THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

PHYS2020
COMPUTATIONAL PHYSICS

SAMPLE FINAL EXAM

SESSION 1 2009

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.

Question 1 (7 marks)

Describe, using a combination of pseudocode and text, how you would write a program to numerically integrate the function

y = cosθ, between θ = 0 and π/2 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.

You do not need to use the exact C syntax, just explain the concepts, but you may find the terms random(), srandom() and RAND_MAX helpful.

Question 2 (9 marks)

The first order ordinary differential equation

$$\frac{dy}{dx} = e^{\frac{x^2}{2}}$$

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

$$y_{i+1} = y_i + (f(x_i, y_i))(h)$$

The numerical solution is then a set of points that approximate the solution curve. A second method of solution is the modified Euler method

$$y_{n+1} = y_n + h[f(x_{n+1/2}, y_n + \frac{h}{2} f(x_n, y_n)] + E(h^3)$$

(a) Explain the operation of these two schemes in geometrical terms, and comment on their relative accuracies.

(b) Apply both the Euler and modified Euler methods to the solution of the above differential equation

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, $y = e^{\frac{(1)^2}{2}}$, where e = 2.7182212. $y = e^{\frac{(1)^2}{2}}$

Question 3 (7 marks)

(a) With the aid of graphs, qualitatively compare the midpoint, trapezoidal and Simpson's approximation techniques for numerically integrating a function, discussing the order of the approximating function used in each case. You should state which method would give the most accurate approximation to the interval.

(b) You wish to integrate the function $y = x^2$ over the interval 0 to 3. Use the rectangular and trapezoidal techniques to evaluate the integral, using 3 "strips" of width 1 in each case. Compare your answer for both methods to analytical evaluation of the integral. Which method is more accurate in this case? Is this what you expect? Explain your answer.

Question 4 (7 marks)

(a) Use pseudocode to write a program which uses the bisection method to find the single root of the equation

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

   a. on the interval $1 \le x \le 2$, to a precision of ±0.1. You should use comments in your program to explain what each section of the code does.

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

Question 5 (10 marks)

When fitting a line of the form

$$y = a + bx$$

$$y = a_0 + a_1 x$$

to a set of data points, the coefficients a_0 and a_1 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) Determine the actual least-squares best-fit straight line to the data points by minimising the error in the coefficients a_0 and a_1. Hence find the matrix equation for the coefficients as functions of the data points.

(c) 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.

Question 5

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					
	2				
2					
	0				
3					
	6				
4					
	56				
5					
	210				
6					
	552				
7					
	1190				
8					
	2256				
9					
	3906				
10					
	6320				

(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.)