UNIVESITY OF ESWATINI FACULTY OF SCIENCE AND ENGINEERING DEPARTMENT OF PHYSICS

Examination 2019/2020

COURSE NAME: ADVANCED COMPUTATIONAL PHYSICS

COURSE CODE: PHY601 TIME ALLOWED: 3 hours

Answer All Questions in Section A. Choose two (2) Questions in section B.

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Section A

Question 1

(a) Match up the following three numerical differentiation schemes, approximating the solution to the ordinary differential equation x'(t) = F(x(t)), with their correct name (Runge-Kutta, Euler or Picard).

A.
$$X_{n+1} = x_n + F(x_n) \triangle t$$

B.
$$X_{n+1} = x_n + \frac{1}{2} [F(x_n) + F(x_{n+1})] \triangle t$$

C.
$$X_{n+1} = x_n + F\left(x_n + \frac{1}{2}F(x_n) \triangle t\right) \triangle t$$

[6 marks]

(b) Consider the finite difference approximation

$$f'(a) = \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h} + O(h^p).$$

What is the value of p?

[2 marks]

(c) Derive the fourth-order Runge–Kutta algorithm for solving the differential equation

$$\frac{dy}{dt} = g(y, t)$$

with a given initial condition. Discuss the options in the selection of the parameters involved.

[5 marks]

Question 2

- (a) The simple program in figure 1 is written to read in the radius and calculate the area of the corresponding circle and volume of the sphere.
 - (i) Modify this program such that it stops with a warning if the radius given is negative.

[5 marks]

```
! ******************************
program Cirle
! *******************************
implicit none
real*8 PI,r,A,V

PI=4.0d0*atan(1.0d0)
write(*,*) 'please enter the value of thr radius,r'
read(*,*) r

A=PI*r**2
V=4*PI*r**3
write(*,*) 'The area is,', A
write(*,*) 'The Volume is,', V
end
```

Figure 1: A program for calculating the area and volume, given the radius.

(ii) Modify the program such that it computes a complex value of the volume and area, given a complex value of the radius.

[10 marks]

(b) Which of the following statements in figure 2 are incorrect declarations and why? (If you think a declaration may be correct in a given situation then say what the situation would be.)

[22 marks]

```
(c) Given
   INTEGER::i=3, j=7
   REAL, DIMENSION(1:20) ::A
   Which of the following are valid array references for the array
   - A(12)
   - A(21)
   - A(1)
   - A(3.0)
   - A(1*J)
   - A(1*INT(4.0*ATAN(1.0)))
```

[10 marks]

```
1.ReAl :: X
2.CHARACTER :: name
3.CHARACTER(LEN=10) :: name
4.REAL :: var-1
5.INTEGER :: 1a
6.CHARACTER(LEN=5) :: town = "Glasgow"
7.CHARACTER(LEN=*) :: town = "Glasgow"
8.CHARACTER(LEN=*), PARAMETER :: city = "Glasgow"
9.REAL :: pi = +22/7
10.LOGICAL :: wibble = .TRUE.
11.CHARACTER(LEN=*), PARAMETER :: "Bognor"
12.REAL, PARAMETER :: pye = 22.0/7.0
13.REAL :: two_pie = pye*2
14.REAL :: a = 1., b = 2
15.LOGICAL(LEN=12) :: frisnet
16.CHARACTER(LEN=6) :: you_know = 'y'know"
17.CHARACTER(LEN=6) :: you_know = "y'know"
18.INTEGER :: ia ib ic id in free format source form
19.DOUBLE PRECISION :: pattie = +1.000
20.DOUBLE PRECISION :: pattie = -1.0E-0
21.LOGICAL, DIMENSION(2) bool
22.REAL :: poie = 4.*atan(1.)
```

Figure 2:

Section B

1. Consider the Poisson equation

$$\nabla^2 \phi(x,y) = -\frac{\rho(x,y)}{\epsilon_0}$$

from electrostatics on a rectangular geometry with $x \in [o, L_x]$ and $x \in [o, L_y]$. Write a program that solves this equation using the relaxation method. Test you program with

(a)
$$\rho(x,y) = 0$$
, $\phi(0,y) = \phi(L_x,y) = \phi(x,0) = 0$, $\phi(x,L_y) = 1V$, $L_x = 1m$ and $L_y = 1.5m$

(b)
$$\frac{\rho(x,y)}{L_x = L_y = 1m} = 1V/m^2$$
, $\phi(0,y) = \phi(L_x,y) = \phi(x,0) = \phi(x,L_y) = 0$,

[20 marks]

2. A point mass that can move along a straight line is attached to an end of an ideal elastic spring. (The other end of the spring is fixed.) A

viscous friction force proportional to the cube of the velocity is acting on the mass. Therefore, the motion of the particle is described by the following differential equation;

$$\ddot{x} + \mu \dot{x}^3 + x = 0,$$

where μ is a positive dimensionless coefficient of nonlinear friction. (The equation is written in dimensionless units). Write a program that solves this equation numerically for the following conditions;

$$-\mu = 0.2$$
, $x(0) = 1$, $\dot{x}(0) = 0$, plot $x(t)$ and $\dot{x}(t)$ for $0 < t < 50$.

[20 marks]

3. The temperature distribution u(x,t) in a thin rod satisfies the equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}$$

together with the boundary conditions

$$u(0,t) = u(1,t) = 0$$

at the ends x = 0, 1. The initial temperature distribution of t = 0 is given by the function

$$u(x,0) = \begin{cases} 0.5, & \text{if } x \in [x_1, x_2] \\ 0.3, & \text{if } x \notin [x_1, x_2], \end{cases}$$

where $x_1 = 0.25$ and $x_2 = 0.75$. Write a program that calculates the temperatire distribution $u(x, t_f)$ for $t_f = 0.0001, 0.001, 0.01, 0.05$. Take $N_x = 100$ and $N_t = 1000$. Do the same for $t_f = 0.1$ by choosing the appropriate N_x and keeping $N_t = 1000$. Plot the functions $u(x, t_f)$ in the same plot.

[20 marks]