3rd Year B.Sc. Honours Examination 2012$_{\text{B1}}$

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 03, 2013

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. A series expansion for the Fresnel integral $C(x) = \int_0^x cos(\pi t^2/2)\mathrm{d}t$ is given by :

$$C(x) \quad = \quad \sum_{k=0}^{\infty} \frac{(-1)^k (\pi/2)^{2k} x^{4k+1}}{(2k)!(4k+1)}$$

where $(2k)! = 1.2.3.4.5 \ldots (2k)$ is the factorial of $(2k)$.

(a) Define a C or C++ function `double fresnel1(double x, int n)` that evaluates the series expansion for the Fresnel integral using the expansion up to the n-th term in the series for a given value of the arguments x and n. You may want to define your own function `factorial(n)` to calculate $n!$ and call it appropriately. [6]

(b) Plot your function `fresnel(x,n)` with $n = 20$, for $x \in [0.0, 2.0]$ using `gnuplot` and save the plot as a postscript file. [2+1]

(c) Can you guess the value of $\lim_{x\to\infty} C(x)$. Using your program above evaluate $\lim_{x\to R} C(x)$ by taking R large and find the asymptotic value. [1]

2. In neutron transport theory the critical length of a fuel rod in a reactor is determined by the roots of thr equation:

$$\cot(x) = (x^2 - 1)/(2x) = (x - 1/x)/2$$

(a) Using `gnuplot` plot $\cot(x)$ (x in radians) and on the same plot, graph $(x^2 - 1)/(2x)$. Plot the functions with different colored lines and save the plot as a postscript file. How many intersections are there? [2+1]

(b) Using any suitable root finding method, write a C or C++ program that finds the the **smallest positive root** of this equation. Does your answer tally with the root(s) that you get from the inspection of the plot above? [6+1]

3. The Bernstein polynomials of degree n are dened by

$$B_{k,n}(x) = \frac{n!}{k!(n-k)!} x^k (1-x)^{n-k}$$

where $k = 0, 1, 2, \ldots n$

(a) Write a `Maple` procedure or function `Bernstein(k,n,x)`, that calculates the Bernstein Polynomial of degree n and index k , using the above relations, at some point x. [2]

(b) Use the above procedure or function `Bernstein(k,n,x)` plot the Bernstein polynomials of degrees $n = 1, 2, 3$ with all possible k-values using `Maple` for $x \in [0, 1]$. [3]

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

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

(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]

1. 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]

2. The electron and the nuclear charge densities of the hydrogen atom are given by

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

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]

3. (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]