THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2120 PAPER 2
PHYS2020 PAPER 1
COMPUTATIONAL PHYSICS

FINAL EXAM

SESSION 1 2012

Answer all questions

Time allowed = 2 hours

Total number of questions = 7

Marks = 75

This paper forms **20%** of the total assessment for **PHYS2120**
This paper forms **40%** of the total assessment for **PHYS2020**

The questions are NOT of equal value.

This paper may be retained by the candidate.

Students must supply their own UNSW approved calculator.

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

Question 1 (10 marks)

(a) What are rounding or round-off errors in the context of a computer program?

(b) What is one simple thing you can do in C to minimize round-off errors? Explain why this measure would not have been such a good idea 20 years ago and what has changed to make it a good idea?

(c) What types of numerical problems are inherently sensitive to round-off errors?

(d) Integer calculations in C are generally exact (as in that the result is what you expect, within the uncertainties). Describe briefly two situations in which integer calculations can go wrong, giving an incorrect result.

(e) Define typecasting and explain how it is useful for getting the correct result for an with integer division operation. Give an example of how you would i) declare variables to divide integer a by integer b giving a non-integer answer c, and ii) give an example of the line of c code you would write for this operation.

(f) If you discover that the result to a calculation from your C program is NaN, what does this signify, and how may it have arisen? What happens to subsequent calculations that include the NaN value?

Question 2 (12 marks)

(a) Describe briefly the principles behind Monte-Carlo integration

(b) Explain how you would generate random numbers in C, including the methods you would use to seed these random numbers. You do not need to write any code.

(c) Explain briefly the main problem associated with generating random numbers using a computer.

(d) Write a brief pseudocode or flow chart algorithm for finding the integral,

$$y = \int_0^{\frac{\pi}{2}} \sin(x)\, dx$$

(e) Assume that you generate just one pair of random numbers to evaluate the integral from part (d). There are a small number of answers that your program may output for the result. Give these values.

Question 3 (20 marks)

The first order ordinary differential equation (ODE)

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

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 $y_{i+1} = y_i + h(f(x_i, y_i))$. The numerical solution is then a set of points that approximate the solution curve.

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

(b) Derive an expression for the simple Euler method using a Taylor series expansion.

(c)

I. Use your result from (b) to derive an expression for the error associated with the simple Euler method.
II. What name is give to this error?
III. Is this error related to the use of a computer in solving an ODE using the simple Euler method?
IV. There is a second type of error that affects numerical integration schemes for ODEs when implemented in a computer program. What is this error generally called, and what is its origin?

(d) Use the simple Euler method to derive an expression for the ith +1 value, knowing the ith value, and the value of the derivative at an initial point (x_i,y_i).

$$y' = -\alpha y$$

(e) Assuming that when x is 0, y=1, find the value of this ODE when x = 4, for a value of α=2. Use steps h of 0.5.

(f) Give the analytical solution to the ODE from part (d), and sketch the function from x = 0 to x = 4.

(g) Using your knowledge of the properties of the equation you found in (f), and your simple Euler method solution from (d), work out the maximum step size, h, that can be used with the simple Euler method, to the introduction of a numerical instability into the solution.

Question 4 (8 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 $f(x_0)$ 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) Write either pseudocode or a flowchart to design an algorithm for finding the single root of the equation $y = x^2 + 2x - 1$ on the interval -1 to 1, to a precision of ± 0.1.

(d) Use the bisection method to find the value of the single root of the equation from part (c) on the interval -1 to 1, to a precision of ± 0.1.

Question 5 (5 marks)

The table below shows experimental measurements 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
1	4				
2	14				
3	36				
4	76				
5	140				
6	234				
7	364				
8	536				
9	756				
10	1030				

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

(c) Use the Gregory Newton equation

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

to approximate the polynomial of whichever order you think is most appropriate. Is the polynomial an exact fit to the measured data?

Question 6 (10 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) To find the best values for the coefficients a and b for a set using a least squares fitting technique, we wish to minimize the error for all points between the measured value of each (x,y) pair, and the value of y predicted for the measured x using the relationship above.

I. Write down an expression that minimizes the error, E, withn respect to the sum of the squares of the differences between the measured and predicted values of y for each x.

II. Explain how mathematically you can use this equation to find the minimum value of E with respect to both a and b, and use the equation you wrote down in (I) to find expressions for the minimum value of both a and b (you will need two separate equations.

(b) If the coefficients a and b are given by

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

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

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

x	y
-1	-2
0	-1
1	0
2	1
3	2

(c) The correlation coefficient is given by

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

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

Question 7 (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) Sketch the both the function and its Fourier transform for the following cases:

I. A top hat function
II. A delta function
III. A Gaussian function

d) 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). Explain how the data should be spaced in time to use a DFT, and be explicit about in what way or ways the DFT varies from a continuous transform that makes this spacing necessary.

e) 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.