Physics 5403: Computational Physics – Project 1

due date: Sep 6, 2022

Potential of a dipole (100 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) Derive the dipole approximation by Taylor expanding the potential for distances large compared to the separation between the charges. Keep the lowest order non-vanishing term.

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

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

d) What behavior do you expect for the difference ΔV as a function of x?

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

f) Run the fit program and plot ΔV vs. x together with the power law resulting from your fit. Compare the fit value of c with the expected value. Discuss the result.

Bonus: 2 Numerical differentiation (10 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.