King’s College London

UNIVERSITY OF LONDON

B.Sc. EXAMINATION

CP2720 Computational Physics

Summer 2003

Time allowed: THREE Hours

Candidates must answer any SIX questions from SECTION A,
and TWO questions from SECTION B.

The approximate mark for each part of a question is indicated in square brackets.

You must not use your own calculator for this paper.
Where necessary, a College calculator will have been supplied.

TURN OVER WHEN INSTRUCTED

In questions asking for descriptions of methods of solution, you are not expected to provide numerical values, or to write computer programs.

SECTION A – Answer SIX parts of this section

1.1) Explain how integers are stored in computer memory and hence write down expressions for the largest and smallest integers that can be stored as 2-byte integers.

[7 marks]

1.2) The Newton-Raphson method for finding the roots of an equation, $f(x) = 0$, states that, if x_1 is a good approximation to a root, then

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

is a better approximation. Starting from a Taylor series about the estimated root, derive this expression. Under what circumstances does this method fail?

[7 marks]

1.3) Describe how the Monte Carlo method could be used to calculate the volume of a sphere.

[7 marks]

1.4) Any N×M matrix, **A**, can be decomposed into the product of an N×M matrix, **U**, whose columns are orthogonal vectors, an M×M diagonal matrix, **W**, and the transpose of an M×M orthogonal matrix $\mathbf{V}^T$.

$$\mathbf{A} = \mathbf{U}.\mathbf{W}.\mathbf{V}^T$$

For the case where **A** is square, explain briefly how this may be used to solve the matrix equation **Ax** = **b** to find the vector **x**, given the constant vector, **b**. If **A** is singular, how can the maximum information be retrieved?
[Note that, for an orthogonal matrix, **U**, the inverse is equal to the transpose, $\mathbf{U}^{-1} = \mathbf{U}^T$.]

[7 marks]

1.5) The recurrence relation for Hermite polynomials, $H_n(x)$, is

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

Show that this is numerically unstable for large n, for all values of x.

[7 marks]

1.6) The equation for the displacement of a bent beam, $y(x)$, is

$$\frac{\mathrm{d}^4 y}{\mathrm{d}x^4} = k\omega(x)$$

where k is a constant characteristic of the properties of the beam and $\omega(x)$ gives the loading of the beam at x. Both ends of the beam are clamped at the same horizontal level. Separate this equation into 4 first-order equations, and state the boundary conditions in terms of any new variables that you have defined. If $\omega(x)$ is given for the whole beam, is there enough information to solve for $y(x)$?

[7 marks]

1.7) The Fresnel integrals are given by

$$C(\omega) = \int_0^\omega \cos\frac{\pi t^2}{2}\mathrm{d}t$$

$$S(\omega) = \int_0^\omega \sin\frac{\pi t^2}{2}\mathrm{d}t$$

Describe how you would use Simpson's method to evaluate these integrals for a given value of ω. Pay particular attention to the choice of step length.

[7 marks]

1.8) A continued fraction expression for $\tan x$ is written as

$$\tan x = \frac{x}{1-}\,\frac{x^2}{3-}\,\frac{x^2}{5-}\,\frac{x^2}{7-}\,\frac{x^2}{9-}\,\frac{x^2}{11-}\cdots$$

Explain what this notation means, and how you would evaluate this expression. What would you notice if you tried to evaluate this expression for one of the values of x at which $\tan x$ is undetermined (e.g. $\tan\pi/2$)?

[7 marks]

SECTION B - answer TWO questions

2) a) The differential equation for damped oscillations of a mass is

$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0{}^2 x = 0 \qquad (2.1)$$

where $x(t)$ is the displacement of the mass as a function of time, γ is a damping factor and ω_0 is the undamped frequency of the oscillator. If the damping factor is a function of velocity, v, then this equation becomes difficult or impossible to solve analytically. In the case where $\gamma(v) = \alpha v^2$, show how equation (2.1) can be separated into two first-order differential equations.

[5 marks]

b) Explain how to use the fourth-order Runge-Kutta method to build up a solution to equation (2.1), given that at t = 0, $x = x_0$ and v = 0, and all constants (x_0, ω_0 and α) have been given numerical values.

[18 marks]

c) If the initial velocity was unknown, but at a time, T, the displacement was zero ($x(T)$ = 0), describe briefly how to build up a solution using the shooting method.

[7 marks]

3) a) Associated Legendre polynomials, $P_l^m(x)$ $(l \geq m)$, obey recurrence relations:

$$(l-m)P_l^m(x) = x(2l-1)P_{l-1}^m(x) - (l+m-1)P_{l-2}^m(x) \qquad (3.1)$$

$$P_l^{m+2}(x) + \frac{2(m+1)x}{\sqrt{x^2-1}}P_l^{m+1}(x) = (l-m)(l+m+1)P_l^m(x) \qquad (3.2)$$

$$P_{m+1}^m(x) = x(2m+1)P_m^m(x) \qquad (3.3)$$

Show that equation (3.1) gives a stable recurrence relation for $|x| \leq 1$ and $l >> m$ but equation (3.2) is unstable for all x and large values of m. Comment on the numerical stability of equation (3.3).

[14 marks]

b) A simple expression for $P_m^m(x)$ is

$$P_m^m(x) = (-1)^m(2m-1)!!(1-x^2)^{m/2} \qquad (3.4)$$

where the notation m!! means the product of all positive **odd** integers less than or equal to m. Describe how these equations allow any associated Legendre polynomial $P_l^m(x)$ to be calculated.

[8 marks]

c) If x >1, equations (3.1) - (3.4) can still be used to derive an analytical polynomial in x for $P_l^m(x)$. Describe how this could be done computationally.

[8 marks]

4) a) When an excess of conduction electrons is generated in a semiconductor, the local concentration, n, is described by the equation

$$\frac{\partial n}{\partial t} = -\frac{(n - n_0)}{\tau} + D\frac{\partial^2 n}{\partial x^2} \qquad (4.1)$$

where n_0 is the equilibrium electron concentration, τ is the electron lifetime and D is the diffusion coefficient for electrons. Express equation (4.1) in finite difference form.

[5 marks]

b) Show that the finite difference equations are stable if the timestep Δt and step length Δx are chosen such that

$$\Delta t\left(\frac{1}{\tau} + \frac{4D}{\Delta x^2}\right) \le 2 \qquad (4.2)$$

You may assume that n >> n_0 for all cases of interest.

[15 marks]

c) At time t = 0, an electron concentration of 10^{11} m^{-3} is generated within 0.3 mm of one end of a 10 cm bar of silicon, where the equilibrium carrier concentration is 10^9 m^{-3}. Given that the lifetime of the carriers is 10^{-6} s, and the diffusion coefficient is 10^{-2} m^2s^{-1}, describe how to calculate the concentration of electrons in the bar in the following 5 μs. State any assumptions that need to be made.

[10 marks]

5) a) Two simultaneous equations:

$$f(x, y) = x^4 + 5x^2y^2 - 3xy - 10 = 0 \qquad (5.1)$$

$$g(x, y) = x^4 - 3xy^3 + 2y^2 = 0 \qquad (5.2)$$

have several solutions in the range $-2 < x < 2, -2 < y < 2$. For x = -1, sketch both functions versus y in this range and hence show that one solution is close to the point (-1, -1).

[6 marks]

b) Describe one method to find a more accurate estimate of this solution.

[14 marks]

c) $f(x, y)$ has a global minimum value in the same range of x and y as that given in part a). Describe briefly one method which would be suitable for finding this minimum. Justify your choice of method.

[10 marks]