THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2020
COMPUTATIONAL PHYSICS

FINAL EXAM

SESSION 1 2010

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.

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

Only UNSW approved calculators may be used.

Question 1 (10 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 your 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) Using pseudocode and / or the C programming language, write a program which uses 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 ± 0.1.

d) Use the bisection method to find the root of equation in part (c), on the given interval. The precision required is ± 0.1.

e) Briefly state why using a computer to generate random numbers might not produce the results expected if many trials for an experiment are conducted? Discuss how this problem can be overcome for generating random numbers in the C language. You do not need to use the C keywords, but you must clearly describe the concepts involved.

Question 2 (10 marks)

a) Explain in simple words, what is meant by a Fourier decomposition of a time-varying signal, y(t).

b) What physical quantity will the Fourier transform F, of the spatially varying signal y(x) be a function of? (i.e. what is the other member of the Fourier transform pair involving a quantity varying as a function of space?)

c) In experimental situations, an analytical form of the function y(t) (i.e. a time-varying signal) is unlikely to be known. Instead, we generally have a series of discrete measurements of y at time t, for which we can use a discrete Fourier transform (DFT).

   i. Explain how the data should be spaced in time to use a DFT.

   ii. If there are m discrete measurements of y as a function of t, how many discrete frequencies will be recoverable from the data.

   iii. State the Nyquist frequency in terms of the time sampling interval, Δt, and explain how this limits the frequencies that may be recovered from the data.

d) Why is a fast Fourier transform (FFT) algorithm usually used instead of a DFT? Your answer should give an approximation in both cases of the number of operations required to transform N data points for both algorithms. What extra constraint do the most common FFT algorithms place on the number of measured data points, N. Is this a hard constraint on the actual number of measurements that needs to be made? Explain why or why not.

e) A general sinusoidal wave has an equation of the form $y(x,t) = A\cos[kx - \omega t + \phi_0]$ where y is the displacement of the medium at time t and position x, A is the amplitude of the wave, k is the wavenumber, ω is the angular frequency and ϕ_0 is the initial phase angle. Starting with this equation, derive a form of the wave equation which is independent of k and ω, but which does depend on the wave speed in the medium.

Question 3 (8 marks)

The first order ordinary differential equation (ODE)

$$\frac{dy}{dx} = 2xy$$

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 simple and modified Euler methods in geometrical terms.

b) Use the simple Euler method to solve the ODE $y' = 2xy$, given that f(0)=1, on the interval $0 \leq x \leq 2$ for a step size of 0.5.

Question 4 (8 marks)

The table below shows experimental measurements of displacement, y, at a time x. Fit an approximating polynomial function to the data by following the steps below to make the fit.

a) Complete the following difference table. Make sure you complete the table in your book, not on this exam paper!

x	y	Δ	Δ^2	Δ^3	Δ^4
0	1				
1	0				
2	3				
3	16				
4	45				
5	96				
6	175				

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

c) Use the Gregory Newton equation

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

to approximate the polynomial of whichever order you think is most appropriate. Is the polynomial an exact fit to the measured data? (Hint: use the first and last x values to see if you can reproduce the exact y value.)

Question 5 (4 marks)

When fitting a line of the form

$$y = ax + b$$

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) The coefficients a and b are given by

$$a = \frac{\sum_{i=1}^{n} x(i) \sum_{i=1}^{n} y(i) - N \sum_{i=1}^{n} (x(i)y(i))}{\left[\sum_{i=1}^{n} x(i)\right]^2 - N\left[\sum_{i=1}^{n} (x(i))^2\right]}$$

$$b = \frac{\sum_{i=1}^{n} x(i) \sum_{i=1}^{n} (x(i)y(i)) - \sum_{i=1}^{n} (x(i))^2 \sum_{i=1}^{n} y(i)}{\left[\sum_{i=1}^{n} x(i)\right]^2 - N\left[\sum_{i=1}^{n} (x(i))^2\right]}$$

Find the equation for the line of best fit for the following data set.

X	Y
-2	-7
-1	-8
0	-2
1	1
2	5

QUESTION CONTINUES ON FOLLOWING PAGE

c) The correlation coefficient is given by

$$r^2 = \frac{a^2\left(\sum_{i=1}^{n}\left(x(i)-\overline{x}\right)^2\right)}{\sum_{i=1}^{n}\left(y(i)-\overline{y}\right)^2}.$$

Calculate the correlation coefficient for the above data. Is the least squares line a good fit to the above data. Give a valid reason for your answer.