Graphene Layer Boundary Condition (Discretized):

$$D_{1\perp} - D_{2\perp} = \sigma \tag{1}$$

$$\mathbf{D} = \varepsilon \mathbf{E} \tag{2}$$

Where ε is the permittivity of the material given by $\kappa\varepsilon_0$ where κ is the dielectric constant of the material and ε_0 is the permittivity of free space. Hence:

$$\varepsilon_1 E_{1\perp} - \varepsilon_2 E_{2\perp} = \sigma \tag{3}$$

Using:

$$\mathbf{E} = -\nabla\phi \tag{4}$$

where $\nabla = \frac{d}{dz}\hat{\mathbf{z}}$ at the boundary, since $E_{\parallel}$ is continuous and hence $\frac{d\phi}{dr} = 0$.

$$\varepsilon_1 \frac{d\phi_1}{dz} - \varepsilon_2 \frac{d\phi_2}{dz} = -\sigma \qquad \begin{cases} \phi(z) = \phi_1 & z_b \leq z \leq z_{max} \\ \phi(z) = \phi_2 & z_0 \leq z \leq z_b \end{cases} \tag{5}$$

Discretizing using forward and backward differences for the gradient of $\phi(z)$ above and below the boundary, respectively gives:

$$\frac{d\phi_1}{dz} \approx \frac{\phi_{i,j+1} - \phi_{i,j}}{h} \qquad \frac{d\phi_2}{dz} \approx \frac{\phi_{i,j} - \phi_{i,j-1}}{h} \tag{6}$$

where i and j and the r and z indices of the boundary and h is the step size.
Then substituting 6 into equation 5:

$$\frac{\varepsilon_1\phi_{i,j+1} - \varepsilon_1\phi_{i,j} - \varepsilon_2\phi_{i,j} + \varepsilon_2\phi_{i,j-1}}{h} = -\sigma$$

$$\varepsilon_1\phi_{i,j+1} - \varepsilon_1\phi_{i,j} - \varepsilon_2\phi_{i,j} + \varepsilon_2\phi_{i,j-1} = -h\sigma$$

$$-(\varepsilon_1 + \varepsilon_2)\phi_{i,j} + \varepsilon_1\phi_{i,j+1} + \varepsilon_2\phi_{i,j-1} = -h\sigma$$

$$\phi_{i,j} = \frac{\varepsilon_1\phi_{i,j+1} + \varepsilon_2\phi_{i,j-1} + h\sigma}{\varepsilon_1 + \varepsilon_2} \tag{7}$$

However, σ is dependent on $\phi_{i,j}$:

$$\sigma = \frac{e\phi_{i,j}^2}{\pi\gamma^2} \tag{8}$$

where e is electron charge and γ is the proportionality constant in the dispersion relation:

$$E = \hbar v_F k = \gamma k \tag{9}$$

expressed in units of $eVnm$. Substituting 8 into equation 7 gives a quadratic equation:

$$\phi_{i,j} = \frac{\varepsilon_1\phi_{i,j+1} + \varepsilon_2\phi_{i,j-1}}{\varepsilon_1 + \varepsilon_2} + \frac{he}{\pi\gamma^2(\varepsilon_1 + \varepsilon_2)}\phi_{i,j}^2 \tag{10}$$

Using the quadratic formula to give the update equation:

$$\phi_{i,j} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad \begin{cases} a = \frac{he}{\pi\gamma^2(\varepsilon_1+\varepsilon_2)} \\ b = -1 \\ c = \frac{\varepsilon_1\phi_{i,j+1} + \varepsilon_2\phi_{i,j-1}}{\varepsilon_1+\varepsilon_2} \end{cases} \tag{11}$$

but get issues with square root. To get it this to work in the code need:

$$\phi_{i,j} = \frac{-b - \sqrt{\mid b^2 - 4ac \mid}}{2a} \tag{12}$$