Project: Elliptic equations in 2D

Introduction

The project aims to develop a code that solves the Laplace and the Poisson's equations in 2D:

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

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

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

The energy of this system can be written as:

$$E = \int_{a_x}^{b_x} dx \int_{a_y}^{b_y} dy \left[\frac{1}{2}(\nabla\phi)^2 - \frac{\rho}{\epsilon}\phi\right] \tag{3}$$

At a solution of Eqs (1) or (2), the energy is stationary under all variations of the potential $\delta\phi$ that respect the boundary conditions imposed. Therefore, it constitutes a convergence criterion (the energy is minimum at a solution).

Discretization

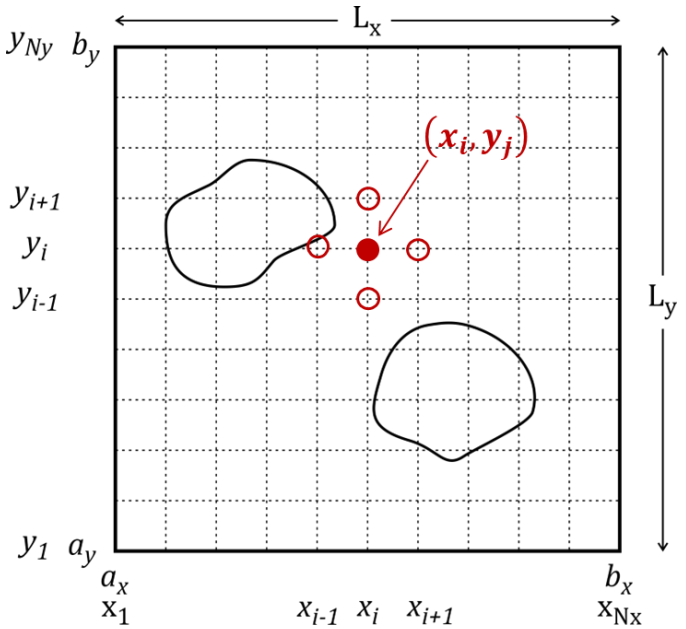

Figure 1 Schematic representation of the cell for a 2D boundary value problem. The values of the potential ϕ are specified on the edges of the cell and perhaps on the surfaces within the box.

We define a mesh covering the area of interest in the xy plane (see Fig. 1). For convenience, we take the spacing h to be uniform and equal in both directions. Nevertheless, a generalization to different spacings in the two directions is straightforward. We also consider that the area of interest is a square with dimensions $L \times L$. If we take N points along each direction, i.e., $N \times N$

points, the spacing is $h = L/(N-1)$. Hence the coordinates of a point (i,j) are $(x_i, y_j) = ((i-1)h, (j-1)h)$.

The Laplacian of the potential in 2D and cartesian coordinates is:

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} \tag{4}$$

We apply the three-point approximation of the second derivatives:

$$\frac{\partial^2\phi}{\partial x^2} = \frac{\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}}{h^2} \text{ and } \frac{\partial^2\phi}{\partial y^2} = \frac{\phi_{i,j+1} + \phi_{i,j-1} - 2\phi_{i,j}}{h^2} \tag{5}$$

Therefore, Eq. (2) is discretized as follows:

$$\phi_{i,j} = \frac{1}{4}\left(\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} + h^2\frac{\rho_{i,j}}{\epsilon}\right) \tag{6}$$

The energy of the system [Eq. (3)] can be approximated as follows:

$$E = \frac{1}{2}\sum_{i=2}^{N}\sum_{j=2}^{N}\left[\left(\phi_{i,j} - \phi_{i-1,j}\right)^2 + \left(\phi_{i,j} - \phi_{i,j-1}\right)^2\right] - h^2\sum_{i=2}^{N-1}\sum_{j=2}^{N-1}\frac{\rho_{i,j}}{\epsilon}\phi_{i,j} \tag{7}$$

Note: Eq. (6) can also be derived from Eq. (7) if we put $\frac{\partial E}{\partial \phi_{i,j}} = 0$.

Boundary conditions

- **Dirichlet boundary conditions**

The value of the potential ϕ is specified on some closed curve (conveniently the boundary of our cell, e.g., the sides of our square box in Figure 1), and probably on some other curves in the box. and perhaps on some additional enclosed curves.

- $\phi_{1,j} = \phi_{\text{Left}}(j), j = 1,2,\dots,N$
- $\phi_{N,j} = \phi_{\text{Right}}(j), j = 1,2,\dots,N$
- $\phi_{i,1} = \phi_{\text{Down}}(i), i = 1,2,\dots,N$
- $\phi_{i,N} = \phi_{\text{Up}}(i), i = 1,2,\dots,N$

(8)

The values of ϕ_{Left} and ϕ_{Right} are prescribed.

- **Neumann boundary conditions:**

The normal derivative of the potential is prescribed on the surfaces (curves in the 2D problem):

$$\frac{\partial\phi}{\partial n} = \hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla}\phi = f \tag{9}$$

If, for the problem depicted in Fig. xx, we want the normal derivative of ϕ on the boundaries $x = a_x$, $x = b_x$, $y = a_y$, and $y = y_x$ to be prescribed, and we take the forward difference approximation for the corresponding derivatives we get:

$$\begin{aligned}
\frac{\phi_{2,j} - \phi_{1,j}}{h} &= f_1(j) \rightarrow \phi_{1,j} = \phi_{2,j} - h\, f_1(j) \\
\frac{\phi_{i,2} - \phi_{i,1}}{h} &= f_2(i) \rightarrow \phi_{i,1} = \phi_{i,2} - h\, f_2(i) \\
\frac{\phi_{Nx,j} - \phi_{Nx-1,j}}{h} &= f_3(j) \rightarrow \phi_{Nx,j} = \phi_{Nx-1,j} + h\, f_3(j) \\
\frac{\phi_{i,Ny} - \phi_{i,Ny-1}}{h} &= f_4(i) \rightarrow \phi_{i,Ny} = \phi_{i,Ny-1} + h\, f_4(i)
\end{aligned} \tag{10}$$

- **Mixed boundary conditions:**

Different types of boundary conditions (i.e., Dirichlet and Neumann) are specified on different subsets of the boundary. E.g., Dirichlet boundary conditions are applied on the boundaries $x = a_x$ and $y = b_y$ and Neumann on the $x = b_x$ and $y = a_y$.

- **Robin boundary conditions:**

These conditions are a weighted combination of Dirichlet and Neumann boundary conditions. E.g., on some boundaries we apply

$$a \cdot \phi + \hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla}\phi = g \tag{11}$$

where a is a constant specified by the problem.

- **Periodic boundary conditions:**

These conditions are relevant when the physical problem has translational symmetry. For the example shown in Fig. 1, the periodic boundary conditions can be written as:

$$\phi\big(x \pm L_x, y \pm L_y\big) = \phi(x, y) \tag{12}$$

And in a discretized from as:

- $\phi_{0,j} = \phi_{Nx,j}, j = 1,2, \dots, N$
- $\phi_{Nx+1,j} = \phi_{1,j}, j = 1,2, \dots, N$
- $\phi_{i,0} = \phi_{i,Ny}, i = 1,2, \dots, N$
- $\phi_{i,Ny+1} = \phi_{i,1}, i = 1,2, \dots, N$

(13)

Gauss-Seidel iteration method

We will use the Gauss-Seidel iteration method to solve the Laplace's and Poisson's equations. Eq. (6) "predicts" the value $\phi_{i,j}$ based on the values of the potential at the four neighboring points. The strategy in the Gauss-Seidel iteration method is to start with an initial guess of the solution and then repeatedly refine the guess until the solution converges to a certain tolerance. This method can be described with the following *relaxation* scheme:

1. Start with an initial guess for the solution $\phi_{i,j}$.
2. Use the current values $\phi_{i,j}$ (i.e., the values from the previous iteration) to "improve" the solution [see Eq. (6)].
3. Calculate the energy [see Eq. (7)].
4. Repeat steps 2 and 3 until the solution or the energy converges to a desired tolerance or a maximum number of iterations is reached.

The convergence efficiency of the Gauss-Seidel iteration method can be enhanced if at each step of the relaxation $\phi_{i,j}$ is replaced by a linear mixture of its old value and the "improved" one. I.e.,

$$\phi_{i,j} = (1-\omega)\phi_{i,j} + \omega\frac{1}{4}\left(\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} + h^2 S_{i,j}\right) \qquad (14)$$

where, ω controls the rate of relaxation and can be adjusted. $\omega < 1$ corresponds to *over-relaxation* and $\omega < 1$ to *under-relaxation*. It can be shown that the method is convergent for $0 < \omega < 2$.

The following figures show the solution of the Poisson's equation for different boundary conditions.

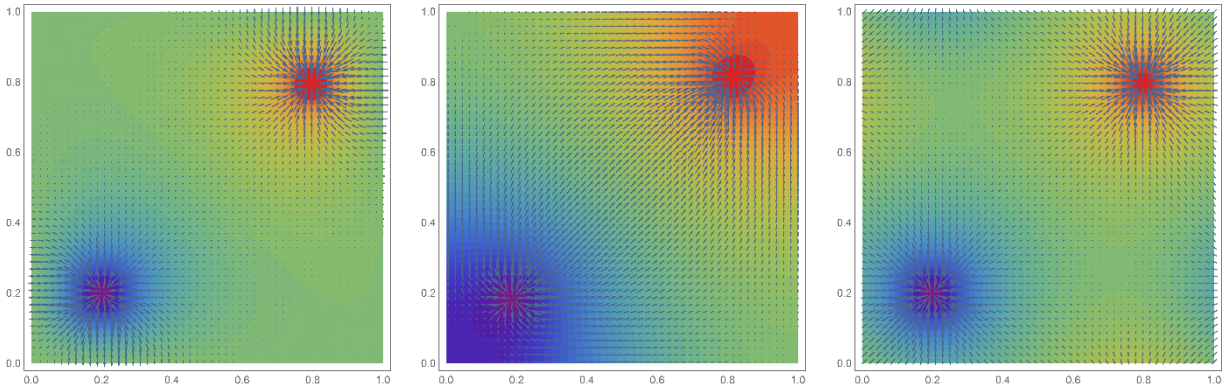

Figure 2 Potential ϕ and vector field derived by the Poisson's equation for a system consisting of positive (placed at the blue-colored region) and negative charges (placed at the red-colored region). The system is charge neutral, i.e., the sum of positive and negative charges is zero. Left: Dirichlet boundary conditions. The value of the potential at the sides of the cell is fixed to 0. Middle: Neumann boundary conditions. The normal derivative on the boundaries is fixed to zero. Right: Periodic boundary conditions. A mesh of 200×200 points has been implemented.

Tasks

15 points	• Develop a code that to numerically solve the Laplace's and Poisson's equations in a rectangular cell using Dirichlet boundary conditions. • Set the potential at the sides of the rectangle to zero. • Start from a simple charge distribution (e.g., dipole consisting of two charges of opposite signs placed at a certain distance) and investigate the effect ω has on the convergence. Try $\omega < 1$, $1 < \omega < 2$, and $\omega > 2$. Do you observe significant differences in the convergence? Adjust the convergence threshold to small values, i.e., 10^{-14}. • Keep the size of the rectangular cell fixed and increase the mesh size (e.g., $N_x = N_y = 10, 100, 1000$, etc. How does this affect the calculated energy [see Eq. (7)]. • Place the dipole at different distances from the boundaries of the cell (keep the distance between the two charges fixed). Does this affect the energy? If you want to calculate the potential around an isolated dipole, what is the best strategy in terms of the dipole's position and the cell's size? • Place the center of mass of the dipole at the center of the cell. Keeping the center of mass fixed, change the distance between the two charges. Are the results you get physically meaningful? • Create a Faraday cage in the cell. Is the calculated potential physically meaningful? • Can you create a capacitor?
10 points	• Implement Neumann and Periodic Boundary conditions. • Calculate the potential arising from a dipole with its center of mass placed at the center of the cell. What differences do you observe in the calculated potential? Can you explain? (hint: it may be helpful to calculate and visualize the corresponding vector field). • If, instead of a dipole, try to solve the Poisson's equation with a single charge (i.e., the system is not charge neutral) and periodic boundary conditions. What do you observe? Can you explain?
	Fill free to try any charge distribution having any shape, profile etc. and plot the corresponding field even if this distribution cannot be considered physically relevant.