King's College London

UNIVERSITY OF LONDON

B.Sc. EXAMINATION

CP1710 Computing for Physical Sciences

Summer 2006

Time allowed: THREE Hours

Candidates should answer ALL parts of SECTION A, and no more than TWO questions from SECTION B. No credit will be given for answering further questions.

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

You must not use your own calculator for this paper. Where necessary, a College calculator will have been supplied.

TURN OVER WHEN INSTRUCTED

Physical Constants

Permittivity of free space	ϵ_0	=	8.854×10^{-12}	$\mathrm{F\,m^{-1}}$
Permeability of free space	μ_0	=	$4\pi \times 10^{-7}$	$\mathrm{H\,m^{-1}}$
Speed of light in free space	c	=	2.998×10^{8}	$\mathrm{m\,s^{-1}}$
Gravitational constant	G	=	6.673×10^{-11}	$\mathrm{N\,m^2\,kg^{-2}}$
Elementary charge	e	=	1.602×10^{-19}	C
Electron rest mass	m_e	=	9.109×10^{-31}	kg
Unified atomic mass unit	m_u	=	1.661×10^{-27}	kg
Proton rest mass	m_p	=	1.673×10^{-27}	kg
Neutron rest mass	m_n	=	1.675×10^{-27}	kg
Planck constant	h	=	6.626×10^{-34}	J s
Boltzmann constant	k_B	=	1.381×10^{-23}	$\mathrm{J\,K^{-1}}$
Stefan-Boltzmann constant	σ	=	5.670×10^{-8}	$\mathrm{W\,m^{-2}\,K^{-4}}$
Gas constant	R	=	8.314	$\mathrm{J\,mol^{-1}\,K^{-1}}$
Avogadro constant	N_A	=	6.022×10^{23}	$\mathrm{mol^{-1}}$
Molar volume of ideal gas at STP		=	2.241×10^{-2}	$\mathrm{m^3}$
One standard atmosphere	P_0	=	1.013×10^{5}	$\mathrm{N\,m^{-2}}$

Where necessary, you may assume that the following *C* functions are declared in the library `math.h`

```
double sqrt( double x);  // Returns the positive square root of x
double erf( double x);   // Returns the value for the
                         //  error function (erf) of x
```

Ensure that any *C* code that you write is clearly laid out, and contains sufficient comments for the reader to understand the code.

SECTION A – Answer ALL parts of this section

1.1) Identify which five of the following names are not valid for *C* variables, giving a reason in each case.

```
convert$        menu.title
False           notfound?
integer         switch
hh:mm:ss        two4[1]
last_entry      2for1
```

[5 marks]

1.2) The following three statements appear *before* the `main()` function of a *C* program is defined:

```
#include <time.h>
#define ARRAY_SIZE 1200
void Delay( unsigned long duration);
```

Briefly describe the consequences of each statement.

[7 marks]

1.3) Write down the output that is generated by the following *C* program, reproducing carefully the layout that the program will produce.

```
#include <stdio.h>  // needed for I/O
int main()
{
   unsigned int n;
   float x, y;
//
   for (n=1, x=2.0, y=1.0; n<=7; n++)
   {
      y *= x;
      printf( "n=%1u, y=%5.1f \n", n, y);
   }
   return 0;
}
```

[7 marks]

1.4) What information does each of the following *C* statements provide to the compiler?

```
struct vector { float x; float y; float z;};
struct vector position;
struct vector Cross_product( struct vector a, struct vector b);
```

[7 marks]

1.5) Define a function in *C* with two real arguments x and y that will return the value of the expression

$$\left|\frac{x-y}{x+y}\right|$$

where the vertical bars $|\ldots|$ denote the absolute value of the expression inside. Comment briefly on how your function deals with any special cases that might arise.

[7 marks]

1.6) A *C* program initialises the variables `a, b, c` and `f` in the following way.

```
int a[3]={10, 20, 30};
int b=4, f;
int *c=a;
```

Determine the values of `f` after the execution of each of the *C* statements below.

```
f = a[0] + (*(a+2));
f = (--b) * (*c);
f = ++(*a) * (*(++c));
```

[7 marks]

SECTION B – Answer TWO questions

2a) The **bisection** method can sometimes be used to locate a real root of the equation $f(x) = 0$. State the conditions that must be satisfied for the bisection method to be successful, and briefly describe the main steps involved in the bisection method.

[10 marks]

b) The equation

$$2x^4 - 4x^2 + 1 = 0$$

has 4 real roots, one of which is known to lie between $x = 0$ and $x = 1$. Estimate how many iterations of the bisection method would be required to locate this root inside an interval of width 1.0×10^{-5}.
Explain briefly why it is certain (without further calculation) that a second root lies between $x = -1$ and $x = 0$.

[6 marks]

c) Write a `main()` *C* program that uses the bisection method to find, and print out, the root of the equation lying between $x = 0$ and $x = 1$, to an accuracy of better than $\pm 5.0 \times 10^{-6}$.

[10 marks]

d) Explain why it is not possible to use the bisection method to find any of the 4 real roots of the very similar equation

$$2x^4 - 4x^2 + 2 = 0$$

[4 marks]

3a) The mean value $\bar{x}$ and standard deviation σ of a set of N data values are given by the formulae

$$\bar{x} = \frac{1}{N}\sum_{n=0}^{N-1} x_n, \qquad \text{and} \qquad \sigma = \sqrt{\left(\frac{1}{N}\sum_{n=0}^{N-1} x_n^2\right) - (\bar{x})^2}$$

where x_n denotes an individual reading.

Provide suitable definitions for two *C* functions that will calculate the mean and standard deviation, respectively, of a one-dimensional array of real data with N elements. Assume that the function declarations are:

```
float Mean( float data[], unsigned long N);
float Stdev( float data[], unsigned long N);
```

[15 marks]

b) Experimental data are stored in a plain text file named `dataset.txt` as a list of 1000 real values, with one value per line. Write a `main()` *C* program that will carry out the following tasks:

(i) Read all the values from the file into a one-dimensional array.

(ii) Calculate the mean and standard deviation of the data using the functions `Mean()` and `Stdev()` declared above, and print out this information to the display, giving all numerical values in scientific notation, accurate to 3 decimal places.

(iii) Search through all the data, counting the number of times that the data value lies within each of the following ranges:
A — no more than 1 standard deviation from the mean,
B — between 1 and no more than 2 standard devations from the mean,
C — more than 2 standard deviations from the mean value.
Print a suitable message to the display providing this information to the user.

[15 marks]

4a) The error function $\mathrm{erf}(x)$ is used in statistics, and has both integral and series representations

$$\begin{aligned}\mathrm{erf}(x) &= \frac{2}{\sqrt{\pi}} \int_0^x \exp(-x^2)\, \mathrm{d}x \\ &= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{n!(2n+1)}\end{aligned}$$

Define a function in C that will return the value of $\mathrm{erf}(x)$ using the first n terms of the series expression given above. The function you define should have the following declaration:

```
double Erf( double x, unsigned n);
```

[12 marks]

b) Write a `main()` program in C that will carry out the following tasks:

(i) Repeatedly prompt the user to supply a value for the variable `x`, exiting when the value zero is supplied.

(ii) Print out the value of $\mathrm{erf}(x)$, calculated by the function `Erf(x, n)` that you have defined above, for all integer values of `n` ≤ 10,

(iii) Calculate $\mathrm{erf}(x)$ using the C library function `erf(x)`, and print this value on the line following the results of the series approximation.

[12 marks]

c) Assuming that $x = 1$, explicitly calculate the first few terms in the series expansion of $\mathrm{erf}(x)$, and hence estimate how many terms would be needed to obtain a value that is accurate to 3 decimal places.

[6 marks]