Problems:

1. This example is a demonstration of the fact that explicit numerical integration methods are incapable of solving even the problem of linearly-graded junctions in thermal equilibrium, for which $N_D - N_A = mx$, where *a* is the edge of the depletion region. To demonstrate this, calculate the following:

- Establish the boundary conditions for the electrostatic potential [$\psi(-a)$ and $\psi(a)$] by taking into account the free carrier terms in the equilibrium 1D Poisson equation:

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{e}{\varepsilon}(p - n + mx) = -\frac{e}{\varepsilon}\left(n_i e^{-\psi/V_t} - n_i e^{\psi/V} + mx\right)$$

- Solve analytically the 1D Poisson equation for $\psi(x)$ within the depletion approximation (no free carriers) and calculate *a* using this result as well as the boundary conditions found in (step 1). What is the expression for absolute value of the maximum electric field?
- Apply the explicit integration method for the numerical solution of the 1D Poisson equation (that includes the free carriers) by following the steps outlined below:
  - Write a Taylor series expansion for $\psi(x)$ around *x=0*, keeping the terms up to the fifth order.
  - Starting from the equilibrium Poisson equation, analytically calculate $\psi''(0)$, $\psi^{(3)}(0)$, $\psi^{(4)}(0)$ and $\psi^{(5)}(0)$.
  - Use the maximum value of the electric field derived in (step 2) to determine from the Taylor series expansion for $\psi(x)$, the terms $\psi(h)$, $\psi(2h)$ and $\psi(3h)$.
  - Compute $\psi(x)$ at x=4h, 5h, 6h, … , up to $x_{\max} = 0.5\mu m$, using the predictor-corrector method in which the predictor formula:

$$\psi_{i+1} = 2\psi_{i-1} - \psi_{i-3} + 4h^2\left(\psi''_{i-1} + \frac{\psi''_i - 2\psi''_{i-1} + \psi''_{i-2}}{3}\right)$$

is applied to predict ψ_{i+1}, which is then corrected by the corrector formula:

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} + h^2\left(\psi_i'' + \frac{\psi_{i+1}'' - 2\psi_i'' + \psi_{i-1}''}{12}\right).$$

- In both, the predictor and the corrector formulas, the second derivatives are obtained from the Poisson's equation. The role of the predictor is to provide ψ_{i+1}'' that appears in the corrector formula.

- Repeat the above procedure for the following values of the first derivative:
  - Trial 1: $\psi'(0)_1 = \psi'(0)$,
  - Trial 2: $\psi'(0)_2 = \psi'(0)_1 / 2$,
  - Trial 3: $\psi'(0)_3 = 0.5[\psi'(0)_1 + \psi'(0)_2]$.
  - Repeat the above described process for several iteration numbers, say up to n=22. Comment on the behavior of this explicit integration scheme.

Use the following parameters in the numerical integration:

$e = 1.602\times10^{-19}C,\ \varepsilon = 12\varepsilon_0 = 1.064\times10^{-12}F/cm,\ T = 300K,$
$n_i = 1.4\times10^{10}cm^{-3},\ \ m = 10^{21}cm^{-4},\ h = 2\times10^{-7}cm.$

2. Write a 1D Poisson equation solver that solves the linearized Poisson equation for a pn-junction under equilibrium condition, with:

(a) $N_A = 10^{15}cm^{-3}, N_D = 10^{15}cm^{-3}$,

(b) $N_A = 10^{16}cm^{-3}, N_D = 10^{16}cm^{-3}$,

(c) $N_A = 10^{16}cm^{-3}, N_D = 10^{18}cm^{-3}$.

For each of these three device structures:

- Calculate analytically the maximum allowed mesh size in each region.
- Plot the conduction band edge versus distance assuming that the Fermi level is the reference energy level ($E_F = 0$).

- Plot the total charge density versus distance.
- Plot the electric field versus distance. Calculate the electric field using centered difference scheme.
- Plot electron and hole densities versus distance.
- Calculate analytically, using the block-charge approximation, the width of the depletion regions and the magnitude of the peak electric field, and compare the analytical with the numerical simulation results. When is the block-charge approximation invalid?