King’s College London

UNIVERSITY OF LONDON

This paper is part of an examination of the College counting towards the award of a degree. Examinations are governed by the College Regulations under the Authority of the Academic Board.

B.Sc. EXAMINATION

CP/2720 Computational Physics

Summer 2000

Time allowed: **THREE HOURS**

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

You are expected to describe the **methods** of solution, not to work out the answers accurately or write a computer program.

Separate answer books must be used for each section of the paper.

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

SECTION A – Answer SIX parts of this section

1.1) Describe how truncation errors and rounding errors arise.

[7 marks]

1.2) The recurrence relation for Legendre polynomials is:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

Show that this relation is unstable for $|x|>1$ when n is large.

[7 marks]

1.3) Show how the "bubble sort" and the "insertion method" can be used to sort the integers: 3, 4, 1, 5, 2 into ascending order. Which of these methods is the more efficient?

[7 marks]

1.4) Show how to use the Newton-Raphson method to find a root of the equation $f(x) = x^3 - 8 = 0$, using a starting value of 3. Why does this method not work if the starting value is 0?

[7 marks]

1.5) By expanding a function $f(x)$ around its minimum in a Taylor series, show that the error in the calculation of the position of its minimum is proportional to the square root of the computer's precision.

[7 marks]

1.6) Show how to calculate a fast Fourier transform (FFT) of a 3 bit step function $f(t)$=0,0,0,0,1,1,1,1 for t=0,1,2 ... 7.

[7 marks]

1.7) Explain how to generate a set of random numbers which fall into the normal distribution, $p(x)dx = \frac{1}{\sqrt{2\pi\sigma}} e^{-(x-\bar{x})^2/2\sigma^2} dx$ from a uniform distribution of random numbers.

[7 marks]

1.8) Explain how to use the Monte Carlo method to evaluate the integral $\int_V \cos(r\cos\theta)\, r\,dr\,d\theta$ where V is the area inside the circle r =1.

[7 marks]

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SECTION B - answer TWO questions

2) Sketch the function $f(x) = x^5 - 5x^2 + 3$ for the range $-1 < x < 2$. Describe two methods that could be used to find the three real roots of this equation:

$$f(x) = x^5 - 5x^2 + 3 = 0.$$

[12 marks]

In what circumstances do these methods fail?

[3 marks]

Separate the similar complex equation: $z^5 - 5z^2 + 3 = 0$, with $z = x + iy$ (where x and y are real) into two simultaneous equations (the real and imaginary parts of this equation) $F(x,y) = 0$, $G(x,y) = 0$.

[5 marks]

Hence, show how the roots of this complex equation can be determined.

[10 marks]

3) The Bessel functions, $J_n(x)$ (with integer values of n) have the following recursion relation:

$$J_{n+1}(x) = \frac{2n}{x} J_n(x) - J_{n-1}(x)$$

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

[6 marks]

Bessel functions can be determined from the series:

$$J_n(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{s!(n+s)!} \left(\frac{x}{2} \right)^{n+2s}$$

Describe how to evaluate $J_0(x)$ for the range $0 \le x \le 8$.

[10 marks]

Bessel functions can be calculated from the continued fraction:

$$\frac{J_{n+1}}{J_n} = \frac{1}{2(n+1)/x -} \; \frac{1}{2(n+2)/x -} \; \frac{1}{2(n+3)/x -} \cdots$$

Explain how to evaluate $J_1(x)$ for the range $0 \le x \le 8$.

[10 marks]

What is the best way to calculate Bessel functions with $n = 2$ and 3 in the range $4 \le x \le 8$?

[4 marks]

4) A beam of length l is supported at each end and loaded in the middle. The differential equation which determines the deflection downwards, y, at distance x from one end is:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -K$$

where K is a constant. The support of the beam means that $y(0) = y(l) = 0$, but we have no knowledge of the values of $\frac{\mathrm{d}y}{\mathrm{d}x}$ at the ends.

Separate this differential equation into two first order ordinary differential equations.

[4 marks]

Show how the fourth order Runge-Kutta method can be used to find the deflection of the beam as a function of the distance along it, assuming that $\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_{x=0} = a,$ where a is some initial estimate.

[20 marks]

Briefly explain how the "shooting method" can be used to find $y(x)$ for $0 \le x \le l$.

[6 marks]

5) The heat flow in a copper bar is determined by the partial differential equation: $\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$, where T is the temperature, x the distance along the bar and κ is a constant.

Express this equation in finite difference form.

[5 marks]

Show that the finite difference equations are stable if $\frac{2\kappa \Delta t}{(\Delta x)^2} \le 1$.

[The identity $(1-\cos 2\theta)=2\sin^2\theta$ may be helpful.]

[15 marks]

One end of the bar is kept at 0º C. At time t=0, the temperature of the other end is raised to 100º C and maintained at that temperature. Explain how the temperature along the bar can be determined as a function of time.

[10 marks]

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