# Computational Physics Lab Continuous Assessment Exam

**Time : 1 hour**

**February 04, 2016 (Session 4)**

*Answer all. Any deviation from instructions will lead to **zero grade***

**1.** The force between the $Na^+$ and $Cl^-$ ions can be modeled as

$$f(r) = -\frac{q^2}{4\pi\epsilon_0 r^2} + \frac{V_0}{r_0}e^{-r/r_0} = 132.276(r_0^2/r^2) + 3303.03e^{-r/r_0} \quad (1)$$

where $q^2/(4\pi\epsilon_0) = 14.4\text{Å}-eV$, $V_0 = 1090eV$ and $r_0 = 0.33\text{Å}$.

(a) Plot $f(x) = -132.276/x^2 + 3303.03e^{-x}$ vs. $x(= r/r_0)$ in the range $x \in [0.15, 10]$ and save the plot as a postscript file.

(b) Using the **Newton-Raphson method** or **Secant method**, write a C++ program that finds the equilibrium length between the $Na^+$ and $Cl^-$ ions. Does your answer tally with the root(s) that you get from the inspection of the plot above?

[4 + 6]

**2.** The Dirac delta function has a representation

$$\delta_n(x - x_0) = \frac{n}{\pi}\frac{1}{1 + n^2(x - x_0)^2}$$

which becomes the exact delta function in the limit $n \to \infty$.

(a) Write a Maple function deltan(n,x,x0) that evaluates the above representation of the delta function.

(b) Plot the functions deltan(n,x,x0) for x in the range $x \in (-10, 10)$ with $x_0 = 2$ and different values of n = 1, 10, 20.

(c) Define a Maple function f(x) where $f(x) = cos(x^2) + sin(x^2)$.

(d) Using Maple, integrate numerically $\delta_n(x - 2)f(x)$ for n = 10, 100, 500 over the range $x \in (-10, 10)$ and compare your results with the numerical value of f (2) in the three cases.

[2.5 + 2.5 + 2 + 2 + 1]