Physics 5403: Computational Physics – Project 1

due date: Sep 3, 2019

Part 1: Potential of a dipole (75 points)

A Na\(^+\) ion (charge +e) is located on the positive x-axis at a distance of 5Å from the origin. A Cl\(^-\) ion (charge −e) is located on the negative x-axis, also a distance of 5Å from the origin. In this project, you will explore the electric potential produced on the x-axis by these two charges. Specifically, you will compare the exact potential with the dipole approximation.

a) Write a program which calculates the exact electric potential \(V_{\text{exa}}\) and the dipole approximation \(V_{\text{dip}}\) of the two charges on the x-axis in the interval \([-x_{\text{max}}, x_{\text{max}}]\) using \(M\) equidistant points. The program should also calculate \(\Delta V = |V_{\text{exa}} - V_{\text{dip}}|\).

b) Think about how to choose reasonable values for the parameters \(x_{\text{max}}\) and \(M\). Run the simulation for your chosen values of \(x_{\text{max}}\) and \(M\). Plot \(V_{\text{exa}}\) and \(V_{\text{dip}}\) vs. \(x\).

c) What behavior do you expect for the difference \(\Delta V\) as a function of \(x\)?

d) Write a program which fits \(\Delta V\) to a power law, \(\Delta V = cx^{-n}\) with given exponent \(n\) but unknown “floating” prefactor \(c\) for all \(x > x_{\text{fit}}\). The answer to c) should tell you which \(n\) to use. Think about reasonable values for \(x_{\text{fit}}\).

e) Run the fit program and plot \(\Delta V\) vs. \(x\) together with the power law resulting from your fit. Compare the fit value of \(c\) with the expected value. Discuss the result.

Part 2 Numerical differentiation (25 points)

Numerically differentiate the function given in the file function.dat on the class web site. Vary the step width \(h\), and analyze how the systematic and random error change.