M.Sc. in Mathematical Modelling and Numerical Analysis

Paper A (Mathematical Modelling)

Thursday 18 April, 1996, 9.30 a.m. – 12.30 p.m.

All candidates are expected to attempt at least three parts of question 1. Having done so, you may attempt as many of the remaining questions (including the remaining part of question 1) as you wish.

Do not turn this page until you are told that you may do so

1. (i) A simple energy balance model for the global average temperature is given by

$$c\dot{T} = Q[1 - \alpha(T)] - \sigma T^4.$$

Explain the meaning of the terms in this equation.

If $\alpha = \alpha_f$ for $T < T_f$ and $\alpha = \alpha_u$ for $T > T_f$, where $1 > \alpha_f > \alpha_u > 0$, show that multiple steady states are possible if $Q_- < Q < Q_+$, where Q_+ and Q_- should be given, and assess their stability.

Hence draw a diagram of equilibrium solutions of T versus Q, and describe what happens if Q slowly oscillates between $Q_{\max}$ and $Q_{\min}$, where $Q_{\max} > Q_+ > Q_- > Q_{\min}$.

(ii) An allosteric enzyme reacts with a substrate S to produce a product P according to the mechanism

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_1 \xrightarrow{k_2} E + P,$$

$$S + C_1 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} C_2 \xrightarrow{k_4} C_1 + P.$$

Write down the equations governing the reaction, and give an interpretation of the terms in these equations. By making a suitable pseudo-steady state assumption, show that the substrate concentration s satisfies the approximate equation

$$\frac{\mathrm{d}s}{\mathrm{d}t} = -s\left[\frac{K_1 + K_2 s}{1 + K_3 s + K_4 s^2}\right],$$

where the constants K_i should be specified.

QUESTION CONTINUES ON NEXT PAGE

1. (CONTINUED FROM PREVIOUS PAGE)

(iii) The equations governing the first order chemical reaction of a gas with a porous catalyst pellet of radius a are given by

$$\begin{aligned}\frac{\partial c}{\partial t} &= D\nabla^2 c - r,\\ \rho c_p\frac{\partial T}{\partial t} &= k\nabla^2 T - r\Delta H.\end{aligned}$$

Explain the meaning of the various terms, and give a suitable expression for r, based on a first order reaction with Arrhenius kinetics. What are suitable boundary conditions at the pellet boundary?

By nondimensionalising the equations, show that the reaction is controlled by the dimensional parameters

$$Le = \frac{\kappa}{D},\quad \delta = \frac{\Delta T}{T_0},\quad \mu = \frac{r_0 a^2}{c_0\kappa},\quad \beta = \frac{E\Delta T}{RT_0^2},$$

where $\kappa = k/\rho c_p$, T_0 is the external temperature, and ΔT should be determined. What happens if $\mu \ll 1$, $Le \gg 1$?

(iv) Write down the equations governing groundwater flow of subsurface water beneath the water table $z = h(x, y, t)$, where z is the vertical coordinate. Explain (great detail is not required) how the Dupuit-Forchheimer approximation allows the reduction of the model to the evolution equation

$$\frac{\partial h}{\partial t} = \boldsymbol{\nabla}.[h\boldsymbol{\nabla}h],$$

when h, $\mathbf{x}$ and t are suitably scaled.

A well of radius r_0 is drilled through a cylindrical aquifer of depth 1 and radius R (all units are dimensionless). If a water flux q $(= h\partial h/\partial r)$ is taken from the well, show that the well will run dry if

$$q > \frac{1}{2r_0 \ln(R/r_0)}.$$

[You may assume that the aquifer is surrounded by water.]

2. $\mathcal{L}$ is a linear operator and u an unknown function. State the *Fredholm Alternative* (i.e. the possibilities concerning existence and uniqueness) for the solution of the inhomogeneous problem $\mathcal{L}u = f \neq 0$ in terms of the solution of a homogeneous problem. Illustrate your statement

(i) in a vector space when $\mathcal{L} = \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}$, $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$, $f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$;

(ii) in a suitable function space with $\mathcal{L} = \dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$ on $0 < x < 1$ with $\dfrac{\mathrm{d}u}{\mathrm{d}x}(0) = \dfrac{\mathrm{d}u}{\mathrm{d}x}(1) = 0$, and $f = f(x)$.

When $\mathcal{L}$ is a second order differential operator with boundary conditions at $x = 0, 1$, show that

$$\mathcal{L}^{-1} f(x) = \int_0^1 G(\xi, x) f(\xi) \mathrm{d}\xi$$

where the function G satisfies certain conditions that you should specify. What happens when the boundary conditions are both at $x = 0$?

When $\mathcal{L} = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$ in $-\infty < x,\ y < \infty$, show that

$$\mathcal{L}^{-1} f(x, y) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi, \eta) \log[(x-\xi)^2 + (y-\eta)^2] \mathrm{d}\xi \mathrm{d}\eta.$$

When $\mathcal{L} = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$ in $-\infty < x < \infty$, $y > 0$ and

$$\mathcal{L}u = 0 \quad \text{with} \quad \frac{\partial u}{\partial y}(x, 0) = f(x),$$

show that

$$\mathcal{L}^{-1} f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\xi) \log[(x-\xi)^2 + y^2] \mathrm{d}\xi.$$

3. (i) Write down the conditions that are necessary for $\sum_0^\infty f_n(\varepsilon)$ to be an *asymptotic expansion* of a function $f(\varepsilon)$ as $\varepsilon \to 0$. Illustrate the nonuniqueness of such expansions by giving two different ones for

$$f(\varepsilon) = \int_0^\infty [\mathrm{e}^{-t}/(1+\varepsilon t)]\mathrm{d}t, \quad \varepsilon > 0.$$

(ii) Suppose A is a real, constant 2 by 2 matrix, $\mathbf{x} = (x, y)$ and

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = A\mathbf{x} + O(|\mathbf{x}|^2) \text{ as } |\mathbf{x}| \to 0.$$

Sketch the phase plane near $\mathbf{x} = \mathbf{0}$ when the eigenvalues of A are (i) real and distinct, (ii) complex conjugates. If the initial data $\mathbf{x}(0) = O(\varepsilon)$ and $t \geq 0$, under what circumstances is $\mathbf{x} \sim \varepsilon\mathbf{x}_0(t)$, where $\mathrm{d}\mathbf{x}_0/\mathrm{d}t = A\mathbf{x}_0$, a good approximation for *all* $t > 0$?

(ii) Given the Fourier series $f(x) = \frac{1}{2}a_0 + \sum_1^\infty a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}$ where $a_n + \mathrm{i}b_n = \frac{1}{L}\int_{-L}^{L} f(x)\mathrm{e}^{\mathrm{i}n\pi x/L}\mathrm{d}x$, show that

$$f(x) = \sum_{-\infty}^{\infty} C_n \mathrm{e}^{\mathrm{i}n\pi x/L} \text{ where } C_n = \frac{1}{L}\int_{-L}^{L} f(x)\mathrm{e}^{-\mathrm{i}n\pi x/L}\mathrm{d}x.$$

Hence show formally that if $\bar{f}(k) = \int_{-\infty}^{\infty} f(x)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x$, then

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \bar{f}(h)\mathrm{e}^{\mathrm{i}kx}\mathrm{d}k. \qquad (*)$$

Describe very briefly any method you know for evaluating $\int_a^b \bar{f}(k)\mathrm{e}^{\mathrm{i}xg(k)}\mathrm{d}k$ asymptotically as $x \to \infty$ when a, b and g are all real.

4. (i) Define a *characteristic* of the hyperbolic quasi-linear system $A\mathbf{u}_x + B\mathbf{u}_y = \mathbf{c}$ and show that the characteristics are given by $\dfrac{\mathrm{d}y}{\mathrm{d}x} = \lambda$ where λ satisfies $|A\lambda - B| = 0$. If the vector $\mathbf{p}$ is such that $\mathbf{p}^T(A\lambda - B) = 0$, show that along a characteristic $\mathbf{p}^T A\dfrac{\mathrm{d}u}{\mathrm{d}x} = \mathbf{p}^T C$.

(ii) Find the equations of the characteristics for the system

$$\left.\begin{aligned} u_x + 2(u-4v)u_y + 8(v-u)v_y &= 0, \\ v_x + 2(v-u)u_y + 2(u-4v)v_y &= 0, \end{aligned}\right\} \qquad (*)$$

and show that the Riemann Invariants are $u \pm 2v$.

(iii) Show that system (*) can be written in conservation form and, by defining a weak solution, deduce that across a discontinuity

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{[u^2 - 8uv + 4v^2]}{[u]} = -\frac{[u^2 - 2uv + 4v^2]}{[v]}$$

where $[u]$ represents the jump in u across the discontinuity.

5. In each of the following problems define a Green's function and show how it can be used to find a solution:

(a) $u_{xx} + u_{yy} = g$ for $-\infty < x < \infty,\ y > 0$ with $u(x,0) = f$ and $u = O(r^{-k})$ as $r^2 = x^2 + y^2 \to \infty$; and

(b) $u_{xx} - \lambda u_y = g$ for $-\infty < x < \infty,\ y > 0$ with $u(x,0) = f$, $u \to 0$ as $x \to \pm\infty$.

Explain clearly the assumptions you need to make about the constants k and λ to be sure the problems are well-posed.