3rd Year B.Sc. Honours Examination 2012B3

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 04, 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 error function $\mathrm{erf}(x) = (2/\sqrt{\pi}) \int_0^x \exp(-t^2)\mathrm{d}t$ has the following infinite sum representation containing finite product as :

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \left(x + \sum_{i=1}^{\infty} \frac{x}{2i+1} \prod_{k=1}^{i} \frac{(-x^2)}{k} \right)$$

   (a) Write a `C` or `C++` function `double error(double x, int n)` that evaluates the series expansion of the error function from the above expansion usin up to the n-th term in the series for a given value of the arguments x and n. Call the function in a complete `C` or `C++` code. [5]

   (b) Write the values of your function `error(x,n)` with $n = 5, 10, 20$, for $x \in [0.0, 2.0]$ in three columns of a file and plot the data for the three cases in a single plot using `gnuplot` and save the plot as a postscript file. [2+1]

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

2. Suppose that for a mass-spring system, the force is given by the usual spring force $F = -kx$ but the inertia is dependent on the speed i.e. $m = M \exp(v/w)$. The differential equation of motion of such an oscillator is given by

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} + (k/M)x \exp\Big(- (\mathrm{d}x/\mathrm{d}t)/w \Big) = 0$$

   where $v = \mathrm{d}x/\mathrm{d}t$ is the speed of the particle, w is a characteristics speed of the particle in the system. Take $M = 1.0$, $k = 1.0$ and $w = 5.0$. Consider the initial conditions $x(0) = 1$ and $v(0) = \dot{x}(0) = 0$.

   (a) Using the fourth order Runge-Kutta (RK4) method solve the above differential equation (you can **not** apply Euler's method for this problem). [6]

   (b) Plot the position x vs time t graph and from there determine the time period of oscillations when the maximum amplitude equals to (a) $x(0) = 0.1$ (b) $x(0) = 1$ and (c) $x(0) = 10$. Save the plots for each case as postscript files. [3]

   (c) Can we make a good clock using a mass connected to a such a "mass"-spring system ? For a simple harmonic oscillator, does the period depend on the amplitude of oscillation? Justify your claim. [2]

3. An integral representation for the Hermite polynomials $H_n(x)$ is given by:

$$H_n(x) = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} (x + it)^n \exp(-t^2)\mathrm{d}t$$

   (a) Write a `Maple` function `Hermi(n,x)`, that evaluates the Hermite polynomials $H_n(x)$, using the above definition, at some point x. [2]
   [Hint: The `Maple` symbol for $i = \sqrt{-1}$ is `I` and that for π is `Pi`].

   (b) Using `Maple`, plot $H_n(x)$ for $n = 1, 2, 3, 4$ in the same plot for $x \in [0, 2]$. [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]