3rd Year B.Sc. Honours Examination 2012$_{\text{B2}}$

Programming and Scientific Computation - PH306

2.00 pm- 5.00 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. Random numbers may be used to calculate integrals. This method is known as Monte Carlo Integration. Consider the following integral

$$I = \int_0^\pi \frac{1}{1+\sin^2(x)} \mathrm{d}x$$

   (a) Generate a sequence of pair of random numbers (x, y) with $x \in [0, \pi]$ 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 $y = 1/(1 + \sin^2(x))$ and that of the rectangular region with sides π and 1 using N pairs of random numbers, i.e. N points. [5]

   (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 $\pi/\sqrt{2}$. [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 differential equation of motion of a particle of unit mass moving in an anharmonic potential is given by

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + kx\Big(1 + \exp(-x/a)\Big) = 0$$

   where $k = 1.0$ and $a = 0.05$. 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). [5]

   (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 "spring" ? For a simple harmonic oscillator, does the period depend on the amplitude of oscillation? Justify your claim. [2]

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

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

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

   (a) Write two `Maple` functions `fresnelint(x)` and `fresnelser(x)` that evaluates the integral and series expansions of Fresnel integrals using the above definitions. [2+2]

   (b) Plot your functions `fresnelint(x)` and `fresnelser(x)` using `Maple` and save the plots. [0.5+0.5]

   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]