Homework #8

20152052

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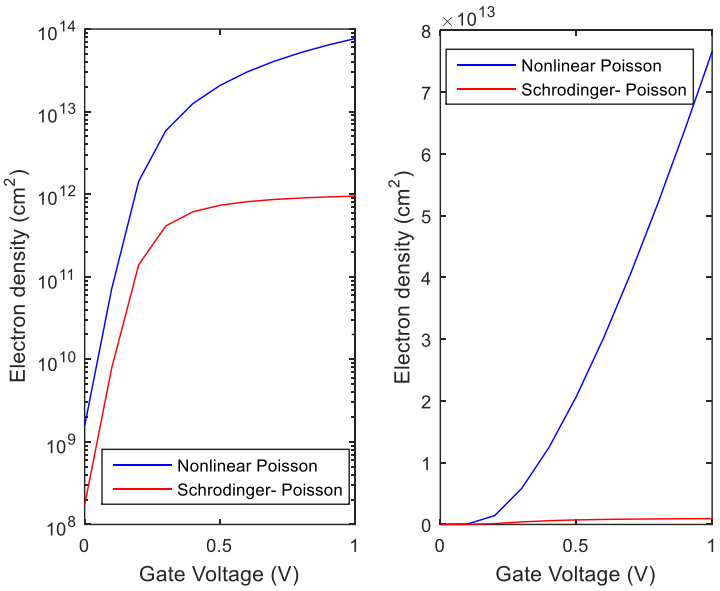
1. Compare the 2D electron density obtained by nonlinear Poisson (NP) solver with Schrodinger-Poisson (SP) solver.

First, I tried to calculate electron density with simple Poission equation solver.

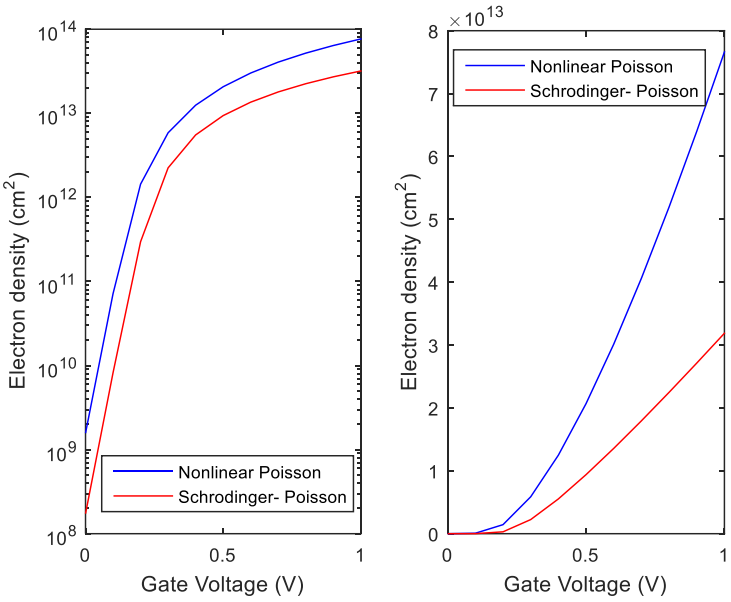
The result little change of electron density in high voltage in SP solver.

(wrong result)



This is because electrostatic potential did not included the difference of electron density calculated by Schrodinger-Poisson solver. Thus, as applied voltage becomes larger, the error becomes larger.

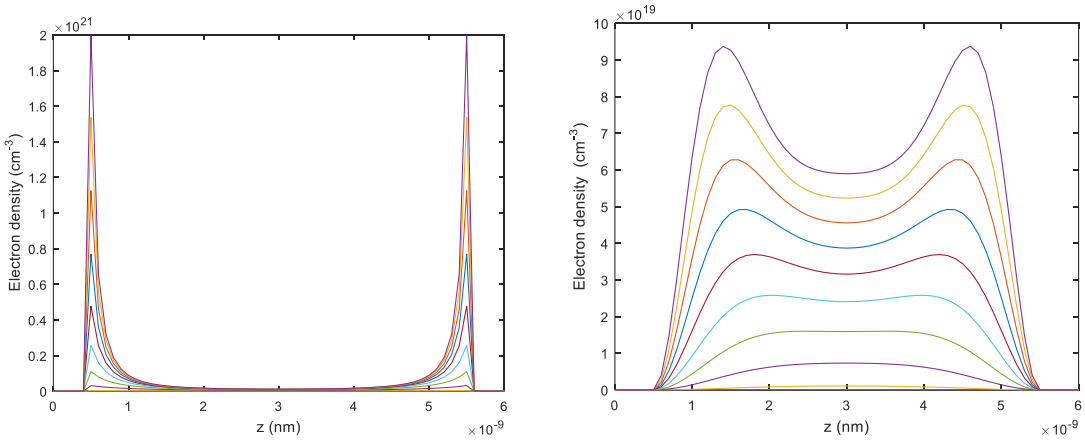
The Newton method is used as second trials to complement SP solver.



Since the method has Jacobian and reside terms, the calculated electron density changes as difference of updated electrostatic potential.

Nonetheless, the difference in density of electrons calculated in NP solver and SP solver is too large.

2. Compare the 3D electron density obtained by nonlinear Poisson solver with Schrodinger-Poisson solver



Left and right figure represent the electron density calculated by NP and SP solver.