

Quiz 4 : Solutions

Problem 1

a) Derive the approximation functions $\phi_I^e(\xi)$ for a master element with nodes at $\xi = -1$, $\xi = 0$, and $\xi = 1$, and show that it meets the typical criteria for approximation functions.

Solution (2 points): We derive the approximation functions based on the first typical criterion:

$$\phi_I^e = \delta_{IJ}, J = 1, 2, \dots, nen,$$

where nen is the number of nodes in the element. Based on this, the approximation functions can be defined as

$$\begin{aligned}\phi_1^e &= \frac{(0 - \xi)(1 - \xi)}{(0 - (-1))(1 - (-1))} = \frac{(-\xi)(1 - \xi)}{2}, \\ \phi_2^e &= \frac{(-1 - \xi)(1 - \xi)}{(-1 - 0)(1 - 0)} = (1 + \xi)(1 - \xi), \\ \phi_3^e &= \frac{(-1 - \xi)(0 - \xi)}{(-1 - 1)(0 - 1)} = \frac{(1 + \xi)(\xi)}{2}.\end{aligned}$$

Now, checking the second typical criterion for shape functions yields the following:

$$\begin{aligned}\sum_{I=1}^{nen} \phi_I^e &= 1, \Omega^e = [-1, 1] \\ &= \frac{(-\xi)(1 - \xi)}{2} + (1 + \xi)(1 - \xi) + \frac{(-1 - \xi)(-\xi)}{2}, \\ &= \frac{-\xi + \xi^2}{2} + \frac{2 - 2\xi^2}{2} + \frac{\xi + \xi^2}{2}, \\ &= \frac{2}{2} = 1,\end{aligned}$$

for all values of ξ .

Thus, the shape functions meet the typical criteria.

b) Write down the map $x = M(\xi)$ for an element in physical space with nodes at x_1 , x_2 , and x_3 .

Solution (2 points): This is fairly straightforward, as follows:

$$\begin{aligned}
x &= \sum_{I=1}^{nen} N_I^e x_I, \\
&= N_1^e x_1 + N_2^e x_2 + N_3^e x_3, \\
&= \frac{(-\xi)(1-\xi)}{2} x_1 + (1+\xi)(1-\xi) x_2 + \frac{(-1-\xi)(-\xi)}{2} x_3.
\end{aligned}$$

c) A desirable property of the isoparametric mapping is that it is invertible for all points in the element. State the mathematical condition that expresses this property.

Solution (2 points): Invertability of the map over the whole element would be guaranteed if

$$J = \det \left[\frac{\partial \mathbf{x}}{\partial \xi} \right] \neq 0, \forall \xi,$$

(for a system where the number of spatial dimensions > 1) and, in particular, we would like J to be strictly positive, to prevent elements from being overly distorted.

For 1D, this reduces to

$$J = \frac{\partial x}{\partial \xi} \neq 0, \forall \xi.$$

d) Consider an element in *physical* space with nodes 1, 2, and 3 at positions x_1 , x_2 , and x_3 , such that $x_1 < x_2 < x_3$. What restriction must be placed on x_2 , in terms of x_1 , x_3 , for the element to be "well-behaved"?

Solution (6 points): First, calculate an expression for J :

$$\begin{aligned}
J &= \det \left(\frac{\partial \mathbf{x}}{\partial \xi} \right), \\
&= \frac{\partial x}{\partial \xi}, \\
&= \frac{\partial N_1}{\partial \xi} x_1 + \frac{\partial N_2}{\partial \xi} x_2 + \frac{\partial N_3}{\partial \xi} x_3, \\
&= \left(\frac{-1+2\xi}{2} \right) x_1 + (-2\xi) x_2 + \left(\frac{1+2\xi}{2} \right) x_3.
\end{aligned}$$

Next, state the problem we would like to answer. In this case, we want to know where we can place x_2 in physical space, in terms of x_1 and x_3 , so that the element is well-behaved (i.e., J is positive, $\forall \xi$). To this end, let us first look at how J varies over the master element (i.e., how J varies with respect to ξ):

$$\frac{\partial J}{\partial \xi} = x_1 - 2x_2 + x_3.$$

So, for fixed values of x_1 , x_2 , and x_3 , the slope is a constant, i.e., $J(\xi)$ is a straight line. Also, we note that J is continuous in the variable ξ . So, let's look at the three cases:

- The slope equals zero: This corresponds to $x_2 = x_1 + \frac{1}{2}(x_3 - x_1)$. In this case, we only need to verify that J is positive, for any value of ξ . Indeed:

$$J(\xi = 0) = \frac{x_3 - x_1}{2}.$$

So, x_2 can be at the midpoint of the element, no problem.

- The slope is positive: This corresponds to $x_2 = x_1 + \alpha(x_3 - x_1)$, where $\alpha < \frac{1}{2}$. To ensure that J is positive everywhere, we only need to choose x_2 so that J is positive at the left endpoint of the domain. Letting $J = 0$ results in

$$J = 0 \Rightarrow x_2 = \frac{\left(-\frac{1}{2} + \xi\right)x_1 + \left(\frac{1}{2} + \xi\right)x_3}{2\xi}.$$

Now, evaluating that at $\xi = -1$ yields

$$x_2(\xi = -1) = \frac{\left(-\frac{1}{2} - 1\right)x_1 + \left(\frac{1}{2} - 1\right)x_3}{2(-1)} = \frac{3}{4}x_1 + \frac{1}{4}x_3 = x_1 + \frac{1}{4}(x_3 - x_1).$$

So, α cannot actually equal $\frac{1}{4}$, since that would result in $J = 0$, so the condition for this case must be $x_2 > x_1 + \frac{1}{4}(x_3 - x_1)$.

- The slope is negative: This corresponds to $x_2 = x_1 + \alpha(x_3 - x_1)$, where $\alpha > \frac{1}{2}$. Now, to ensure that J is positive everywhere, we only need to choose x_2 so that J is positive at the right endpoint of the domain. A similar calculation as the previous case yields

$$x_2(\xi = 1) = \frac{\left(-\frac{1}{2} + 1\right)x_1 + \left(\frac{1}{2} + 1\right)x_3}{2} = \frac{1}{4}x_1 + \frac{3}{4}x_3 = x_1 + \frac{3}{4}(x_3 - x_1).$$

Again, in this case, α cannot actually equal $\frac{3}{4}$.

Thus, the final condition on x_2 required to make the Jacobian positive at the endpoints (and thus everywhere in the domain) is

$$x_1 + \frac{1}{4}(x_3 - x_1) < x_2 < x_1 + \frac{3}{4}(x_3 - x_1).$$

Problem 2

Consider the system described by the strong form

$$\begin{aligned} \frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \tau c(x, t) &= \dot{c}(x, t) \quad \text{in } \Omega \times I = (0, L) \times (0, T], \\ c &= \bar{c} \quad \text{on } \Gamma_u \times I, \\ -D(x) \frac{\partial c}{\partial x} &= \bar{q}(t) \quad \text{on } \Gamma_q \times I, \\ c &= c_0 \quad \text{on } \Omega \times 0. \end{aligned}$$

a) Derive the weak form for this system.

Solution (6 points): This calculation will have an added twist: the inclusion of \dot{c} in the PDE. However, at this point, we can proceed with all of the usual steps:

$$\begin{aligned} \frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \tau c(x) - \dot{c}(x, t) &= 0, \\ w(x) \left[\frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \tau c(x, t) - \dot{c}(x, t) \right] &= 0, \\ \int_{\Omega} w(x) \left[\frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \tau c(x, t) - \dot{c}(x, t) \right] d\Omega &= 0, \\ \int_{\Omega} w(x) \frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \tau w(x)c(x, t) - w(x)\dot{c}(x, t) d\Omega &= 0, \\ \int_{\Omega} -\frac{\partial w}{\partial x} D(x) \frac{\partial c}{\partial x} - \tau w(x)c(x, t) - w(x)\dot{c}(x, t) d\Omega &= - \int_{\Omega} \frac{\partial}{\partial x} \left(w(x) D(x) \frac{\partial c}{\partial x} \right) d\Omega, \\ \int_{\Omega} \left[D(x) \frac{\partial w}{\partial x} \frac{\partial c}{\partial x} + \tau w(x)c(x, t) + w(x)\dot{c}(x, t) \right] d\Omega &= \int_{\Gamma_q} w(x) D(x) \frac{\partial c}{\partial x} n_x d\Gamma, \\ \int_{\Omega} \left[D(x) \frac{\partial w}{\partial x} \frac{\partial c}{\partial x} + \tau w(x)c(x, t) + w(x)\dot{c}(x, t) \right] d\Omega &= -w(L)\bar{q}(t). \end{aligned}$$

Note that that last line uses the assumption that $\Gamma_q = L$.

b) Define a (simple) approximation to calculate \dot{c} . Use that, along with the appropriate approximations for $c(x, t)$ and $w(x)$, to calculate the system of equations. Show the matrix form of the system of equations, similar to $\mathbf{K}\mathbf{u} = \mathbf{f}$ for time-independent problems, and show the entries for each matrix of the equation, e.g.,

$$\mathbf{K} = \begin{bmatrix} \int_{\Omega} A_1 \frac{\partial \phi_1}{\partial x} \frac{\partial \phi_1}{\partial x} d\Omega & \cdots \\ \vdots & \ddots \end{bmatrix}, \mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \end{bmatrix}, \mathbf{f} = \begin{bmatrix} \int_{\Omega} f(x)\phi_1 d\Omega \\ \vdots \end{bmatrix}.$$

To make things easier, make the following assumptions: 1) the approximation functions are defined over the whole domain (i.e., don't worry about elements), 2) the approximation functions are defined in terms of x (i.e., don't worry about parametric space), and 3) don't apply the Dirichlet BCs to the matrix system of equations.

Solution (8 points): Define a simple time integrator as

$$\dot{c}_{n+1} = \frac{c_{n+1} - c_n}{\Delta t}.$$

The typical approximations are as follows:

$$\begin{aligned} c(x, t) &= \sum_{I=1}^{nmp} N_I c_I, \\ \dot{c}(x, t) &= \sum_{I=1}^{nmp} N_I \dot{c}_I, \\ w(x) &= \sum_{I=1}^{nmp} N_I w_I, \end{aligned}$$

where nmp is the number of nodal points in the domain. Note that the spatial and time dependencies are split, with the approximation functions being defined as $N_I = N_I(x)$, and the nodal values of c being defined as $c_I = c_I(t)$.

So, substituting in the time integrator and the approximation for w yields the following:

$$\begin{aligned} \sum_{I=1}^{nmp} w_I \left[\int_{\Omega} \left[D(x) \frac{\partial N_I}{\partial x} \frac{\partial c_{n+1}}{\partial x} + \tau N_I c_{n+1} + N_I \left(\frac{c_{n+1} - c_n}{\Delta t} \right) \right] d\Omega \right] &= \sum_{I=1}^{nmp} w_I [-N_I(L) \bar{q}_{n+1}], \\ \sum_{I=1}^{nmp} w_I \left[\int_{\Omega} \left[D(x) \frac{\partial N_I}{\partial x} \frac{\partial c_{n+1}}{\partial x} + \tau N_I c_{n+1} + N_I \frac{c_{n+1}}{\Delta t} \right] d\Omega \right] &= \sum_{I=1}^{nmp} w_I \left[-N_I(L) \bar{q}_{n+1} + \int_{\Omega} N_I \frac{c_n}{\Delta t} d\Omega \right]. \end{aligned}$$

and since w is arbitrary, we have a system of equations

$$\int_{\Omega} \left[D(x) \frac{\partial N_I}{\partial x} \frac{\partial c_{n+1}}{\partial x} + \tau N_I c_{n+1} + N_I \frac{c_{n+1}}{\Delta t} \right] d\Omega = -N_I(L) \bar{q}_{n+1} + \int_{\Omega} N_I \frac{c_n}{\Delta t} d\Omega, \quad I = 1, 2, \dots, nmp.$$

Now, substitute in the approximation for $c(x, t)$:

$$\int_{\Omega} \left[D(x) \frac{\partial N_I}{\partial x} \sum_{J=1}^{nmp} \frac{\partial N_J}{\partial x} c_{J_{n+1}} + \tau N_I \sum_{J=1}^{nmp} N_J c_{J_{n+1}} + N_I \frac{1}{\Delta t} \sum_{J=1}^{nmp} N_J c_{J_{n+1}} \right] d\Omega = -N_I(L) \bar{q}_{n+1} + \int_{\Omega} N_I \sum_{J=1}^{nmp} N_J \frac{c_{Jn}}{\Delta t} d\Omega,$$

$I = 1, 2, \dots, nmp.$

So, finally, we can write out the matrix equation as

$$\mathbf{K} \mathbf{c}_{n+1} = \mathbf{f},$$

where

$$\mathbf{K} = \begin{bmatrix} \int_{\Omega} \left[D(x) \frac{\partial N_1}{\partial x} \frac{\partial N_1}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_1 N_1 \right] d\Omega & \int_{\Omega} \left[D(x) \frac{\partial N_1}{\partial x} \frac{\partial N_2}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_1 N_2 \right] d\Omega & \cdots & \int_{\Omega} \left[D(x) \frac{\partial N_1}{\partial x} \frac{\partial N_{nmp}}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_1 N_{nmp} \right] d\Omega \\ \int_{\Omega} \left[D(x) \frac{\partial N_2}{\partial x} \frac{\partial N_1}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_2 N_1 \right] d\Omega & \int_{\Omega} \left[D(x) \frac{\partial N_2}{\partial x} \frac{\partial N_2}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_2 N_2 \right] d\Omega & \cdots & \int_{\Omega} \left[D(x) \frac{\partial N_2}{\partial x} \frac{\partial N_{nmp}}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_2 N_{nmp} \right] d\Omega \\ \vdots & \vdots & \ddots & \vdots \\ \int_{\Omega} \left[D(x) \frac{\partial N_{nmp}}{\partial x} \frac{\partial N_1}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_{nmp} N_1 \right] d\Omega & \int_{\Omega} \left[D(x) \frac{\partial N_{nmp}}{\partial x} \frac{\partial N_2}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_{nmp} N_2 \right] d\Omega & \cdots & \int_{\Omega} \left[D(x) \frac{\partial N_{nmp}}{\partial x} \frac{\partial N_{nmp}}{\partial x} + \left(\tau + \frac{1}{\Delta t} \right) N_{nmp} N_{nmp} \right] d\Omega \end{bmatrix},$$

$$\mathbf{c}_{n+1} = \begin{bmatrix} c_{1n+1} \\ c_{2n+1} \\ \vdots \\ c_{nmpn+1} \end{bmatrix},$$

and $\mathbf{f} = \mathbf{t} + \mathbf{A}\mathbf{c}_n$, where

$$\mathbf{t} = \begin{bmatrix} -N_1(L)\bar{q}_{n+1} \\ -N_2(L)\bar{q}_{n+1} \\ \vdots \\ -N_{nmp}(L)\bar{q}_{n+1} \end{bmatrix},$$

where all entries except one will be zero, and

$$\mathbf{A} = \frac{1}{\Delta t} \begin{bmatrix} \int_{\Omega} N_1 N_1 d\Omega & \int_{\Omega} N_1 N_2 d\Omega & \cdots & \int_{\Omega} N_1 N_{nmp} d\Omega \\ \int_{\Omega} N_2 N_1 d\Omega & \int_{\Omega} N_2 N_2 d\Omega & \cdots & \int_{\Omega} N_2 N_{nmp} d\Omega \\ \vdots & \vdots & \ddots & \vdots \\ \int_{\Omega} N_{nmp} N_1 d\Omega & \int_{\Omega} N_{nmp} N_2 d\Omega & \cdots & \int_{\Omega} N_{nmp} N_{nmp} d\Omega \end{bmatrix}.$$

Problem 3

Consider a linear system of equations, given as

$$\mathbf{A}\mathbf{u} = \mathbf{b}.$$

a) Define *conjugacy* of the vectors \mathbf{a} and \mathbf{b} with respect to a matrix \mathbf{A} .

Solution (2 points): Conjugacy of the vectors \mathbf{a} and \mathbf{b} with respect to the matrix \mathbf{A} is defined as

$$\mathbf{a}^T \mathbf{A} \mathbf{b} = 0.$$

b) State the requirements on a linear system of equations that need to exist for the method of conjugate gradients to work, and define those requirements mathematically.

Solution (2 points): The system must be representable as a symmetric, positive-definite matrix. Symmetry is defined as

$$\mathbf{A} = \mathbf{A}^T,$$

and positive-definiteness of the matrix \mathbf{A} is defined as

$$\mathbf{a}^T \mathbf{A} \mathbf{a} > 0, \forall \mathbf{a}.$$

There are various other sufficient conditions for positive definiteness. The other one most often stated was that

$$\min(\lambda_i(\mathbf{A})) > 0,$$

where λ_i are the eigenvalues of \mathbf{A} , which implies that *all* of the eigenvalues of \mathbf{A} are positive.

c) Show that the solution to an appropriate system of equations is the minimizer of its *quadratic form, or potential*.

Solution (4 points): The quadratic form (or potential) of a system of equations can be defined as

$$f(x) = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{b}.$$

The minimizer of this potential can be found by setting the derivative equal to zero, as follows:

$$\begin{aligned} \text{grad } f = \mathbf{0} &= \frac{\partial f}{\partial \mathbf{x}} = \frac{1}{2} \mathbf{A}^T \mathbf{x} + \frac{1}{2} \mathbf{A} \mathbf{x} - \mathbf{b}, \\ &= \mathbf{A} \mathbf{x} - \mathbf{b}, \text{ (for symmetric } \mathbf{A}) \end{aligned}$$

which is the definition of the solution to the system of equations.

d) Given the system

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}, \mathbf{u}^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

derive the conjugate gradient method via example (i.e., show where all of the numbers go). By *derive*, I mean 1) define each necessary step, and 2) describe steps whose rationale or purpose is not obvious. Perform two complete iterations, with a final calculation of $\mathbf{u}^{(3)}$.

Note: Carry around any fractions, i.e., do not try to convert fractions to decimals.

Solution (6 points): Note that, during the quiz, it was stated to ignore preconditioning. Now, start by defining the *residual* as

$$\mathbf{r}^{(i)} = \mathbf{b} - \mathbf{A}\mathbf{u}^{(i)},$$

$$\mathbf{r}^{(1)} = \begin{bmatrix} 0 \\ 3 \end{bmatrix} - \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \end{bmatrix},$$

and the iteration to calculate the solution as

$$\mathbf{u}^{(i+1)} = \mathbf{u}^{(i)} + \lambda^{(i)}\mathbf{z}^{(i)}.$$

To be able to iterate for \mathbf{u} , we need to know λ and \mathbf{z} .

Lets define \mathbf{z} as follows:

$$\mathbf{z}^{(1)} = \mathbf{r}^{(1)} = \begin{bmatrix} 0 \\ 3 \end{bmatrix},$$

$$\mathbf{z}^{(i)} = \mathbf{r}^{(i)} + \theta^{(i)}\mathbf{z}^{(i-1)}.$$

Even though we don't need it yet, lets define θ so that $\mathbf{z}^{(i)}$ is \mathbf{A} -conjugate to $\mathbf{z}^{(i-1)}$, which results in

$$\theta^{(i)} = -\frac{\mathbf{r}^{(i)T}\mathbf{A}\mathbf{z}^{(i-1)}}{\mathbf{z}^{(i-1)T}\mathbf{A}\mathbf{z}^{(i-1)}}.$$

Choosing λ to minimize the potential energy results in

$$\lambda^{(i)} = \frac{\mathbf{z}^{(i)T}\mathbf{r}^{(i)}}{\mathbf{z}^{(i)T}\mathbf{A}\mathbf{z}^{(i)}},$$

$$\lambda^{(1)} = \frac{\begin{bmatrix} 0 & 3 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \end{bmatrix}}{\begin{bmatrix} 0 & 3 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \end{bmatrix}} = \frac{1}{2}.$$

Thus,

$$\mathbf{u}^{(2)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 \\ 3 \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{3}{2} \end{bmatrix}.$$

Now, lets do one more iteration:

- Calculate $\mathbf{r}^{(2)}$:

$$\mathbf{r}^{(2)} = \begin{bmatrix} 0 \\ 3 \end{bmatrix} - \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ \frac{3}{2} \end{bmatrix} = \begin{bmatrix} \frac{3}{2} \\ 0 \end{bmatrix}$$

- Calculate $\theta^{(2)}$:

$$\theta^{(2)} = -\frac{\begin{bmatrix} \frac{3}{2} & 0 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \end{bmatrix}}{\begin{bmatrix} 0 & 3 \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \end{bmatrix}} = \frac{1}{4}$$

- Calculate $\mathbf{z}^{(2)}$:

$$\mathbf{z}^{(2)} = \begin{bmatrix} \frac{3}{2} \\ 0 \end{bmatrix} + \frac{1}{4} \begin{bmatrix} 0 \\ 3 \end{bmatrix} = \begin{bmatrix} \frac{3}{2} \\ \frac{3}{4} \end{bmatrix}$$

- Calculate $\lambda^{(2)}$:

$$\lambda^{(2)} = \frac{\begin{bmatrix} \frac{3}{2} & \frac{3}{4} \end{bmatrix} \begin{bmatrix} \frac{3}{2} \\ 0 \end{bmatrix}}{\begin{bmatrix} \frac{3}{2} & \frac{3}{4} \end{bmatrix} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} \frac{3}{2} \\ \frac{3}{4} \end{bmatrix}} = \frac{2}{3}$$

- Finally, update \mathbf{u} :

$$\mathbf{u}^{(3)} = \begin{bmatrix} 0 \\ \frac{3}{2} \end{bmatrix} + \frac{2}{3} \begin{bmatrix} \frac{3}{2} \\ \frac{3}{4} \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$