3rd Year B.Sc. Honours Examination 2011 B6

Programming and Scientific Computation - PH306

2.00 pm- 5.00 pm. May 10, 2012

Instructions: Answer the following questions. The mark for each part of a question is indicated on the right. Once done writing and executing codes, **please copy them in the exam book**. Any plot that you make, **must be saved for later viewing**.

Time: 3 hours. **Total Marks**: 25

1. Consider the simple Logistic Map defined by the recursive relation

$$x_{n+1} = a - x_n^2$$

where a is a parameter.

(a) Write a `C` or `C++` function `double logistic(double a, double x0, int n)` that calculates the n-th order iterated value of x starting from a given $x0$ and using a given a. [3]

(b) In the `main()` function, call the function `logistic(a,x0,n)` with $a = 0.5$, $a = 1.476$ and $a = 2.0$ starting from $x_0 = 0.5$ for $n \in [0, 100]$. Write the value of n in the first column of a file, and successive values x_n for different a in different columns of the file. [3]

(c) Plot the successive values of x_n with respect to n for different a using `gnuplot`. Save the file(s) as postscript file. [2]

(d) Now change the program and write the values of x_{n-1} and x_n in two different columns of another datafile. Plot x_n vs x_{n-1} for $a = 2$ using `gnuplot` and save the plot in a postscript file. [2]

2. In Fluid dynamics, the Navier-Stokes equations may be reduced to a set of three coupled first order ordinary differential equations, known as the Lorenz Model:

$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t} &= \sigma(y - x) \\
\frac{\mathrm{d}y}{\mathrm{d}t} &= -xz + rx - y \\
\frac{\mathrm{d}z}{\mathrm{d}t} &= xy - bz
\end{aligned}$$

where, x, y, z are called the Lorenz variables, derived from the temperature, density, and velocity variables in the original Navier-Stokes equations. The parameters σ (Prandtl number), r(Rayleigh number) and b (Physical proportion) are measures of the temperature difference across the fluid and other fluid parameters. Take, $\sigma = 10$ and $b = 8/3$, which correspond to cold water.

(a) Write a C or C++ program that solves the above coupled differential equations to get x, y and z as functions of the the time t. Take, the initial conditions $x_0 = 1$, $y_0 = z_0 = 0$ and the parameter $r = 5$. Write the values of t, x, y and z on the first four columns of a datafile. [5]

(b) Plot (i) z versus time t and (ii) z versus x for $t \in [0, 100]$ using `gnuplot` for three values of $r = 5, 10, 25$. Save the plots as postscript files. Which plot is qualitatively different from the other two for one particular value of r? [3]

3. For extremely relativistic particles at high density, the energy can be approximated as $\epsilon = pc$, where p is the momentum and c is the speed of light. The element of momentum space is $\mathrm{d}p = 4\pi(\epsilon^2/c^3)\mathrm{d}\epsilon$. For bosons and fermions, the distribution laws are:

$$f_{\mathrm{BE}}(\epsilon) = \frac{1}{\exp(\epsilon/kT) - 1} \quad , \quad f_{\mathrm{FD}}(\epsilon) = \frac{1}{\exp(\epsilon/kT) + 1}$$

(a) Define $\eta = \epsilon/(kT)$. Using `Maple`, plot f_{BE} and f_{BE} as functions of η for $\eta \in [-2, 3]$ and $y \in [0, 2]$. [2]

(b) Using `Maple`, evaluate the total number of particles N in a volume V at temperature T for both bosons and fermions using the formula: $N = (gV/h^3)\int_0^\infty f(\epsilon)\mathrm{d}p$. Here, g is the degeneracy and h is Planck's constant. [1+1]

(c) Using `Maple`, evaluate the total internal energy U of particles in a volume V at temperature T for both bosons and fermions using the formula: $U = (gV/h^3)\int_0^\infty \epsilon f(\epsilon)\mathrm{d}p$. [1+1]

(d) For photons, degeneracy $g = 2$. Using `Maple`, plot the energy density $\rho = U/V$ as a function of energy ϵ in the range $[0, 20]$. Take $c = h = 1$. This is the famous Planck's distribution law. [1]

Save the worksheet that contains the `Maple` commands that you wrote and the plot(s).

$$P_n(x) = \frac{1}{\pi}\int_0^{\pi}\left[x + \sqrt{x^2-1}\cos\phi\right]^n \mathrm{d}\phi$$

(a) Write a `Maple` procedure or function, `legendre(n,x)`, that evaluates the Legendre Polynomial of order n, using the above relations, at some point x. [3]

(b) Using `Maple`, evaluate

$$\int_{-1}^{1} P_m(x)P_n(x)\mathrm{d}x$$

for $m \neq n$ and $m = n$. Take $m, n = 1, 2, 3, \ldots$ etc. [2]

(c) Using `Maple`, plot $P_3(x)$ and $P_5(x)$. [2]

(d) Using `Maple`, find the zeros of $P_3(x)$. [1]

2. The generating function for the Legendre polynomials $P_n(x)$ is $g(x,t) = 1/\sqrt{1-2xt+t^2}$, with $0 < t < 1$ such that

$$\sum_{n=0}^{\infty} P_n(x)t^n = g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}}$$

(a) Use the `taylor` command to generate the first five Legendre polynomials from the above definition of the generating function. [2]

(b) Use the `coeftayl` command to write a `Maple` function, `legendre(n,x)`, that evaluates the Legendre polynomials of order n, using the above relation, at some point x. [2]

(c) Using `Maple`, plot $P_3(x)$ and $P_5(x)$. [1]

(d) Using `Maple`, find the zeros of $P_3(x)$. [2]

Save the worksheet that contains the `Maple` commands that you wrote and the plot .

1. Random numbers may be used to calculate integrals. This method is known as Monte Carlo Integration. Consider the following integral

$$I = \int_{-1}^{1} \frac{2}{1+x^2}\mathrm{d}x$$

(a) Generate a sequence of pair of random numbers (x, y) with $x \in [-1, 1]$ and $y \in [0, 1]$. Write a `C` or `C++` function `double integral2(int N)` to calculate the value of the integral by comparing the area under the curve $y = \frac{2}{1+x^2}$ and that of the rectangular region with sides 2 and 1 using N pairs of random numbers, i.e. N points. [4]

(b) Increase the number of points used to evaluate the area and find the errors in each case. Take $N \in [10, 10^7]$. The exact value of the integral is π. [2]

(c) Write the number of points and the errors in two columns of a file. Plot the error vs the number of points used and the save the plot as a postscript file. [2+1]

2. The Euler's method for solving the second order ordinary differential equation $\mathrm{d}^2x/\mathrm{d}t^2 + \omega^2 x = 0$, written as a set of coupled first order difference equations is

$$\begin{aligned} x_{n+1} &= x_n + f(x_n, t_n)(t_{n+1} - t_n) = x_n + z_n h \\ z_{n+1} &= z_n + g(z_n, x_n, t_n)h = z_n - \omega^2 x_n h \end{aligned}$$

Consider the initial conditions $x_0 = 0$, $z_0 = 1$.

(a) Write a C/C++ code that solves the above initial value problem. Your code should write the values of t, x and z in different columns of a file. [6]

(b) Plot the values of $z = \frac{\mathrm{d}x}{\mathrm{d}t}$ vs. x for $\omega = 1, 4, 9, 16$. [3]

$$\rho_e(r) = -\frac{q}{\pi}e^{-2r}, \qquad \rho_p(r) = q\delta(\vec{r})$$

where we have adopted the system of units in which the Bohr radius $a_0 = 1$ and $k_e = 1/(4\pi\epsilon_0) = 1$. The system is spherically symmetric and hence volume integration of a radial function $f(r)$ can be expressed as $\int f(r)\mathrm{d}^3r = 4\pi\int_{r=0}^{\infty} f(r)\,r^2\mathrm{d}r$. Also, recall that $\int \delta(\vec{r})\mathrm{d}^3r = 1$
Hint: The `Maple` function for the Dirac delta function $\delta(r)$, is `Dirac(r)`. Use `Pi` for π in `Maple` instead of `pi`.

(a) Using `Maple` find the total positive and negative charges of the atom. Do your answers make sense? [2]

(b) Using `Maple` evaluate

$$\int_{-\infty}^{\infty} j_m(x)j_n(x)\mathrm{d}x, \qquad m,\, n \geq 0$$

for (a) $m \neq n$ and (b) $m = n$ taking $m, n = 0, 1, 2, \ldots$ etc. Can you interpret the result? Can you guess the value of the integral for general m, n? [2+0.5+0.5]

4. (a) Using `Maple`, evaluate the magnetic field at a distance D for in infinitely long wire procedure `laguerre:=proc(n,x)`, that recursively calculates the Laguerre Polynomial of order n, using the above relations, at some point x. [5]

(b) Use the above procedure `laguerre(n,x)` to calculate the values of $n!L_n(x)$ for $n = 1, 2, \ldots 4$ and plot them. [2]