SCHOOL OF MATHEMATICS AND STATISTICS

Computational Engineering Mathematics

*Marks will be awarded for answers to your best FIVE questions*
In the following, a repeated index in any of \( i, j \) or \( k \) only indicates that the summation convention is to be used. Given the stress state, defined in MPa, \( \sigma_{xx} = 6.0000, \sigma_{xy} = 1.2247, \sigma_{xz} = 1.2247, \sigma_{yy} = 4.5000, \sigma_{yz} = -0.5000 \) and \( \sigma_{zz} = 4.5000 \) together with the transformation matrices

\[
T_x \equiv \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \theta_x & -\sin \theta_x \\ 0 & \sin \theta_x & \cos \theta_x \end{bmatrix}, \quad T_y \equiv \begin{bmatrix} \cos \theta_y & 0 & -\sin \theta_y \\ 0 & 1 & 0 \\ \sin \theta_y & 0 & \cos \theta_y \end{bmatrix},
\]

\[
T_z \equiv \begin{bmatrix} \cos \theta_z & -\sin \theta_z & 0 \\ \sin \theta_z & \cos \theta_z & 0 \\ 0 & 0 & 1 \end{bmatrix},
\]

then

- find the new stress state (to the nearest KPa) corresponding to the rotation \( \theta_z = \pi/2 \) followed by \( \theta_y = \pi/4 \) and finally by \( \theta_x = \pi/3 \). Remember that, after a rotation described by the rotation matrix \( T \), then the new stress state is related to the old stress state by

\[
\sigma^{(\text{new})} = T \sigma^{(\text{old})} T'
\]

where \( T' \) denotes transpose; \( \text{ (14 marks) } \)

- Find:
  - the mean (average) stress \( \sigma_{kk}^{(\text{new})}/3; \) \( \text{ (2 marks) } \)
  - the deviatoric stresses defined by

\[
\sigma_{ij}^{(\text{new})} = \sigma_{ij}^{(\text{new})} - \frac{1}{3} \delta_{ij} \sigma_{kk}^{(\text{new})},
\]

where \( \delta_{ij} \) represents the usual \( 3 \times 3 \) unit matrix; \( \text{ (2 marks) } \)

- and \( \sigma_{kk}^{(\text{new})}. \) \( \text{ (2 marks) } \)
The second order PDE

\[ A \frac{\partial^2 \Phi}{\partial x^2} + B \frac{\partial^2 \Phi}{\partial x \partial y} + C \frac{\partial^2 \Phi}{\partial y^2} + D = 0, \]

where \( A, B, C \) and \( D \) are arbitrary constants, can be classified as being either elliptic, parabolic or hyperbolic.

(i) Define the three classes in terms of the signature of \( B^2 - 4AC \) and hence classify each of the following three PDEs:

- \( U_{xx} + 2U_{xy} + U_{yy} - U_y = f ; \)
- \( 2U_{xx} + U_{xy} + 7U_{yy} = U_x + 5x^2 ; \)
- \( U_{xx} + U_{xt} - U_{tt} = 0. \)

(6 marks)

(ii) The one-dimensional diffusion equation is given by

\[ \frac{\partial U}{\partial t} = \alpha \frac{\partial^2 U}{\partial x^2}, \]

where \( \alpha \) is the diffusion coefficient. Use the standard finite difference approximations, given on the formulae sheet, together with the notation \( k = \Delta t / \Delta x^2 \), to derive the implicit scheme

\[ \alpha k U_{i+1,j} - (1 + 2\alpha k) U_{ij} + \alpha k U_{i-1,j} = -U_{ij-1} , i = 1, 2, \ldots n, j = 1, 2, \ldots \]

which approximates this equation. (3 marks)

(iii) Given that the diffusion equation is to be solved over the range \( 0 \leq x \leq 1 \) for the temperature distribution along a given steel billet with boundary conditions \( U(0, t) = 0^\circ C \) and \( U(1, t) = 100^\circ C \) and initial conditions \( U(x, 0) = 100x \), and assuming that the units have been normalized so that \( \alpha = 1 \), then, with the aid of a diagram:

- use the implicit scheme with \( \Delta x = 0.25 \) and \( \Delta t = 0.1 \) to write down the system of algebraic equations for the temperatures at \( x = 0.25, 0.5, 0.75 \) at time \( t = 0.1 \); (8 marks)

- express your equations in the form \( Ax = b \), and write a Scilab (or Matlab) program to solve these equations. Your program should define \( A \) and \( b \) explicitly and then print out the solution \( x \). Note: this is a very short program! (3 marks)
3 (i) A vanishingly small force, $\Delta f$, acts on a surface of vanishingly small area, $\Delta A$, drawn on the interior of a solid body. Using a diagram to clarify things, define what is meant by the stress at a point $P$ in $\Delta A$ and explain, briefly, why a complete mathematical description of stress requires it to be defined as a two-index tensor.

(6 marks)

(ii) A concrete slab, of unit thickness in the z-direction, is loaded with body-forces $f$ and is in a state of plane stress so that $\sigma_{xx} = \sigma_{yy} = \sigma_{xy} = F_z = 0$. By considering only the balance of forces in the x-direction, use a diagram to derive the x-component of the equations of static equilibrium and hence infer the full set of force-balance equations for a three-dimensional body.

(14 marks)

4 The velocity field in an unsteady moving fluid is given by $\mathbf{V} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$ where $u \equiv u(x, y, z, t)$, $v \equiv v(x, y, z, t)$ and $w \equiv w(x, y, z, t)$.

(i) By considering the density, $\rho(x, y, z, t)$, an infinitesimal control volume, $\delta V$, in the fluid moving from a point $(x_1, y_1, z_1)$ at time $t_1$ to a point $(x_2, y_2, z_2)$ at time $t_2$ then derive the substantial (or total) derivative

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} + w \frac{\partial \rho}{\partial z}$$

of $\rho$ and interpret the meanings of the first two terms on the right-hand side of this latter expression.

(12 marks)

(ii) Given that the divergence of $\mathbf{V}$ is defined by

$$\nabla \cdot \mathbf{V} \equiv \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = \lim_{\delta V \rightarrow 0} \frac{1}{D(\delta V)} D_{t}^{\delta V},$$

then, by considering the mass of the moving control volume, $\delta m = \rho \delta V$, derive the equation of continuity (that is, of mass conservation) for a compressible fluid and show that this can be rearranged in conservative form as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0.$$

(8 marks)
Figure 1 shows an 8-noded isoparametric hexahedral finite element with a local coordinate system, \((\alpha, \beta, \gamma)\), having its origin at the geometric centre of the element, as indicated. The shape function for the first node of this element is given by

\[ N_1 = \frac{1}{8}(1 - \alpha)(1 - \beta)(1 - \gamma). \]

Figure 1: Isoparametric finite element and its local coordinate system

(i) Write down the shape functions for the remaining nodes. \hspace{1cm} (8 marks)

(ii) If the global coordinate system is denoted by \((x, y, z)\) and the global coordinates of nodes 1, 2, ... 8 of the finite element are given by \((0, 0, 0)\), \((1, 0, 0)\), \((1, 1, 0)\), \((0, 1, 0)\), \((1, 1, 2)\), \((2, 1, 2)\), \((2, 2, 3)\) and \((1, 2, 2)\) respectively, then find the \((x, y, z)\) coordinates of the point \((\alpha, \beta, \gamma) = (0.5, 0.1, -0.7)\) using the shape functions \(N_1, N_2, ..., N_8\). Work correct to four decimal places. \hspace{1cm} (12 marks)
Figure 2 shows an L-shaped plate made of an homogeneous isotropic material. The temperature distribution in this plate satisfies the indicated boundary conditions and has reached a steady-state condition so that it is described by Laplace’s equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0.$$  

(i) Draw a sketch of the solution domain showing clearly the line of symmetry for the temperature distribution. \( (3 \text{ marks}) \)

(ii) Use the finite difference formulae on the formulae sheet to formulate the finite difference equations required to find estimates of the nodal temperatures \( T_A, T_B, T_C, T_D \) and the temperatures at the two circled locations, taking care to treat the Neumann boundary conditions, \( \partial T / \partial y = -0.5^\circ C \text{ mm}^{-1} \) and \( \partial T / \partial x = -0.5^\circ C \text{ mm}^{-1} \), at the circled locations using the central difference formulae. \( (7 \text{ marks}) \)

(iii) Solve these equations using the method of Gaussian Elimination. \( (10 \text{ marks}) \)
The boundary value problem

\[ \mathcal{L}(u) \equiv \frac{d^2u}{dx^2} - 9u - 3x = 0, \text{ given } u(0) = 0 \text{ and } u(1) = 1 \]

is to be solved by the weighted residual method.

(i) Determine which of the two trial functions, \( U_1(x) \) or \( U_2(x) \), automatically satisfies the boundary conditions:

\[ U_1(x) = (1 - x) + c_1x(1 - x) + c_2x(1 - x^2) \]
\[ U_2(x) = x + c_1(x^2 - x) + c_2(x^3 - x) \]

(3 marks)

(ii) Determine the residual \( \mathcal{L}(U) = R(x) \) associated with your chosen trial function and then, by applying the weight functions \( w(x) = 1 \) and \( w(x) = x \) in turn, use the condition

\[ \int_0^1 w(x) R(x) \, dx = 0 \]

to derive two algebraic equations for \( c_1 \) and \( c_2 \). Solve these equations working correct to four decimal places. (12 marks)

(iii) Given that the exact solution is given by

\[ u(x) = Ae^{-3x} + Be^{3x} - \frac{x}{3} \]

where \( A \approx -0.06656, \ B \approx 0.06656, \)

then perform a check on your approximate solution, \( U(x) \), by computing the difference \( u(0.5) - U(0.5) \). (5 marks)

End of Question Paper
Formulae Sheet

Notation:

\[ U(x_i, t_j) = U_{ij} \]

Forward difference formula for \( U_t \):

\[ \frac{\partial U}{\partial t} \approx \frac{U_{ij+1} - U_{ij}}{\Delta t} \]

Backward difference formula for \( U_t \):

\[ \frac{\partial U}{\partial t} \approx \frac{U_{ij} - U_{ij-1}}{\Delta t} \]

Central difference formula for \( U_x \):

\[ \frac{\partial U}{\partial x} \approx \frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x} \]

Central difference formula for \( U_{xx} \):

\[ \frac{\partial^2 U}{\partial x^2} \approx \frac{U_{i,j+1} - 2U_{ij} + U_{i,j-1}}{\Delta x^2} \]