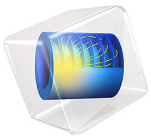
Created in COMSOL Multiphysics 6.2



Density-Gradient and Schrödinger–Poisson Results for a Silicon Inversion Layer

This tutorial demonstrates the use of the density-gradient formulation to include the effect of quantum confinement in the device physics simulation of a silicon inversion layer. This formulation requires only a moderate increase of computational resources as compared to the conventional drift–diffusion equation. Thus, it allows much speedier engineering investigation than other more sophisticated quantum mechanical methods. The result of the density-gradient theory is compared with the solution of the Schrödinger–Poisson equation. The computed electron density profiles from both theories show the expected behavior of quantum confinement and both agree well with the published figures in the reference paper.

Introduction

As the semiconductor fabrication technology progresses to produce smaller and smaller devices, the effect of quantum confinement becomes more and more important. This tutorial follows the approach described in Ref. 1 to compute the electron density distribution of a Si inversion layer using the density-gradient theory (as reviewed in Ref. 2) and to compare with the result from the self-consistent Schrödinger–Poisson theory.

Model Definition

The model aims to reproduce Fig. 4 in Ref. 1, which plots the electron density profiles underneath the gate oxide as computed with each of the two theories. Not all simulation details are given in the paper, especially the Schrödinger–Poisson simulator. Nevertheless, the approach described in the paper is followed as closely as possible. When a parameter is not listed, a typical value found in the literature is used in the model: the material properties of silicon and oxide are taken from Ref. 3; the parameters used for the Schrödinger–Poisson theory are taken from Ref. 4. The section Modeling Instructions lists all the parameters used in the model.

The oxide thickness is 3.1 nm and the doping concentration is $3.8{\cdot}10^{16}$ cm^{-3}. The effective mass for the density-gradient formulation is $1/3$ of the electron mass. The temperature is assumed to be 300 K. Fermi–Dirac statistics is used. The gate metal work function of 4.01 V is selected to match the peak electron densities shown in Fig. 4 in Ref. 1.

The Schrödinger–Poisson simulator used in Ref. 1 does not quantize the holes according to the author. Thus in this model we take the following strategy to treat the holes classically. First, both electron and hole concentrations are solved for using the density-gradient theory. Then, in the Schrödinger–Poisson equation, only the electron wave functions are solved for, with the hole concentration fixed to be the same as in the solution

of the density-gradient study. In other words, only the behavior of the electron gas is solved for using the two different methods and the two solutions will be compared.

See the comments in the section Modeling Instructions for more detailed discussions on the model construction, solution processes, and result visualization.

Results and Discussion

Figure 1 and Figure 2 show the electron density profiles for two values of gate voltage as computed by the two theories and at two different levels of zoom. They compare well with Fig. 4(a) and 4(b) in Ref. 1, respectively. The only difference is in the behavior of the Schrödinger–Poisson solution, which shows an abrupt drop off in the paper but not in this model. The drop off is just an artifact caused by the fact that an insufficient number of wave functions were used in the Schrödinger–Poisson simulator in the paper.

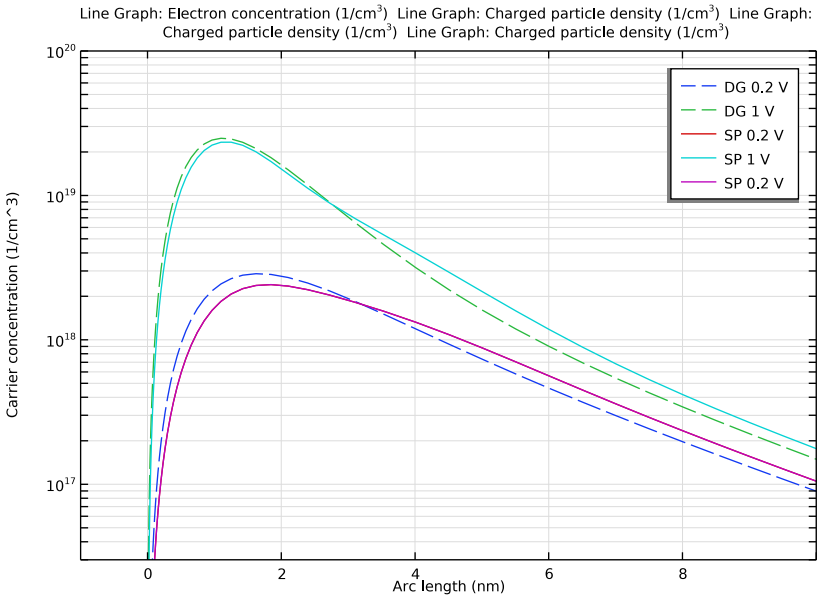


Figure 1: Electron density profiles for two values of gate voltage as computed using the two theories.

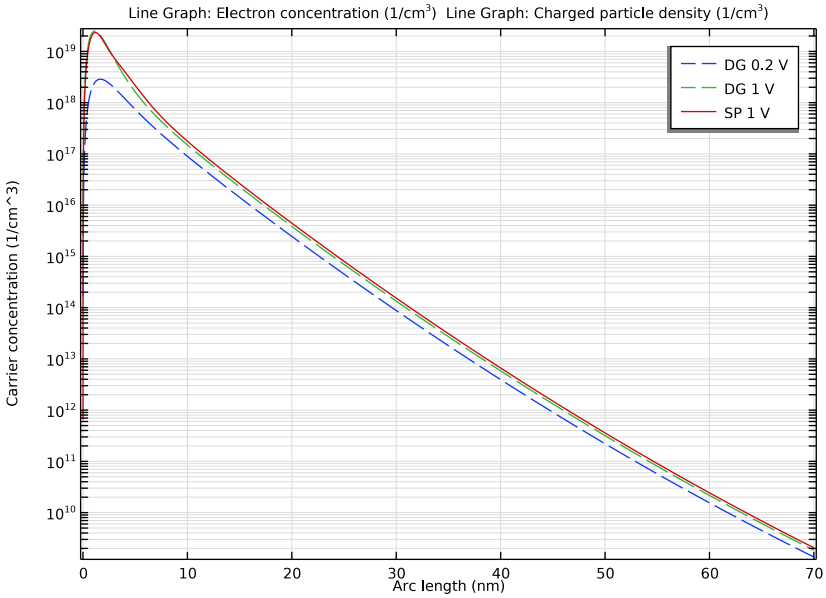


Figure 2: Zoomed-in version of the plot above.

References

1. M.G. Ancona, "Equations of State for Silicon Inversion Layers," *IEEE Trans. Elec. Dev.*, vol. 47, no. 7, p. 1449, 2000.

2. M.G. Ancona, "Density-gradient theory: a macroscopic approach to quantum confinement and tunneling in semiconductor devices," *J. Comput. Electron.*, vol. 10, p. 65, 2011.

3. S.M. Sze and K.K. Ng, *Physics of Semiconductor Devices*, 3rd ed., Wiley, 2007.

4. F. Stern, "Self-Consistent Results for n-Type Si Inversion Layers," *Phys. Rev. B*, vol. 5, no. 12, p. 4891, 1972.

Application Library path: `Semiconductor_Module/Device_Building_Blocks/si_inversion_layer_density_gradient_and_schrodinger_poisson`

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

Select the **Semiconductor** interface first. We will add the **Schrödinger-Poisson Equation** multiphysics interface later.

2 In the **Select Physics** tree, select **Semiconductor>Semiconductor (semi)**.

3 Click **Add**.

4 Click **Study**.

The **Semiconductor Equilibrium** study step is suitable and easier to solve for systems known to be in thermal equilibrium.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Semiconductor Equilibrium**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard starts the COMSOL Desktop at the **Geometry** node. Use this chance to select a convenient length unit. Then create the 1D geometry with a few consecutive intervals for easily plotting the results in various regions of interest.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **nm**.

Interval 1 (i1)

1 Right-click **Component 1 (comp1)>Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 From the **Coordinate source** list, choose **Vector**.

4 In the **Coordinates** text field, type `0, 10, 70, 300, 1e3`.

GLOBAL DEFINITIONS

Parameters for Density-Gradient

Enter the parameters for the density-gradient model.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Parameters for Density-Gradient` in the **Label** text field.

3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
T0	300[K]	300 K	Temperature
mnDG	me_const/3	3.0365E-31 kg	Density-gradient effective mass
Na0	3.8e16[1/cm^3]	3.8E22 1/m³	Doping concentration
Vg	0[V]	0 V	Gate voltage
epsrOx	3.9	3.9	Oxide dielectric constant
dOx	3.1[nm]	3.1E-9 m	Oxide thickness
Phi0	4.01[V]	4.01 V	Gate metal work function

Add a blank material and then fill in the material data.

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Electron mobility	mun	1450[cm^2/(V*s)]	m²/(V·s)	Semiconductor material
Hole mobility	mup	500[cm^2/(V*s)]	m²/(V·s)	Semiconductor material

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 0	11.9	1	Basic
Band gap	Eg0	1.12[V]	V	Semiconductor material
Electron affinity	chi0	4.05[V]	V	Semiconductor material
Effective density of states, conduction band	Nc	2.80e19[cm^-3]	1/m³	Semiconductor material
Effective density of states, valence band	Nv	2.65e19[cm^-3]	1/m³	Semiconductor material

Set up physics formulations and parameters.

SEMICONDUCTOR (SEMI)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.

2 In the **Settings** window for **Semiconductor**, locate the **Model Properties** section.

3 From the **Carrier statistics** list, choose **Fermi–Dirac**.

4 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element density-gradient (quadratic shape function)**.

Semiconductor Material Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Semiconductor (semi)** click **Semiconductor Material Model 1**.

2 In the **Settings** window for **Semiconductor Material Model**, locate the **Model Input** section.

3 In the T text field, type `T0`.

4 Locate the **Material Properties, Density-Gradient** section. In the $\mathbf{m}_e^{DG}$ text field, type `mnDG`.

The holes are not treated quantum mechanically in the reference paper. Use an arbitrary large effective mass to minimize the effect of the density-gradient contribution from holes.

5 In the $\mathbf{m}_h^{DG}$ text field, type `10*me_const`.

Analytic Doping Model 1

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Impurity** section. In the N_{A0} text field, type `Na0`.

Metal Contact 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Metal Contact**.

2 Select Boundary 5 only.

Thin Insulator Gate 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Thin Insulator Gate**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Thin Insulator Gate**, locate the **Terminal** section.

4 In the V_0 text field, type `Vg`.

5 Locate the **Gate Contact** section. In the ε_{ins} text field, type `epsrOx`.

6 In the d_{ins} text field, type `dOx`.

7 In the Φ text field, type `PhiO`.

The Schrödinger-Poisson computation in the reference paper assumes an infinite barrier height at the oxide interface. Use a large barrier height for electrons to approximate the infinite barrier limiting case. On the other hand, use zero barrier height for the holes to suppress the quantum confinement effect from the density-gradient formulation.

8 Locate the **Density-Gradient** section. From the **Formulation** list, choose **Potential barrier**.

9 In the $\Phi_n{}^{Ox}$ text field, type `1e4[V]`.

10 In the $\Phi_p{}^{Ox}$ text field, type `0[V]`.

MESH 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Fine**.

Remove artificial interior boundaries from the auto-generated list for mesh refinement.

Size 1

1 In the **Model Builder** window, click **Size 1**.

2 Select Boundary 5 only.

Specify a small mesh element size at the oxide interface to resolve the very large gradient there.

Size 2

1 In the **Model Builder** window, click **Size 2**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section.

5 Select the **Maximum element size** check box. In the associated text field, type `1e-4`.

Add a **Size** node to prevent the mesh element size from growing too large in the regions of interest in which the results will be plotted.

Size 3

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.

2 Right-click **Size 3** and choose **Move Up**.

3 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

4 From the **Geometric entity level** list, choose **Domain**.

5 Select Domains 1–3 only.

6 Locate the **Element Size** section. From the **Calibrate for** list, choose **Semiconductor**.

7 From the **Predefined** list, choose **Finer**.

8 Click the **Custom** button.

9 Locate the **Element Size Parameters** section.

10 Select the **Maximum element size** check box. In the associated text field, type `0.5`.

STUDY 1: DENSITY-GRADIENT

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1: Density-Gradient` in the **Label** text field.

Step 1: Semiconductor Equilibrium

1 In the **Model Builder** window, under **Study 1: Density-Gradient** click **Step 1: Semiconductor Equilibrium**.

2 In the **Settings** window for **Semiconductor Equilibrium**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click + **Add**.

Start the gate voltage sweep at a value close to the flat band condition for easier convergence.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`-1 0.2 1`	V

6 In the table, click to select the cell at row number 1 and column number 3.

7 In the **Home** toolbar, click = **Compute**.

RESULTS

Net Dopant Concentration (semi)

The model has a uniform p-doping therefore, we remove the generated default plot, Net Dopant Concentration.

1 In the **Model Builder** window, under **Results** right-click **Net Dopant Concentration (semi)** and choose **Delete**.

Duplicate the plot group **Carrier Concentrations** to plot the electron density in the regions of interest to be compared with Fig.4 in the reference paper.

Carrier Concentrations (semi)

In the **Model Builder** window, under **Results** right-click **Carrier Concentrations (semi)** and choose **Duplicate**.

Electron Concentration Comparison

1 In the **Model Builder** window, under **Results** click **Carrier Concentrations (semi) 1**.

2 In the **Settings** window for **1D Plot Group**, type `Electron Concentration Comparison` in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (Vg)** list, choose **Manual**.

4 In the **Parameter indices (1-3)** text field, type `2 3`.

Hole Concentration

1 In the **Model Builder** window, expand the **Electron Concentration Comparison** node.

2 Right-click **Hole Concentration** and choose **Delete**.

Density-Gradient

The region of interest can be conveniently specified by selecting the domains to be plotted.

1 In the **Model Builder** window, under **Results>Electron Concentration Comparison** click **Electron Concentration**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 Click to select the **Activate Selection** toggle button.

4 Select Domains 1 and 2 only.

5 In the **Label** text field, type `Density-Gradient`.

For easier comparison, make the plot line style the same as the one in the reference paper.

6 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

7 Click to expand the **Legends** section. From the **Legends** list, choose **Automatic**.

8 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `DG ` .

Electron Concentration Comparison

1 In the **Model Builder** window, right-click **Electron Concentration Comparison** and choose **Duplicate**.

Alternatively, the region of interest for plotting can be specified using the option **Manual axis limits**.

2 In the **Model Builder** window, click **Electron Concentration Comparison**.

3 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

4 Select the **Manual axis limits** check box.

5 In the **x minimum** text field, type `-1`.

6 In the **x maximum** text field, type `10`.

7 In the **y minimum** text field, type `3e16`.

8 In the **y maximum** text field, type `1e20`.

For the Schrödinger-Poisson study, we take the approach that it shares the same hole and ionized dopant concentrations as the density-gradient study, such that the only difference between the two studies is the treatment of the electron distribution. As such, various results from the previous study will be taken as the inputs to the following setup steps where appropriate.

Now add the **Schrödinger-Poisson Equation** multiphysics interface. Remember to exclude **Study 1** from the newly added interface.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1: Density-Gradient**.

4 In the tree, select **Semiconductor>Schrödinger–Poisson Equation**.

5 Click **Add to Component 1** in the window toolbar.

6 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

SCHRÖDINGER EQUATION (SCHR)

Add the parameters used by the **Schrödinger-Poisson Equation** multiphysics interface.

GLOBAL DEFINITIONS

Parameters for Schrödinger-Poisson

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters for Schrödinger-Poisson` in the **Label** text field.

3 Locate the **Parameters** section. In the table, enter the following settings:

Name	Expression	Value	Description
nv	2	2	Valley degeneracy
fm3	0.916	0.916	Longitudinal effective mass factor
fm1	0.190	0.19	Transverse effective mass factor 1
fm2	0.190	0.19	Transverse effective mass factor 2
m3	fm3*me_const	8.3442E-31 kg	Longitudinal effective mass
m1	fm1*me_const	1.7308E-31 kg	Transverse effective mass 1
m2	fm2*me_const	1.7308E-31 kg	Transverse effective mass 2
md	sqrt(m1*m2)	1.7308E-31 kg	Density of states effective mass

Restrict the **Schrödinger-Poisson Equation** domain selection to a reasonable range near the oxide interface.

SCHRÖDINGER EQUATION (SCHR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.

2 Select Domains 1–3 only.

ELECTROSTATICS (ES)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electrostatics (es)**.

2 Select Domains 1–3 only.

SCHRÖDINGER EQUATION (SCHR)

Effective Mass 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Schrödinger Equation (schr)** click **Effective Mass 1**.

2 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

3 In the $\mathbf{m}_{\mathrm{eff,e,11}}$ text field, type `m3`.

Electron Potential Energy 1

1 In the **Model Builder** window, click **Electron Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

3 From the V_e list, choose **User defined**. In the associated text field, type `0`.

Specify the **Zero Probability** boundary condition at the oxide interface, to match the infinite barrier limiting case assumed by the reference paper.

Zero Probability 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Zero Probability**.

2 Select Boundary 1 only.

Use the density-gradient result for the initial guess electron density distribution, as well as the (fixed) space charge contribution from the holes and ionized dopants.

ELECTROSTATICS (ES)

In the **Model Builder** window, under **Component 1 (comp1)** click **Electrostatics (es)**.

Space Charge Density 1: initial electron density

1 In the **Physics** toolbar, click **Domains** and choose **Space Charge Density**.

2 In the **Settings** window for **Space Charge Density**, type `Space Charge Density 1: initial electron density` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Space Charge Density** section. In the ρ_v text field, type `-e_const*semi.N`.

5 Right-click **Space Charge Density 1: initial electron density** and choose **Duplicate**.

Space Charge Density 2: holes and ionized dopants

1 In the **Model Builder** window, under **Component 1 (comp1)>Electrostatics (es)** click **Space Charge Density 1: initial electron density 1**.

2 In the **Settings** window for **Space Charge Density**, type `Space Charge Density 2: holes and ionized dopants` in the **Label** text field.

3 Locate the **Space Charge Density** section. In the ρ_v text field, type `e_const*(semi.P+semi.Ndplus-semi.Naminus)`.

Similarly use the density-gradient result for the electrostatics boundary conditions.

Electric Potential 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Potential**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the V_0 text field, type `-semi.Ec`.

Electric Displacement Field 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Displacement Field**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Electric Displacement Field**, locate the **Electric Displacement Field** section.

4 Specify the $\mathbf{D}_0$ vector as

`epsilon0_const*epsrOx*(Vg-(PhiO-semi.chi_semi)-V2)/dOx`	`x`

Set up the multiphysics coupling, again borrowing the result from the density-gradient simulation where appropriate.

MULTIPHYSICS

Schrödinger–Poisson Coupling 1 (schrp1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Schrödinger–Poisson Coupling 1 (schrp1)**.

2 In the **Settings** window for **Schrödinger–Poisson Coupling**, locate the **Model Input** section.

3 In the T text field, type `T0`.

The variable for the equilibrium Fermi level is not available in the current evaluation context. Thus we need to use the **withsol** operator to retrieve its value.

4 Locate the **Particle Density Computation** section. In the E_f text field, type `e_const*withsol('sol1',semi.Ef_0,setval(Vg,Vg))`.

5 In the m_d text field, type `md`.

6 In the g_i text field, type `nv`.

First use a **Stationary** study step to solve only the electrostatics physics to obtain a good initial condition for the fully coupled problem.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Semiconductor (semi)** and **Schrödinger Equation (schr)**.

5 Find the **Multiphysics couplings in study** subsection. In the table, clear the **Solve** check box for **Schrödinger–Poisson Coupling 1 (schrp1)**.

6 Click **Add Study** in the window toolbar.

7 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

Use a **Parametric Sweep** node to set the gate voltage of 0.2 V for both subsequent study steps (one of them soon to be added).

STUDY 2

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	0.2	V

5 In the table, click to select the cell at row number 1 and column number 3.

Use the **Values of variables not solved for** section to inherit the solution from the previous study. Make sure to select the solution corresponding to the same gate voltage of 0.2 V as the one specified in the **Parametric Sweep** node previously.

Step 1: Stationary

1 In the **Model Builder** window, click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

3 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1: Density-Gradient, Semiconductor Equilibrium**.

6 From the **Parameter value (Vg (V))** list, choose **0.2 V**.

7 In the **Model Builder** window, click **Study 2**.

8 In the **Settings** window for **Study**, type `Study 2: Schrödinger-Poisson Vg=0.2V` in the **Label** text field.

9 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Add the dedicated **Schrödinger-Poisson** study step. For a completely new problem, it is often necessary to use the default **Manual** search option to find the range of the eigenenergies. Once the range is found, switch to the **Region** search option with appropriate settings for the range and number of eigenvalues, in order to ensure that all significant eigenstates are found by the solver.

Step 2: Schrödinger–Poisson

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Schrödinger–Poisson**.

2 In the **Settings** window for **Schrödinger–Poisson**, locate the **Study Settings** section.

3 From the **Eigenvalue search method** list, choose **Rectangle**.

4 In the **Approximate number of eigenvalues** text field, type `100`.

5 In the **Maximum number of eigenvalues** text field, type `300`.

6 Find the **Elliptic search region** subsection. From the **Unit** list, choose .

7 Find the **Rectangle search region** subsection. In the **Smallest real part** text field, type `-0.1`.

8 In the **Largest real part** text field, type `1`.

9 In the **Smallest imaginary part** text field, type `-1e-7`.

10 In the **Largest imaginary part** text field, type `1e-7`.

Disable the space charge density contribution from the initial guess of the electron concentration.

11 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

12 In the tree, select **Component 1 (comp1)>Electrostatics (es)> Space Charge Density 1: initial electron density**.

13 Click **Disable**.

14 Locate the **Iterations** section. From the **Termination method** list, choose **Minimization of global variable**.

15 In the **Global variable** text field, type `schrp1.global_err`.

16 In the **Absolute tolerance** text field, type `1e-6`.

17 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

18 Click **Add**.

19 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
nv (Valley degeneracy)	`2 4`	

20 Click **Add**.

21 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
fm3 (Longitudinal effective mass factor)	`0.916 0.190`	

22 Click **Add**.

23 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
fm2 (Transverse effective mass factor 2)	`0.190 0.916`	

24 In the **Study** toolbar, click **Compute**.

Add the result to the electron concentration comparison plots.

RESULTS

Density-Gradient

In the **Model Builder** window, under **Results>Electron Concentration Comparison** right-click **Density-Gradient** and choose **Duplicate**.

Schrödinger-Poisson Vg=0.2V

1. In the **Model Builder** window, click **Density-Gradient 1**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Dataset** list, choose **Study 2: Schrödinger-Poisson Vg=0.2V/Solution 2 (sol2)**.
4. In the **Label** text field, type `Schrödinger-Poisson Vg=0.2V`.
5. Locate the **y-Axis Data** section. In the **Expression** text field, type `schrp1.n_sum`.
6. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.
7. Locate the **Legends** section. From the **Legends** list, choose **Manual**.
8. In the table, enter the following settings:

Legends
SP 0.2 V

9. Right-click **Schrödinger-Poisson Vg=0.2V** and choose **Copy**.

Electron Concentration Comparison

In the **Model Builder** window, right-click **Electron Concentration Comparison** and choose **Paste Line Graph**.

Schrödinger-Poisson Vg=0.2V

Duplicate the steps with some modifications for the case of gate voltage of 1.0 V.

ADD STUDY

1. In the **Study** toolbar, click **Add Study** to open the **Add Study** window.
2. Go to the **Add Study** window.
3. Find the **Studies** subsection. In the **Select Study** tree, select **Empty Study**.
4. Click **Add Study** in the window toolbar.
5. In the **Study** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2: SCHRÖDINGER-POISSON VG=0.2V

Parametric Sweep, Step 1: Stationary, Step 2: Schrödinger–Poisson

1 In the **Model Builder** window, under **Study 2: Schrödinger-Poisson Vg=0.2V**, Ctrl-click to select **Parametric Sweep**, **Step 1: Stationary**, and **Step 2: Schrödinger–Poisson**.

2 Right-click and choose **Copy**.

STUDY 3: SCHRÖDINGER-POISSON VG=1.0V

1 In the **Model Builder** window, right-click **Study 3** and choose **Paste Multiple Items**.

2 In the **Model Builder** window, click **Study 3**.

3 In the **Settings** window for **Study**, type `Study 3: Schrödinger-Poisson Vg=1.0V` in the **Label** text field.

4 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Parametric Sweep

1 In the **Model Builder** window, under **Study 3: Schrödinger-Poisson Vg=1.0V** click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	1.0	V

4 In the table, click to select the cell at row number 1 and column number 3.

Step 1: Stationary

1 In the **Model Builder** window, click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Values of Dependent Variables** section.

3 Find the **Values of variables not solved for** subsection. From the **Parameter value (Vg (V))** list, choose **1 V**.

4 In the **Study** toolbar, click **Compute**.

RESULTS

Schrödinger-Poisson Vg=0.2V

In the **Model Builder** window, under **Results>Electron Concentration Comparison** right-click **Schrödinger-Poisson Vg=0.2V** and choose **Duplicate**.

Schrödinger-Poisson Vg=1.0V

1 In the **Model Builder** window, under **Results>Electron Concentration Comparison** click **Schrödinger-Poisson Vg=0.2V 1**.

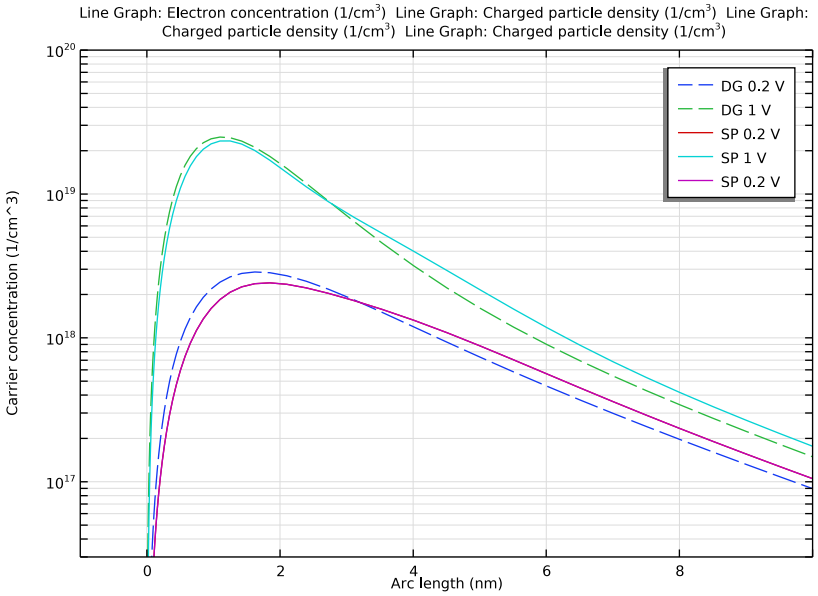
2 In the **Settings** window for **Line Graph**, type `Schrödinger-Poisson Vg=1.0V` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Schrödinger-Poisson Vg=1.0V/Solution 8 (sol8)**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
SP 1 V

5 In the **Electron Concentration Comparison** toolbar, click **Plot**.



6 Right-click **Schrödinger-Poisson Vg=1.0V** and choose **Copy**.

Electron Concentration Comparison 1

In the **Model Builder** window, under **Results** right-click **Electron Concentration Comparison 1** and choose **Paste Line Graph**.

Schrödinger-Poisson Vg=1.0V

1 In the **Model Builder** window, click **Schrödinger-Poisson Vg=1.0V**.

2 In the **Electron Concentration Comparison 1** toolbar, click **Plot**.