned} \tag{22}$$

<u>Int_{11}</u>

$$\begin{aligned}
Int_{00} &= \int_{-1}^{1} \psi_1 \psi_1 \; d\zeta \\
&= \int_{-1}^{1} \Big(\frac{1+\zeta}{2}\Big)^2 d\zeta \\
&= \Big[\frac{1}{3}\Big(\frac{1+\zeta}{2}\Big)^3 .2\Big]_{-1}^{1} \\
&= \frac{2}{3}
\end{aligned} \tag{23}$$

Putting the results of the integrals into the matrix for from equation 20 we get the result shown by equation 24. This result is used by the LinearReactionElemMatrix.m function. As per equation XXXX we will need to subtract this result from the local diffusion element matrix result given by equation 16 in order to get the overall local element matrix which we can then assemble into an global matrix.

$$J\lambda \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} \end{bmatrix} \tag{24}$$

1.2.2 Solving Laplace With Dirichlet Boundaries

We will use the finite element solver to solve Laplace's equation:

$$\frac{\partial^2 c}{\partial x^2} = 0 \tag{25}$$

over the domain $x = 0$ to $x = 1$ with the Dirichlet boundary conditions:

$$c = 2 \quad at \quad x = 0 \tag{26a}$$
$$c = 0 \quad at \quad x = 1 \tag{26b}$$

The analytical solution is given by equation 27.

$$c = 2(1 - x) \tag{27}$$

The result of the analytical solution has been plotted in **??** with the FEM results overlaid. The FEM solution is very accurate here because we have used linear approximations as our basis functions and the analytical solution is also linear. This means we can achieve good results even with a low resolution 4 element mesh.

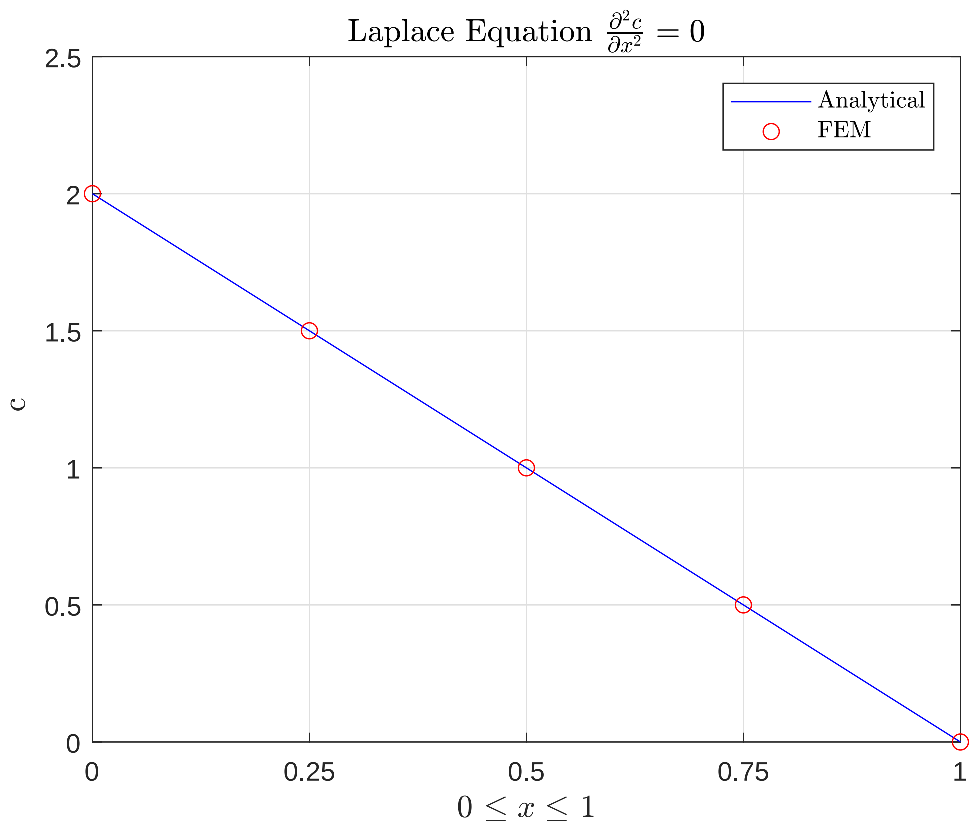


Figure 1: Comparison of Analytical and Finite Element Solutions of Laplace's Equation

1.2.3 Add a Neumann Boundary

Now we will change the initial boundary condition to a Neumann boundary, the conditions are given by equations 28.

$$\frac{dc}{dx} = 2 \quad at \quad x = 0 \tag{28a}$$

$$c = 0 \quad at \quad x = 1 \tag{28b}$$

2 Part 2

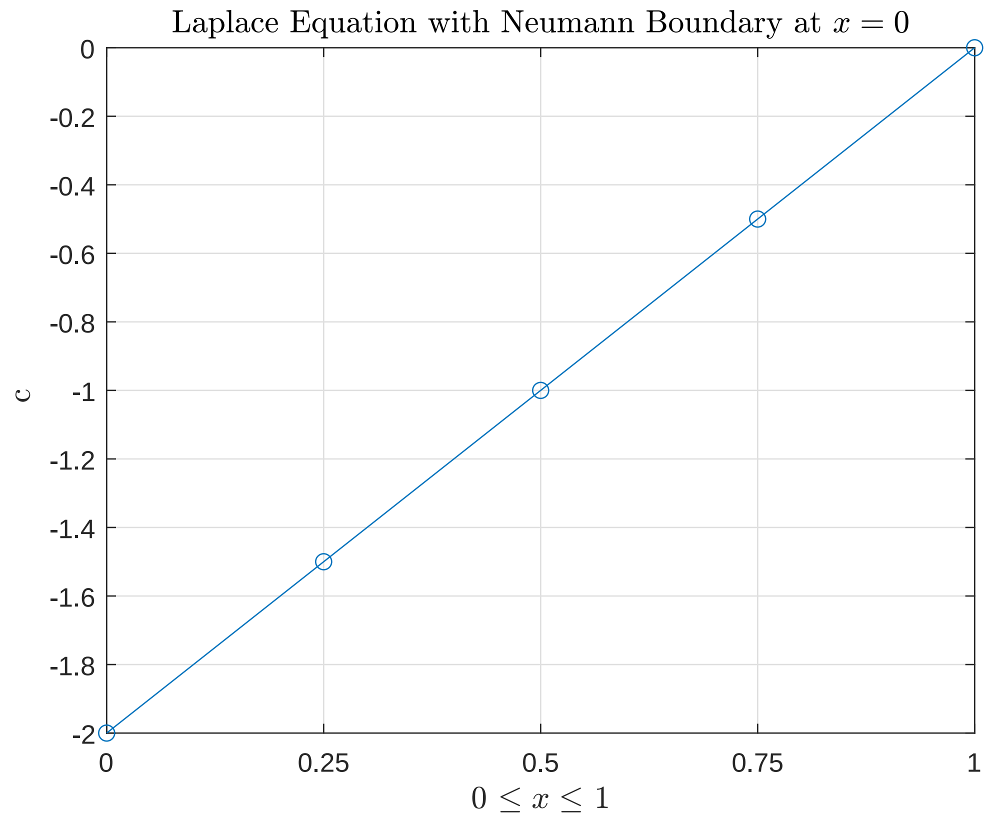


Figure 2: Comparison of Analytical and Finite Element Solutions of Laplace's Equation