THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2020
COMPUTATIONAL PHYSICS

FINAL EXAM

SESSION 1 2007

Answer all questions

Time allowed = 2 hours

Total number of questions = 5

Marks = 40

The questions are NOT of equal value.

This paper may be retained by the candidate.

Candidates may not bring their own calculators.

Calculators will be provided by the Enrolment and Assessment Section.

Answers must be written in ink. Except where they are expressly required, pencils may only be used for drawing, sketching or graphical work.

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**Question 1 (9 marks)**

(a) From geometric considerations, derive an expression for the Newton-Raphson (Newton's) method for finding the roots of a non-linear equation for which you have the explicit form of the equation,
$y = f(x)$,
and an initial approximation to the root of $x_0$.

The expression should clearly show how to find the next approximation to the root, $x_1$, in terms of $f(x)$ and $x_0$. Illustrate you answer with a clear sketch (or sketches) showing how Newton's method works. Mark on your sketch the position of both $x_0$ and $x_1$, and show how they are related.

(b) Briefly state the main differences between the bisection method and Newton's method for finding the roots of an equation in terms of robustness and time taken to converge.

(c) Use the bisection method to find the single root of the equation
$$x^3 - 2x - 2$$
on the interval $1 \le x \le 2$, to a precision of $\pm 0.1$.

**Question 2 (6 marks)**

(a) With the aid of graphs, qualitatively compare the rectangular, trapezoidal and Simpson's approximation techniques for numerically integrating a function. You should state which method would give the most accurate approximation to the interval.

(b) Describe, using a combination of pseudocode and text, how you would write a program to numerically integrate the function
$y = \cos(\theta)$, between $\theta = 0$ and $\theta = \pi$ using Monte Carlo integration.

You must set out all steps logically using pseudocode. You need to explain clearly

- how you will generate random numbers between the appropriate values using the C language,
- how you will ensure that these numbers are as truly random as possible,
- which C function you will use,
- how you will seed it, and
- how your program calculates the answer to the integration.

Illustrate your answer with a diagram.

**Question 3 (12 marks)**

The first order ordinary differential equation

$$\frac{dy}{dx} = f(x, y)$$

can be solved using Euler's method. Given an initial condition ($x_0$, $y_0$), successive points on the solution curve (x, y(x)) can be generated by taking equal steps of size $h$ in the independent variable $x$, and determining the new $y$ value using $y_{i+1} = y_i + hf(x_i, y_i)$. The numerical solution is then a set of points that approximate the solution curve. A second method of solution is the modified Euler method

$$y_{i+1} = y_i + hf\left[x_i + \frac{h}{2}, y_i + \frac{h}{2} f(x_i, y_i)\right]$$

(a) Explain the operation of the Euler method in geometrical terms.

(b) Apply the Euler method to the solution of

$$f(x, y) = x^2 y$$

with the initial condition ($x_0$, $y_0$) = (0,1). Use a step size of 0.5, and calculate the value of y at x = 1. Compare with the exact result at x = 1, y = $e^{\frac{1}{3}}$, where e = 2.7182212.

(c) Use a Taylor series expansion to derive the expressions given above for the Euler and modified Euler methods.

(d) The modified Euler method is part of a general class called Runge-Kutta methods. What order Runge-Kutta method is the modified Euler method, and of what order will be the error term associated with this method.

**Question 4 (7 marks)**

You are programming a new scenario in the game *World of Warcraft*, and you want to make the motion of a thrown object seem as real as possible. The table below shows experimental measurements of the displacement of an odd-shaped object, $y$, at a time $x$. You would like to be able to use these measured values to predict the displacement at times that have not been measured, and so want to fit an approximating polynomial function to the data. Follow the following steps to make the fit.

(a) Complete the following difference table.

| x | y | $\Delta$ | $\Delta^2$ | $\Delta^3$ | $\Delta^4$ |
|---|---|---|---|---|---|
| 1 | 3 | | | | |
| 2 | 12 | | | | |
| 3 | 33 | | | | |
| 4 | 72 | | | | |
| 5 | 135 | | | | |
| 6 | 228 | | | | |
| 7 | 357 | | | | |
| 8 | 528 | | | | |
| 9 | 747 | | | | |
| 10 | 1020 | | | | |

(b) What order polynomial would you consider the most appropriate to fit the above data set? Why?

(c) Use the Gregory Newton equation

$$y = f(x) = f(a) + \frac{1}{h}(x-a)\Delta + \frac{1}{2!}\frac{1}{h^2}(x-a)(x-a-1)\Delta^2 + \frac{1}{3!}\frac{1}{h^3}(x-a)(x-a-1)(x-a-2)\Delta^3 + \ldots$$

to approximate the polynomial of whichever order you think is most appropriate.

(d) Could the above data set have been generated from actual experimental measurements? Discuss why this may or may not be likely. You answer should only be a few sentences in length.

**Question 5 (6 marks)**

When fitting a line of the form

$$y = a + bx$$

to a set of data points, the coefficients $a$ and $b$ can be determined via the technique of least squares.

(a) Briefly describe how the least-squares criteria determine an objective "line of best fit" for a data set. You may assume that we are concerned with the uncertainty in the "y" value only. Illustrate your answer with a hypothetical graph with 5 points scattered around a line-of-best-fit by drawing on this graph the geometric quantity to be minimised.

(b) Assume that for each measurement y in the above problem you have an uncertainty $\sigma$. Describe qualitatively how you would take into account this uncertainty when using the method of least squares to obtain a line-of-best-fit to the data. Explain why this makes the least squares minimisation more robust if a few very noisy measurements (measurements with large uncertainties) are included in the data. Why is it better to include the noisy measurements with weighting rather than just discarding the measurements? Illustrate you answer by drawing a second diagram, this time including error bars.