UNIVERSITY OF ESWATINI

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION: 2021

TITLE OF THE PAPER: COMPUTATIONAL PHYSICS-II

COURSE NUMBER: PHY482/P482

**TIME ALLOWED:**
SECTION A: 1 HOUR
SECTION B: 2 HOURS

**INSTRUCTIONS**:
THERE 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 FOR 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 4 PAGES, INCLUDING THIS PAGE.

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

## Section A

### Question 1

(a) **(3 marks)** What are some of desired properties of a random number generator

(i) High performance
(ii) Long period
(iii) Unpredictability
(iv) All of the above
(v) None of the above

(b) **(2 marks)** Write the master equation for a one-dimensional random walks on linear lattice.

(c) **(5 marks)** Show that the master equation can be reduced to a diffusion equation in the limit in which the lattice spacing $l$ and the time-step $\tau$ go to zero.

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### Question 2

a) **(5 marks)** In numerical analysis, the Euler method ...

(i) is a first-order numerical procedure for solving initial value problem for ordinary differential equations
(ii) is a third-order numerical procedure for solving initial value problem for ordinary differential equations
(iii) is very fast and accurate and thus should always be the first method to try when solving ordinary differential equations
(iv) all of the above
(v) none of the above

b) **(5 marks)** The diffusion equation for a density field $c(x,t)$ is given by a partial differential equation

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial^2 x} \tag{1}$$

where $D$ is a diffusion constant. Given the initial and boundary condition, this equation can be solved numerically using the finite difference schemes. Show that alternatively, the Eq. (1) can be transformed into a first-order *ordinary differential equation* by the application of a Fourier transform.

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## Question 3

a) **(4 marks)** The rectangle and trapezoid methods of integration give identical results for the integral of any function $f(x)$ in the interval $[a, b]$, if $f(a) = f(b)$. In other words, the two methods have the same error with respect to the correct value, even though they have different rates of convergence. How do you reconcile these two results?

b) **(2 marks)** Name one condition under which the Monte Carlo integration method is most suitable compared to the standard numerical methods such as the Trapezoidal and the Simpson rule.

c) **(4 marks)** As part of the solution of a particular problem you need (repeated) calculation of the following expression

$$\frac{1}{1 - \sqrt{1-x}} \qquad (2)$$

for small $x$ such that $x \approx \epsilon$ where $\epsilon$ is the machine epsilon.

(i) Briefly describe what trouble you expect when using Eq. (2).

(ii) Rewrite Eq. (2) to avoid the trouble

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## Question 4

a) **(10 marks)** The general one-dimensional Poisson equation reads as

$$\frac{d^2u(x)}{d^2x} = f(x), \quad x \in (0,1), \quad u(0) = u(1) = 0$$

Show that this equation in a discretized approximations can be given as

$$\frac{u_{i+1} + v_{i-1} - 2u_i}{h^2} = f_i \text{ for } i = 0, \ldots, N$$

where $f_i = f(x_i)$, $u_i = u(x_i)$, with the grid points $x_i = ih$ and the grid spacing $h = 1/N$

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## Section B – Question 5 (Computer based problem)

The Landau-Ginzburg model that describe the dynamics of the ferromagnetic ordering from the paramagnetic state close to the critical temperature ($T_c$) is given as:

$$\frac{\partial}{\partial t}m(x,y,t) = K\nabla^2 m(x,y,t) - am(x,y,t) - bm^3(x,y,t) \tag{3}$$

where $m$ is the magnetization, $K$ coupling strength between neighboring spins and $b = (1 - T_c/T)$ is the temperature-like control parameter..

(i) **(3 marks)** What is the phenomenon or physical process that is described by Eq. (3) in the limit where $a = b = 0$.

(ii) **(15 marks)** Consider the attached `Fortran` code, `ferromagnets.f95` that utilized the Euler algorithm

$$m_{i,j}^{n+1} = m_{i,j}^{n}\Delta t \cdot \nabla^2 m_{i,j}^{n} + \Delta t \cdot (m_{i,j}^{n} - (m_{i,j}^{n})^3) \tag{4}$$

where the the Laplacian

$$\nabla^2 m_{i,j}^{n} = (m_{i+1,j}^{n} + m_{i-1,j}^{n} + m_{i,j+1}^{n} + m_{i,j-1}^{n} - 4m_{i,j}^{n})/\Delta x^2$$

where $m_{i,j}^{n} = m(i\Delta x, j\Delta x, n\Delta t)$ is a discretized variable to compute the time dependent solutions. In the code $m(x, y, t = 0)$ consists of random fluctuation and the periodic boundary applied with $a = -1$, $K = b = 1$ . Run the code and plot the snapshots of the magnetization at $t = 0$, $t = 25$, and $t = 50$.

(iii) **(10 marks)** Modify the code by replacing the five-point Laplacian with the nine-point difference method

$$\begin{aligned}\nabla^2 m_{i,j}^{n} &= (m_{i+1,j}^{n} + m_{i-1,j}^{n} + m_{i,j+1}^{n} + m_{i,j-1}^{n})/(2\Delta x^2) \\ &+ ((m_{i+1,j+1}^{n} + m_{i-1,j+1}^{n} + m_{i+1,j-1}^{n} + m_{i-1,j-1}^{n})/4 - 3m_{i,j}^{n}))/\Delta x^2 \end{aligned} \tag{5}$$

Rerun the code and plot the snapshots of the magnetization at $t = 0$, $t = 25$, and $t = 50$. Are there any qualitative difference between the results of the two methods

(iv) **(15 marks)** Modify the code plot the $m(x, y, t)$ at $t = 50$ for three different systems with: $K = 0.1$, $1.0$, and $K = 10$.

(v) **(7 marks)** What describe the nature of the magnetization patterns that are recovered in the small $K$ limit compared those at the larger $K$ values. Are these results meaningful?

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