SAINT MARY'S UNIVERSITY

FACULTY OF SCIENCE

DEPARTMENT OF ASTRONOMY AND PHYSICS

PHYS3210, COMPUTATIONAL METHODS IN PHYSICS

MOCK FINAL EXAMINATION

APRIL 2009

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**Instructions**
This exam is TWO (2) HOURS in length. A non-programmable calculator is allowed. A total of THREE (3) questions should be answered from the two sections in the examination. All questions carry equal weighting and the total marks are 75. No additional credit for answering more than three questions is available. There are THREE (3) pages in the exam. **Vague answers that do not specifically address the question will be given zero marks.**

- **Part 1:** Answer at minimum one of these two questions.
- **Part 2:** Answer at most two questions from this section.

**Please put your student number on all answer booklets and sheets. To receive full credit all assumptions must be cleary stated.**

GOOD LUCK!

PLEASE NOTE: The candidate is urged to submit with the answer paper a clear statement of any assumptions made if doubt exists as to the interpretation of any question.

## Part 1. Answer at least one question from this section.

Answer any questions requiring detailed explanations in *bullet* form.

**(1)** (a) Define the concepts of commutativity, associativity and distributivity. Do floating-point numbers satisfy these mathematical concepts? (**6 marks**).
(b) The general quadratic formula is

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

What is catastrophic cancellation? Under what conditions will the general quadratic exhibit this problem? If you needed to implement the general formula in a code what changes could you make to ensure your results do not suffer from catastrophic cancellation? (**8 marks**).
(c) Outline the types of errors that can occur in computational science. Ensure you mention approaches that can help reduce these kinds of errors. Note that for full credit you should consider issues beyond programming and floating-point representations. (**11 marks**).

**(2)** (a) The following FORTRAN program gives incorrect output. How would you fix the code? (**5 marks**)

```
c
c Input number of integers into n
c Read all the numbers and then calculate the average
c
      PROGRAM AVERAGE
      READ *,N
      DO 10, I=1,N
         READ *,NUM
         SUM = SUM + NUM
10    CONTINUE
      PRINT *,'AVERAGE IS ‘,(1/N)*SUM
      STOP
      END
```

```
Input: 5

1

2

3

4

5

Output:

AVERAGE IS 0.0000000E+00
```

(b) What do the following UNIX commands do? (**5 marks**)

- `pwd`

- `wc`
- `chmod u+x`
- `diff`
- `head`

(c) Describe the Von Neumann architecture (a diagram is probably the best way). What was the great conceptual advance, related to instructions, underlying this architecture? What is the main bottleneck in this computer architecture? What are registers? How does the speed of registers compare to that of main memory? (**15 marks**)

## Part 2. Answer at most 2 questions from this section.

Answer any questions requiring detailed explanations in *bullet* form.

**(3)** (a) Discuss polynomial fitting methods. Give as many examples as you can. What are the primary applications of these methods, are some better than others in certain circumstances? (**15 marks**)
(b) Outline how tridiagonal matrices can be solved by back substitution methods. Be sure to indicate the important parts of tridiagonal matrices. Also state how Gaussian elimination is applied. You do not have to derive the formulae for the back substitution to achieve full marks, however answers that do derive the substitution formulae will automatically be awarded full marks. (**10 marks**)

**(4)** (a) Derive the formula for the composite trapezoid rule over n trapezoids. (**10 marks**).
(b) Use the composite trapezoid rule to calculate

$$\int_0^2 (2x^2 + 2)dx$$

using partitions at 0,1,2. (**8 marks**)
(c) Outline how Richardson extrapolation can be applied to the Trapezoid rule to yield Romberg Integration. Ensure you mention Romberg Tables and also convergence checks. (**7 marks**)

**(5)** (a) Draw a diagram of a general function f(x) that passes through the y=0 axis. On this diagram give a representation of the algorithm used in the Newton-Raphson root finding method. Give the formula for the $x_{n+1}$ iteration as a function of $x_n$ in the Newton-Raphson scheme. What are some of the advantages and disadvantages of N-R? Draw, if you can, a function which would converge very slowly under the N-R algorithm. (**15 marks)**
(b) Use N-R to find an approximate root of the function

$$f(x) = x^3 + 2x^2 - 5$$

where you take $x_0 = 1$ as your initial guess. You should carry out at least two steps of the iteration scheme. **(10 marks)**