P.S.

THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF PHYSICS

FINAL EXAMINATION

JUNE/JULY 2002

PHYS2020

Computational Physics

Time Allowed – 2 hours

Total number of questions - 4

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

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. (25 marks)

a) A set of data points obtained from a projectile experiment consists of a list of vertical heights at particular times, that is $\{t_i, y_i\}$. The data is believed to show that y is a quadratic function of t, $y = a_0 + a_1 t + a_2 t^2$. If we define the error between the data, and the quadratic fit to the data, to be

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

then derive a set of equations for the coefficients a_0, a_1, and a_2, that minimise the total error $E(a_0, a_1, a_3)$. Hence write down the matrix equation for the coefficients of the least squares best fit to the data.

b) For the root finding problem $f(x) = x^3 - 13x + 18$, write down three different functional forms for the $g(x)$ for the fixed point problem $s = g(s)$, that are equivalent. Why is the transformation from root finding to fixed point problem not unique?

c) Find the first four terms in the Taylor series for $f(x) = \cos x$. The definition of the Taylor series is

$$f(x) = f(x_0) + (x - x_0) f'(x_0) + \cdots + (x - x_0)^n \frac{f^{(n)}(x_0)}{n!} + R(x)$$

where

$$R(x) = (x - x_0)^{n+1} \frac{f^{(n+1)}(\xi)}{(n+1)!} \quad \text{with} \quad x_0 \le \xi \le x .$$

d) Using the Taylor series for $\cos(x)$ with $x_0 = 0$, find an estimate for $\cos\left(\frac{\pi}{2}\right)$ and the associated error estimate.

QUESTION 2. (25 marks)

The divided differences are defined by

0 $$f[x_0] = f(x_0)$$

1 $$f[x_1, x_0] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$$

2 $$f[x_2, x_1, x_0] = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0}$$

3 $$f[x_3, x_2, x_1, x_0] = \frac{f[x_3, x_2, x_1] - f[x_2, x_1, x_0]}{x_3 - x_0}$$

and Newton's fundamental formula for divided differences is

$$\begin{aligned} p_n(x) &= f[x_0] + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0] \\ &+ (x - x_0)(x - x_1)(x - x_2) f[x_3, x_2, x_1, x_0] + \ldots \end{aligned}$$

and these can be used to generate polynomial approximations.

a) If the x_i are equally spaced, so that $x_i = x_0 + ih$, determine the relation between each of the divided differences and the forward difference of the same order, where the forward differences are defined by

$$\begin{aligned} \Delta^0 f(x_0) &= f(x_0) \\ \Delta^1 f(x_0) &= \Delta^0 f(x_0 + h) - \Delta^0 f(x_0) \\ \Delta^2 f(x_0) &= \Delta^1 f(x_0 + h) - \Delta^1 f(x_0) \\ \Delta^3 f(x_0) &= \Delta^2 f(x_0 + h) - \Delta^2 f(x_0) \end{aligned}$$

b) Hence show that the third order polynomial approximation from Newton's fundamental formula for divided differences $p_3(x)$ gives the first four terms of Newton's formula for forward differences

$$f(x_0 + \alpha h) = \Delta^0 f(x_0) + \alpha \Delta^1 f(x_0) + \frac{\alpha(\alpha - 1)}{2!} \Delta^2 f(x_0) + \frac{\alpha(\alpha - 1)(\alpha - 2)}{3!} \Delta^3 f(x_0) + \ldots$$

where $x = x_0 + \alpha h$.

QUESTION 2. (continued)

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

x_i	$f(x_i)$	$\Delta^1 f$	$\Delta^2 f$	$\Delta^3 f$
0	0			
1	2			
2	6			
3	13			

d) Newton's fundamental formula for the interpolating polynomial is

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

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

QUESTION 3. (25 marks)

Newton's forward formula for 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 $\Delta f(x_0) = f(x_1) - f(x_0)$. The error term is

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

a) Using the linear polynomial approximation for $f(x)$ given above, show that the single strip trapezoidal approximation to the integral and the error term, is given by

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

b) Calculate the one strip trapezoidal rule estimate, with error bars, for the integral

$$I = \int_0^{\pi/2} dx \sin(x)$$

c) Derive the error term for an n strip trapezoidal rule integration. How many strips are required to ensure that the error for the integral in b) is less than 10^{-2}?

d) Richardson extrapolation using n and $2n$ strips is given by

$$I^* = \frac{1}{3}\left(4I_{2n} - I_n\right).$$

Calculate the value of the integral in b) using this method and $n = 1$.

e) Describe the relation between Richardson's extrapolation of the trapezoidal rule and Simpson's rule.

QUESTION 4. (25 marks)

a) The first order ordinary differential equation

$$\frac{dy}{dx} = f(x,y) \tag{1}$$

can be solved using a 2nd order Runge-Kutta method. This involves evaluating the derivative at two places per step of size h. The second order method can be written as

$$y_{i+1} = y_i + h\{A_1 f(x_i, y_i) + A_2 f(x_i + \beta h, y_i + \alpha h f(x_i, y_i))\} \tag{2}$$

where A_1, A_2, α and β are constants, yet to be determined.

The Taylor expansion of the function y about $x = x_i$ is

$$y_{i+1} = y_i + h\left.\frac{dy}{dx}\right|_{x=x_i} + \frac{1}{2!}h^2\left.\frac{d^2y}{dx^2}\right|_{x=x_i} + \ldots \tag{3}$$

Using equation (1) above, and the fact that

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_i} = \left.\frac{d}{dx}f(x,y)\right|_{x=x_i} = f_x(x_i, y_i) + f_y(x_i, y_i)\left.\frac{dy}{dx}\right|_{x=x_i} \tag{4}$$

show that, for equations (2) and (3) to give the same value for y_{i+1}, then

$$A_1 + A_2 = 1, \qquad A_2\beta = \tfrac{1}{2}, \qquad A_2\alpha = \tfrac{1}{2}.$$

Hence show that the general 2nd order Runge-Kutta method is

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

b) Explain the operation of the Euler method and the Runge Kutta methods in geometrical terms, and comment on their relative accuracies.

c) Apply the 2nd order Runge-Kutta method with $\alpha = \frac{1}{2}$ to the solution of $f(x,y) = xy$ with the initial condition $y(0) = 1$. Make one step using $h = 1$.