A Quasi–Variational Inequality Model for Semiconductor Simulation

M. Morandi Cecchi - Roberto Bertelle

Department of Pure and Applied Mathematics,
University of Padova, Via Trieste 63, Padova, Italy

Workshop on
Multiscale Analysis for Quantum Systems and Applications

Istituto Nazionale di Alta Matematica (INDAM),
Roma, Italy, October 24-26, 2007

Introduction

In this talk we present a new algorithm for the computation of the electrostatic and the quasi—Fermi potentials inside a p—n junction.

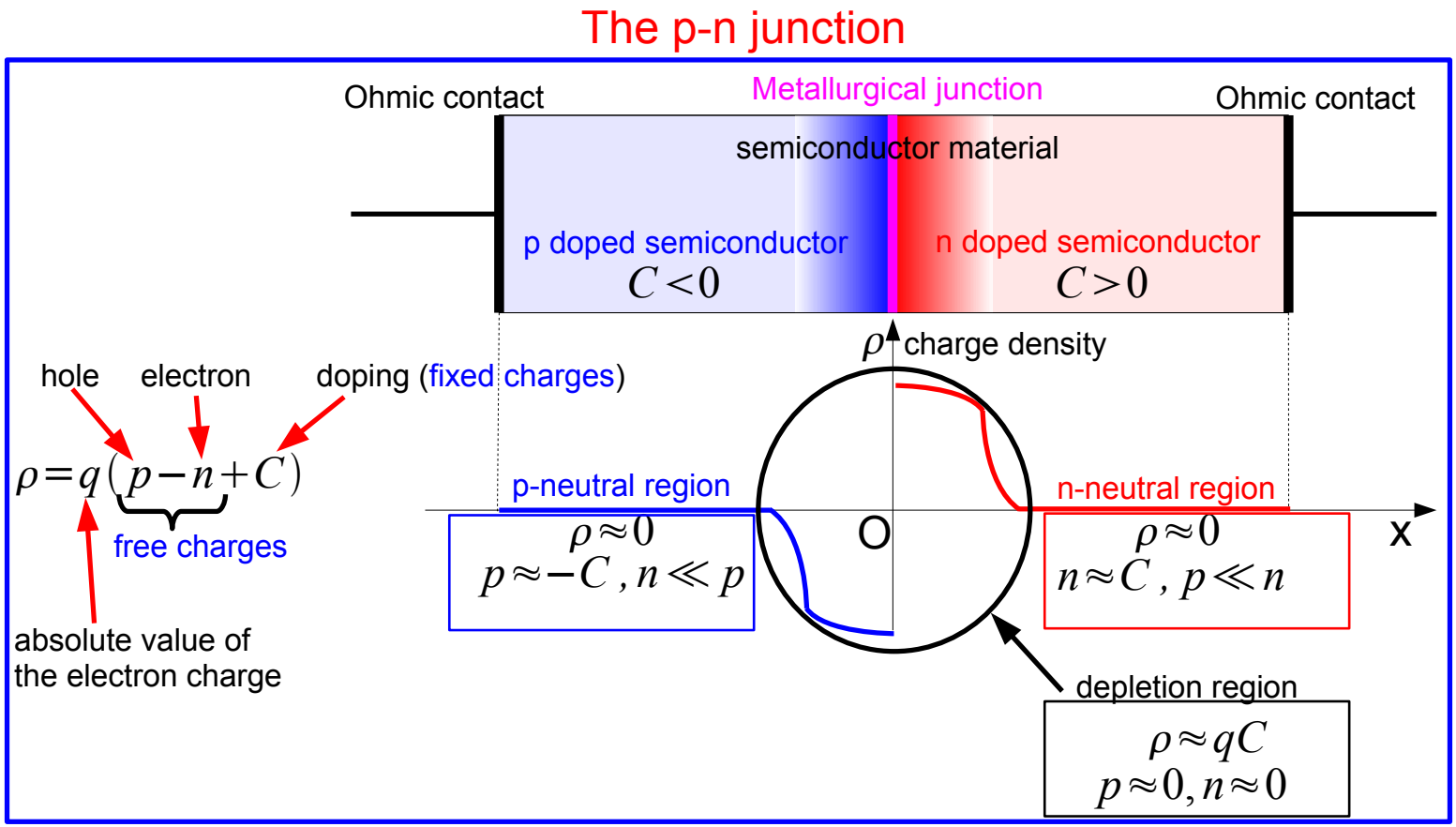
This algorithm is based on a Quasi—Variational Inequality Model.

We take care to relate the derivation of this model to the underline physic of the p—n junction.

The algorithm gives good solutions and has interesting properties, such as low computation time and good robustness.

The p-n junction

In a doped semiconductor the concentration of added impurities C is used to control, in a fine way, the concentrations of electron and holes, p and n, respectively.

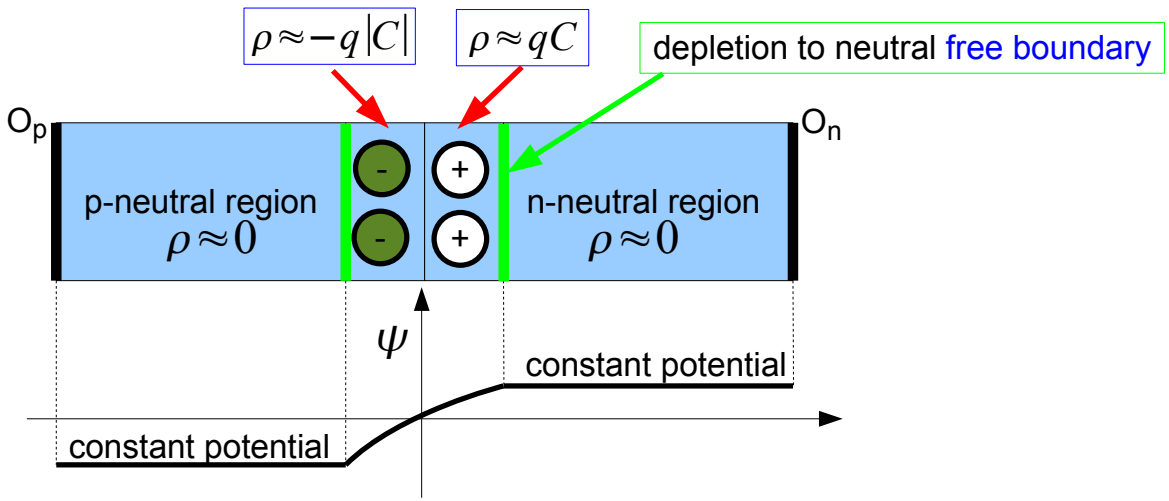


The p-n junction as a free boundary problem

From the physic of a p-n junction, we may assume the following three statements

- Near the metallurgical junction, we have a depletion region.
- Far away from the metallurgical junction the semiconductor is neutral (neutral regions).
- The semiconductor is globally neutral.

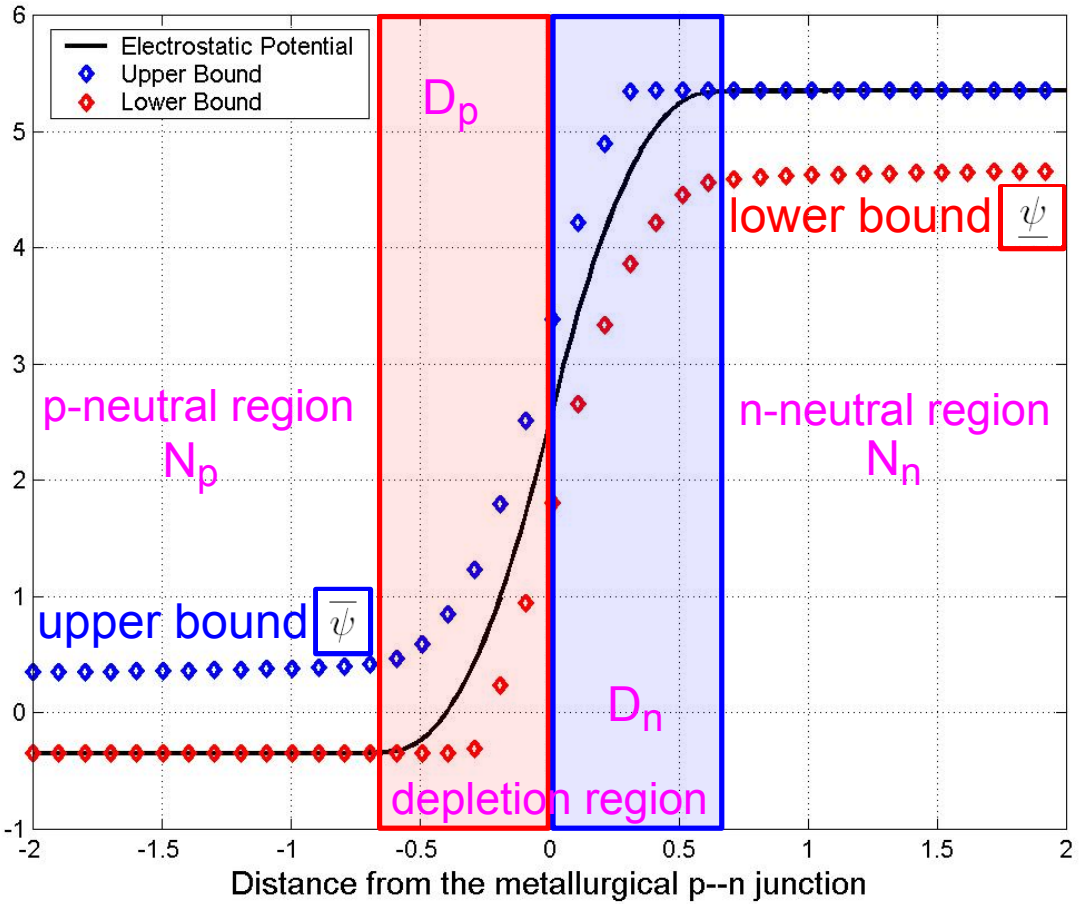
So, we may subdivide the p-n junction into neutral and depletion regions only!



We know the values for the charge density but we do not know where these values are assumed, since we do not know the location of the two free boundaries.

⇒ free boundary problem!

The potential is lower and upper bounded



quasi—Fermi potentials

$$\begin{cases} \overline{\psi} = \phi_n + V_{bi,n} \\ \underline{\psi} = \phi_p + V_{bi,p} \end{cases}$$

built—in potentials

The potential is bounded

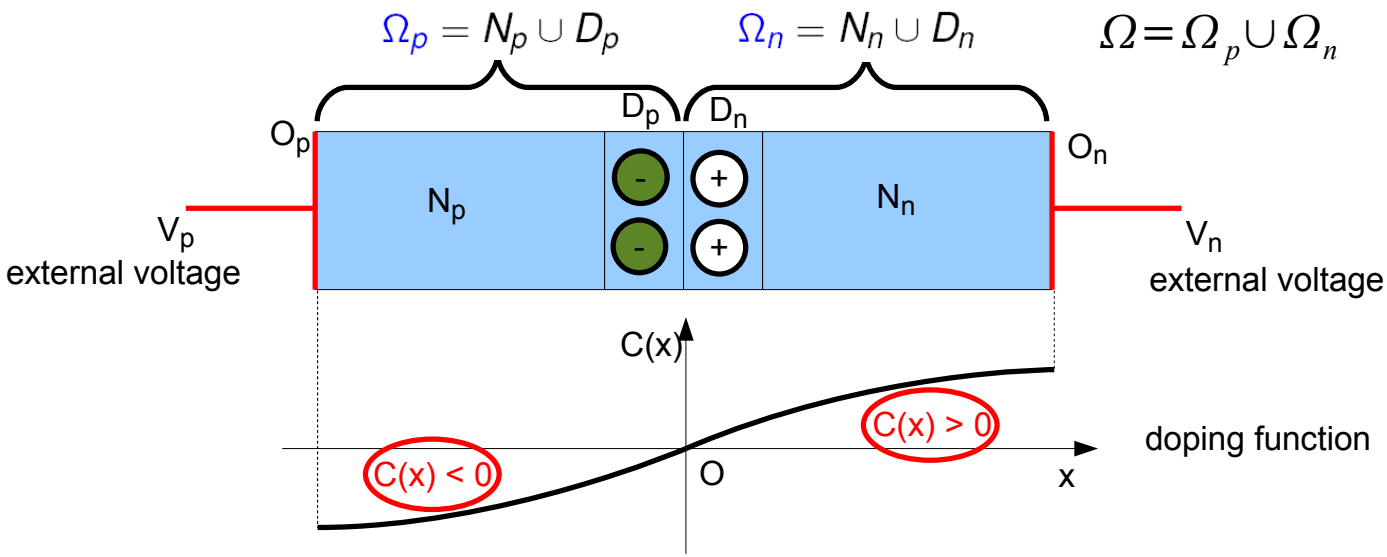
$$\psi = \underline{\psi} \quad \text{in } N_p$$

$$\psi > \underline{\psi} \quad \text{in } D_p$$

$$\psi = \overline{\psi} \quad \text{in } N_n$$

$$\psi < \overline{\psi} \quad \text{in } D_n$$

The Quasi-Variational Inequality Model: notations



electrostatic potential at O_p | electrostatic potential at O_n

built-in potentials at O_p and O_n

$$V = \left\{ u \in H^1(\Omega) : u(O_p) = \psi_p,\ u(O_n) = \psi_n \right\} \quad \text{where} \quad \begin{cases} \psi_p = V_p + V_{bi,p} \\ \psi_n = V_n + V_{bi,n} \end{cases}$$

$$K = \left\{ u \in V : \underline{\psi} \leq u, \text{ in } \Omega_p,\ u \leq \overline{\psi}, \text{ in } \Omega_n \right\}$$ It's a convex set!

A Quasi-Variational Inequality for ψ–part A

Let $u \in K$.

These integrals are zero, since $\Delta\psi = 0$ inside the neutral regions.

$$\begin{aligned}\int_\Omega \Delta\psi(u-\psi)dx &= \int_{N_p} \Delta\psi(u-\psi)dx + \int_{D_p} \Delta\psi(u-\psi)dx \\ &+ \int_{D_n} \Delta\psi(u-\psi)dx + \int_{N_n} \Delta\psi(u-\psi)dx \\ &= \int_{D_p} \Delta\psi(u-\psi)dx + \int_{D_n} \Delta\psi(u-\psi)dx\end{aligned}$$

Recalling that $-\varepsilon\Delta\psi = q(p-n+C)$, we have

C(x) < 0 and so -qC(x) > 0!
$u - \underline{\psi} > 0$ inside N_p!

$$\begin{aligned}\int_{D_p} \varepsilon\Delta\psi(u-\psi)dx &= \int_{D_p} -qC(u-\psi)dx \\ &\le \int_{N_p} -qC(u-\underline{\psi})dx + \int_{D_p} -qC(u-\psi)dx \\ &= \int_{N_p} -qC(u-\underline{\psi})dx + \int_{D_p} -qC(u-\psi)dx \\ &= \int_{\Omega_p} -qC(u-\psi)dx.\end{aligned}$$

$\psi = \underline{\psi}$ inside N_p

In the same way, we have $\int_{D_n} \varepsilon\Delta\psi(u-\psi)dx \le \int_{\Omega_n} -qC(u-\psi)dx$

A Quasi-Variational Inequality for ψ–part B

Using the Green equation we get

$$\int_\Omega -\Delta\psi v dx = \int_\Omega \nabla\psi\cdot\nabla v dx - \int_{\partial\Omega} \frac{\partial\psi}{\partial\vec{\nu}} v d\gamma$$

$\partial\Omega = \Gamma_D \cup \Gamma_N$

$$= \int_{\Gamma_D} \frac{\partial\psi}{\partial\vec{\nu}} v d\gamma + \int_{\Gamma_N} \frac{\partial\psi}{\partial\vec{\nu}} v d\gamma = 0\ !$$

Ohmic contacts are inside the neutral regions!

At Neumann boundary conditions we take $\partial\psi/\partial\vec{\nu}=0$!

Collecting all the results

$$\begin{aligned}
\int_\Omega -\varepsilon\nabla\psi\cdot\nabla(u-\psi)dx &= \int_\Omega \varepsilon\Delta\psi(u-\psi)dx \\
&= \int_{D_p} \varepsilon\Delta\psi(u-\psi)dx + \int_{D_n} \varepsilon\Delta\psi(u-\psi)dx \\
&\leq \int_{\Omega_p} -qC(u-\psi)dx + \int_{\Omega_n} -qC(u-\psi)dx \\
&= \int_\Omega -qC(u-\psi)dx \qquad \text{since} \qquad \Omega = \Omega_p \cup \Omega_n
\end{aligned}$$

So, we obtain the quasi-variational inequality

$$\int_\Omega \varepsilon\nabla\psi\cdot\nabla(u-\psi)dx - \int_\Omega qC(u-\psi)dx \geq 0, \quad \forall u \in K(\psi)$$

The idea to solve the Quasi-Variational Inequality

We define the map $S : U \to U$ using the following steps.

Let $w \in U$. Then, $S(w)$ is

$$\begin{cases} \nabla \cdot (\mu_n n_i e^{w-\phi_n} \nabla \phi_n) = R(w, \phi_n, \phi_p) \\ \phi_n(-L) = V_L, \quad \phi_n(L) = V_R, \end{cases}$$

Electron continuity equation
solve for ϕ_n

$$\begin{cases} \nabla \cdot (\mu_p n_i e^{\phi_p - w} \nabla \phi_p) = R(w, \phi_n, \phi_p) \\ \phi_p(-L) = V_L, \quad \phi_p(L) = V_R. \end{cases}$$

Hole continuity equation
solve for ϕ_p

$$\begin{cases} \overline{\psi} = \phi_n + V_{bi,n} \\ \underline{\psi} = \phi_p + V_{bi,p} \end{cases} \Rightarrow K(w)$$

$$\int_\Omega \epsilon \nabla \psi \cdot \nabla (u - \psi) dx - \int_\Omega qC(u - \psi) dx \geq 0, \ \forall \ u \in K(w)$$

$$\Rightarrow S(w)$$

Now we note that, since ψ solve the quasi-variational inequality, it is a fixed point for the map S(w)! That is, $\psi = S(\psi)$.

This last result suggests an iterative algorithm!

For each function w, we have to solve a variational inequality!

The iterative algorithm

set $\psi^{(0)}$, $\phi_n^{(0)}$, $\phi_p^{(0)}$
compute $\overline{\psi}^{(0)}$, $\underline{\psi}^{(0)}$

$k \leftarrow 0$
$\varepsilon^{(k)} \leftarrow 2\varepsilon$
while $(\varepsilon^{(k)} > \varepsilon)$
  solve the EVI for $\psi^{(k+1)}$ using $K(\psi^{(k)})$
  solve the ECE for $\phi_n^{(k+1)}$
  solve the HCE for $\phi_p^{(k+1)}$
  compute $\overline{\psi}^{(k+1)}$, $\underline{\psi}^{(k+1)}$
  $k \leftarrow k+1$
  compute $\varepsilon^{(k)}$
endwhile

Starting guesses.

Check for stop.

Update the potential solving a variational inequality!

Update lower and upper obstacles using the continuity equations.

Note that, at the beginning of each iteration, we have known values for both obstacles and thus we are able to compute the set $K(\psi^{(k)})$.

The Variational Inequality as a minimun problem

The variational inequality is equivalent to a constrained minimization problem

$$\begin{cases} \psi = \arg\min_{u \in K} J(u) \\ J(u) = \int_\Omega \frac{\varepsilon}{2} |\nabla u|^2 dx - \int_\Omega qCu dx \end{cases}$$

Energy functional!

We are right!

We are dealing with a physical system which naturally get towards the condition of minimum energy. Thus we have a minimization problem. But this system is not free, since we have the boundary conditions. Thus the constrained in the minimization problem!

The problem is discretized using finite element method. For N unknowns, we get

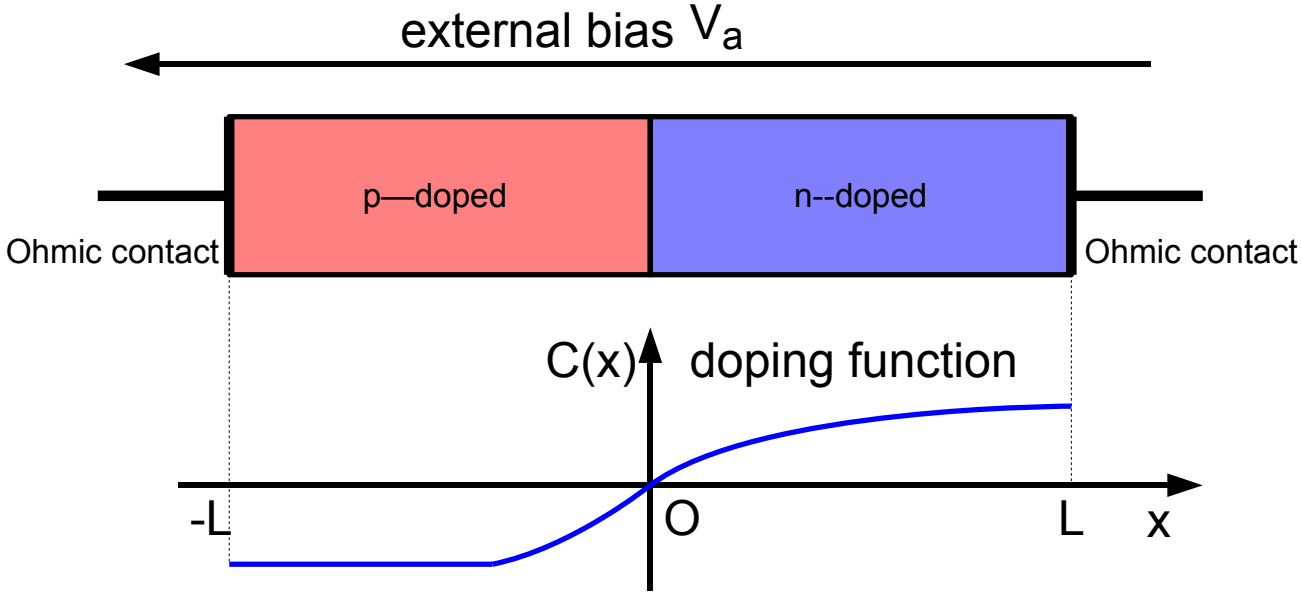
$$\begin{cases} \Psi = argmin_{U \in K} J(U) \\ J(U) = \frac{1}{2} U^T P U + b^T U \end{cases}$$

subset of R^N !

symmetric and positive semidefinite

where $U = [u_1, ..., u_N]^T$.

The framework for the examples

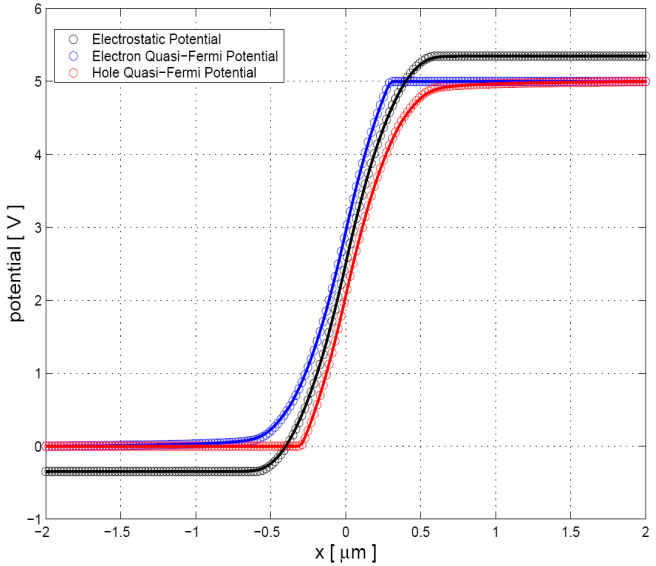


The device has a length equal to 2L and the metallurgical junction is located at x = 0.

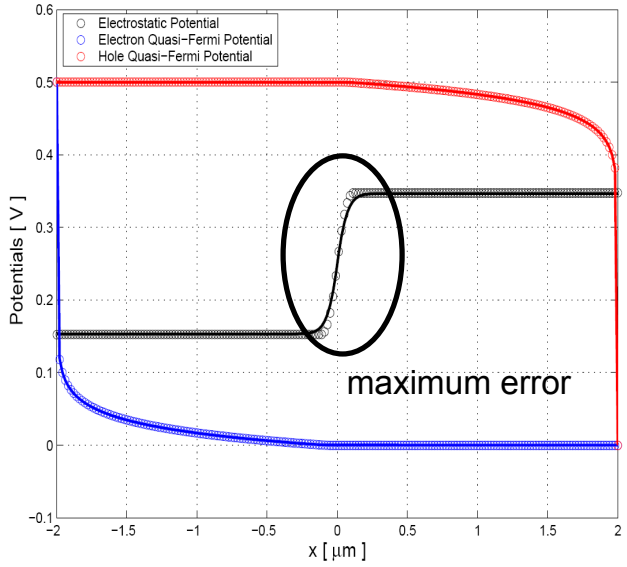
The numerical solution is carried out using a uniform grid with N_p points. The continuity equations are solved using the Sharfetter—Gummel stabilization scheme.

The abrupt p–n junction at low bias

5 V reverse bias



0.5 V forward bias



Computation time [s]

N_p	t_{QVI}	t_{DDM}
25	0.7	3.5
50	1.4	5.1
100	4.2	7.7
200	25.1	14.9
400	252	37.8

Drift Diffusion Model

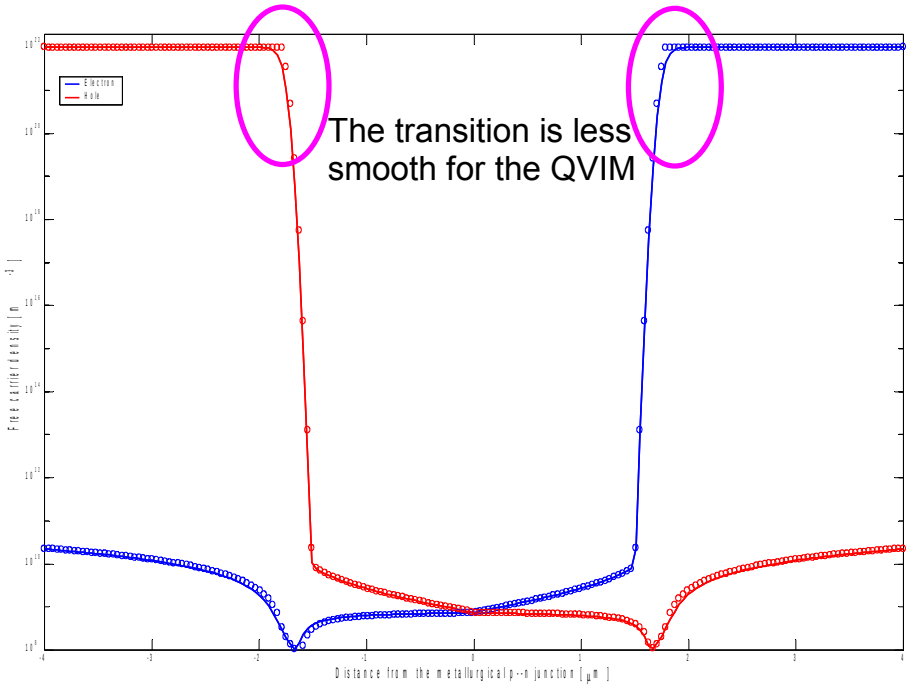
N_p	t_{QVI}	t_{DDM}
25	0.7	0.7
50	1.4	0.8
100	4.5	1.2
200	30.7	2.3
400	-	5.1

few iterations since V_a is low!

For high N_p values, the non-linear Poisson equation may become ill conditioned.

The abrupt p–n junction at high reverse bias

The applied voltage is V_a = 50 V and the doping is $N_a = N_d = 10^{22}$ m^{-3}.



computation time [s]

N_p	t_{QVI}	t_{DDM}
50	1.5	22.1
100	4.4	34.3
200	46.4	66.3

This times are obtained using a continuation scheme with 0.5 V step

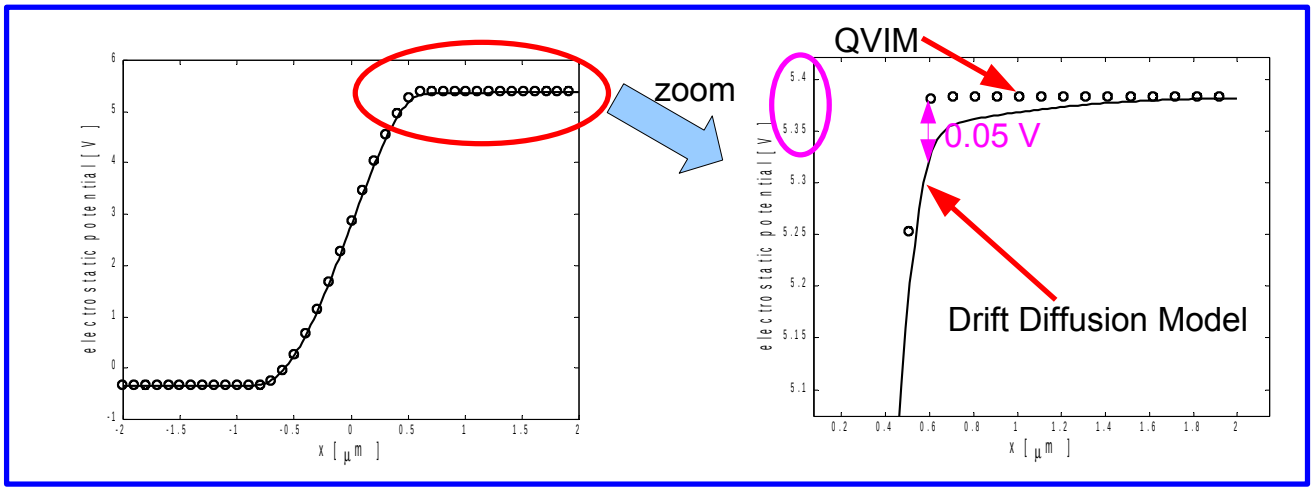
The Gaussian doped p–n junction

Doping function

$$C = -N_a + N_p e^{-\frac{1}{2}\left(\frac{x-L}{\sigma}\right)^2}$$

$$\begin{cases} N_a &= 10^{22}\ m^{-3} \\ N_p &= 5 \cdot 10^{22}\ m^{-3} \\ L &= 2 \cdot 10^{-6}\ m \\ \sigma &= L/\sqrt{2\ln(N_p/N_a)} \end{cases}$$

Potential (at reverse bias with V_a = 5V)



The QVIM does not capture the small slope in the potential due to the gradient of the impurities C. Otherwise, the solution is very good.

Notes

- The algorithm gives the complete solution of the p—n junction, that is the potential as well as the quasi—Fermi potentials.
- The algorithm does not solve the non—linear Poisson equation.
- From our test, we have the following

  The algorithm have good convergence properties even for high applied voltages and does not any continuation scheme.

  The solutions are very good in a reverse bias condition.

  The solutions are still good even in a forward bias condition. In this case, a small error appears near the neutral/depletion regions transition. This is a limit of this kind of model.

  The computational time are low for sparse meshes and rises to high values for dense meshes.

Conclusions

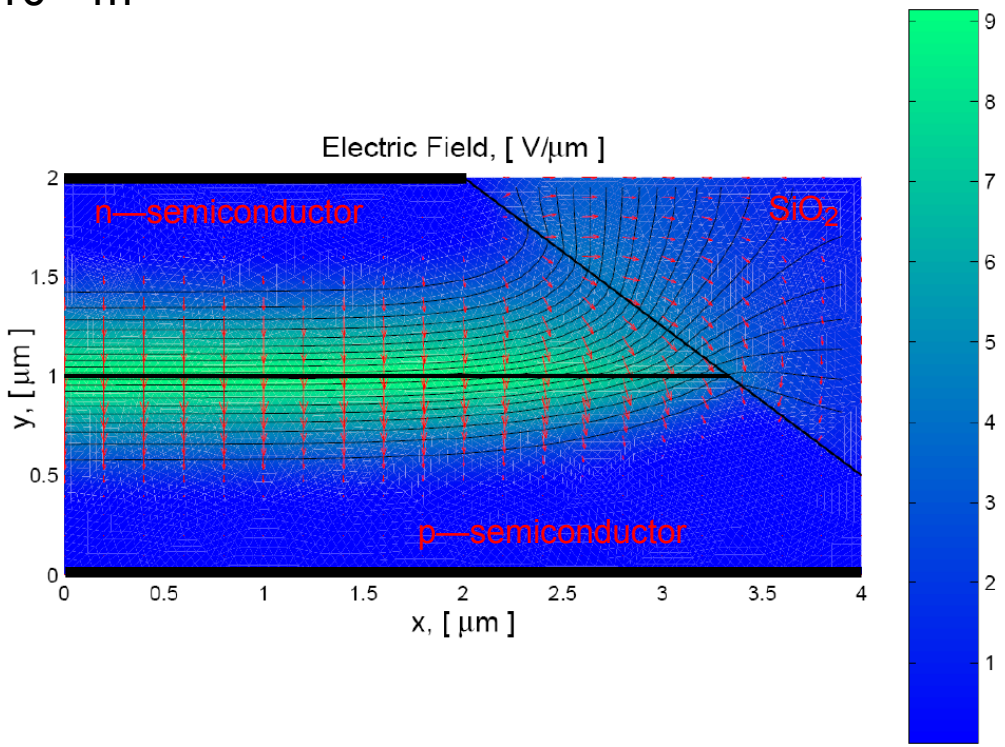
In this talk we have presented the Quasi—Variational Inequality Model for the simulation of a p—n junction.

We have shown an algorithm for the solution of the QVIM for which we have

- Good solutions both for reverse and forward bias.
- Works for an arbitrarily doped p—n junction.
- Good computational time for sparse meshes.

Bevelled p–n junction

$N_a = N_d = 10^{22}\ m^{-3}$



The mesh has 10944 triangles and 5605 points.

The CPU time using a proper quadratic solver is about 2 seconds!

The potential is lower and upper bounded

We start by introducing the two obstacle functions

$$\begin{cases} \overline{\psi} = \phi_n + V_T \ln(|C|/n_i), & \text{in } \Omega_n \\ \underline{\psi} = \phi_p - V_T \ln(|C|/n_i), & \text{in } \Omega_p \end{cases}$$

upper obstacle

lower obstacle

Recalling the definitions of the quasi-Fermi potentials

$$\begin{cases} \phi_n = \psi - V_T \ln(n/n_i) \\ \phi_p = \psi + V_T \ln(p/n_i) \end{cases}$$

electron quasi-Fermi potential

hole quasi-Fermi potential

and neglecting the minority free carriers, we obtain the two bounds for the potential

charge neutrality

$\cancel{p}$-$\cancel{n}$-|C| = 0

$$\begin{cases} p = |C| \text{ in } N_p \Rightarrow \psi = \underline{\psi} \text{ in } N_p \\ p < |C| \text{ in } D_p \Rightarrow \psi > \underline{\psi} \text{ in } D_p \end{cases}$$

charge neutrality

$\cancel{p}$-$\cancel{n}$+|C| = 0

$$\begin{cases} n = |C| \text{ in } N_n \Rightarrow \psi = \overline{\psi} \text{ in } N_n \\ n < |C| \text{ in } D_n \Rightarrow \psi < \overline{\psi} \text{ in } D_n \end{cases}$$