Physics 305 – Computational Physics, Fall 2020
Term Project
Full project submission Due Date: Tuesday December 15, 5pm
Presentation Phase: November 30 - December 11

The program in your term project can be either submitted as a python program or ipython notebook, where the latter is preferred. The program, an explanation of what the program does, along with answers to **all** questions asked should be uploaded to d2l.

You are expected to write a term paper (in word or Latex) on your project that discusses the problem you are trying to solve, the basic equations that govern the problem, includes plots that show the solutions, and describes the solution and the numerical method involved. In addition, you must demonstrate that your solution is correct by showing that the code converges at the expected order. If your code does not converge at the expected order you should try to identify potential reasons for why this is the case. You are expected to work on your term project by yourself..

Your term project will receive full credit **only** if: (a) the program runs successfully without errors using python 3, (b) the programs have explanatory comments and variable names that identify with the problem equations you are trying to solve, (c) give the correct output, and (d) demonstrate the validity of the solution through convergence plots. No credit will be given to late term projects.

The term paper is as important as the code (50% of the term project credit will go to the code and the other 50% to the paper). Answers to the questions and analysis requested below should be elaborated in the report. Plots should be clearly labeled and be properly described in the report, and not just shown. You will need to explain what each and every plot demonstrates. A polished paper written in word or LaTex (preferred, e.g. please try overleaf) is expected to get full credit.

Note: Before you present results from numerical integrations that answer the questions in the project, it is critical to *first* perform the convergence tests for one case, and to estimate errors. This will tell you how small a step size is necessary for accurate solutions. Only after errors are estimated, does it make sense to run your code for producing results that help you learn more about the system you study.

I. THE POISSON–BOLTZMANN EQUATION IN NEUTRAL PLASMAS: DEBYE SCREENING

You will be examining solutions to the Poisson-Boltzman (PB) equation in neutral plasmas.

In a system of N different species of charges, with the j-th species carries charge q_j and has concentration $n_j(\mathbf{r})$ at position $\mathbf{r}$, the electric potential from the distribution of charges is given by

$$\varepsilon \nabla^2 \Phi(\mathbf{r}) = -\sum_{j=1}^{N} q_j\, n_j(\mathbf{r}) - \rho_{\rm ext}(\mathbf{r}) \tag{1}$$

where $\rho_{\rm ext}$ is a charge density external (logically, not spatially) to the medium. Assuming thermodynamic equilibrium with a heat container at constant temperature T, the concentration of the j-th charge species is described by the Boltzmann distribution

$$n_j(\mathbf{r}) = n_j^0 \exp\left(-\frac{q_j\,\Phi(\mathbf{r})}{k_{\rm B}T}\right) \tag{2}$$

with $k_{\rm B}$ being Boltzmann's constant and n_j^0 is the mean concentration of charges of species j. If one plugs Eq. (2) in Eq. (1) one obtains the non-linear Poisson-Boltzman equation. To simplify the equation one assumes that the potential energies are small, i.e.,

$$\exp\left(-\frac{q_j\,\Phi(\mathbf{r})}{k_{\rm B}T}\right) \approx 1 - \frac{q_j\,\Phi(\mathbf{r})}{k_{\rm B}T}. \tag{3}$$

Under this approximation we obtain the linearized Poisson-Boltzmann equation

$$\varepsilon \nabla^2 \Phi(\mathbf{r}) = \left(\sum_{j=1}^{N} \frac{n_j^0\, q_j^2}{k_{\rm B}T}\right) \Phi(\mathbf{r}) - \sum_{j=1}^{N} n_j^0 q_j - \rho_{\rm ext}(\mathbf{r}) \tag{4}$$

For neutral plasmas $\sum_{j=1}^{N} n_j^0 q_j = 0$, thus one arrives at

$$\nabla^2\Phi(\mathbf{r}) = \lambda_{\mathrm{D}}^{-2}\Phi(\mathbf{r}) - \frac{\rho_{\mathrm{ext}}(\mathbf{r})}{\varepsilon}, \tag{5}$$

where

$$\lambda_{\mathrm{D}} = \left(\frac{\varepsilon\, k_{\mathrm{B}} T}{\sum_{j=1}^{N} n_j^0\, q_j^2}\right)^{1/2} \tag{6}$$

is called the Debye length. We will be consider an external point charge $\rho_{\mathrm{ext}} = Q\delta(r)$ ($\delta(r)$ is the Dirac δ function) and will adopt spherical symmetry. Then Eq. (5) becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = \lambda_{\mathrm{D}}^{-2}\Phi - \frac{Q\delta(r)}{\varepsilon}, \tag{7}$$

The goal is to solve Eq. (7), which although an ordinary differential equation, it actually is a boundary value problem. Before doing so, it is important to non-dimensionalize it as much as possible. First introduce a new dimensionless radius $\tilde{r} = r/\lambda_{\mathrm{D}}$, and rewrite the equation.

The potential has dimensions of Q/ϵ/length. Thus, one can introduce a new dimensionless potential $\tilde{\Phi} = \Phi\epsilon\lambda_D/Q$. Introduce the dimensionless potential in the equation to write the final dimensionless form of the equation (keeping in mind that the Dirac delta has dimensions of 1/length^3 so introduce the non-dimensional Dirac delta $\tilde{\delta} = \delta\lambda^3$, and rewrite the final equation that should have no constants in it.

$$\frac{1}{\tilde{r}^2}\frac{d}{d\tilde{r}}\left(\tilde{r}^2\frac{d\tilde{\Phi}}{d\tilde{r}}\right) = \tilde{\Phi} - \tilde{\delta}(r). \tag{8}$$

The equation admits a solution which becomes singular at $\tilde{r} = 0$. For this reason the goal will be to start the integration at some large $\tilde{r}$ and integrate inward, i.e., for decreasing $\tilde{r}$, but not all the to $\tilde{r} = 0$. You will start at $\tilde{r}_0 = 10$ and integrate to $\tilde{r} = 0.001$. To solve the normalized and dimensionless version of the PB for neutral plasmas you will need to cast it to first order form. Show your work in the report. You will also need to specify initial conditions: Use $\tilde{\Phi}(\tilde{r}_0) = 3.6128116188621609369589 07 \times 10^{-7}$ and $\frac{d\tilde{\Phi}}{dr}|_{\tilde{r}=\tilde{r}_0} = -3.9740927807483770306547 98 \times 10^{-7}$. Do the following:

1. Use RK4 to integrate numerically the dimensionless of the PB equation from $\tilde{r}_0 = 10$ to $\tilde{r} = 0.001$. Show a plot of your solution and compare it to the potential of the same point charge *in vacuum*, i.e., $\tilde{\Phi}_{\mathrm{vacuum}} = 1/4\pi\tilde{r}$.
   - What do you notice? Is the potential of a point charge in a neutral plasma the same as that of a point charge in vacuum? Do they agree within a certain region? If yes, at what value of $\tilde{r}$ do you start to see significant deviations between the two?
   - Make also a plot of the ratio of your numerical solution to $\tilde{\Phi}_{\mathrm{vacuum}}$. Is the ratio a powerlaw, exponential? Show the appropriate plot (log-log, log-linear, linear-log) that justifies your conclusion. Is the slope of the straight line you see -1? Since $\tilde{r} = r/\lambda_D$, what does that tell you about the lengthscale beyond which the vacuum point charge potential deviates significantly from the point charge potential in a neutral plasma?

   Use your judgement as to how small a step size you need to solve this system accurately. If you cannot figure this out from pure thought, experiment with different step sizes and use the solution $\tilde{\Phi}$ at the final $\tilde{r}$ and choose the step size such that $\tilde{\Phi}$ at that $\tilde{r}$ does not change appreciably.

2. **Convergence**: Use a number of step sizes and the difference between your $\tilde{phi}$ at a $\tilde{r}$ of your choosing, and the value of the function $\frac{e^{-\tilde{r}}}{4\pi\tilde{r}}$ evaluated at the same $\tilde{r}$. Does the difference converge to 0? Does the order of convergence match your expectation? If not, try to explain why.

3. **Self-convergence**: Use a number of step sizes and for a specific choice make a plot to demonstrate that the code solution for $\tilde{\Phi}$ at $\tilde{r} = 3$ self-converges. Does the order of convergence match your expectation? If not, try to explain why.

4. Using the order of convergence you determined, employ Richardson extrapolation to determine an error for the solution for $\tilde{\Phi}(\tilde{r})$ at $\tilde{r} = 0.001$.