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UNIVERSITY OF SWAZILAND

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION: 2016/2017

TITLE OF THE PAPER: COMPUTATIONAL METHODS-II

COURSE NUMBER: P482

TIME ALLOWED:
SECTION A: 1.5 HOURS
SECTION B: 1.5 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.
- You may proceed to do Section B only after you have submitted your answer book for Section A

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 6 PAGES, INCLUDING THIS PAGE.

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

Section A

Question 1

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(a) Using the information about precedence/associativity of operators in Fortran evaluate each of the following F95 expressions

(i) $2 * *3 * 4 + 2$
(ii) $6/5 + 1$
(iii) $(9 - 3 * 2)/2$
(iv) $2.3 * (3/2) - 5$
(v) $10/(1.0 * 3) - 10/3$

[5 marks]

(b) Compute the period of the sequence $\{ x_n\}$ defined below. Give two reasons why it would make a bad random number generator.

$$x_n = (x_{n-1} + x_n n - 2) \bmod 8 \quad (1)$$
$$x_0 = 3 \quad (2)$$
$$x_1 = 7 \quad (3)$$
$$(4)$$

[5 marks]

Question 2

a) A sleep-deprived P482 student (working late on an assignment) is trying to compute the kinetic energy $p^2/(2m)$ of a particle of mass $m = 0.5$ and momentum $p = 4$. His four attempts yield to the following Fortran snippets. In each case, determine the value assigned to kin_en:

```
  real*8::  m,v, kin_en

m=0.5d0
p = 4.d0
i) kin_en =(1/2)* m* p* p
ii) kin_en =p**2/2* m
```

```
iii) kin_en =0.5d0 p* p /m
iv) kin_en =0.d0* p* p/ m
```

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[4 marks]

b) A quantum particle living in one dimension is characterized by its wavefunction $\psi(x)$. If the particle interacts with nothing else and is subject to no confining potential, then it is free and its energy is given

$$E = -\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}.$$

i) Show that a finite difference approximation for the kinetic energy is as follows:

$$E = -\frac{\hbar^2}{2ma^2}(\psi_{i-1} + \psi_{i+1} - 2\psi_i).$$

where $\psi_i = \psi(x_i)$ at discrete points $x_i = i \cdot a$. for integer i

[4 marks]

ii) In what parameter regime is the continuum result recovered?

[2 marks]

Question 3

Consider a one-dimensional random walker on a linear lattice. The walker starts at the origin and moves non-stop for M steps.

a) Write an algorithm to simulate the movement of the random walker. Assume the random walker takes a unit step at each instant and that he/she moves to the left or right with equal probabilities.

[4 marks]

b) Show that a basic random walk can be rewritten as a continuum diffusion equation by taking the limit in which the lattice spacing l and the time-step τ to go to zero.

[6 marks]

Question 4

a) Write a Fortran 95 function for 170

$$\text{sinc}(x) \equiv \frac{\sin x}{x}$$

Make sure that your function handles $x = 0$ correctly.

[4 marks]

b) A magnet can be modelled by a set of N 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 with $N = 20$ spins:

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

Compute the magnetization $m = \sum_{i=1}^{N} S_i/N$ and the average energy $\langle E \rangle = \sum_{i=1}^{N} E_i/N$ of the system, assuming that the left-end and the right-end spins are connected, i.e., periodic boundary conditions.

[6 marks]

Section B

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

Question 5

Ferromagnetism:- The evolution of the magnetization $m(x,t)$ of a material very close to the demagnetization temperature (T_c), where the ferromagnetism of the material is destroy by heat, can be described by the following model

$$\frac{\partial m(x)}{\partial t} = \frac{\partial^2 m(x)}{\partial x^2} + rm(x) - m^3(x)$$

in one dimension. Here r is a temperature dependent parameter. The spatial average magnetization is nonzero below T_c and vanishes above T_c. The corresponding difference formula the above dynamics equation is given as ,

$$m_i^{n+1} = m_i^n + \frac{\Delta t}{(\Delta x)^2} \cdot (m_{i+1}^n + m_{i-1}^n - 2m_i^n) + \Delta t[rm_i^n - (m_i^n)^3] \qquad (5)$$

where $m_i^n = m(i \cdot \Delta x, n \cdot \Delta t)$. The code *ferroM.f95* implements the above difference formula to determine the dynamics of a system with $r = 0.5$ with random initial conditions and periodic boundary conditions.

(i) **(10 marks)** Rerun the code with a different seed of the random number generator. Plot the configuration of the magnetization $m(x, t = 0)$, i.e., m_i^0 for $i = 1$ to 100.

(ii) **(20 marks)** Using the program calculate how the magnetization of the system evolves with time t_n. Create plots of the magnetization $m_i \equiv m(x_i)$ for $i = 1...100$ at $t_0 = 0$, t_{700} and t_{5000}. Superimposed these results into one graph use proper labels to differentiate each case.

(iii) **(30 marks)** Modify your code in order to compute the average magnetization of the system at each given time step: $\bar{m}(t_n) = \frac{1}{100}\sum_{i=1}^{100} m(x_i, t_n)$. Plot $\bar{m}$ vs t_n, for n =1 to 5000 for two cases: when $r = -0.5$ and $r = 0.5$. From your results can you conclude that negative r corresponds to temperatures below the demagnetization temperature? Explain.