UNIVERSITY OF SWAZILAND

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION: 2009/2010

TITLE OF THE PAPER: COMPUTATIONAL METHODS-II

COURSE NUMBER: P482

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

INSTRUCTIONS:
THE ARE TWO SECTIONS IN THIS PAPER:

- **SECTION A** IS A WRITTEN PART. ANSWER THIS SECTION ON THE ANSWER BOOK. IT CARRIES A TOTAL OF **30** MARKS.
- **SECTION B** IS A PRACTICAL PART WHICH YOU WILL WORK ON A PC AND SUBMIT THE PRINTED OUTPUT. IT CARRIES A TOTAL OF **70** MARKS.

Answer **any** two questions from **section A** and
all the questions from **section B**.
Marks for different sections of each Question are shown in the right hand margin.

THE PAPER HAS 7 PAGES, INCLUDING THIS PAGE.

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Section A

Question 1

(a) In the two dimensional Ising model for magnetic systems, the magnetic spin at site (i, j) is given by $S_{i,j} = \pm 1$. The plus represents a spin-up and the minus represents a spin-down. In the paramagnetic state (non-magnetic state), the spins' orientation at the lattice sites is random. Write down algorithm that generates the paramagnetic state for the Ising model on a lattice with 10×10 lattice points.

[5 marks]

(b) Consider a random walker in two dimensions on a square lattice. The walker starts at the origin (0,0) and moves non-stop for $N_s = 100$ steps. Write an algorithm to simulate the movement of the random walker. Assume the random walker takes a step unit, either along the x-direction or y-direction at each instant.

[10 marks]

Question 2

(a) The electric potential $V(x,y)$ in some region of space with a charge density $\rho(x,y)$ is given by the Poisson equation:

$$\frac{\partial^2 V(x,y)}{\partial x^2} + \frac{\partial^2 V(x,y)}{\partial y^2} = \frac{\rho(x,y)}{\epsilon_0}$$

(i) Express this Poisson equation in discrete space, i.e, transform $V(x,y)$ into $V(i,j) = V(x_i, y_j)$, where the discretized spatial variables: $x_i = i\Delta x$ and $y_i = j\Delta y$. For convenience let the stepsize $\Delta x = \Delta y$. And solve for $V(i,j)$.

[6 marks]

(ii) State two types of plots, that could be used to plot the data from the numerical computation of $V(i,j)$.

[3 marks]

(b) The corresponding electric field in the region with a potential $V(x,y)$ is given by the relation

$$\vec{E}(x,y) = -\left(\hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y}\right) V(x,y).$$

where $\hat{x}$ and $\hat{y}$ are unit vectors point along the x-and y-directions, respectively.

(i) Using the finite difference method write the expression for $E_x[i,j]$ and $E_y[i,j]$, the components of the discretized electric field $E(i,j)$ along $\hat{x}$ and $\hat{y}$ direction, respectively.

[4 marks]

(ii) Write the Maple commands to plot the electric vector field

$$\vec{E}(i,j) = E_x[i,j]\hat{x} + E_y[i,j]\hat{y},$$

for $i = 0..10$, and $j = 0..10$.

[2 marks]

Question 3

(a) Suppose a computational physicist wants to simulate some spatial noise $\zeta(j)$ at a point j of a physical system. $\zeta(j)$ has a uniform distribution and fluctuates in the range $[-\pi/4, \pi/4]$. Write some maple commands to generate $\zeta(j)$, for N points.

[5 marks]

(b) The realistic projectile motion of a spherical ball with mass m can be described by a set of four first-order ODEs:

$$\begin{aligned}
\frac{dv_x(t)}{dt} &= Av_x(t) - B[v_x^2(t) + v_y^2(t)]^{1/2}v_x(t)/m, \\
\frac{dv_y(t)}{dt} &= -gAv_y(t) - B[v_x^2(t) + v_y^2(t)]^{1/2}v_y(t)/m, \\
v_x(t) &= \frac{dx(t)}{dt} \\
v_y(t) &= \frac{dy(t)}{dt}
\end{aligned}$$

where $x(t)$ and $y(t)$ are the horizontal and vertical coordinates of the projectile, respectively. A is the coefficient of the viscous force, B is the coefficient of the drag force, and g is the acceleration due to gravity.

Rewrite these equations using the Euler discretization scheme, i.e, into a form that can used to obtain their numerical solutions. Explain your notation carefully.

[10 marks]

Section B

Question 4

Consider a second order differential equation,

$$\frac{d^2y(x)}{dx^2} = G\left(\frac{dy(x)}{dx}, y(x), x\right),$$

where G is some function. This equation can be decomposed into two equations suitable for the Euler algorithm, i.e., into

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

and

$$\frac{dz(x)}{dx} = G(z(x), y(x), x)$$

Use of the Euler method in the interval $0 \leq x \leq h$ gives us the following algorithm for calculating $y[i]$ and $z[i]$ at N_p points:

$$\begin{aligned} x[i] &= i * \Delta x \\ y[i+1] &= y[i] + \Delta x * z[i] \\ z[i+1] &= z[i] + \Delta x * G(z[i], y[i], x[i]) \end{aligned}$$

where $\Delta x = h/N_p$ and $i = 0, 1, 2, 3..N_p - 1$, with $y[0] = \alpha$, $z[0] = \beta$. Using this algorithm, write a program to calculate the *angular displacement* $\theta(t)$ and *velocity* $\omega(t) = d\theta/dt$ of a driven pendulum. The driven pendulum is described by the Newton's equation

$$\frac{d^2\theta(t)}{dt^2} + q\frac{d\theta(t)}{dt} + \sin[\theta(t)] = b\cos(At)$$

where q is the coefficient of the damping force, b and A are the amplitude and frequency of the driving force respectively. Given $A = 2/3$, $b = 0.3$ and $q = 1/2$. Assume the initial conditions to be $\omega(t = 0) = 2.$ and $\theta(t = 0) = 0$. Find the numerical solution of $\theta(t)$ and $\omega(t)$ on the interval $0 \leq t \leq 20\pi$ at $N_p = 1000$ points.

[10 marks]

(a) Plot $\theta(t)$ and $\omega(t)$ against t on the interval $0 \leq t \leq 20\pi$.

[4 marks]

(b) The behavior of the pendulum can be easily analyzed in phase space ($\omega - \theta$ space). Plot the trajectory of the pendulum in phase-space.

[6 marks]

(c) Base on your graphical results, describe the characteristic of the pendulum.

[3 marks]

Question 5

Calculate and plot the power spectrum of the following signal:

$$\rho(t) = \cos(3t) + \cos(t/2).$$

You may need to discretize the variable t into $t_i = i\Delta t$, where $i = 1, 2, 3....N$ and Δt is the time-step. You may take $\Delta t = 1$ and $N = 256$. In this case, the power spectrum of the function $\rho(t_i)$ is given by

$$P(\omega_i) = |\rho(\omega_i)|^2$$

where $\rho(\omega_i)$ is the Fourier transform of the $\rho(t_i)$, and the frequency $\omega_i = 2\pi i/(N\Delta t)$.

[12 marks]

Question 6

(a) Write a procedure *Rwalker1d(I,N_s)*, that returns the trajectory of the a *one-dimensional* random walker after N_s steps. The other input variable I is the initial displacement of the walker with respect to the origin.

[15 marks]

(b) On one graph, plot the trajectory of three random walkers: $X_1(t = 0) = 0$, $X_2(t = 0) = +10$, and $X_3(t = 0) = -10$, i.e., $X_j(t = 0)$ being the initial position of the random walker j with respect to the origin $x = 0$. Assume that each walker takes $N_s = 1000$ steps.

[6 marks]

(c) Consider a system with $N_w = 100$ *one-dimensional* random walkers. Assume that each random walker j, begins his/her journey from the origin, i.e, $X_j[t = 0] = 0$. Each random walker takes $N_s = 1000$ steps.

(i) Use the procedure *Rwalker1d(I,N_s)* to calculate $X_j[n]$, the position of the random walker j after n steps for $j = 1..N_w$, and also compute the mean square displacements of the walkers,

$$X2(n) = \frac{1}{N_w}\sum_{j=1}^{N_w} X_j^2(n),$$

for $n = 0...N_s$ steps.

[10 marks]

(ii) Verify that the movement of the N_w walkers results to a diffusion process, that is the mean square displacement $X2(n)$ is directly proportional to number of steps n.

[4 marks]