King’s College London

UNIVERSITY OF LONDON

This paper is part of an examination of the College counting towards the award of a degree. Examinations are governed by the College Regulations under the Authority of the Academic Board.

B.Sc. EXAMINATION

CP/1710 COMPUTING FOR PHYSICAL SCIENCES

JANUARY 1998

Time allowed: **THREE HOURS**

Candidates must answer any SIX questions from SECTION A, and TWO questions from SECTION B.

Separate answer books must be used for each section of the paper

The approximate mark for each part of a question is indicated in square brackets.

Good answers to the questions in Section B will consist of plans or explanations in addition to Fortran code. You can gain marks for later sections of a question even if you cannot do the earlier sections.

π=3.1415927

TURN OVER WHEN INSTRUCTED

SECTION A – Answer SIX parts of this section

1.1) The same memory allocation of 4 bytes may be used to store a real or an integer variable. Explain the difference in the way they are stored. What consequences does this have on the possible precision and magnitude of the two types of variables?

[7]

1.2) What is the difference between a function and a subroutine in Fortran 90? What are the advantages of splitting a long program into separate functions and subroutines?

[7]

1.3) What is printed out by the following section of Fortran 90 code? Mark the spaces as well as the characters.

```
integer :: x=4
real :: y=0.75, z=.0012
character*6 :: a ='metres'
write(*,10)x,y,z,a
10 format(' x=',i4,', y=',f5.2,', z=',e10.3,a6)
```

[7]

1.4) Write down two methods of passing an integer array containing 10 elements into a subroutine, using Fortran 90. What are the advantages of each method?

[7]

1.5) What is printed out by the following section of code?

```
do i=0,8,2
     do j=1,i/2
          print*,i,j
     enddo
enddo
```

[7]

1.6) Write lines of Fortran 90 code that read in 10 real numbers from a file called `data.dat`, and print out their sum and mean.

[7]

1.7) Write the lines of Fortran 90 code which would set up a 3x3 matrix called *A* and allocate the values as shown:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

[7]

1.8) If the integer `n=2` and the real `a=4.0`, what are the values of the real variable `x` after the following statements?

a) `x=n/3+a`
b) `x=n/(3+a)`
c) `x=real(n)/3.+a`
d) `x=a**2/n`
e) `x=sqrt(a)`
f) `x=int(-2.9)`
g) `x=nint(-2.9)`

[7]

SECTION B – Answer TWO questions

2) Write a function (or subroutine) in Fortran 90 that takes as its argument a value of x (in radians) and calculates to 5 significant figures, the value of the function, erf(x) (known as the error function) which is given by the convergent series:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{n!(2n+1)}$$

Note that erf(x) converges to the value 1 for large x, such that erf(3.5)=.999999

[30]

3) The results of an experiment give you a list of 100 data points (in the form (x_i , y_i) where i=1, 2…,100), which should follow a polynomial equation:

$$y = a_1 + a_2 x + a_3 x^2 \ldots a_{n+1} x^n$$

where a_i are constants which you would like to determine from your results. There is a library subroutine called `polyfit`, which fits a polynomial of order n to the data points given. Its specification is:

`SUBROUTINE polyfit(x,y,m,a,n+1)`
`n, m` are integers. `m` is the number of points, `n` is the order of the polynomial.
`x(m), y(m), a(n+1)` are real arrays of the size indicated. The i^{th} point to be fit to the curve is given by `(x(i), y(i))`. `a` is the array of coefficients, such that, on exit from the subroutine, `a(i)`= a_i.

Write a program which reads in the 100 data points from a file called `data.dat` and uses the library routine to find the best values of the constants a_i, i =1…4, when the points are fitted to a cubic polynomial.

[20]

Explain, without writing any more code, how you might investigate numerically how closely the polynomial curve fits the data points.

[10]

4) The Newton-Raphson numerical method finds the roots of an equation. It states that if x_1 is an approximation to a root of the equation, $f(x)=0$, then x_2 is a better approximation, where:

$$x_2 = x_1 - \frac{f(x_2)}{f'(x_1)}$$

and $f'(x)$ is the first derivative of $f(x)$.

Write a program in Fortran 90, which uses the Newton-Raphson method to find the first two non-zero, positive roots of:

$$f(x) = \tan x - x = 0\,.$$

[20]

What precautions do you have to take when using this method to find the roots of a general equation?

[10]

5) Write a Fortran 90 function which calculates the value of:

$$f(x) = \frac{x^2 + x - 5}{x^2 - 1}$$

for a given value of x.
Your function should print out a warning if x has a value that makes $f(x)$ difficult to compute.

[15]

How would you alter this code to calculate a more general function:

$$f(x) = \frac{ax^2 + bx + c}{x^2 + d}$$

Explain how you would pass the constants a, b, c and d to your function.

[15]

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