P5

THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

EXAMINATION – JUNE/JULY 2001

PHYS2020

Computational Physics

Time Allowed – 2 hours

Total Number of Questions – 5

Answer all Questions

All questions are of equal value

This paper may be retained by the candidate

Candidates may not bring their own calculators

The following materials will be provided by the

Enrolment and Assesment Section: Calculators

All answers must be written in ink. Except where they

are expressly required, pencils may be used

only for drawing, sketching or graphical work.

QUESTION 1. (20 marks)

a) The following piece of fortran code has been written to find the roots of a function using the bisection method.

```
      f(x) = x**4 - 4*x**3 + 4.75*x**2 - 1.5*x
      eps = 1.e-5
      READ(*,*) a,b
c
      DO i = 1, 20
      xm = 0.5*(a+b)
      WRITE(*,*) a, xm, b
c
      IF (ABS(f(xm)) < eps) THEN
       WRITE(*,*) 'Root is ',xm,i
       PAUSE
       STOP
      ENDIF
c
      IF (f(a)*f(xm) < 0.0) THEN
       b = xm
      ELSE
       a = xm
      ENDIF
      ENDDO
c
      WRITE(*,*) i,' End of loop'
c
      PAUSE
      END
```

The function $f(x) = x^4 - 4x^3 + \frac{19}{4}x^2 - \frac{3}{2}x = x\left(x - \frac{1}{2}\right)\left(x - \frac{3}{2}\right)(x-2)$

has roots at $x = 0, \frac{1}{2}, \frac{3}{2}$ and 2. If for input we choose $a = 0$ and $b = 2$, determine the output from the program, and hence determine which root the bisection scheme converges to.

b) The forward-difference operators are defined by

$$\Delta f(x) = f(x+h) - f(x)$$
$$\Delta^2 f(x) = \Delta f(x+h) - \Delta f(x)$$
$$\Delta^3 f(x) = \Delta^2 f(x+h) - \Delta^2 f(x)$$

Calculate all forward-differences for the following set of function values:

x_i	$f(x_i)$	Δf	$\Delta^2 f$	$\Delta^3 f$
0	0			
1	1			
2	6			
3	16			

Newton's fundamental formula for the interpolating polynomial is

$$f(x_0 + \alpha h) = f(x_0) + \alpha \Delta f(x_0) + \frac{\alpha(\alpha-1)}{2!}\Delta^2 f(x_0) + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}\Delta^3 f(x_0) + \ldots$$

Find the third order polynomial approximation to the function using the values in the table above.

QUESTION 2. (20 marks)

a) Using Newton's forward formula, the linear polynomial approximation to a function $f(x)$ is given by

$$f(x) = f(x_0) + \alpha \Delta f(x_0) + R_1(x)$$

where $x = x_0 + \alpha h$, $h = x_1 - x_0$, the forward difference $\Delta f(x_0) = f(x_1) - f(x_0)$, and the error term is

$$R_1(x) = h^2 \frac{\alpha(\alpha - 1)}{2!} f''(\xi) \qquad \text{where} \qquad x_0 \le \xi \le x_1$$

Using the linear polynomial approximation for $f(x)$ given above, show that the single strip trapezoidal approximation to the integral $I(p_1)$, is given by

$$I(p_1) = \int_{x_0}^{x_1} f(x)\, dx = \frac{h}{2}\big(f(x_0) + f(x_1)\big) - \frac{h^3}{12} f''(\xi)$$

b) Calculate the one strip trapezoidal rule estimate for the integral

$$I = \int_0^1 dx \tan\left(\frac{\pi x}{4}\right)$$

c) Derive the n strip trapezoidal approximation error term.

d) How many strips are required to calculate this integral to an accuracy of ± 0.0001?

Note that, $\quad \dfrac{d^2}{dt^2} \tan\left(\dfrac{\pi x}{4}\right) = \left(\dfrac{\pi}{4}\right)^2 \dfrac{2 \sin x}{\cos^3 x}.$

QUESTION 3. (20 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 improved Euler method

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

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

b) Apply both the Euler and improved Euler methods to the solution of $f(x,y) = nx^{n-1}y$ with the initial condition $(x_0, y_0) = (0,1)$. Use a step size of $h = 1.0$, and calculate the value of y at $x = 1$. Compare with the exact result at $x = 1$, $y = e$, where $e = 2.718212$. What is special about the value $n = 1$?

c) Is the modified Euler scheme,

$$y_{i+1} = y_i + hf(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}hf(x_i, y_i))$$

a better method for this function?

QUESTION 4. (20 marks)

a) A given set of data points $\{x_i, y_i\}$ obtained from an experiment are believed to obey a quadratic law, $y = a_0 + a_1 x + a_2 x^2$. The equation for a parabola has three coefficients a_0, a_1, and a_2. If we define the total error $E(a_0, a_1, a_2)$, as

$$E(a_0, a_1, a_2) = \sum_{i=1}^{n} \left\{a_0 + a_1 x_i + a_2 x_i^2 - y_i\right\}^2,$$

determine the least squares best fit parabola by minimising the total error with respect to variations in the coefficients a_0, a_1, and a_2. Hence find the matrix equation for the coefficients as functions of the data points.

b) To construct Newton-Cotes open integration formulas that use equally spaced base points we consider Newton's fundamental formula based on x_1, rather than x_0. That is

$$f(x_1 + \alpha h) = f(x_1) + \alpha \Delta f(x_1) + \frac{\alpha(\alpha-1)}{2!}\Delta^2 f(x_1) + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}\Delta^3 f(x_1) + \ldots$$

Show how the first two open formulas are obtained by integrating this function. That is, derive

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1)$$

and

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{2}\left(f(x_1) + f(x_2)\right)$$

QUESTION 5. (20 marks)

For Gaussian integration on the interval [-1,1] we can use the polynomials

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = x^2 - \tfrac{1}{3}, \quad p_3(x) = x^3 - \tfrac{3}{5}x.$$

The polynomial $p_j(x)$ can be shown to have exactly j distinct roots in the interval. Moreover, the roots of $p_j(x)$ are interleaved with the roots of $p_{j+1}(x)$.

a) Explain why Gaussian integration with two basis points is more accurate than any of the usual Newton-Cotes methods with two basis points.

b) Construct a numerical scheme to find all the roots of the polynomials for $j = 1$ to 10. Discuss any standard methods you use and justify the particular choice of method.

DO NOT write any FORTRAN CODE for this question.