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UNIVERSITY OF SWAZILAND

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION: 2013/2014

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 **40** MARKS.
- **SECTION B** IS A PRACTICAL PART WHICH YOU WILL WORK ON A PC AND SUBMIT THE PRINTED OUTPUT. IT CARRIES A TOTAL OF **60** MARKS.

Answer **all** the 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 5 PAGES, INCLUDING THIS PAGE.

DO NOT OPEN THIS PAGE UNTIL PERMISSION HAS BEEN GIVEN BY THE INVIGILATOR

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Section A

Question 1

(a) A magnet can be modeled by a set of N_s spins interacting classically via an interaction energy

$$E_i = -J \sum_j s_i s_j$$

where the Ising spin at site i can take two values $s_i = +1$ ($\uparrow$) or $s_i = -1$ ($\downarrow$) and the sum is over the j nearest neighbors of i. Consider the following one-dimensional lattice $N_s = 11$ spins.

$\uparrow \uparrow \downarrow \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow$

(i) Compute the magnetization $m = \frac{1}{N_s} \sum_{i=1}^{N_s} s_i$ and the average energy $\langle E \rangle = \frac{1}{N_s} \sum_{i=1}^{N_s} E_i$ of the 1D Ising spin system.

[4 marks]

(ii) Compute the change in the magnetization and the average energy of the system when the spin at the right-end of the lattice is flipped.

[4 marks]

(b) In a paramagnetic state (non-magnetic state), the spins are randomly oriented on the lattice. Write a short $f95$ program that generates the paramagnetic state for the Ising model on a square with N^2 lattice points, where $N = 200$.

[6 marks]

(c) A sleep-deprived P482 student (working late on an assignment) is trying to compute the kinetic energy $\frac{1}{2}mv^2$ of a particle of mass $m = \frac{3}{2}$ and velocity $v = 4$. His three attempts yield the following Fortran 95 snippets. In each case, determine the value assigned to *kin_en*.

```
real:: m, v, kin_en
m = 1.5; v =4.0
(i) kin_en = (1/2) * m * v * v
(ii) kin_en = 0.5 * mv * *2
(ii) kin_en = 0.5 * m * v * v
```

[6 marks]

Question 2

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(a) Compare the following prescriptions for integrating a differential equation $\frac{dx}{dt} = f(x,t)$. Δt is the time step, x_i is the current point , x_{i+1} is the next point. For each method, state the order of accuracy (as $\mathcal{O}[(\Delta t)]$), where these represent the lowest-order terms that are not predicted correctly.

(i) $x_{i+1} = x_i + \Delta t \cdot f(x_i, t_i)$

(ii) $x_{i+1} = x_{i-1} + 2\Delta t \cdot f(x_i, t_i)$

[6 marks]

(b) A two dimensional space is discretized using a uniform square mesh of grid size Δx i.e, $\psi(i \cdot \Delta x, j \cdot \Delta x) = \psi_{i,j}$. What is an appropriate finite-difference approximation to the Laplacian $\nabla^2\psi$? Explain in detail.

(i) $\frac{1}{(\Delta x)^2}\left[\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{i,j}\right]$

(ii) $\frac{1}{(\Delta x)}\left[\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1} - \psi_{i,j}\right]$

(iii) $\frac{1}{(\Delta x)^2}\left[\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1} - 4\psi_{i,j}\right]$

[4 marks]

(c) The diffusion equation is given as

$$\frac{\partial u(x,t)}{\partial t} = D\left(\frac{\partial^2 u(x,t)}{\partial x^2}\right).$$

Devise a finite difference approximation to the diffusion equation that leads to the discretized field $u(n) = u(i \cdot \Delta x, n \cdot \Delta t)$ being updated according to

$$u_i^{n+1} = u_i^n(1-2s) + s(u_{i+1}^n + u_{i-1}^n)$$

What is the value of s?

[4 marks]

(d) Given a differential equation

$$\frac{d^2y(t)}{dt^2} = -g - \gamma\frac{dy(t)}{dt}$$

where g and γ are constants, detail the algorithm of how to use the Forward Euler method using a fixed stepsize Δt to determine the value of $y(t)$ at a later time t_f. Assume that $y(t=0) = y_0$ and $\frac{dy(t=0)}{dt} = v_0$.

[6 marks]

Section B

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Note: The answers to this question must include the computer code and output, in addition to any writing that might be needed.

Question 3

A radioactive sample contains N_0 radioactive nuclei at $t = 0$. The decay rate of the nuclei is $\lambda = 0.27s^{-1}$. Imagine that the activity of the sample was measure from $t = 0$ at time intervals of $0.1s$ until there are no nuclei left to decay. Note that the probability p of any particle decaying at a given time interval Δt is

$$p = -\frac{N(t+\Delta t) - N(t)}{N(t)} = \lambda \cdot \Delta t$$

Utilize the pseudo-code given below to simulate the radioactive decay experiment and to answer the questions below.

(a) Plot the natural logarithm of the number of radioactive nuclei $\ln N(t)$ versus time for $N_0 = 10^5$, 10^4, 10^3, 10^2, and 10. Which values of N_0 leads to a pronounced stochastic behavior?

[30 marks]

(b) Create a plot showing that the slopes of $\ln N(t)$ versus t is proportional to $-\lambda$.

[10 marks]

(c) Consider a system with a decay rate that fluctuates about an average value over time, i.e $\lambda = [0.27 + r(t)]$ where the fluctuating variable $r(t)$ is uniformly distributed in the range $[-0.1, 0.1]$. Create a plot showing that the slopes of $\ln N(t)$ versus t for this system. Explain your observations.

[20 marks]

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A pseudocode for simulating the decay process is simple:

```
! Declaration of parameters: N is number of radioactive nuclei
!dN is the number of decaying nuclei at a time interval dt
integer:: N, dN, i,m
real*8:: ran3, lambda, dt, p, rd
integer::iseed
open(7,file='output.txt')

!Initialization of parameters:
iseed =-1053
N =10000 ! initial number of radioactive nuclei N0
m =0 ! evolution time = m*dt
lambda =0.27; dt = 0.1
! probability that a radioactive nucleus decay at time t
p = lambda * dt

! computation loop

do while (N.gt.0)
dN=0 !
do i =1,N
rd = ran3(iseed)
if (rd.lt.p) then
dN =dN +1
end if
end do
m =m+1
N =N-dN
! output data is N(t) vs time
write(7,) m*dt, N
end do
```