Laplace's and Poisson's Equations in 2D

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1 Introduction

This project aims to develop a computational code to solve the two-dimensional Laplace and Poisson equations, providing efficient and accurate numerical solutions. Basically:

$$\nabla^2 \phi = 0 \tag{1}$$

$$\nabla^2 \phi = -\frac{\rho}{\epsilon} \tag{2}$$

where $\phi(x, y)$ = potential, $\rho(x, y)$ = charge density, ϵ = dielectric constant of the medium.

In the upcoming sections, I will test a sum of different cases, like the case of a dipole consisting of two charges of opposite signs placed at a certain distance using Dirichlet, Neumann and Periodic Boundary conditions. The mesh size will be limited due to the computationally intensive nature of increasing N (mesh size). To avoid confusion with the units, I will be using arbitrary units (a.u.).

2 Dirichlet Boundary conditions

2.1 A simple charge distribution

Following the Gauss-Seidel iteration method with Dirichlet boundary conditions, defining the energy and a function for gaussian distributions. I created a dipole consisting of two charges of opposite signs placed at a certain distance, where each charge is a Gaussian distribution (see appendix A). The convergence limit set for now is 1 $\times 10^{-10}$.

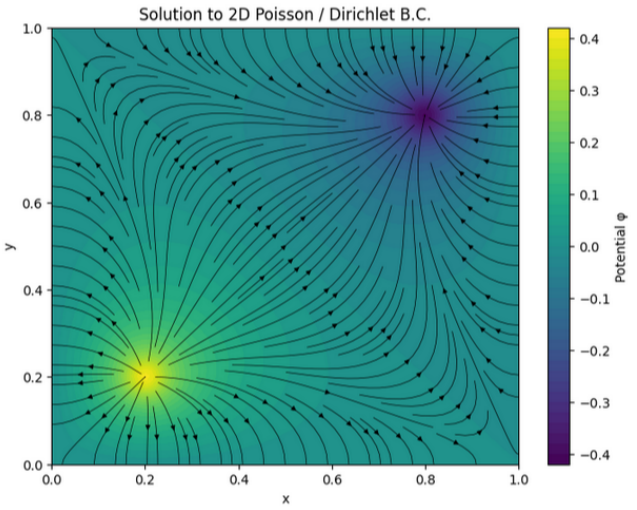

Figure 1: A dipole consisting of two charges of opposite signs, at (0.2,0.2) and (0.8,0,8)

2.2 Effects of the relaxation parameter on the convergence

Here, I investigate the influence of the relaxation parameter ω on the number of iterations required to achieve energy convergence. I do keep a relatively small value of mesh size (N=50) since it is a highly computationally intensive task.

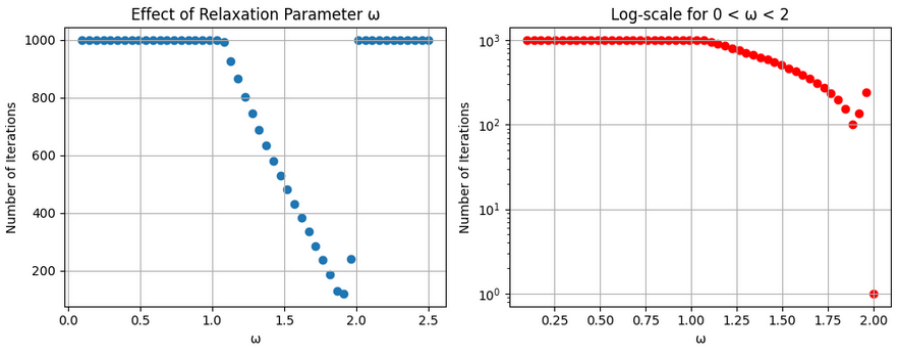

Figure 2: The first plot shows the effect of the relaxation parameter between values of 0 and 2.5. The second plot is limited between 0 and 2, but scaled logarithmically.

The optimal value of ω found, for the least number of iterations is 1.912 (121 iterations).

omega	**Energy value**
0.2	-0.319138
1.2	-0.351183
1.912	-0.351238
2.0	-5.03×10^{-17}
2.2	5.58×10^{13}

Table 1: Energy values for different values of the relaxation parameter

The plot suggests that for ω below 1.0, the energy convergence requires a significant number of iterations. A similar trend is observed for values above 2.0. The results obtained from running the code in Section 2.1 are shown in the table above. For $\omega = 0.2$, the algorithm reached the maximum iteration limit (1000) without achieving convergence. For $\omega = 1.2$ and $\omega = 1.912$, the energy values are nearly identical, with differences only in the number of iterations required for convergence. However, for $\omega = 2$, the energy begins to diverge, approaching zero. For $\omega = 2.2$ the divergence is even more extreme, with the energy value being several orders of magnitude greater than the expected result!

The optimal value of ω that I found from the plot and that I will be using from now on, is 1.912 (121 iterations).

2.3 Effect of mesh size (N) to the Energy

Next task of this project, is to keep the size of the rectangular cell fixed and increase the mesh size, to observe how it affects the Energy.

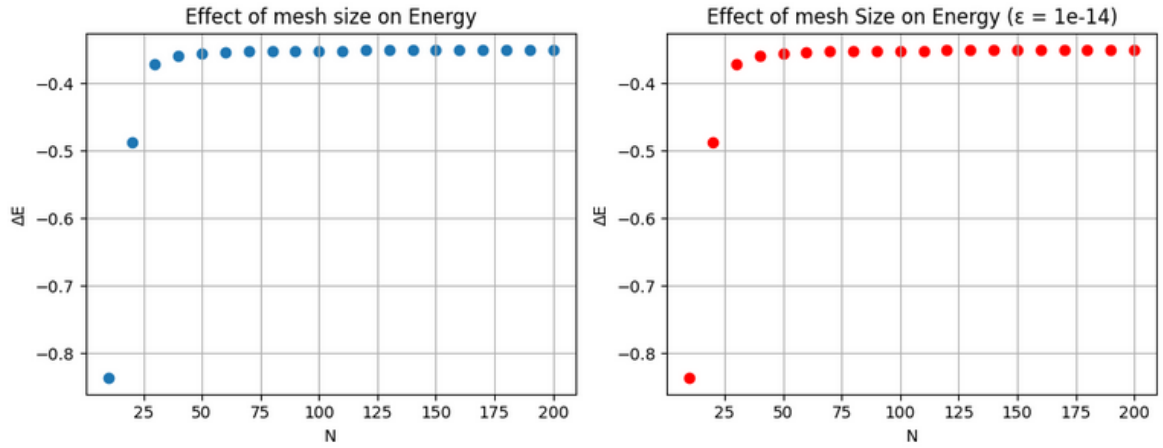

Figure 3: The first plot shows the effect of grid size on Energy for convergence threshold 10^{-10}, while the second for 10^{-14}

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The mesh size does affect the expected energy, particularly for smaller values, but its impact is reduced beyond a certain point. Ultimately, I aim to select the highest N value possible without significantly increasing the computational cost, while maintaining an accurate result. For this reason, I chose N=100.

Now for a different convergence threshold, upon a first look, there seems to be absolutely no change at the energy calculated. Though, by printing out the energy at the 100th iteration we get:

eps	**Energy value**
10^{-10}	-0.3552980467
10^{-14}	-0.3552980472

Table 2: Energy values for different convergence threshold

The two values differ only at the ninth decimal place, which is not significant for most cases, unless precise calculations are required.

2.4 Dipole at different distances

In this subsection, the dipole is placed at different distances from the boundaries of the cell (while keeping the distance between the two charges fixed). The aim once again is to observe any differences in the energy.

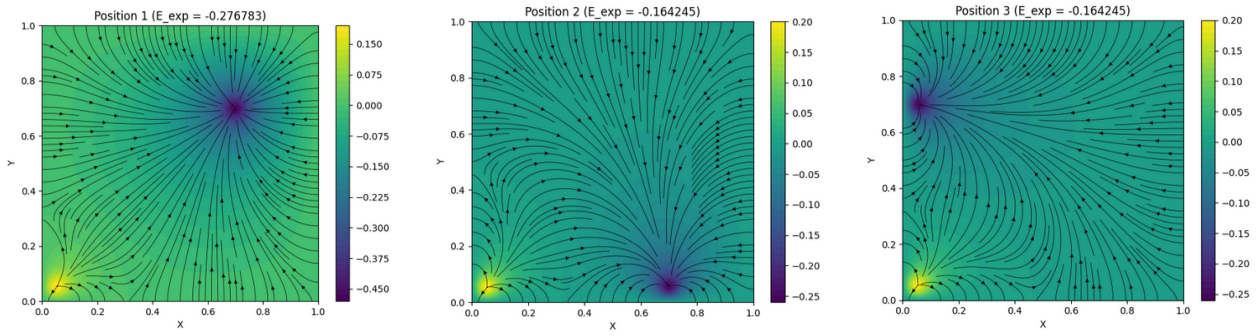

Figure 4: Dipole placed at different distances.

The plots indicate that the energy increases as the charges approach the boundaries. To avoid this, the charges should be positioned in a way that minimizes the influence of the boundary conditions. This implies that the optimal approach for calculating the potential around an isolated dipole is to place it within a sufficiently large box, ensuring it is positioned far enough from the boundaries.

2.5 Faraday cage

Here is the Faraday cage with Dirichlet boundary conditions.

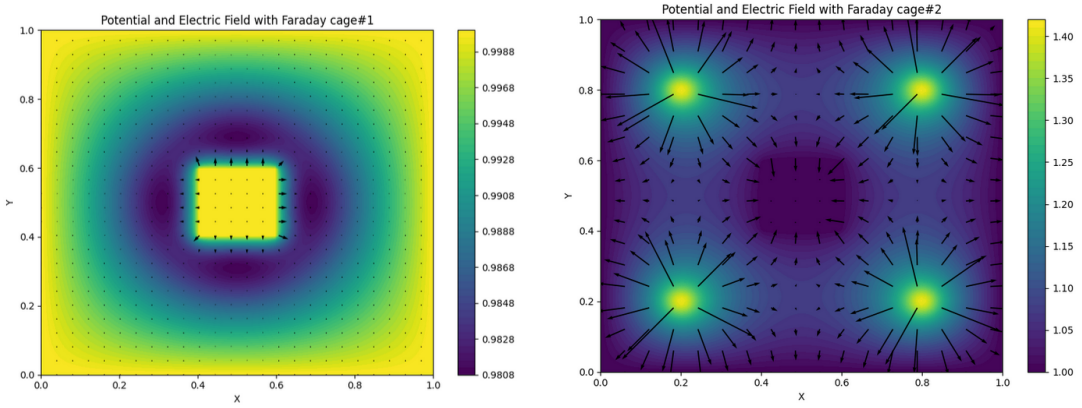

Figure 5: Two cases of a Faraday cage.

The calculated potential is physically meaningful if the Faraday cage correctly implements a zero potential inside. As we can see from the plots above, it works as expected.

2.6 Capacitor

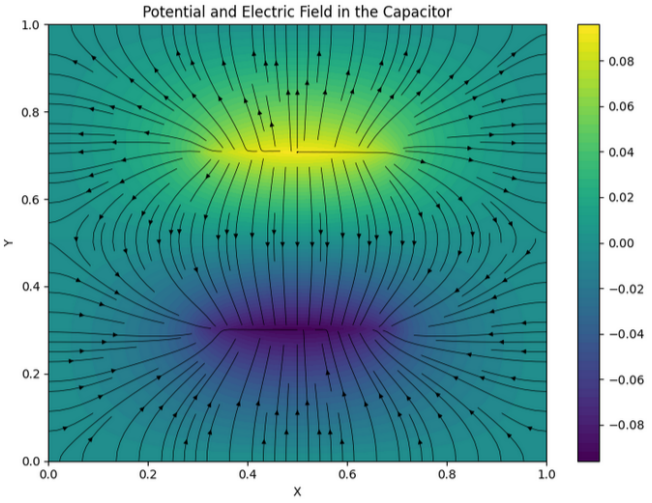

Figure 6: A capacitor

3 Part2

3.1 Neumann and Boundary conditions

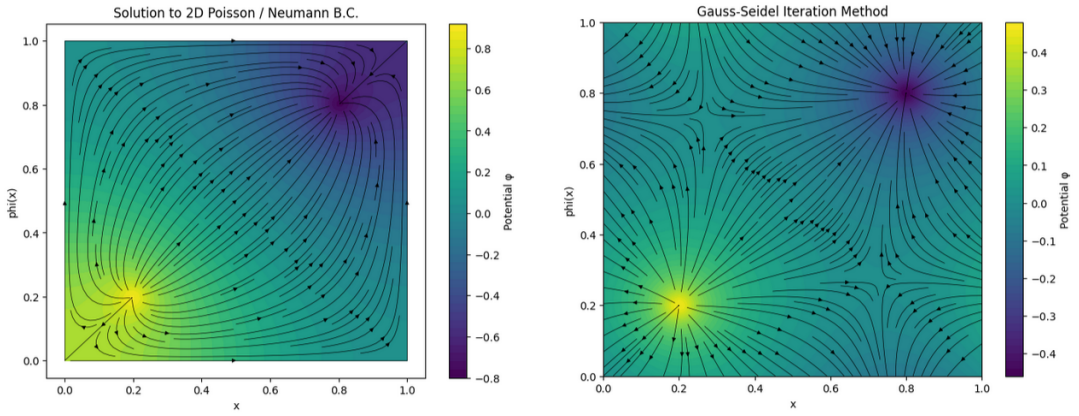

Figure 7: The first plot uses Neumann BC, while the second Periodic BC.

In Appendix B, I show a picture of proof that the periodic boundaries conditions worked as they should have.

3.2 Dipole's CM at center of the cell

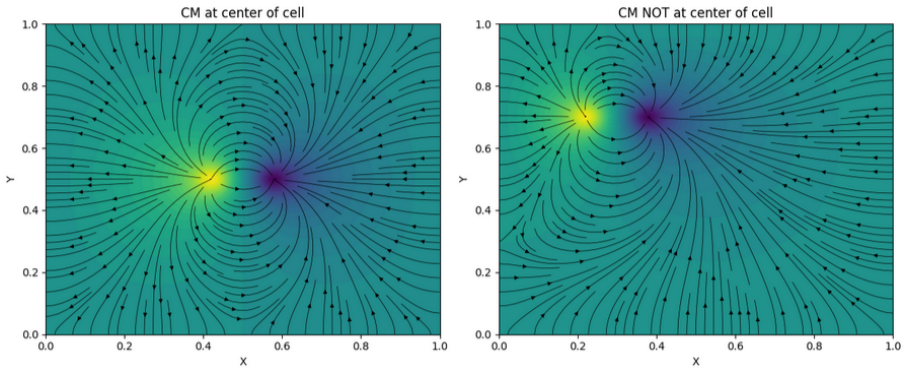

Figure 8: Different center of mass. The CM in the first picture in in the middle of the cell, while in the second it is not.

In this subsection, I examine the observable differences when the dipole's center of mass is either at the center of the cell or not, while maintaining a constant distance. As expected, there is a small difference in the calculated energy. When the center of mass is at the center of the cell, the energy is $E_{cm} = -0.2513$, and when it is displaced from the center (as shown in the figure), the energy is $E_{notcm} = -0.2467$. This results in a 1.83% difference.

These differences are possible attributed to the fact that in the second case, there center of mass/charges are near the boundaries. Furthermore, when the dipole's center of mass is at the center of the cell, the dipole maintains a symmetric field, leading to a slightly lower energy. However, when the center of mass is shifted, the symmetry is broken, causing different interactions with the affected boundary conditions and thus producing a distinct energy result.

3.3 Single charge - Periodic B.C.

This is a unique scenario. For various iteration values (ranging from 1000 to 50,000), the maximum number of iterations is always reached. While we obtain the same plot (as expected), the energy value differs significantly and continues to decrease as the number of iterations increases. In contrast, in the other subsections, convergence was reached within 1000 iterations. Taking this into consideration, the conclusion is that there is no solution to the problem of the monopole under periodic boundary conditions. Possibly, this occurs because the periodic b.c. introduce an ambiguity in the configuration of the monopole which causes serious issues with the convergence.

3.4 Distance vs Energy for different B.C.

In this and final subsection, I tested the effect of the distance on the energy, for different boundary conditions. Below are the results:

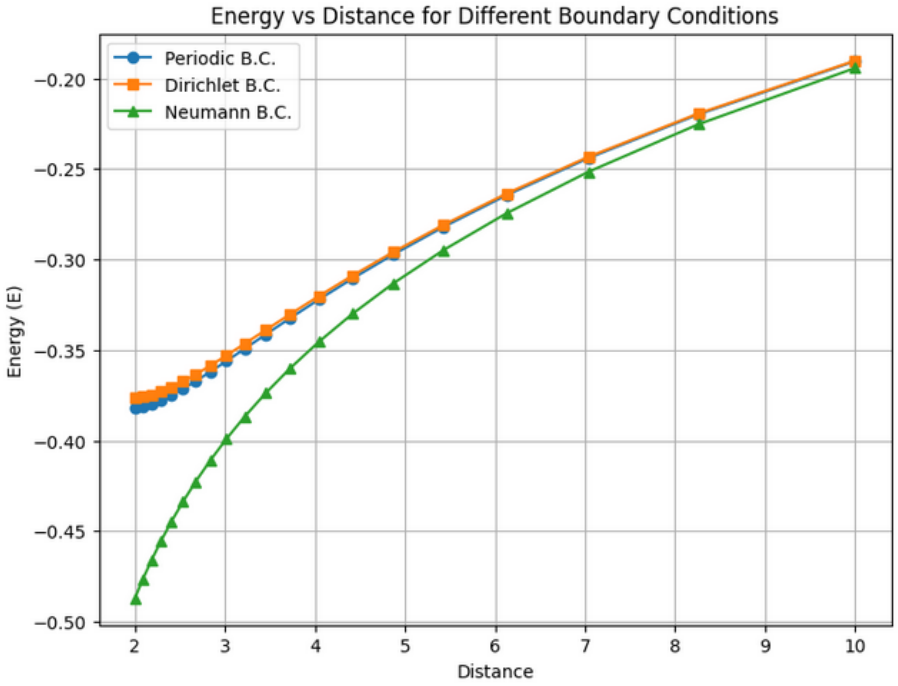

Figure 9: Distance vs Energy for Periodic, Dirichlet and Neumann B.C. (Distance is actually 1/d here)

For all boundary conditions, the energy decreases as the distance between the charges increases, consistent with the expected electrostatic behavior of a dipole (appendix c). Additionally, there is little difference between periodic and Dirichlet boundary conditions, as both similarly constrain the potential. In contrast, Neumann conditions provide more freedom in how the field behaves, as they affect the derivatives rather than directly restricting the potential.

A

Gaussian Function in 2D for modeling charges

$$g(x,y) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{(x-\mu_x)^2 + (y-\mu_y)^2}{2\sigma^2}\right) \tag{3}$$

B

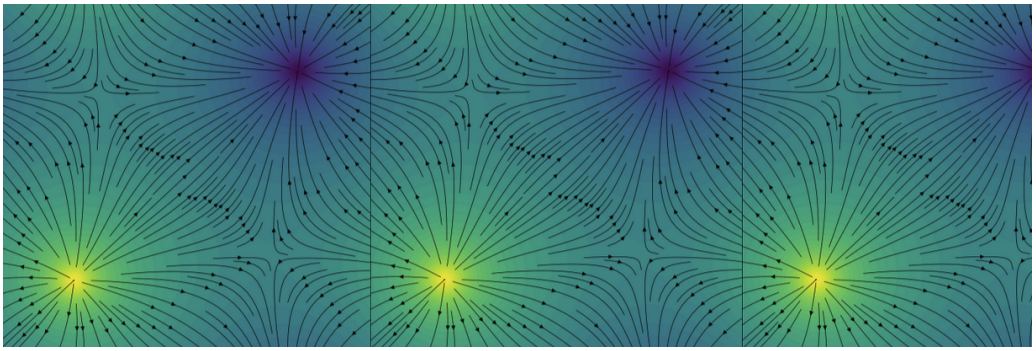

Figure 10: Proof of Periodic B.C.

C

Potential Energy of Dipole

This is the case without any external electric field.

For a dipole with charges $q_1 = +q$ and $q_2 = -q$, separated by a distance d, the potential energy is:

$$U = \frac{1}{4\pi\epsilon_0} \frac{(+q)(-q)}{d} \tag{4}$$

$$U = -\frac{q^2}{4\pi\epsilon_0 d} \tag{5}$$

The negative sign indicates that work is required to separate the charges to infinity.