UNIVERSITY OF SWAZILAND

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION 2007_2008

TITLE OF THE PAPER: COMPUTATIONAL PHYSICS-II

COURSE NUMBER : P482

TIME ALLOWED : *SECTION A: ONE HOUR.*
SECTION B: TWO HOURS.

INSTRUCTIONS:

THERE ARE TWO SECTIONS IN THIS PAPER:

SECTION A **: THIS IS A WRITTEN PART ON YOUR ANSWER BOOK. CARRIES A TOTAL OF 30 MARKS.**

SECTION B**: THIS IS A PRACTICAL PART WHICH YOU WILL WORK ON A PC AND SUBMIT THE PRINTED OUTPUT. CARRIES A TOTAL OF 70 MARKS.**

ANSWER **ANY TWO** QUESTIONS FROM **SECTION A** AND **ALL** THE QUESTIONS FROM **SECTION B.**

MARKS FOR EACH QUESTION ARE SHOWN IN THE RIGHT-HAND MARGIN.

USE THE INFORMATION GIVEN IN THE ATTACHED APPENDIX WHEN NECESSARY.

THIS PAPER HAS SIX PAGES, INCLUDING THIS PAGE.

DO NOT OPEN THE PAPER UNTIL THE INVIGILATOR HAS GIVEN PERMISSION.

SECTION A
(Written Section)

Q.1. Van der Waal's equation for an imperfect gas is given by

$$(P + \frac{a}{V^2})\,(V - b) = RT$$

where R=8.3149 J kg^{-1} $mole^{-1}$ K^{-1} . The constants a and b are related to critical pressure P_c and T_c and are given by the relation

$$a = \frac{27R^2\,T_c^2}{64\,P_c} \quad , \quad b = \frac{R\,T_c}{8\,P_c}$$

For CO_2 , T_c=304.26 K and P_c = 7.40 x 10^6 Pa.

(i) Write Maple commands to calculate V at temperature 304.26 K and pressures 5.0 x 10^6 Pa to 50 x 10^6 Pa with an increment of 1.0 x 10^6 Pa. [6]

(ii) Write a procedure to calculate V at any given temperature T, with critical temperature T_c and critical pressure P_c for any imperfect gas for given initial pressure P_i , final pressure P_f with a given increment dP [9]

Q.2. Under the Block-Gruneissen approximation for the resistance in a mono-valent metal, integrals of the following form need to be calculated;

$$\text{BGintegral} = \int_0^t \frac{x^5}{(e^x - 1)(1 - e^{-x})}\,dx$$

To avoid the singularity at x=0, assume lower limit of integration to be 0.001.

(i) Write a program to calculate the integral using Simpson's Rule for t=2 convergent to a precision of 0.001. This can be checked by initial estimation for some N steps and then with N+2 steps. If the difference between two estimates of the integral is small (in this case less than 0.001) then the integral is convergent. [15]
You may begin with N > 10.

Note: Use the algorithm given in the Appendix.

Q.3. Two dimensional trajectory of a projectile of mass m, in the presence of air resistance is given by the following equations:

$$m\frac{dv_x}{dt} = -f_d\cos(\vartheta) \quad , \quad m\frac{dv_y}{dt} = -mg - f_d\sin(\vartheta)$$

with

$$\frac{dx}{dt} = v_x \quad , \quad \frac{dy}{dt} = v_y$$

Here ϑ = the angle at which the projectile is directed above the horizontal.
v_x= horizontal component of velocity of the projectile.
v_y= vertical component of velocity of the projectile.

f_d =force due to air resistance= $k\,v^2$.
where k= co-efficient of air resistance and $v^2=v_x^2+v_y^2$.
g=acceleration due to gravity=9.8 .

Using the Euler method of solving first order differential equations, we can write the four equations as

$$x(i+1) = x(i) + v_x(i)\,\Delta t$$
$$v_x(i+1) = v_x(i) - \Delta t\, k(v_x(i)^2 + v_y(i)^2)\cos\vartheta / m$$
$$y(i+1) = y(i) + v_y(i)\,\Delta t$$
$$v_y(i+1) = v_y(i) - g\Delta t - \Delta t\, k(v_x(i)^2 + v_y(i)^2)\sin\vartheta / m$$

Given m=7, k=0.01.
Initial conditions are: time t=0 , x(0)=0,y(0)=0,
$v_x(0)$= 30 cos(θ) . $v_x(0)$= 30 sin(θ) .

Write a program to calculate at launching angle θ= 30^0 , x,y,v_x and v_y starting at time t=0 to 10 s at intervals of Δt=0.1 s and determine the range of the projectile. [15]

Note: The range is determined by x(i) when y(i) is negative.
i=0,1,2,......n where n=10/0.1=100 in this case.
All the data given is in SI units as applicable in each individual cases.

SECTION B
(Practical Section)

Q.4. For a charged thin wire along the x-direction which extends from *x= a to b* the potential *V* at any point (x_0, y_0) is given by the integral

$$V = \int_a^b \frac{\sin(\pi k x)}{\left[(x - x_0)^2 + y_0^2\right]^{1/2}} dx$$

Assume that *a= -2.5m* and *b= 2.5m* and *k=0.1* .

(i) Write a program to calculate the potential at x_0=*1.2* , y_0=*1.2* using the Monte-Carlo method. Consider the case for which the number of random numbers N=20 to verify the working of your program. [10]
Note: Use the evaluated value for Pi of Maple. i.e. evalf(Pi).

(ii) Use the program of (i) to include in your program a criterion to confirm that the integral is convergent to a precision of 0.004 , that is, calculate the integral with N steps and then with 2N steps and find the absolute difference between the integrals and if the difference is less 0.004 then the integral is convergent. [10]
Use the starting value of N=1000.

(iii) Convert the program of (i) to a procedure which can be used for any function and any value of a , b, k, x_0, y_0 and precision. Verify the working of the procedure using the data given above. [10]

Note: Use the uniform random number generator in the range (0,1) available in Maple.

Q.5. Consider the random walk problem in two dimensions on a square lattice. The walk starts at the origin which is at a lattice point approximately at the centre of the lattice and assume the length of each step to be of one unit . Each point on the lattice is recognized by the coordinates ***(x,y)*** from the origin. At all the co-ordinates (x,25) and (x,-25) there is a reflection plane. That is if the walker reaches these points, he traces back along the y-direction by one unit if his movement is along the y-direction in his previous step.

Write a program and execute it to find the distance $d = (x^2 + y^2)^{1/2}$ the walker has covered in 1000 steps. Assume the starting point of walk to be at (0,0). [15]

Note: Consider a 100 x 100 matrix to begin with and if need be, increase the matrix dimension.
Use the uniform random number generator in the range (0,1) available in Maple.

Q.6. (i) Consider a second order differential equation of the form

$$\frac{d^2y(x)}{dx^2} + p\frac{dy(x)}{dx} + f(x) = 0$$

where ***p*=constant.** The initial conditions are $y(a) = \alpha$, $\left.\frac{dy}{dx}\right|_{x=a} = \beta$.

This equation can be reduced to two first order differential equations:

$$\frac{dy(x)}{dx} = z(x)$$

$$\frac{dz(x)}{dx} = -pz(x) - f(x)$$

Define $g(x,z) = -pz(x) - f(x)$.

Use of Euler method in the interval $a \le x \le b$ gives us the following algorithm for calculating $y[i]$ at n points:

$$y[i+1] = y[i] + h * z[i]$$

$$z[i+1] = z[i] + h * g(x[i], z[i])$$

$$x[i+1] = x[i] + h \quad where \quad h = (b-a)/n \quad , and \quad i = 0,1,2,3.........n$$

$$with\ y[0] = \alpha\ ,\ z[0] = \beta$$

Write program for a procedure using the above algorithm to calculate the sequence x[i], y[i] for $i = 0...n$, for any $f(x)$ with n steps. [10]

(ii) The Duffing oscillator differential equation is given by

$$\frac{d^2y}{dx^2} + k\frac{dy}{dx} + x^3 = B\cos(x)$$

Given B=5, k=0.01.

Assume initial conditions to be at x=*0* , *y(0)=0.5* and $\left.\frac{dy}{dx}\right|_{x=0} = 0$.

(a) Write Maple commands to solve this equation numerically. [5]

(b) Find the solution y(x) numerically on the interval $0 \le x \le 25$ at 200 points using the procedure of (i). [5]

(iii) Plot the solutions of (a) and (b) on the same graph. [5]

@@@@END OF EXAMINATION@@@@

APPENDIX

1. Solution of First Order Differential Equation with initial Conditions:

The equation is of the form $\frac{dy}{dx} = f(x,y)$ with $y(x_0) = \alpha$.

(i) Euler's Method:

$$y_{i+1} = y_i + h\,f(x_i, y_i) \qquad \textit{where } h = x_{i+1} - x_i$$

(ii) Fourth Order RK-Method:

$$y_{i+1} = y_i + (k_1 + 2k_2 + 2k_3 + k_4)/6$$

where

$k_1 = h\,f(x_i, y_i)$
$k_2 = h\,f(x_i + 0.5\,h, y_i + 0.5\,k_1)$
$k_3 = h\,f(x_i + 0.5\,h, y_i + 0.5\,k_2)$
$k_4 = h\,f(x_i + h, y_i + k_3)$ *and* $h = x_{i+1} - x_i$

2. Solution of Second Order Differential Equation with initial Conditions:

The equation is of the form $\frac{d^2y}{dx^2} + p(x)\frac{dy}{dx} + q(x)y = r(x)$ with initial conditions at x=a,

$y(a) = \alpha$, $\left.\frac{dy}{dx}\right|_{x=a} = \beta$.

The second order equation can be reduced into two first order differential equations given below:

$$\frac{dy}{dx} = z(x)$$

$$\frac{dz}{dx} + p(x)z + q(x)y = r(x)$$

The two first order equations can be solved numerically using Euler or RK-methods given in (1) above.

3. Numerical Integration:

(A) Simpson Rule:

$$\int_a^b f(x)dx = \frac{h}{3}[f(a)+f(b)+4(f_1+f_3+f_5+.....+f_{n-1})+2(f_2+f_4+f_6+..+f_{n-2})]$$

where $f_0 = f(a)$, $f_n=f(b)$, $f_1=f(a+h)$, $f_2=f(a+2h)$......*etc. and* n=*even integer.*

(B) Monte Carlo Evaluation of Integrals:

Integral of the form F= $\int_a^b f(x)dx$ is given by

$$F = \frac{(b-a)}{n}\sum_{i=1}^{n} f(x_i)$$

where x_i is the i^{th} random number of n random numbers distributed uniformly in the interval (a,b). The standard deviation can be estimated from the points sampled in evaluating the integral by

$$\sigma_n = \left[\frac{\frac{1}{n}\sum_{i=1}^{n}[f(x_i)]^2 - [\frac{1}{n}\sum_{i=1}^{n} f(x_i)]^2}{n-1}\right]^{1/2}$$

with 68.3% confidence.