THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2020
COMPUTATIONAL PHYSICS

FINAL EXAM

SESSION 1 2011

Answer all questions

Time allowed = 2 hours

Total number of questions = 6

Marks = 50

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 (8 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?

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

(d) What are underflow and overflow errors?

(e) 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?

(f) Rounding errors are part of a general class of errors known as quantization errors. Another type of quantization error can occur when using Euler's method to solve a differential equation. Consider for example using Euler's method to solve a differential equation which involves radioactive decay with time, explain how the order of the error at each step varies with Δt (the time step of the measurements) and how this error can be minimized using the simple Euler method. What order will the error have after N steps are calculated?

(g) Does the quantization error in part (f) explain why the simple Euler method is a poor choice for solving problems involving periodic motion? Give the reasoning behind you answer.

Question 2 (14 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 $y_{i+1} = y_i + h(f(x_i, y_i))$. The numerical solution is then a set of points that approximate the solution curve.

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

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

(c) A simple pendulum has equation of motion

$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}\theta$$

where θ is the angular displacement of the pendulum with time, t, from the equilibrium position,
g is the acceleration due to gravity, and
l is the length of the string.

You wish to use the simple Euler method to solve this differential equation. To do this, you will need to replace the 2nd order differential equation by two first order differential equations that can be solved using Euler's method. Write down two suitable equations that can be solved in conjunction using simple Euler method, to find θ as a function of t. [Hint: You will need to use ω in both equations, where ω is the angular velocity.

(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).

(e) Considering the motion of a simple pendulum, show that the simple Euler method does not conserve energy. [Hint: use the expressions from part (d) to look at the energy at time t, and at time t+ΔT.] Explain why this renders the simple Euler method unsuitable for use in solving this particular problem.

$$E = \frac{1}{2}ml^2(\omega^2 + \frac{g}{l}\theta^2)$$

Question 3 (6 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) Use the bisection method to find the single root of the equation

$$2x^3 - 4x^2 - 3$$

on the interval $1 \le x \le 3$, to a precision of ± 0.2.

Question 4 (4 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
0	2				
1	1				
2	4				
3	17				
4	46				
5	97				
6	176				

(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. 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 (8 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(i) in the above problem you have an uncertainty σ(i). 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.

(c) 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
-9	-2
-7	-1
-5	0
0	1
2	2

(d) 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 6 (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.