

HW 7.

2020년 9월 24일 목요일 오전 11:25

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Find a root of $N^+ + n_{int} e^{-\frac{\epsilon \phi}{k_B T}} - n_{int} e^{\frac{\epsilon \phi}{k_B T}} = 0$.

Let be a residue $r(\phi) = N^+ + n_{int} e^{-\frac{\epsilon \phi}{k_B T}} - n_{int} e^{\frac{\epsilon \phi}{k_B T}}$
 $= N^+ - 2n_{int} \sinh\left(\frac{\epsilon \phi}{k_B T}\right),$

$$\frac{dr(\phi)}{d\phi} = -2n_{int} \frac{\epsilon}{k_B T} \cosh\left(\frac{\epsilon \phi}{k_B T}\right) \Rightarrow \phi_{new} = \phi_{old} - r(\phi_{old}) / \left. \frac{dr(\phi)}{d\phi} \right|_{\phi=\phi_{old}}$$

$$= \phi_{old} + \left[\frac{N^+ k_B T}{2n_{int} \cosh\left(\frac{\epsilon \phi}{k_B T}\right) \epsilon} - \frac{k_B T}{\epsilon} \tanh\left(\frac{\epsilon \phi}{k_B T}\right) \right]$$

$$\equiv \delta \phi$$

* Numerical algorithm : $|\delta \phi| < \epsilon = 10^{-7}$ 이면 loop termination.

* Exact solution

$$\phi_{root} = \frac{k_B T}{\epsilon} \sinh^{-1}\left(\frac{N^+}{2n_{int}}\right)$$

Results.

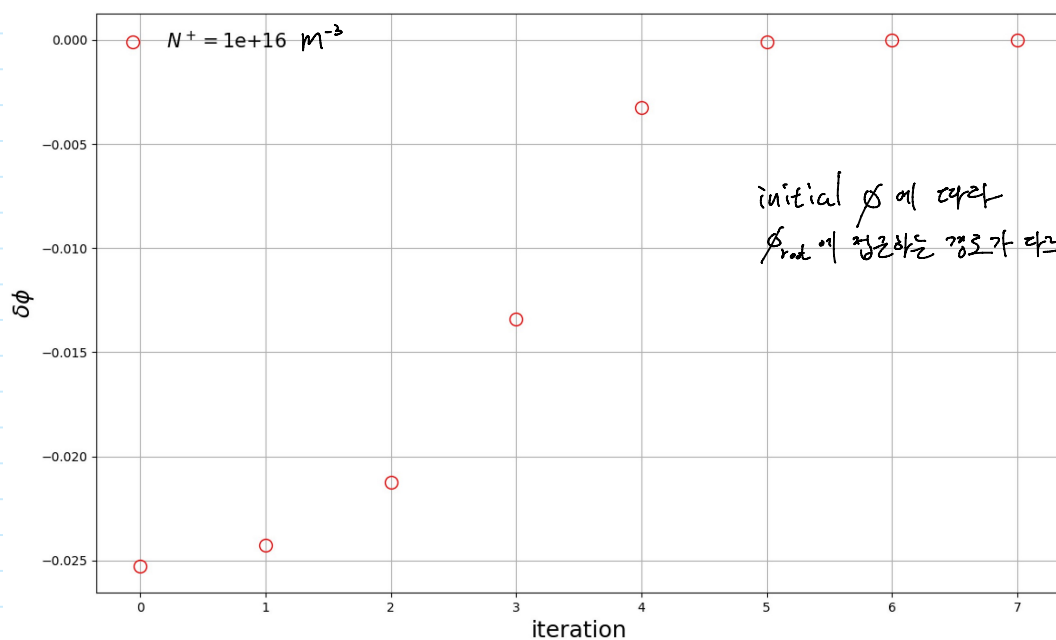
$n_{int} = 10^{16} \text{ m}^{-3}$, $N^+ = 10^{16} \text{ m}^{-3} \sim 10^{24} \text{ m}^{-3}$, $T = 300 \text{ K}$

1) $N^+ = 10^{16} \text{ m}^{-3}$

Exact ϕ : 0.012440283776141349

Numerical ϕ : 0.012440283776141349

, $\phi_0 = 0.1$

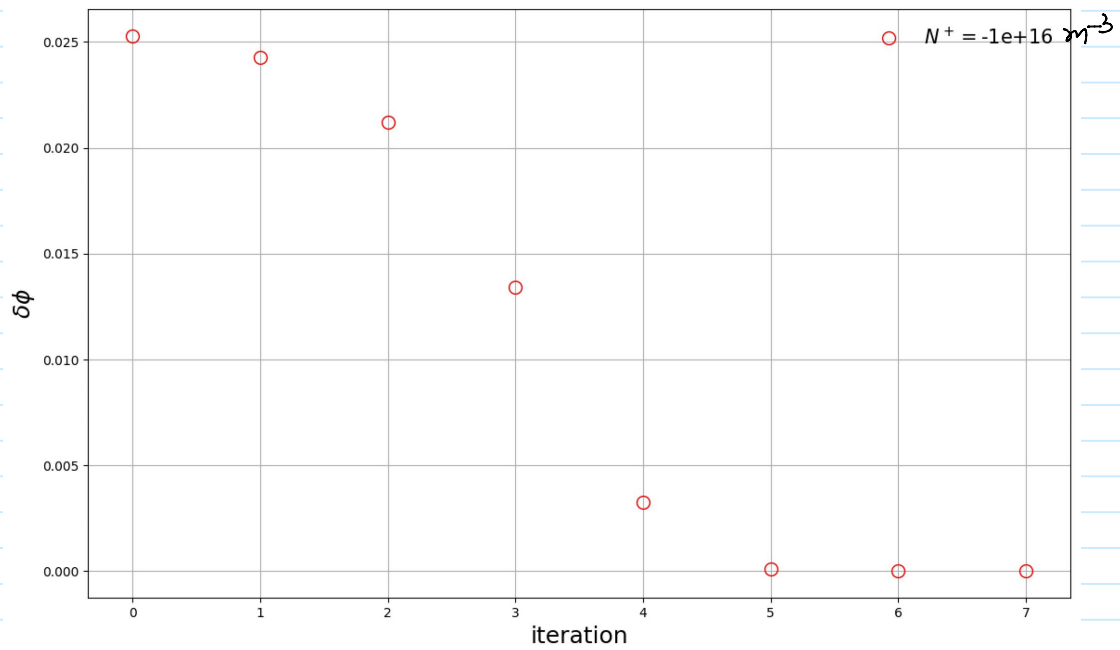


initial ϕ 에 따라
 ϕ_{root} 에 접근하는 경로가 다르다.

$$N^+ = -10^{16} \text{ m}^{-3}$$

Exact ϕ : -0.012440283776141349

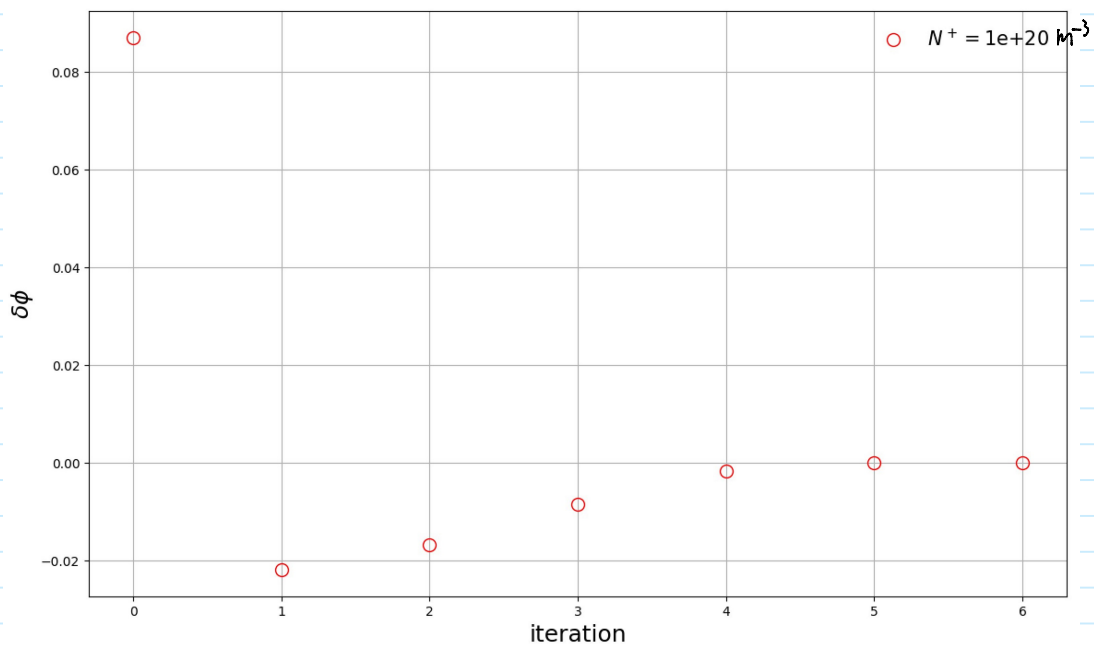
Numerical ϕ : -0.012440283776141349 , $\phi_0 = -0.1$



$$2) N^+ = 10^{20} \text{ m}^{-3}$$

Exact ϕ : 0.23810563676910038

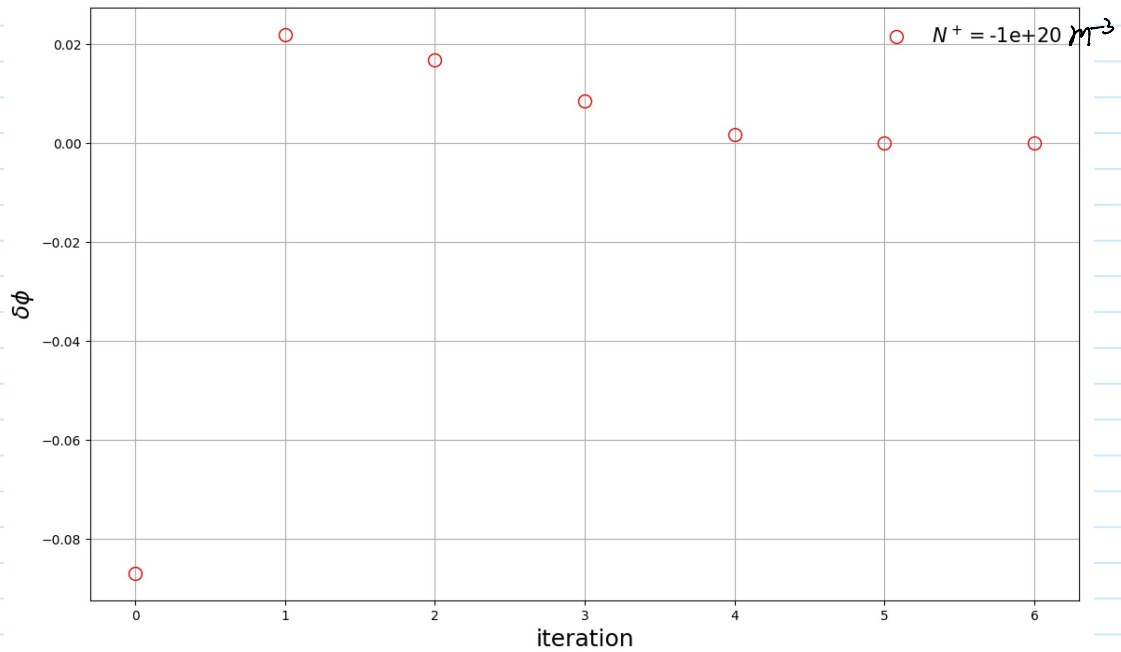
Numerical ϕ : 0.23810563676919358 , $\phi_0 = 0.2$



$$N^+ = -10^{20} \text{ m}^{-3}$$

Exact ϕ : -0.23810563676910038

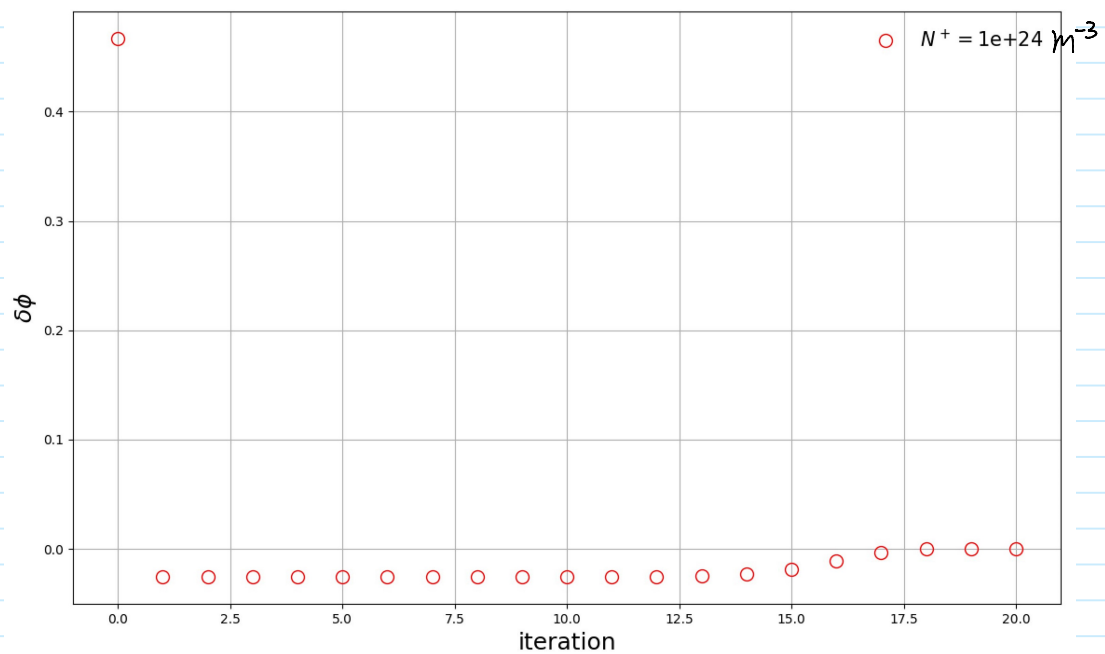
Numerical ϕ : -0.23810563676919358 , $\phi_0 = -0.2$



$$3) N^+ = 10^{24} \text{ m}^{-3}$$

Exact ϕ : 0.47621127302116095

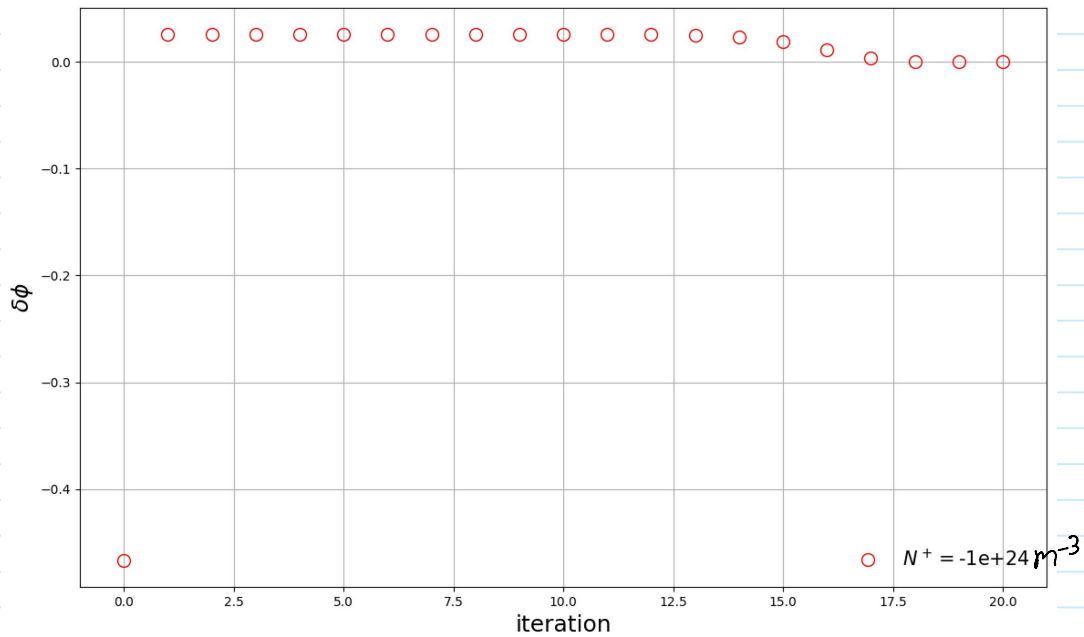
Numerical ϕ : 0.4762112730211609 , $\phi_0 = 0.4$



$$N^+ = -10^{24} \text{ m}^{-3}$$

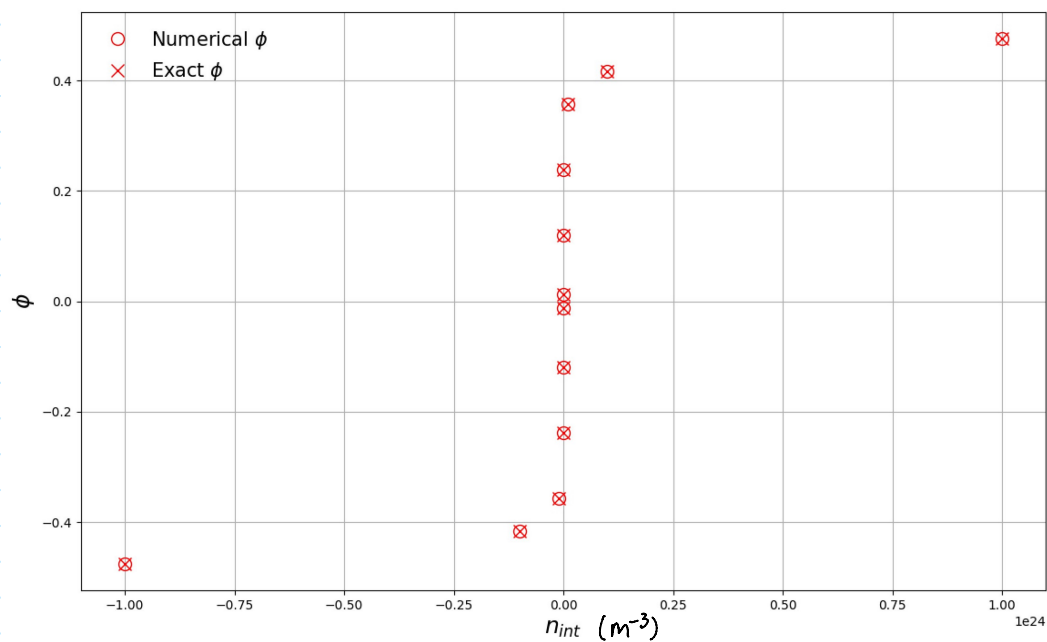
Exact ϕ : -0.47621127302116095

Numerical ϕ : -0.4762112730211609 , $\phi_0 = -0.4$



전체적으로 Newton method가 정확한 값으로 빠르게 수렴이 됨을 알 수 있다.

$$4) N^+ = -10^{24} \sim 10^{24} \text{ m}^{-3}$$



Numerically 구한 $\phi_{\text{root}}(N^+)$ 가 $\sinh(N^+)$ 을 따르는 것 알 수 있다.