Computational Physics Project Report

Yu Ziyang
UID:3030057277

November 21, 2018

1 Title

Using random Walk model to solve Poisson's Equation in different situations

2 Introduction

It is known that there exists many kind of linear or nonlinear partial equations in different kinds of fields in physics. Sometimes it's difficult to get the analytical solutions for these equations. However the numerical or seminumerical/analytical solutions have been extensively studied. One kind of problem is to solve the Poisson's equation in dielectric material in electromagnetism.

In any electric field generated by a set of charges can be written as the gradient of a scalar potential, which is:

$$\mathrm{E} = -\nabla\Phi \tag{1}$$

This equation can be combined with the field equation:

$$\nabla \cdot \mathrm{E} = \frac{\rho}{\epsilon_0} \tag{2}$$

to give a partial differential equation for the scalar of electric potential:

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0} \tag{3}$$

This is an example of a very famous type of partial differential equation called Poisson's equation.

Random walk model is known as a stochastic process describing a path that consists of a succession of random steps in some mathematical spaces. A object can move to every direction by a special length step at one mathematical time. It can be used to simulate many complex physical or mathematical problems if we set the proper probability about which direction the particle will move towards.

In my project, I use random walk methods to calculate the electric potential in diaelectric material thus get the solution of Poisson's equation. In one dimension situation, I analyse the potential at each location quantitively. Then I extend it to two dimension situation and get the qualitive results. In further study, I can extend this method to solve three dimension Poisson's equation.

3 Physics background

In electromagnetism, if there is a charge density $\rho(x, y, z)$ in the region, we could rewrite Poisson's equation as:

$$\nabla^2 V(\mathrm{r}) = \frac{\partial^2 \mathrm{V}}{\partial \mathrm{x}^2} + \frac{\partial^2 \mathrm{V}}{\partial \mathrm{y}^2} + \frac{\partial^2 \mathrm{V}}{\partial \mathrm{z}^2} = -4\pi\rho(\mathrm{r}) \tag{4}$$

here $\rho(\boldsymbol{r})$ is the charge density. The difference form of Poisson's equation in two dimensions is:

$$\phi(x, y) \approx \frac{1}{4}[\phi(x + \Delta x, y) + \phi(x - \Delta x, y) + \phi](x, y + \Delta y) + \phi(x, y - \Delta y)] + \frac{1}{4}\Delta x \Delta y 4\pi\rho(x, y) \tag{5}$$

The general idea is that the electric potential at any point equals to the average of the potential beside the point.

To make the expression briefly, we rewrite the equation(5) as:

$$\phi_0 = \sum_{k=1}^{4} p_{0,k}\phi_k - h^2 q_0/4, p_{0,k} = 1/4 \tag{6}$$

here $p_{0,k}$ is the probability of moving from point 0 to k.

If we choose a particle located at 0 point (i, j) and perform random walk, we assume in next step, this particle moves to the neighbour point m randomly. So the electric potential is $\phi_0 = \phi_m - h^2 q_0/4$; then this particle again randomly moves to neighbour point n, we can also get $\phi_m = \phi_n - h^2 q_m/4$. We can represent the potential at 0 point as $\phi_0 = \phi_n - h^2(q_0 + q_m)/4$. We perform this procedure K times until the particle reaches s point on the edge where the potential $\Phi(s)$is fixed in boundry condition. So we have:

$$\phi_0 = \Phi(s) - \frac{h^2}{4}\sum_{k=1}^{K-1} q_k \tag{7}$$

This is what we get from one single simulation. To make the numerical results more reliable, we repeat this simulation N times, and get statistical average value:

$$\langle\phi_0\rangle = \frac{1}{N}\sum_{n=1}^{N}\phi_0^{(n)} = \frac{1}{N}\sum_{n=1}^{N}\{\Phi(s^(n)) - \frac{h^2}{4}\sum_{k=1}^{K^(n)-1} q_k^{(n)}\} \tag{8}$$

4 Algorithm Presentation

4.1 One dimension algorithm

First we implement a rather simple one dimension Poisson's equation problem. We use a 1 x n array to build a one dimension space, and let particle move inside this space. In more general situation, the space contains two kinds of dielectric material. So actually when the particle reaches the interface, the probability of turning left or right is different. We should take this character into consideration.

When implementing this on the computer, we must consider the time consumption. The length of selected one dimension space is 50, then we focus on the interface. The boundary condition of interface is :

$$\begin{cases} \phi_1 = \phi_2 \\ \varepsilon_1\frac{\partial\phi_1}{\partial n} = \varepsilon\frac{\partial\phi_2}{\partial n} \end{cases} \tag{9}$$

The continuity condition has already been satisfied for computer simulation, we need to use finite-difference method to implement the normal continuity of electric displacement:

$$\begin{aligned} \varepsilon_1\frac{\partial\phi_1}{\partial n} = \varepsilon_1\frac{\phi_1^n - \phi_1^{n-1}}{h} = \varepsilon_2\frac{\phi_2^n - \phi_2^{n-1}}{h} = \varepsilon_2\frac{\partial\phi_2}{\partial n}; \\ \Rightarrow \phi_1^n = \frac{\varepsilon_1}{\varepsilon_1+\varepsilon_2}\phi_1^{n-1} + \frac{\varepsilon_2}{\varepsilon_1+\varepsilon_2}\phi_1^{n+1} = p_{1,n-1}\phi_1^{n-1} + p_{1,n+1}\phi_1^{n+1}; \\ \Rightarrow p_{1,n-1} = \frac{\varepsilon_1}{\varepsilon_1+\varepsilon_2}; p_{1,n+1} = \frac{\varepsilon_2}{\varepsilon_1+\varepsilon_2} \end{aligned} \tag{10}$$

As is shown above, when particle moves inside one dielectric material, the probability of moving right or left is 0.5. But the probability will differ when it reaches the interface, the probability of moving into material 1 is $p_{1,n-1} = \frac{\varepsilon_1}{\varepsilon_1+\varepsilon_2}$,the probaility of moving into material 2 is $p_{1,n+1} = \frac{\varepsilon_2}{\varepsilon_1+\varepsilon_2}$ We can do some simple adjustments in the program.

Besides we also need to consider the effect of electric charge fixed in the material represented in the equation(8). In one dimension situation, the coefficient of the electric charge term is 1/2 but not 1/4.

In my program, after setting some constants like the space length N and the repeat random walk times M. The relative permittivity of dielectric material 1 and 2 is 2 and 1 respectively in my example. I also set a positive unitive charge at 1/4 N and a negative unit charge at 3/4 N. It's important to notice that this is not

two traditional point charges, in my example, the potential where the charge located is not an infinite value but a finite value.

For every position in the one dimension space, we use a unit random number generator to generate [0,1] random number to deside whether the particle moves right or left. This will continue until the particle reaches the edge, i.e, position = 0 or N. When the particle moves through where the charge located, the potential of particle will change. When particle reaches the interface of two dielectric materials, the random walk probability will change. In other situation, the particle will simply follow the random walk rules and moves left or right with same probability.

We repeat above procedure M times and calculate the mean value. Finally we get our approximate potential numerical results.

4.2 Two dimension algorithm

After we have explained one dimension algorithm, it's easy to extend it into two dimension situation. In two dimension plate, left part is filled with dielectric material 1 and right part is filled with dielectric 2. The relative permittivity is $\varepsilon_1 = 2$ and $\varepsilon_2 = 1$ respectively. We also set a positive charge and a negetive charge in the cent of two dielectric material areas.

When particle reaches the interface of two material, the probabilities differ a little bit from one dimension situation. Here $p_1 = \frac{\varepsilon_1}{\varepsilon_1+\varepsilon_2}; p_2 = \frac{\varepsilon_2}{\varepsilon_1+\varepsilon_2}; p_3 = 1/4; p_4 = 1/4$, 1,2,3,4 represents left, right, up, down. In any other position, particle could move to four directions with the probilities all equals to 1/4.

5 Simulation Results and discussion

5.1 One dimension Poisson's equation

First we discuss that the space contains two kinds of dielectric material without fixed charge. To make the analytical solution simpler, we choose such condition:

$$\begin{cases} \varepsilon_1 = 2, 0 < x < 25 \\ \varepsilon_2 = 1, 25 < x < 50 \\ \phi_1 = 0 \\ \phi_{50} = 5 \end{cases} \tag{11}$$

We can present the theoretical derivation:

$$\frac{d^2\phi_a}{dx^2} = 0, (0 < x < 25) \Rightarrow \phi_a = Ax + B,$$
$$\frac{d^2\phi_b}{dx^2} = 0, (25 < x < 50) \Rightarrow \phi_b = Cx + D,$$

We take boundary condition into consideration:

$$\phi_{a,25} = \phi_{b,25}; \varepsilon_1 \frac{\partial \phi_a}{\partial x}|_{x=25} = \varepsilon_2 \frac{\partial \phi_b}{\partial x}|_{x=25}; \phi_1 = 0; \phi_{50} = 5;$$
$$\Rightarrow \begin{cases} A = \frac{1}{15} \\ B = -\frac{1}{15} \end{cases} ; \begin{cases} C = \frac{2}{15} \\ D = -\frac{5}{3} \end{cases} ; \Rightarrow \phi_a = \frac{1}{15}x - \frac{1}{15}; \phi_b = \frac{2}{15}x - \frac{5}{3} \tag{12}$$

That is the general solution in the whole one dimension space. We could compare this to the numerical calculation result: It can be observed that the slope of the potential curve differs in two dielectric material areas. We focus on each part:

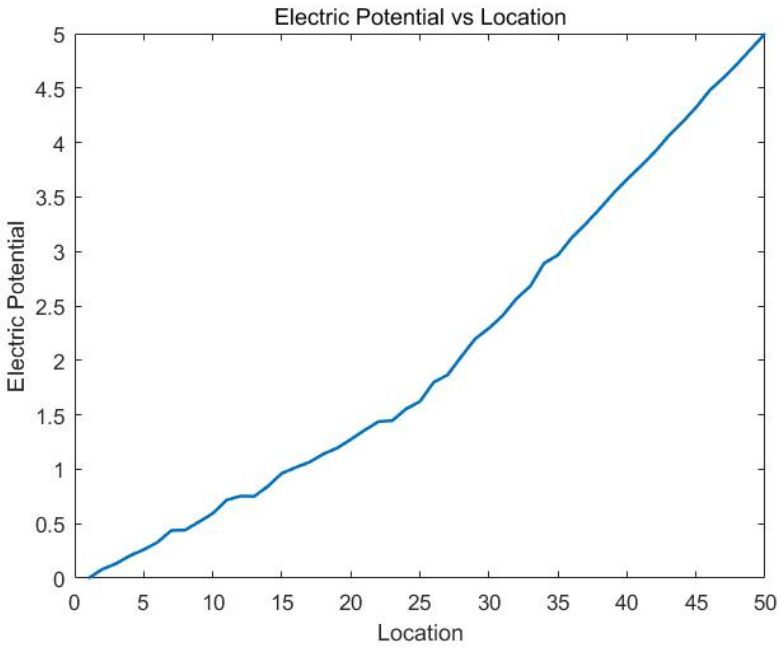
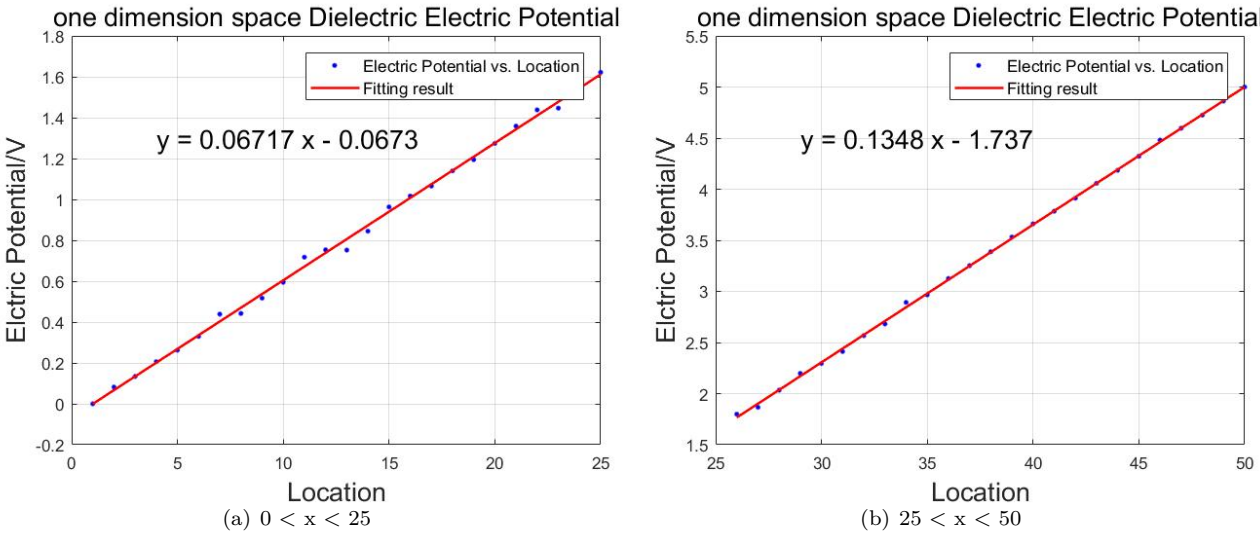


Figure 1: Potential simulation result without charge in one dimension



(a) 0 < x < 25 (b) 25 < x < 50

Figure 2: The fitted potential in one dimension space without charges

The numerical experiment result is:

$$\begin{cases} \phi_a = 0.06717x - 0.0673, 0 < x < 25 \\ \phi_b = 0.1348x - 1.737, 25 < x < 50 \end{cases} \tag{13}$$

this result is in fairly good accordance with the theoritical result. The main source of error is the repetition times we choose to perform random walks is not infinite large. In my program, I repeat 10000 times for each model. It's obvious the result will be more accurate if the repetition time is larger.

Hence we can talk about when the unit charges is set in the material. The Poisson's equations become:

$$\frac{d_a^\phi}{dx^2} = -\frac{\delta(12)}{\varepsilon_1}, (0 < x < 25)$$
$$\frac{d_b^\phi}{dx^2} = -\frac{\delta(37)}{\varepsilon_2}, (25 < x < 50)$$

These equations satisfy the boundary condition:

$$\begin{gathered}\phi_{1,12} = \phi_{2,12}; \phi_{2,25} = \phi 3, 25; \phi_{3,37} = \phi_{4,37}; \\ \varepsilon_1 \frac{\partial \phi_2}{\partial x}|_{x=25} = \varepsilon_2 \frac{\partial \phi_3}{\partial x}|_{x=25}; \\ \phi_{1,1} = 0; \phi_{4,50} = 50\end{gathered} \tag{14}$$

So as before, we could give the theoretical results:

$$\begin{cases}\phi_1 = \frac{47}{148}x - \frac{47}{148}, 0 < x < 12 \\ \phi_2 = -\frac{27}{148}x + \frac{841}{148}, 12 < x < 25 \\ \phi_3 = \frac{27}{74}x + \frac{379}{37}, 25 < x < 37 \\ \phi_4 = \frac{47}{74}x - \frac{990}{37}, 37 < x < 50\end{cases}$$

Then we take a look at the numerical experiment results, the general potential in the whole space is shown below:

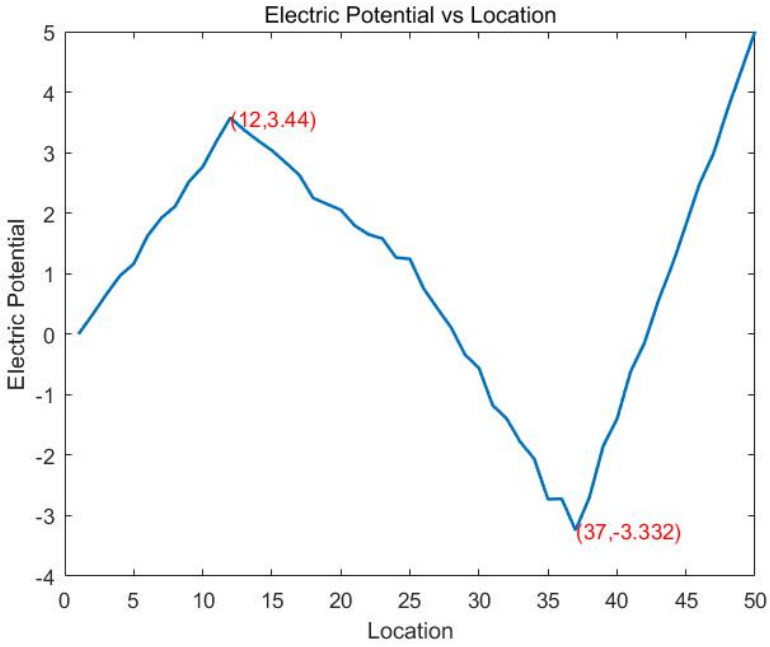
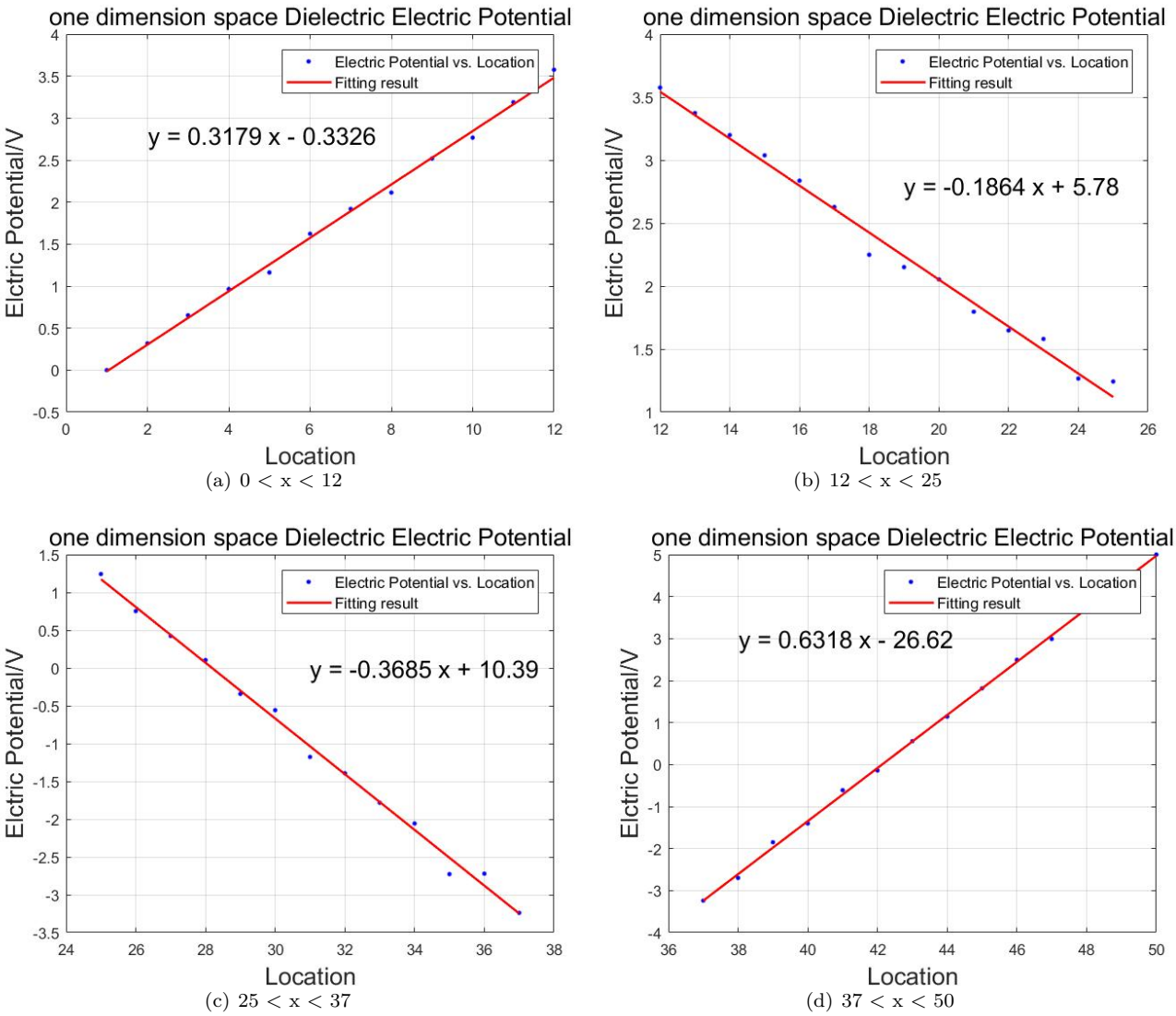


Figure 3: Potential simulation result with charge in one dimension

We focus on four specific part of this curve. We could compare these two results:

$$\begin{cases}\phi_1 = 0.3176x - 0.3176, 0 < x < 12 \\ \phi_2 = -0.1824x + 5.6824, 12 < x < 25 \\ \phi_3 = -0.3649x + 10.2432, 25 < x < 37 \\ \phi_4 = 0.6351x - 26.7568, 37 < x < 50\end{cases} theoreticalresults; \begin{cases}\phi_1 = 0.3179x - 0.3326, 0 < x < 12 \\ \phi_2 = -0.1864x + 5.78, 12 < x < 25 \\ \phi_3 = 0.3685x + 10.39, 25 < x < 37 \\ \phi_4 = 0.6318x - 26.62, 37 < x < 50\end{cases} numericalresults$$

We could find the numerical results are good enough to simulate theoretical results. There of course exists some error, it mainly comes from the length of the space and the repetition times.



(a) $0 < x < 12$ (b) $12 < x < 25$

(c) $25 < x < 37$ (d) $37 < x < 50$

Figure 4: The fitted potential in one dimension space with charges

5.2 Two dimension Poisson's equation

In two dimension simulation, we consider the area was divided equally by two part. Left part is filled with dielectric material $\varepsilon_1 = 2$ and right part is filled with dielectric material $\varepsilon_2 = 1$. A positive unit charge is located in the center of left part and a negative unit charge is located in the center of right part.

We know that the potential distribution in vaccum area caused by a unit charge pair in two-dimensional is as below: When the area cotains different dielectric material. It's intuitive that the distribution will change a little bit but in general they are similar.

First, we consider the electric potential on edge is all fixed to 0 V. The simulation result is shown in Fig(6) and Fig(7): We can find that when ε is larger, the absolute value of potential is supressed, which is in accordance with theoretical prediction.

Then we consider changing the boundary condition, here I choose to set the potential on one edge where x = 30 to 1 V. Let's first take a look at how it looks like without fixed charge pair in Fig(8): This is not so accurate because the width of the system we choose is 100 and the length is 30.They can't be too large due to the constraint of the computer calculation capability. But we can observe the property of potential distribution qualitatively.

Finally we could combine the above two situation, we set potential on one edge to a exact value 1 V, and set a charge pair to see what is the potential distribution in this situation. The result of homocharge pair and

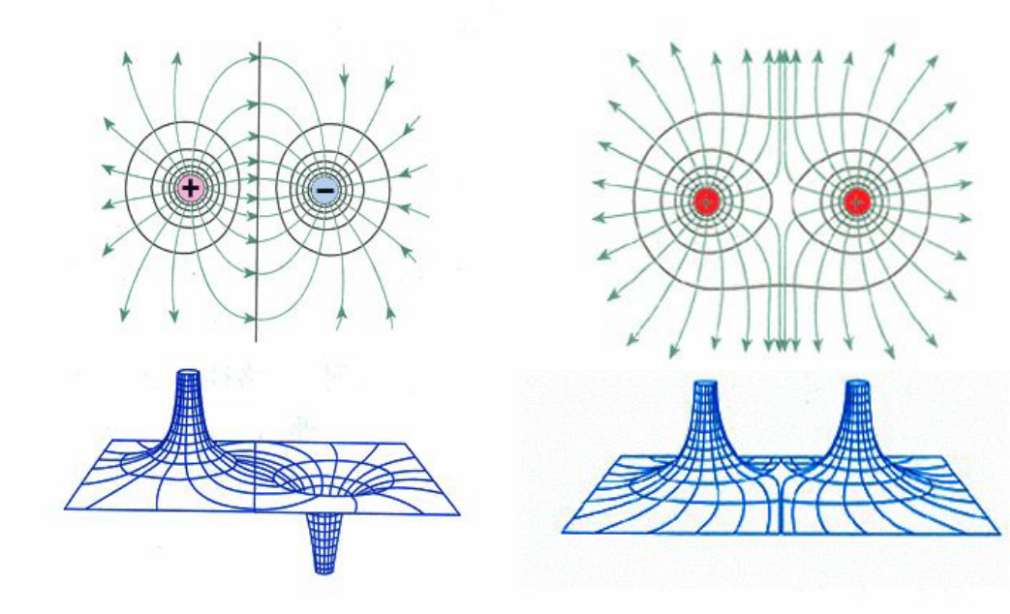
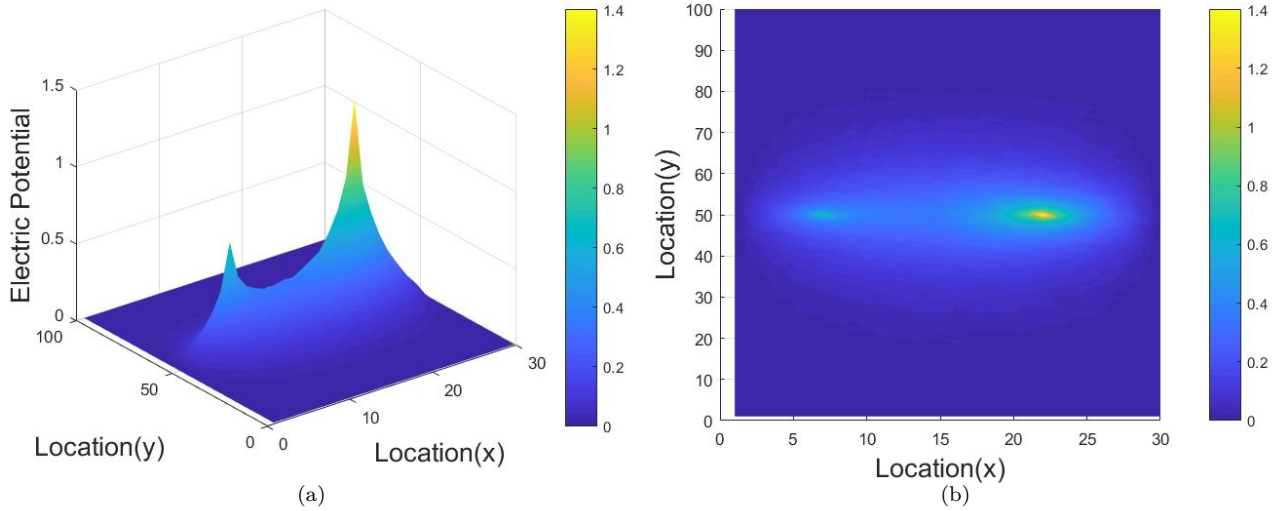


Figure 5: Potention distribution caused by unit positive-negative charge pair



(a) (b)

Figure 6: The potential in two-dimensional area with homocharges and 0 edge potential

hetrocharge pair are all displayed in Fig(9) and Fig(10) respectively.

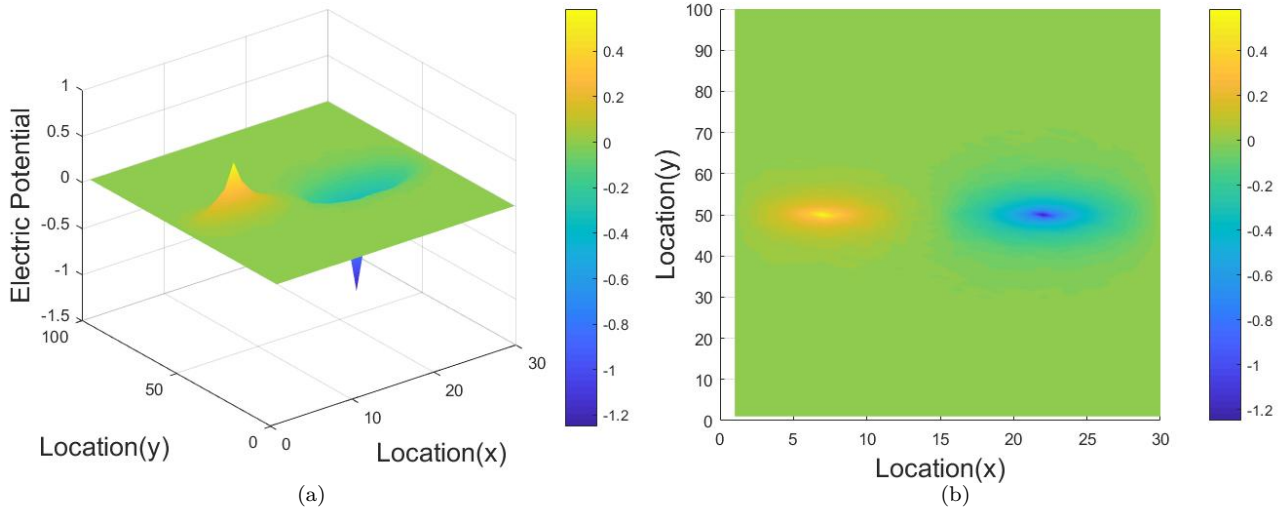
Compare Fig(5) to Fig(6) and Fig(7), we can find the potential distributionn is changed due to the influence of dielectric material. The relative permittivity of left dielectric material is larger than right part, and the absolute value is smaller. This is in accordance with the theoretical result.

Compare Fig(6) and Fig(7) to Fig(8) and Fig(9), we can see the influence of specific voltage added to one edge of the material plate.

6 Summary

With the help of random walk model, we get the numerical solution of one dimension and two dimension Poisson's equation, which is the electric potential distribution.

In one dimension situation, we fitted the potential-location relation curve, which is very close to the



(a) (b)

Figure 7: The potential in two-dimensional area with hetrocharges and 0 edge potential

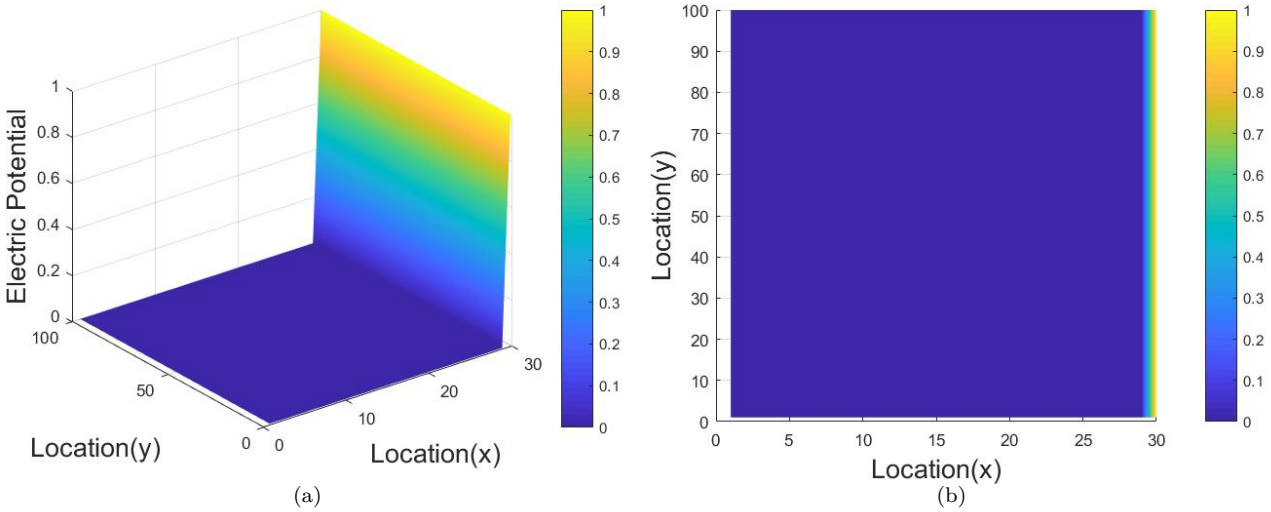
theoretical result. In two dimension situation, we display the potential distribution by surface picture. We can compare the results in different situation by changing the boundary condition to see the influcence of fixed charge pair and specific voltage added to one edge of the area.

I think it's a interesting project, I have a better understanding of random walk model and Poisson's equation. I'm sure this experience will help me in further research life.

Reference

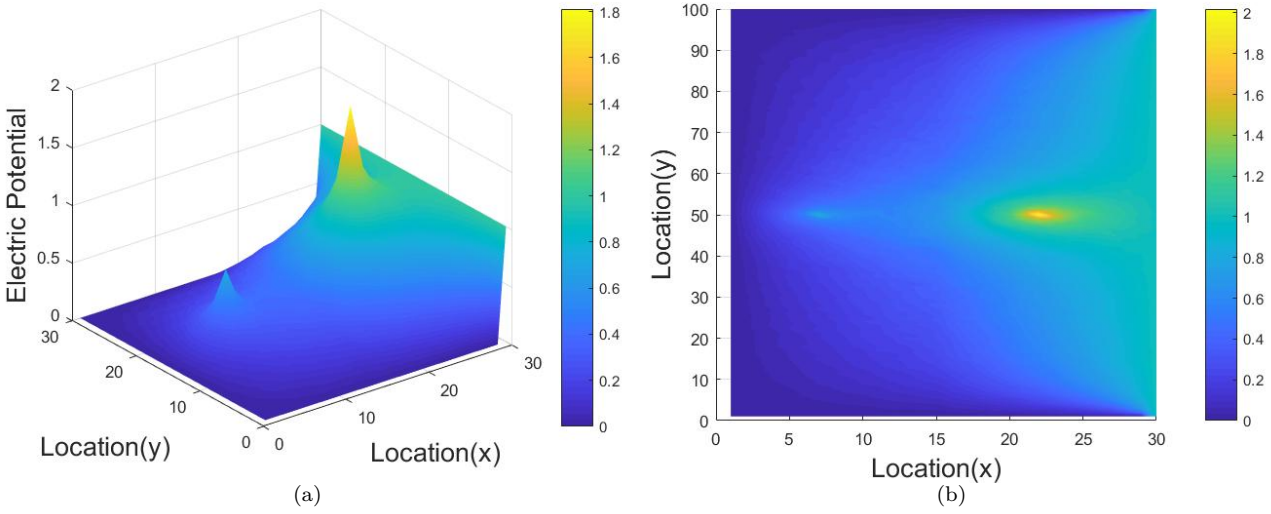
[1] A. M. Winslow, "Numerical solution of the quasilinear poisson equation in a nonuniform triangle mesh," *Journal of computational physics*, vol. 1, no. 2, pp. 149–172, 1966.

[2] H. Gould, J. Tobochnik, and W. Christian, *An introduction to computer simulation methods*, vol. 1. Addison-Wesley New York, 1988.



(a) (b)

Figure 8: The potential in two-dimensional area with homocharges and 0 edge potential



(a) (b)

Figure 9: The potential in two-dimensional area with homocharges and special edge potential

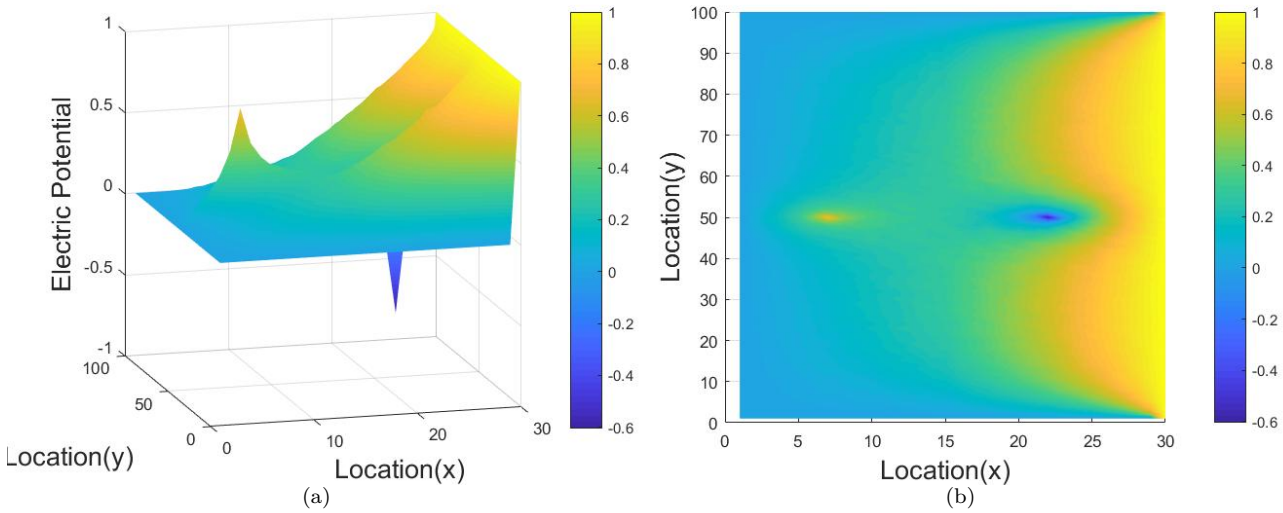


Figure 10: The potential in two-dimensional area with hetrocharges and special edge potential