Problem Set 7

CIVIL-425: Continuum Mechanics and Applications

17 April 2025

Problem 1: Finite element formulation

Consider a two-dimensional simplex element which, in its deformed configuration, occupies a triangular region Ω whose corners, or 'nodes', are labelled 1,2 and 3 consecutively and counterclockwise. The element lies in the $x_1 - x_2$ plane. Let $\mathbf{x}_a$, $a = 1, 2, 3$, be the coordinates of the nodes and $\mathbf{x} \in \Omega$ a point in the element. Denote $\mathbf{r}_a = \mathbf{x}_a - \mathbf{x}, a = 1, 2, 3$. Define 'shape functions' of the form:

$$
\begin{aligned}
N_1(\mathbf{x}) &= [\mathbf{e}_3, \mathbf{r}_2, \mathbf{r}_3] /(2A) \\
N_2(\mathbf{x}) &= [\mathbf{e}_3, \mathbf{r}_3, \mathbf{r}_1] /(2A) \\
N_3(\mathbf{x}) &= [\mathbf{e}_3, \mathbf{r}_1, \mathbf{r}_2] /(2A)
\end{aligned}
$$

where A is the area of the element and $\mathbf{e}_3$ is the unit vector normal to the plane of the element.

i) Show that $N_1 + N_2 + N_3 = 1$.

Incremental displacements $\mathbf{u}(\mathbf{x})$ and accelerations $\ddot{\mathbf{u}}(\mathbf{x})$ over the element are defined by interpolation,

$$
\begin{aligned}
\mathbf{u}(\mathbf{x}) &= \sum_{a=1}^{3} \mathbf{u}_a N_a(\mathbf{x}) \\
\ddot{\mathbf{u}}(\mathbf{x}) &= \sum_{a=1}^{3} \ddot{\mathbf{u}}_a N_a(\mathbf{x})
\end{aligned}
$$

where $\mathbf{u}_a$ and $\ddot{\mathbf{u}}_a, a = 1, 2, 3$, are the nodal displacements and accelerations. The Cauchy stresses $\boldsymbol{\sigma}$ are taken to be constant over the element. The element is under the action of body forces $\mathbf{b}$ defined over Ω, and boundary tractions $\bar{\mathbf{t}}$ applied over a part $\partial\Omega_\tau$ of the boundary of the element.

ii) Using the principle of virtual work and restricting virtual displacements to be of the form (2), show that the equation of linear momentum balance for the element reduces to:

$$
\mathbf{M}\ddot{\mathbf{u}} + A\mathbf{B}^T\boldsymbol{\sigma} = \mathbf{f}
$$

where $\ddot{\mathbf{u}} = \{\ddot{u}_1, \ddot{u}_2, \ddot{u}_3\}$ is an array which collects all nodal accelerations, $\mathbf{M}$ is a 6×6 'mass' matrix, $\boldsymbol{\sigma}$ is redefined as the array $\{\sigma_{11}, \sigma_{22}, \sigma_{12}\}$, $\mathbf{B}$ is a 3×6 matrix, and $\mathbf{f}$ is a 6-dimensional 'nodal force' array. Compute the arrays $\mathbf{M}, \mathbf{B}$ and $\mathbf{f}$ in terms of the nodal coordinates, the mass density $\rho, \mathbf{b}$ and $\bar{\mathbf{t}}$.

Solution

$$
N_a = \frac{A_a}{A} \Rightarrow \sum_{a=1}^{3} N_a = \frac{1}{A}\sum_{a=1}^{3} A_a = 1
$$

Note that $N_a(\mathrm{x}_b) = \delta_{ab}$. Also,

$$
\begin{aligned}
N_1 &= (x_{2\alpha} - x_\alpha)(x_{3\beta} - x_\beta)\,\epsilon_{\alpha\beta 3} = (x_{2\alpha}x_{3\beta} - x_\alpha x_{3\beta} - x_{2\alpha}x_\beta)\,\epsilon_{\alpha\beta 3} \\
N_2 &= (x_{3\alpha} - x_\alpha)(x_{1\beta} - x_\beta)\,\epsilon_{\alpha\beta 3} = (x_{3\alpha}x_{1\beta} - x_\alpha x_{1\beta} - x_{3\alpha}x_\beta)\,\epsilon_{\alpha\beta 3} \\
N_3 &= (x_{1\alpha} - x_\alpha)(x_{2\beta} - x_\beta)\,\epsilon_{\alpha\beta 3} = (x_{1\alpha}x_{2\beta} - x_\alpha x_{2\beta} - x_{1\alpha}x_\beta)\,\epsilon_{\alpha\beta 3}
\end{aligned}
$$

since $x_\alpha x_\beta \epsilon_{\alpha\beta 3} = 0$. Hence, the shape functions N_a are linear in $\mathbf{x}$. The gradients of the shape functions follow as:

$$N_{1,\alpha} = (x_{3\beta} - x_{2\beta})\,\epsilon_{\alpha\beta 3}$$

$$N_{2,\alpha} = (x_{1\beta} - x_{3\beta})\,\epsilon_{\alpha\beta 3}$$
$$N_{3,\alpha} = (x_{2\beta} - x_{1\beta})\,\epsilon_{\alpha\beta 3}$$

and they are constant. From virtual work:

$$\int_{\Omega} \left[\sigma_{\alpha\beta}\eta_{(\alpha,\beta)} + \rho\left(\ddot{u}_{\alpha} - b_{\alpha}\right)\eta_{\alpha}\right] dV - \int_{\partial\Omega_{\tau}} \bar{t}_{\alpha}\eta_{\alpha} dS = 0$$

Inserting interpolation:

$$\int_{\Omega} \left[\sigma_{\alpha\beta} \sum_{a=1}^{3} \frac{1}{2}\left(\eta_{a\alpha}N_{a,\beta} + \eta_{a\beta}N_{a,\alpha}\right) + \rho\left(\sum_{a=1}^{3}\eta_{a\alpha}N_{a}\right)\left(\sum_{b=1}^{3}\ddot{u}_{b\alpha}N_{b}\right)\right] dV$$
$$-\int_{\Omega}\rho b_{\alpha}\left(\sum_{a=1}^{3}\eta_{a\alpha}N_{a}\right) dV - \int_{\partial\Omega}\bar{t}_{\alpha}\left(\sum_{a=1}^{3}\eta_{a\alpha}N_{a}\right) dS = 0$$

which must hold for all $\eta_{a\alpha}$. Arrange in matrix form. Define:

$$\{\eta\}^{T} = (\eta_{11}, \eta_{12}, \eta_{21}, \eta_{22}, \eta_{31}, \eta_{32})$$
$$\{\ddot{u}\}^{T} = (\ddot{u}_{11}, \ddot{u}_{12}, \ddot{u}_{21}, \ddot{u}_{22}, \ddot{u}_{31}, \ddot{u}_{32})$$
$$\{\sigma\}^{T} = (\sigma_{11}, \sigma_{22}, \sigma_{12})$$

Then:

$$\sigma_{\alpha\beta}\sum_{a=1}^{3}\frac{1}{2}\left(\eta_{a\alpha}N_{a,\beta} + \eta_{a\beta}N_{a,\alpha}\right) = \{\eta\}^{T}B^{T}\{\sigma\}$$

where:
Likewise,

$$B = \begin{bmatrix} N_{1,1} & 0 & N_{2,1} & 0 & N_{3,1} & 0 \\ 0 & N_{1,2} & 0 & N_{2,2} & 0 & N_{3,2} \\ N_{1,2} & N_{1,1} & N_{2,2} & N_{2,1} & N_{3,2} & N_{3,1} \end{bmatrix}$$

where:

$$\int_{\Omega}\rho\left(\sum_{a=1}^{3}\eta_{a\alpha}N_{a}\right)\left(\sum_{b=1}^{3}\ddot{u}_{b\alpha}N_{b}\right) d\Omega = \{\eta\}^{T}M^{T}\{\ddot{u}\}$$

Define nodal forces:

$$M_{a\alpha b\beta} = \int_{\Omega}\rho N_{a}N_{b}\delta_{\alpha\beta} d\Omega$$

$$f_{a\alpha} = \int_{\Omega}\rho b_{\alpha}N_{a} dV + \int_{\partial\Omega}\bar{t}_{\alpha}N_{a} dS$$

and arrange into force array:

$$\{f\}^{T} = \{f_{11}, f_{12}, f_{21}, f_{22}, f_{31}, f_{32}\}$$

With these definitions, the virtual work expression becomes:

$$\{\eta\}^{T}\left(M\{\ddot{u}\} + AB^{T}\{\sigma\} - \{f\}\right) = 0$$

Enforcing this constraint for all $\{\eta\}$ gives:

$$M\{\ddot{u}\} + AB^{T}\{\sigma\} = \{f\}$$

bonus: Entropy and concentration equilibrium

Consider two perfectly miscible solid solutions placed in contact through an adiabatic but permeable boundary. The combined system is otherwise isolated from the rest of the world. Suppose that the subsystems have N_1 and N_2 intersticial locations, and, initially, n_1 and n_2 atoms, respectively. We proceed to compute the equilibrium concentrations in the two subsystems.

i) Show that $c_1^{eq} = c_2^{eq} = c^{eq}$ at equilibrium.

ii) Compute the internal entropy $S_{int} \geq 0$ produced in going from the initial conditions to equilibrium and show that $\triangle S_{int} \geq 0$.

Solution: The total number of interstiticial location is $N = N_1 + N_2$ and the total number of atoms $N = N_1 + N_2$. The equilibrium condition is when the entropy is maximum. The total entropy is:

$$S = S_1 + S_2 \,. \tag{1}$$

For it to be maximum it must be a stationary point of either n_1 or n_2.

Let us choose n_1 (even though this does not change the solution) and take the derivative:

$$\frac{\partial S(n_1, n)}{\partial n_1} = \frac{\partial S_1(n_1, n)}{\partial n_1} + \frac{\partial n_2}{\partial n_1}\frac{\partial S(n_1, n)}{\partial n_2} \implies \frac{\partial S_1}{\partial n_1} = \frac{\partial S_2}{\partial n_2} \tag{2}$$

or

$$\frac{\partial}{\partial c_1}\Big(\frac{S_1}{N_1}\Big) = \frac{\partial}{\partial c_2}\Big(\frac{S_2}{N_2}\Big) \tag{3}$$

But S_1/N_1 and S_2/N_2 are identical functions of c_1 and c_2, respectively. Hence, at equilibrium,

$$c_1^{eq} = c_2^{eq} = c^{eq} \tag{4}$$

Since, in addition, $n_1 + n_2 = n$ or $c_1 N_1 + c_2 N_2 = n$, it follows that

$$c^{eq} = \frac{n}{N_1 + N_2} = \frac{N_1}{N_1 + N_2} c_1 + \frac{N_2}{N_1 + N_2} c_2 \equiv \alpha_1 c_1 + \alpha_2 c_2 \tag{5}$$

where c_1 and c_2 are the initial concentrations of solute systems. We may also compute the internal entropy production

$$\triangle S_{int} = S_1^{eq} + S_2^{eq} - (S_1 + S_2) \tag{6}$$

resulting from mass transfer. To this end, write $\eta(c) = S/N$. Since, at equilibrium, $\eta_1^{eq} = \eta_2^{eq} = \eta(c^{eq})$, it follows that

$$\triangle S_{int} = (N_1 + N_2)\eta(c^{eq}) - \Big[N_1 \eta(c_1) + N_2 \eta(c_2)\Big] \tag{7}$$

or

$$\frac{\triangle S_{int}}{N_1 + N_2} = \eta(\alpha_1 c_1 + \alpha_2 c_2) - \Big[\alpha_1 \eta(c_1) + \alpha_2 \eta(c_2)\Big] \tag{8}$$

But, η is a concave function of c, which implies that $\triangle S_{int} \geq 0$, in agreement with the second law.