Homework #5

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Calculating electrostatic potential with Newton method

Introduction

I calculated the electrostatic potential, ϕ, with equation

$$\mathrm{N}^{+} + n_{int}e^{-\frac{q\phi}{k_B T}} - n_{int}e^{\frac{q\phi}{k_B T}} = 0$$

by using the Newton's method.

The parameters I used is

$$\mathrm{k_B} = \ 1.380648521 \times 10^{-23}\mathrm{m^2kg\ \ s^{-2}K^{-1}}$$

$$\mathrm{q\ \ =\ \ 1.602192\ \ 10^{-19}\ \ C}$$

$$\mathrm{N^{+}\ \ =\ \ \pm\ 10^{10}\ \sim\ 10^{18}\ \ cm^{-3}}$$

$$\mathrm{n_{int}\ \ =\ \ 10^{18}\ \ cm^{-3}}$$

$$\mathrm{T\ \ =\ \ 300\ \ K}$$

Result

First, I compared numerical solution with analytical solution when loop repetition time i = 1000.

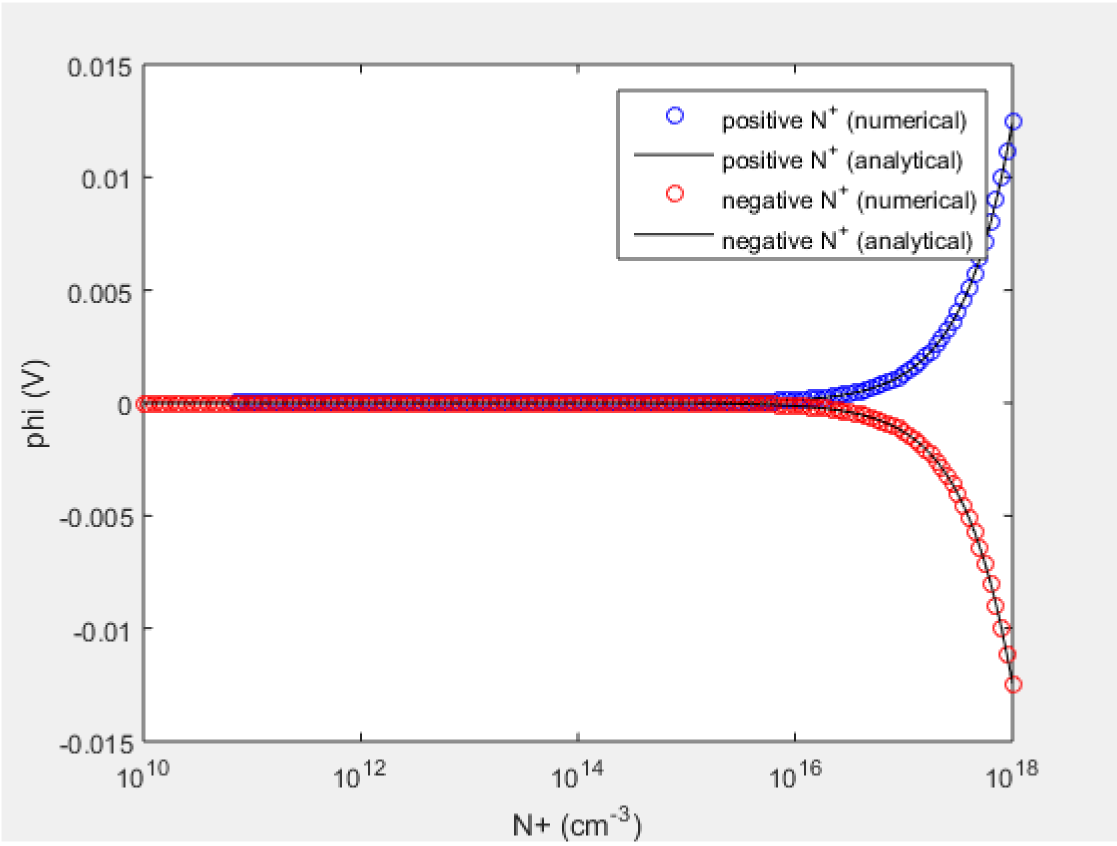

Figure 1. electrostatic potential, ϕ, by using the Newton method (repetition time i = 1000).

We can see that numerically calculated value is almost same with analytically calculated value.

I also estimated the error calculated with the equation

$$error = \frac{\text{Analytical solution} - \text{Numerical solution}}{\text{Analytical solution}} \times 100(\%)$$

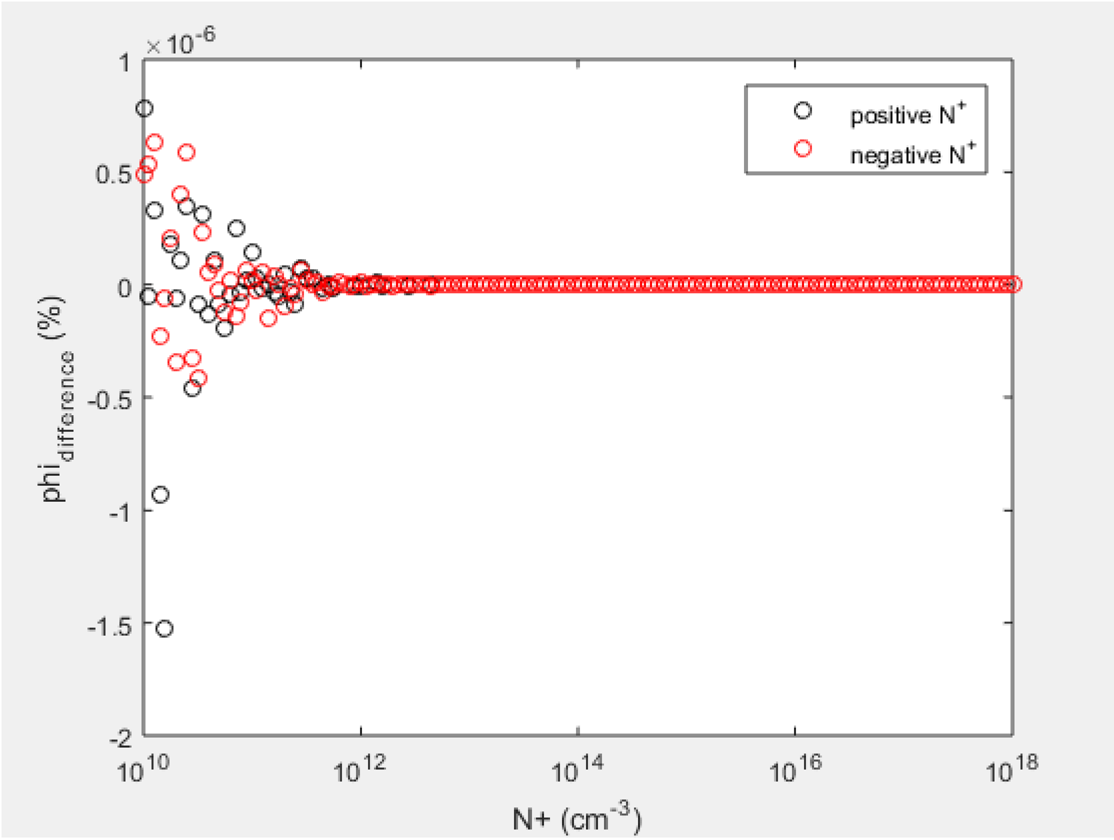

Figure 2. Calculated error.

Here we can clearly see that error is less than 10^{-5} % in every N+. However, error of small N+ is comparatively high than large N+. This is because potential of low N+ is significantly low. Therefore, numerical calculation cannot follow the resolution.

Finally, I also see the numerical solution approach to the analytical solution if we increase the repetition time i.

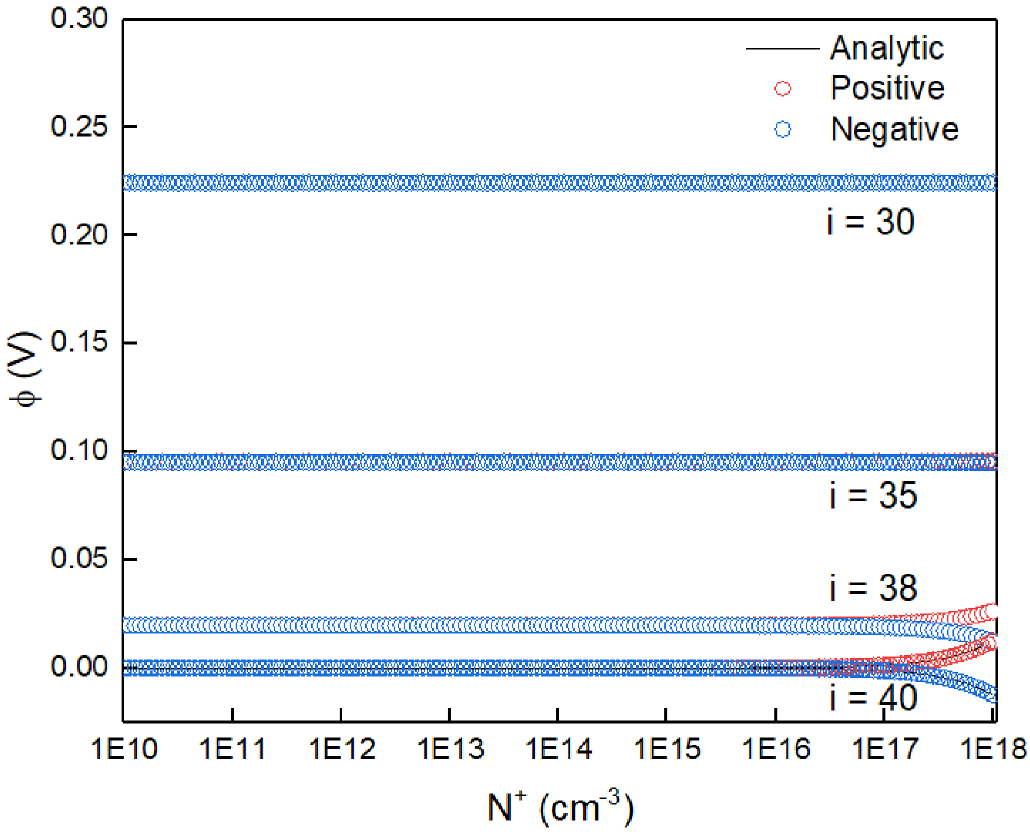

Figure 3. numerical solution approach to the analytical solution