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 2004

Time allowed: THREE Hours

Candidates should answer no more than SIX questions from SECTION A, and no more than TWO questions from SECTION B.
No credit will be given for answering further questions.

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

Physical Constants

Permittivity of free space	ε_0	=	8.854×10^{-12}	$\mathrm{F\ m^{-1}}$
Permeability of free space	μ_0	=	$4\pi \times 10^{-7}$	$\mathrm{H\ m^{-1}}$
Speed of light in free space	c	=	2.998×10^{8}	$\mathrm{m\ s^{-1}}$
Gravitational constant	G	=	6.673×10^{-11}	$\mathrm{N\ m^{2}\ kg^{-2}}$
Elementary charge	e	=	1.602×10^{-19}	C
Electron rest mass	m_e	=	9.109×10^{-31}	kg
Unified atomic mass unit	m_u	=	1.661×10^{-27}	kg
Proton rest mass	m_p	=	1.673×10^{-27}	kg
Neutron rest mass	m_n	=	1.675×10^{-27}	kg
Planck constant	h	=	6.626×10^{-34}	J s
Boltzmann constant	k_B	=	1.381×10^{-23}	$\mathrm{J\ K^{-1}}$
Stefan-Boltzmann constant	σ	=	5.670×10^{-8}	$\mathrm{W\ m^{2}\ K^{-4}}$
Gas constant	R	=	8.314	$\mathrm{J\ mol^{-1}\ K^{-1}}$
Avogadro constant	N_A	=	6.022×10^{23}	$\mathrm{mol^{-1}}$
Molar volume of ideal gas at STP		=	2.241×10^{-2}	$\mathrm{m^{3}}$
One standard atmosphere	P_0	=	1.013×10^{5}	$\mathrm{N\ m^{-2}}$

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) Distinguish between truncation and rounding errors and describe how they can affect the accuracy of the evaluation of a series.

[7 marks]

1.2) Why would the numerical evaluation of a definite integral normally be expected to be more accurate using Simpson's method rather than the trapezium rule, for the same number of steps? When would both methods fail?

[7 marks]

1.3) Describe how to evaluate $\Gamma(0) = \int_0^\infty e^{-t} t^{-1} \mathrm{d}t$ numerically.

Note that the integrand converges quickly towards a value of zero as t increases.

[7 marks]

1.4) A recurrence relation for Hermite polynomials (with $k \geq 1$)) is:

$$H_{k+1}(x) = 2xH_k(x) - 2kH_{k-1}(x)\,.$$

Show that this relation is unstable for all values of x.

[7 marks]

1.5) A continuous waveform $f(t)$ is stored digitally by sampling at intervals of Δt. Show, graphically or otherwise, how this will lead to aliases in the frequency spectrum, when the frequency is greater than $1/\Delta t$.

[7 marks]

1.6) Define the Newton-Raphson method and explain why when one attempts to find a root of the equation

$$\tan x = x$$

with a starting value of x = 5.0, this method gives a divergent result. Suggest a starting value which would lead this method to converge to the lowest non-zero positive root of the equation.

[7 marks]

1.7) A square matrix **A** can be deconvolved into a lower triangular matrix **L** and an upper triangular matrix **U** such that **A** = **L.U**. Explain the terms "upper triangular" and "lower triangular" matrices, and show how to solve the simultaneous equations **Ax** = **b**, where **b** is a known vector of the same length as the dimension of **A**.

[7 marks]

1.8) In SI units the time-independent Schrödinger equation for the hydrogen atom is $\left(\frac{-\hbar^2}{2m_\mathrm{e}}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}\right)\varphi = E\varphi$, but in atomic units (where $\frac{e^2}{4\pi\varepsilon_0}$, m_e and $\hbar\,(= h/2\pi)$ are defined as equal to one) it is $\left(-\tfrac{1}{2}\nabla^2 - \frac{1}{r}\right)\varphi = E\varphi$.

Explain why the use of atomic units may make numerical solutions more reliable. By noting that each separate term in the two versions of the Schrödinger equation above have the same dimensions, calculate the values of the atomic units of energy and length in SI units.

[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) Sketch the two equations

$$y^2 + 1 = x^2$$

$$(x-1)^2 + (y-1)^2 = 2$$

on the same axes. How many solutions are there? Give a rough estimate of their values.

[10 marks]

These equations can be expressed as a 2-dimensional vector equation **F**(**x**)=0 where $\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}$. Derive an expression for the Jacobian **J**.

[6 marks]

Hence show how to use the multi-dimensional version of the Newton-Raphson method to find the solution(s) more accurately.

[14 marks]

3) Explain how a quadrature method could be used to evaluate the integral

$$\int_D \frac{\exp(-x^2)}{1+y^4}\,\mathrm{d}x\,\mathrm{d}y,$$

where D is the region bounded by $-1 \le x \le 1, \quad 0 \le y \le (1-x^2)$.

[15 marks]

Describe how the same integral could be evaluated using a Monte Carlo method.

[10 marks]

Which method would give the more accurate result? For what class of problems would the other method be more suitable? [5 marks]

4) A block is sliding down a rough ramp which is at an angle α to the horizontal. The block's position, x, is described by

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = g(\sin\alpha - \mu\cos\alpha)$$

where μ is the coefficient of friction, which is proportional to the velocity of the block. Express this equation as two first order equations.

[8 marks]

The block starts from rest. Describe how the fourth-order Runge Kutta method could be used to predict the position of the block as a function of time, if the values of the constants are known.

[14 marks]

If the block has a velocity of 10 ms^{-1}, after 10 seconds, but the coefficient of friction (still proportional to the velocity) is unknown, explain how to adapt the method to find the subsequent position and velocity of the block as a function of time.

[8 marks]

5) The Fick equation, which describes the diffusion of impurities into a solid is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

where the impurity concentration is given by $C(x,t)$ and the diffusion constant is D. Express this equation in finite difference form.

[5 marks]

Use a Von Neumann stability analysis to establish the limits on the choice of the size of the finite elements.

[15 marks]

The impurity concentration is zero throughout the solid at time t = 0, except for a region of width 10 μm where the concentration is C_0. Describe how to solve the Fick equation numerically to show how the impurities diffuse as a function of time.

[10 mark]