UNIVERSITY OF SWAZILAND

FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

MAIN EXAMINATION: 2015/2016

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 6 PAGES, INCLUDING THIS PAGE.

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Section A

Question 1

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

(i) $2 + 3 * 4 + 2$

(ii) $5 * *2 * 4$

(iii) $4 * *(1/2.)$

(iv) $2.3 * (3/2) - 5$

(v) $10/(1.0 * 3) - 10/3$

[5 marks]

(b) Indicate which of the following declaration statements are valid. For invalid declaration statements describe why they are invalid:
i) $y + 2 = x$
ii) $Dist := y2 - y1$
iii) $NUM = NUM + 1$

[3 marks]

(c) The following code fragment shows a potential infinite loop:

```
i =0
do
i =i+1
write(*,*), i**2
end do
```

Present two alternatives for of the above do loop that will cause it to be executed precisely 100 times.

[2 marks]

Question 2

a) **Catalan numbers:** The Catalan numbers C_n are a sequence of integers 1, 1, 2, 5, 14, 42, 132. . . that play an important role in quantum mechanics and the theory of disordered systems. (They were central to Eugene Wigners proof of the so-called semicircle law.) They are defined by

$$C_0 = 1, C_{n+1} = \frac{4n+2}{n+2} C_n.$$

Write a program that prints in increasing order all Catalan numbers less than or equal to one billion.

[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.

$$\begin{aligned} x_n &= (x_{n-1} + x_{n-2}) \bmod 12 \\ x_0 &= 3 \\ x_1 &= 7 \end{aligned}$$

[5 marks]

Question 3

a) Write a program to calculate an approximate value for the integral

$$\int_0^2 (x^4 - 2x + 1)dx$$

using the Trapezoidal rule with 10 slices.

[5 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

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

Devise a finite difference approximation to evaluate E given the wavefunction $\psi(i) = \psi(x_i)$ at discrete points $x_i = i * h$, (for integer i).

[5 marks]

Question 4

a) Consider two $N \times N$ matrices A and B. Which loop is more efficient for reading the sum of the two matrices in Fortran 90/95. Explain.

i)
```
DO i =1, N
DO j =1, N
S(i,j) = A(i,j)+B(i,j)
END DO
END DO
```

ii)
```
DO j =1, N
DO i =1, N
S(i,j) = A(i,j)+B(i,j)
END DO
END DO
```

[2 marks]

b) In nuclear physics the semi-empirical mass formula gives an approximate value for the binding energy B of a nucleus with atomic number Z and a mass number A:

$$B = a_1 A - a_2 A^{2/3} - a_3 \frac{Z^2}{A^{1/3}} - a_4 \frac{(A-2Z)^2}{A} + \frac{a_5}{A^{1/2}},$$

where, in units of MeV, the constants are $a_1 = 5.67$, $a_2 = 17.23$, $a_3 = 0.75$, $a_4 = 93.2$, and

$$a_5 = \begin{cases} 12.0 & \text{if Z and A -Z are both even,} \\ -12.0 & \text{if Z and A-Z are both odd,} \\ 0 & \text{otherwise} \end{cases}$$

Write a F95/C++ program that asks the user to enter A and Z and then calculates and returns the binding energy per nucleon B/A.

[8 marks]

Section B

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

Question 5

The dynamics of a cyclist:- The equation of motion of a cyclist exerting a force on his bicycle corresponding to a constant power P and moving against the force of air resistance is given by

$$\frac{dv(t)}{dt} = \frac{P}{mv(t)} - \frac{C\rho A v(t)^2}{m},$$

where m = mass of the rider, $v(t)$ is the velocity which is *always positive*, ρ is the air density C= coefficient of the air drag force, and A is the cross-sectional area of the cyclist. The Euler algorithm give the approximate solution:

$$v(i+1) = v(i) + \Delta t\left(\frac{P}{mv(i)} - \frac{C\rho A v^2(t)}{m}\right)$$

for i =0, 1, ..., N with the corresponding time $t \equiv t_i = i \cdot \Delta t$

a) Write a F95/C++ program that calculate the speed v as function of time in the case of zero air resistance and then in the case of non-vanishing air resistance. What do you observe. Assume that m = 70 kg, v(0) =4.0m/s, ρ = 1.2 kg/m^3, Δt = 0.1s, P =200 Watts, A = 0.33m^2 and the cyclist starts at time t= 0 and stops t =200s. What do you observe if you change the drag coefficient and/or the power.

[30 marks]

b) An even more realistic model considers that the cyclist may face either a head or tail wind. The improved model is given as

$$\frac{dv(t)}{dt} = \frac{P}{mv(t)} - \frac{C\rho A}{m}(v(t) - v_w)|v(t) - v_w|,$$

where v_w is the wind speed. Determine the $v(t)$ for v_w = 3.5 m/s (tail wind) and v_w = −3.5 m/s (head wind). Plot these results on the same figure.

[10 marks]

Question 6

a) Write a program to calculate an approximate value for the integral:

$$\int_0^1 x^{1/2} e^x dx,$$

using the Simpson's rule. Recall that according to the Simpson's rule the integral of $f(x)$ over the interval $[a,b]$ is given as:

$$\int_a^b f(x)dx \sim \frac{h}{3}\left(f(a) + f(b) + 4\sum_{k=1}^{N/2} f(a+(2k-1)h) + 2\sum_{k=1}^{N/2-1} f(a+2kh) \right)$$

where $h = (b-a)/N$, where N is positive even number. Run the program for N =10 and compare your result to the exact results of 1.255630082......

[10 marks]

b) Modify the program to increase N, the number of sampling points. Comment on the improvement in the result, compared with the exact solution.

[10 marks]

For a full credit hand in your program, your results, and a brief discussion of the results.