

PHY 312/628 - Numerical Methods and Programming

(Hands-on session)

Problem 1: Write programs to find the root of $f(x) = e^{-x} - x$ using bisection, false-position method and Newton-Raphson methods (True root = 0.56714329). Plot the "true error" in all the cases as a function of iteration to show which of them converges faster.

Problem 2: Determine the positive real root of $x^{20} - 1$ using bisection, false-position method and Newton-Raphson methods. Plot the "approximate error" in all the cases as a function of iteration to show which of them converges faster. Use different initial conditions and show this.

Problem 3: In a diatomic molecule NaCl, the interaction potential between the Na^+ and Cl^- ions can be modelled as: $V(r) = -\frac{e^2}{4\pi\epsilon_0 r} + V_0 \exp(-r/r_0)$.

At equilibrium the force between the ions is: $f(r) = -\frac{dV(r)}{dr} = -\frac{e^2}{4\pi\epsilon_0 r^2} + \frac{V_0}{r_0} \exp(-r/r_0)$. Find the root of $f(r) = dg(r)/dr = 0$ with $g(r) = -V(r)$. This will give us the equilibrium distance between the ions. Use $V_0 = 1.09 \times 10^3 eV$, $r_0 = 0.330 \text{ \AA}$ and, $e^2/4\pi\epsilon_0 = 14.4 \text{ \AA}^2 eV$.