3rd Year B.Sc. Honours Examination 2012 B5

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 13, 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. The spherical Bessel function of the first kind $j_n(x)$ is defined by the infinite series representation as:

$$j_n(x) = x^n \sum_{k=0}^{\infty} \frac{(-x^2/2)^k}{k!(2n+2k+1)!!}$$

where $k! = 1.2.3.\ldots k$ is the factorial of k and $(2s+1)!!$ is the double factorial of $2s+1$ defined as $(2s+1)!! = (2s+1).(2s-1).(2s-3).\ldots.3.1.$

(a) Write a `C` or `C++` function `double jn(double x, int n,int M)` that evaluates the spherical Bessel function of the first kind $j_n(x)$ using the above definitions and using the first $(M+1)$ terms in the infinite series. Take suitable value of M for evaluating the function `jn(x)`. You may want to define your own factorial and double factorial functions in evaluating the series. [4+1+1]

(b) In a complete `C` or `C++` program write the values of x in the first column and the values of the function $j_n(x)$ in consecutive columns for different values of n. Plot, using `gnuplot` the functions $j_n(x)$ in the range $x \in [0, 10]$ using the above C/C++ function for $n = 0, 1, 2, 3$ in the same plot. Save the two plot as postscript files. [2+2]

2. The modified Besssel function of the first kind $I_\nu(x)$ has the integral representation given by

$$I_\nu(x) = \frac{1}{\pi^{1/2}(\nu - \frac{1}{2})!}\left(\frac{x}{2}\right)^\nu \int_{-1}^{1} \exp{(xp)}(1-p^2)^{\nu-1/2}\,\mathrm{d}p$$

where $\nu > -1/2$. For this problem, take $\nu = n = 1, 2, 3, 4, \ldots$ etc.

(a) Using any suitable numerical integration scheme, write a `C` or `C++` function `double BesselI(double x, int n)` that evaluates the modified Besssel function of the first kind $I_n(x)$, where n is a positive integer. Use suitable number of grid points beetwen the interval $[-1, 1]$. You need to define your own function for calculating the factorial. [6]

(b) Call the above function `BesselI(x,n)` in a complete `C` or `C++` program and write the values of x in the first column and the function values $I_n(x)$ in consecutive columns for $n = 1, 2, 3, \ldots$ for $x \in [0, 3]$ in a file. Plot $I_n(x)$ versus x for $n = 1, 2, 3$ using `gnuplot` in a single plot and save the plot as a postscript file. [3+2]

3. An integral representation for the Kelvin functions $\mathrm{ber}_n(x)$ and $\mathrm{bei}_n(x)$ are given by:

$$\mathrm{ber}_n(x) = \frac{(-1)^n}{\pi}\int_0^\pi \cos{(x\sin{(t)}/\sqrt{2} - nt)}\cosh{(x\sin{(t)}/\sqrt{2})}\mathrm{d}t$$

$$\mathrm{bei}_n(x) = \frac{(-1)^n}{\pi}\int_0^\pi \sin{(x\sin{(t)}/\sqrt{2} - nt)}\sinh{(x\sin{(t)}/\sqrt{2})}\mathrm{d}t$$

(a) Write `Maple` functions `ber(n,x)` and `bei(n,x)`, that evaluates the Kelvin functions $\mathrm{ber}_n(x)$ and $\mathrm{bei}_n(x)$, using the above definition, at some point x. [1+1]
[Hint: The `Maple` symbol for π is `Pi`].

(b) Using `Maple`, plot $\mathrm{ber}_0(x)$ and $\mathrm{bei}_0(x)$ in the same plot for $x \in [0, 2]$. [1]

(c) Using `Maple` evaluate the first derivatives of the Kelvin functions i.e. $\mathrm{ber'}_n(x)$ and $\mathrm{bei'}_n(x)$ for $n = 0, 1$. [0.5+0.5]

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

$$csch(x) = \frac{1}{x} + 2x \sum_{k=1}^{\infty} \frac{(-1)^k}{x^2 + (k\pi)^2}$$

for $x \neq 0$

(a) Define a C or C++ function `double cosech(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. [5]

(b) Plot your function `cosech(x,n)` with $n = 20$, for $x \in [0.1, 1.0]$ using `gnuplot` and save the plot as a postscript file. [2+1]

2. The Legendre Polynomials have the integral representation

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

(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]