MATH 4311 Spring 2025

Program 3 Due: April 3, 2025

This project considers the Poisson–Boltzmann equation (PBE) which describes the distribution of electric potential and ion concentration around charged surfaces in solutions. This equation has been widely and successfully applied in energy devices such as lithium battery and super-capacitor, and in biology such as DNA and protein functionality and structure.

For simplicity, we consider a capacitor whose two planar electrodes are located at $x = 0$ and $x = L$. The region $0 \le x \le L$ is occupied by electrolyte solution. There are only 2 types of ions, with valence $\pm z$. For example, $NaCl$ solution dissolves into Na^+ and Cl^- with valence ± 1. The electrostatic potential of this system can be described by the following BVP,

$$\begin{cases} \phi_{xx} = z \sinh(z\phi), \\ \phi(0) = 0, \\ \phi(L) = V. \end{cases}$$

Here V represents the voltage of the capacitor. The surface charge density on the electrodes can be calculated as $\sigma_L = \phi_x(0)$ and $\sigma_R = -\phi_x(L)$. Here we should see $\sigma_L = -\sigma_R = \sigma$. Then the capacitance of this capacitor can be calculated as

$$C(V) = \frac{\sigma}{V}.$$

Notice, for different voltage applied to the capacitor, the capacitance might be different.

(A) Write a program using finite difference method to solve the equation.

(B) For $z = 1$, $L = 6$, Plot the curve $\phi(x)$ and the curve $C(V)$ using the data from $V = -5,\ -4,\ -3,\ \cdots\ ,\ 3,\ 4,\ 5$. You might use spacing $h = 0.01$.

Hint: With $\phi(x)$ solved, we might use finite difference formula to approximately estimate $\sigma \approx \dfrac{\phi(h) - \phi(0)}{h} \approx \dfrac{\phi(L) - \phi(L-h)}{h}$.

(C) Repeat Part (B) using $z = 1$, $L = 3$. This corresponds to compressing the size of capacitor.

(D) Repeat Part (B) using $z = 2$, $L = 6$. This corresponds to using divalent ions instead of multivalent ions.

(E) Write a program using finite element method to solve the linearized PBE,

$$\begin{cases} \phi_{xx} = z^2\phi, \\ \phi(0) = 0, \\ \phi(L) = V. \end{cases}$$

(F) Repeat Part (B)(C)(D) using the program from Part (E).