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

CP2720/Computational Physics

Summer 2002

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

SECTION A – Answer SIX parts of this section

In questions asking for descriptions of methods of solution, you are not expected to work out accurate answers or write a computer program.

1.1) Discuss the significance of "rounding errors" and "truncation errors" in the evaluation of the series $\sum_{n=1}^{\infty} \frac{1}{n^2}$ which has the exact sum of $\pi^2/6$.

[7 marks]

1.2) If the sum of n terms of a convergent series is S_n show, by comparing it to a geometric series, that a good estimate of its infinite sum is

$$S_{n+1} - \frac{(S_{n+1} - S_n)^2}{S_{n+1} - 2S_n + S_{n-1}}.$$

Note that the sum of a geometric series is $\sum_{j=0}^{n} ar^j = a\frac{1-r^{n+1}}{1-r}$.

[7 marks]

1.3) 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.

[7 marks]

1.4) Describe how Simpson's rule could be used to evaluate

$$\int_0^2 x^4 \log\left(x + \sqrt{x^2 + 1}\right) \mathrm{d}x.$$

[7 marks]

1.5) Describe how the Monte Carlo method could be used to evaluate the double integral

$$\int_A \exp(-|x|y^3)\,\mathrm{d}x\mathrm{d}y,$$

where the area A is the area bounded by the lines $y = x^2$ and $y = 1$.

[7 marks]

1.6) Describe the method of bisection by showing how it would be used to find the root of the following equation in the range $0<x<1$:

$$\cosh x = 2\sqrt{x^3} \, .$$

[7 marks]

1.7) By expanding $f(x+\Delta x)$ in a Taylor series, explain why the centred difference approximation for $f'(x)$ is more accurate than the one-sided difference expression.

[7 marks]

1.8) Explain, briefly, one method to find the complex roots of the equation

$$z^3 - z^2 = 1$$

where z is complex.

[7 marks]

SECTION B - answer TWO questions

Descriptions of methods of numerical or computational solution are required, not computer programs or actual numerical answers.

2) A set of N spheres, which may have different radii, are to be packed into a container of square cross-section and arbitrary height. For any arrangement of spheres, one can calculate the total potential energy. The problem is to find the arrangement with the lowest total potential energy.

Select the lateral positions (x_i, y_i) of each sphere randomly and allow it to drop vertically until it touches another sphere or the container, when its height is z_i. A further reduction in energy can be reached (a local minimum) by allowing each sphere to roll laterally, if this reduces z_i, among the other spheres (which are considered to be fixed). Describe how you would design a computational procedure which would calculate such a local minimum of the potential energy.

[12 marks]

Describe the simulated annealing, or a similar, technique which could be used in order to find a global minimum of potential energy by rearranging the positions of the spheres more drastically. Include in your explanation a justification for using this method.

[18 marks]

3) The gamma function is defined as $\Gamma(a) = \int_0^\infty e^{-t} t^{a-1} \mathrm{d}t$.

It has the properties that:

i) for all values of *a* $\Gamma(a+1) = a\Gamma(a)$;

ii) when a is an integer $\Gamma(a) = (a-1)!$

iii) $\Gamma(0.5) = \sqrt{\pi}$.

Discuss how you would evaluate $\Gamma(a)$, for values of a in the range $1 < a \leq 2$.

[10 marks]

The incomplete gamma function, $P(x,a)$, is defined as:

$$P(x,a) = \frac{1}{\Gamma(a)} \int_0^x e^{-t} t^{a-1} \mathrm{d}t \qquad \text{for } a > 0.$$

There is a series expansion, given by:

$$P(x,a) = e^{-x} x^a \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(a+1+n)} ,$$

which is convergent for all $x > 0$ and $a > 0$, but it converges quickly when $x < a+1$.

There is also a continued fraction expansion

$$P(x,a) = \frac{e^{-x} a^x}{\Gamma(a)} \left(\frac{1}{x+} \frac{1-a}{1+} \frac{1}{x+} \frac{2-a}{1+} \frac{2}{x+} \frac{3-a}{1+} \cdots \right),$$

which is also convergent for all $x > 0$ and $a > 0$, but which converges quickly for $x > a+1$.

Explain how you would evaluate $P(x,a)$ in the range $0 < x \leq 4$, in the most economical way from the information given above, for $a = 1.0$ and $a = 2.25$.

[20 marks]

4) The differential equation of the deflection of a beam, $y(x)$, at a distance x from one end, is given by

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

where the function $K(x)$ is determined by the properties of the beam and its loading.

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

[5 marks]

The beam is supported at both ends, $x = 0$ and $x = l$. This means that $y(0) = y(l) = 0$, but the values of $\frac{\mathrm{d}y}{\mathrm{d}x}$ at the ends are unknown. $K(x)$ is known at 100 evenly spaced positions along the beam.

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 by assuming that $\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)_{x=0} = a$, where a is some initial estimate.

[20 marks]

Explain how the shooting method can be used to find the deflection $y(x)$ of the beam for $0 < x < l$.

[5 marks]

5) The time-dependent Schrodinger equation in one space dimension is given by

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = H\psi \qquad (1)$$

for a suitable choice of units. Express equation 1 in finite difference form, using forward time, centred space (FTCS) expressions.

[5 marks]

Show, by using a von Neumann analysis, that this expression is not stable.

[10 marks]

This problem is usually circumvented by using the backward time expression:

$$i\left(\frac{\psi_p^{n+1} - \psi_p^n}{\Delta t}\right) = H\psi_p^{n+1} \qquad (2)$$

where $\psi_p^n \equiv \psi(n\Delta t, p\Delta x) = \psi(x,t)$ and n and p are positive integers.
Show that this is stable for all choices of Δt and Δx.

[5 marks]

The formal solution to equation 1 is $\psi(x,t) = e^{-iHt}\psi(x,0)$. Step forward in time by Δt, to find ψ^{n+1} in terms of ψ^n and H, which may be treated as a constant, to first order in Δt, for both equations 1 and 2.

[5 marks]

Hence, show that even when ψ^n is normalised, neither equation 1 nor 2 gives physically sensible, normalised solutions satisfying

$$\int_{-\infty}^{\infty} \left|\psi^{n+1}\right|^2 \mathrm{d}x = 1.$$

[5 marks]