3rd Year B.Sc. Honours Examination 2012B7

Programming and Scientific Computation - PH306

2.00 pm- 5.00 pm. April 19, 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 Chebyshev polynomial of type I of order n is defined by the series expansion

$$T_n(x) = \frac{n}{2} \sum_{m=0}^{[n/2]} (-1)^m \frac{(n-m-1)!}{m!(n-2m)!} (2x)^{n-2m}$$

where $[n/2]$ denotes the greatest positive integer less than (when n is odd) or equal to (when n is even) $n/2$. (For example, $[n/2] = 2$, when $n = 4$ and $[n/2] = 2$, when $n = 5$.)

   (a) Write a `C` or `C++` function `double mycheb(double x, int n)` that evaluates the Chebyshev polynomial of type I, $T_n(x)$ using the above definition. (Hint: You may want to define your own function `double fact(int n)` to evaluate the factorials in the series or do otherwise.) [4+2]

   (b) Call `mycheb(n,x)` in a complete `C` or `C++` program to write the values of $T_n(x)$ for $n = 1, 2, 3, 4$ in different columns of a file for $x \in [-1, 1]$. Plot the functions $T_n(x)$ for $n = 1, 2, 3, 4$ with respect to x using `gnuplot` and save the file as a postscript file. [2+2]

2. The modified Struve's function $M_\nu(x)$ has the integral representation given by

$$M_\nu(x) = -\frac{2(x/2)^\nu}{\sqrt{\pi}(\nu - 1/2)!} \int_0^1 \exp(-xt)\ (1-t^2)^{\nu-1/2}\, \mathrm{d}t$$

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 modstruv(double x, int n)` that evaluates the modified Struve's function $M_n(x)$, where n is a positive integer. Use suitable number of grid points for $t \in [0, 1]$. You need to define your own function for calculating the factorial. [6]

   (b) Call the above function `modstruv(x,n)` in a complete `C` or `C++` program and write the values of x in the first column and the function values $M_n(x)$ in consecutive columns for $n = 1, 2, 3, \ldots$ for $x \in [-2, 2]$ in a file. Plot $M_n(x)$ 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 Struve's function $H_\nu(x)$ is given by:

$$H_\nu(x) = \frac{2(x/2)^\nu}{\sqrt{\pi}(\nu - 1/2)!} \int_0^\pi \sin(x\cos(t))\ (\sin(t))^{2\nu}\, \mathrm{d}t$$

   (a) Write `Maple` functions `struv(n,x)` that evaluates the Struve's function $H_\nu(x)$, using the above definition, at some point x. [2]
   [Hint: The `Maple` symbol for π is `Pi`].

   (b) Using `Maple`, plot $H_\nu(x)$ for $\nu = 0, 1/2, 1, 3/2, 2, 3$ in the same plot for $x \in [0, 10]$. [2]

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]