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 2001

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 the Monte Carlo method can be used to find the value of π.
[7 marks]

1.2) The recurrence relation for Chebyshev polynomials, $T_n(x)$ is:

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad \text{where} \quad n \geq 1$$

Show that this relation is only stable for $0 < |x| < 1$.
[7 marks]

1.3) Use a Taylor series expansion of $f(x+\Delta x)$ to show that a numerical evaluation of $f'(x)$ using $f'(x) = \dfrac{f(x+\Delta x) - f(x)}{\Delta x}$ introduces errors of the order of Δx.
By using the symmetric difference formula $f'(x) = \dfrac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$,
how is the accuracy improved?
[7 marks]

1.4) Suppose that x_1 is an approximate value of the root of an equation $f(x) = 0$.
Show that a more accurate estimate is given by $x_2 = x_1 - \dfrac{f(x_1)}{f'(x_1)}$ (Newton-Raphson method). When does this method fail?
[7 marks]

1.5) An equation for the conservation of a quantity u, in one dimension, can be expressed as:

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}$$

where v is a constant.
Show that for this equation, the finite difference equations in the forward time, centred space (FTCS) scheme are unstable for any choice of Δt and Δx.
[7 marks]

1.6) A continuous waveform $F(t)$ is digitally sampled at intervals of Δ. Show graphically that two waves with frequencies f_1 and (f_1+1/Δ) cannot be distinguished as components of the digitally sampled waveform $F(t)$.
[7 marks]

1.7) Explain, as a series of steps, how you would use the simulated annealing technique to find an estimate of the global minimum of a function of N variables, $F(x_1, x_2, x_3, \ldots x_N)$ with respect to those N variables. (You need not discuss the choice of the "temperature" variable or the step size.)

[7 marks]

1.8) Illustrate the method of Gaussian elimination, by using it to solve the following equations:

$$\begin{aligned} x + \quad y + \quad z &= 2 \\ x - \quad y - \quad z &= 0 \\ 2x + \quad 2y + \quad z &= 5 \end{aligned}$$

Under what circumstances does this method fail or become unreliable?

[7 marks]

SECTION B – Answer TWO questions

Explain how you would solve the problems numerically. A detailed description of the method of solution is required, not a computer program or an actual solution.

2) A circular drumskin is fixed around its circumference. When it is struck in the centre, the vertical displacement $z(r, \theta, t)$ of the drumskin satisfies the (circularly symmetric) wave equation.:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial z}{\partial r}\right) = \frac{1}{u^2}\frac{\partial^2 z}{\partial t^2}$$

Express this equation in finite difference form.

[5 marks]

Show that these finite difference equations are stable if $\frac{u\Delta t}{\Delta x} \leq 1$.

[15 marks]

If the initial displacement of the drumskin is a cone shape, with the maximum displacement at the centre, explain how you would use the finite difference equations to find the subsequent displacement of the centre of the drumskin.

[10 marks]

3) The equation of motion of a simple pendulum, of fixed length l, is

$$\frac{d^2\theta}{dt^2} + \frac{g}{l}\sin\theta = 0,$$

where θ is the angle to the vertical.

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

[4 marks]

The pendulum is released from rest at an angle of θ_0. Show how the fourth order Runge-Kutta method can be used to find the angle of the pendulum as a function of time.

[20 marks]

Describe how you would use the “shooting method” in order to find the value of the angle θ_0 such that the period of the pendulum is exactly 2.25 s.

[6 marks]

4) Sketch the function $\frac{\sin x}{x}$ in the range $-\pi \le x \le \pi$.

[4 marks]

Which value of x might be expected to cause problems in the numerical evaluation of this function? How could these problems be overcome?

[4 marks]

Describe how you would evaluate $\int_{-\pi}^{\pi} \frac{\sin x}{x}\, dx$ using:

a) the trapezium rule,

[6 marks]

b) the expansion of $\frac{\sin x}{x}$ as a series,

[6 marks]

c) a Monte Carlo technique.

[6 marks]

Explain which of a), b) or c) you would expect to be the most accurate and efficient evaluation method?

[4 marks]

[The series for $\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} \cdots$]

5) Explain what is meant by an "unstable recursion relation". [3 marks]

A recursion relation for Legendre polynomials, $P_n(x)$, is:

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

Show that this recursion relation (for large n) is stable for $|x|<1$, but unstable for $|x| >1$.

[10 marks]

Given that $P_0(x) = 1$ and $P_1(x) = x$, derive $P_4(x)$.

[5 marks]

The summation formula for Legendre polynomials is:

$$P_n(x) = 2^{-n} \sum_{m=0}^{[n/2]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} x^{n-2m}$$

where $\binom{n}{m} = \frac{n!}{m!(n-m)!}$ are the binomial coefficients, and $[n/2]$ is the integer produced by rounding $n/2$ down.

Describe how you would use the summation formula to calculate $P_4(x)$ with $x = 10$.

[10 marks]

What are the most reliable and efficient methods for calculating $P_4(x)$ for $x < 1$ and $x >10.0$? Justify your answer.

[2 marks]

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