A NEW HYBRID METHOD FOR SHAPE OPTIMIZATION WITH APPLICATION TO SEMICONDUCTOR EQUATIONS

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ABSTRACT. The aim of this work is to reconstruct the depletion region in pn junction. Starting with famous drift diffusion model, we establish the simplified equation for the considered semiconductor. There we call the shape optimization technique to formulate a minimization problem from the inverse problem at hand. The existence of an optimal solution of the optimization problem is proved. The proposed numerical algorithm is a combined Domain Decomposition method with an efficient hybrid conjugate gradient guided by differential evolution heuristic algorithm, the finite element method is used to discretize the state equation. At the end we establish several numerical examples, to prove the validity of theoretical results using the proposed algorithm, in addition we show some simulation of the depletion region approximation under two different functioning modes.

1. Introduction. Free boundary problems are defined as the problem of finding an optimal domain satisfying a given model. Their application appears in different scientific areas such as identification of cavities and cracks in solid bodies, semiconductor framework [2, 5, 6, 13]. In this paper we study the pn-junction[21], which is a semiconductor device considered as bipolar transistor, composed from two electrode semiconductors a p-type and n-type. When some voltages are applied on the terminals (electrodes), the free electrons and the holes spread toward each other, thus a new region called the depletion region $D$ is created (Figure 1, the region limited with blue boundary).

The thickness of this depletion region varies with respect to the applied voltages at each terminal, that makes it an unknown region, limited by two free layers. Our purpose is to construct a numerical scheme to identify the geometry of the unknown depletion region. In order to understand the working of the pn junction it is important to perform a study of the depletion region as a function of the applied voltages, the material properties of the semiconductor.

The pn-junction domain is $\Omega = [0, L] \times [0, H]$, we assume that $\partial \Omega$ is smooth, the depletion region is the zone denoted by $\Omega$, $C_1$ and $C_2$ are the conductivity regions. We set $\Gamma_N = \Gamma_1 \cup \Gamma_3$ and $\Gamma_D = \Gamma_2 \cup \Gamma_4$, where $\Gamma_2$ and $\Gamma_4$ are the negative and the positive terminals respectively. $I_1$ and $I_2$ represent the depletion layers or the

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interfaces. The electrostatic potential $V$ satisfies the drift diffusion [12] model that reads in $\Omega$:

$$
\begin{align*}
-\varepsilon \Delta V &= \zeta \\
J_n &= q(d_n \nabla n + \mu_n n \nabla V) \\
J_p &= -q(d_p \nabla p + \mu_p p \nabla V) \\
\text{div}(J_n) &= \text{div}(J_p) = qR(n, p, V)
\end{align*}
$$

(1)

with $\zeta = q(n - p - m)$. The physical constants are $q$ the electron charge and $\varepsilon$ the permittivity constant of the pn junction. The quantities $n$, $p$ and $m$ are the electrons, holes concentration and the impurity distribution respectively. $J_n$ and $J_p$ are the charge concentrations. $d_n$ and $d_p$ are the electron and hole diffusivity constants, and $\mu_n$, $\mu_p$ stand for their corresponding mobilities.

To complete the model we add the following boundary conditions

$$
\begin{align*}
n &= n_d, \quad p = p_d, \quad \text{and} \quad V = V_d \text{ on } \Gamma_D \\
\nabla_{\nu} n &= \nabla_{\nu} p = \nabla_{\nu} u = 0 \text{ on } \Gamma_N
\end{align*}
$$

(2)

To reduce the problem in a single carrier transport equation, we suppose that the current density is negligible. Inside the depletion region of the pn junction, we assume that the current is carried only by the electrons, which implies that $J_p = 0$ and $R(n, p, V) = 0$. In addition, it means, that the depletion region $D$ does not contain mobile charges, the conductivity regions $C_1$ and $C_2$ the pn junction are neutral. Which leads to the next equations

$$
\zeta = qN \text{ in } D \quad \text{and} \quad \zeta = 0 \text{ in } C_1 \cup C_2
$$

With simple calculus we can summarize the above equations in the next partial differential equation:

$$
\begin{align*}
-\Delta u &= 0 \quad \text{in } C_1 \cup C_2 \\
-\Delta u &= \zeta \quad \text{in } D \\
u = V_d \quad \text{on } \Gamma_2 \cup \Gamma_4 \\
\nabla_{\nu} u &= 0 \quad \text{on } \partial\Omega,
\end{align*}
$$

(3)

where $V$ is the applied voltage, it equals $V^+$ on $\Gamma_2$ and $V^-$ on $\Gamma_4$, $\nu$ is the unit normal outer vector and $\zeta = q(N_d - N_a)$, $N_a$ and $N_d$ are the hole and the electron densities respectively.

Figure 1. The geometry of the PN-Junction

Figure 1. the geometry of the PN-Junction
To this end, we consider the next inverse problem, which is a bilateral free boundary problem derived from the simplified pn junction model, we write

\[
\begin{align*}
\text{Find } (u, I_1, I_2) \text{ such that:} \\
-\Delta u &= f \text{ in } \Omega \\
u &= j \text{ on } \Gamma_2 \cup \Gamma_4 \\
\nabla_{\nu} u &= g \text{ on } \partial \Omega,
\end{align*}
\]

It is easy to return to pn junction model by taking \( f = 0 \text{ on } C_1 \cup C_2, f = \zeta \text{ on } D, \)
g \( = V_d \text{ and } h = 0. \) The reason of this consideration is to have the ability to validate the numerical approach when the layers \( I_1 \) and \( I_2 \) are given, then we apply it to identify the depletion layers the pn junction model. Since we will simulate an real application, where the datum are always not exact, they are infected by machine errors, we must consider noisy data, for this reason we consider the new form

\[
\begin{align*}
\text{Find } (u, I_1, I_2) \text{ such that:} \\
-\Delta u &= f \text{ in } \Omega \\
u &= j^\delta \text{ on } \Gamma_2 \cup \Gamma_4 \\
\nabla_{\nu} u &= g^\delta \text{ on } \partial \Omega,
\end{align*}
\]

with \( \delta \) is the noise level and \( \|j - j^\delta\| + \|g - g^\delta\| \leq \delta. \)

In this paper, the shape optimization technique [15, 22] is used to formulate the free boundaries problem (5) as a minimization problem, it is based on the definition of a cost functional and the optimal solution will be the critical point of this functional. In this formulation, the analysis of the cost functional is needed to prove the existence of an optimal solution for the minimization problem.

During the last years, many works have studied inverse problems arising in semiconductor theory, such the work [3] where the authors survey the numerical solution of a single free boundary problem in MOSFET semiconductor, using variational inequalities. In the work [8] they studied the optimal semiconductor design using a second order scheme based on Newton’s method. There are some few works that study the case of a two free boundaries problem [4, 13, 10], where they have used numerical schemes based on gradient methods. Although they reach good results.

In this contribution, we propose to use a hybrid algorithm based on the differential evolution guided conjugate gradient. The idea behind using heuristic method, is to find the best initial guess for the conjugate gradient, moreover the convergence of gradient based methods depends on the choice of the initial guess. It is harder to pick it manually, it may be overcome by some gentle hybridization with some heuristic method, such in the work [2] they used genetic algorithm to generate the best initial guess for the gradient method.

This paper is organized as follows, the next section we give some existence results of the shape optimization problem, then we establish the discretization of the optimization problem in section 3. The shape gradient and first optimality condition are computed in section 4. In section 5 concern the description of the proposed method. In section 6 we establish some numerical examples in order to show the performance of the proposed algorithm and we finish by giving a numerical approach for the depletion region.

2. Shape optimization problem. In this section, we will introduce an energy functional to design a shape optimization problem associated to the inverse problem.
at hand. First we parameterize the free layers as the following:

$$I_1(\varphi) = \{(\varphi(y), y) / y \in [0, H] \text{ and } L^1_1 \leq \varphi(y) \leq L^1_2\}$$

$$I_2(\psi) = \{(\psi(y), y) / y \in [0, H] \text{ and } L^2_1 \leq \psi(y) \leq L^2_2\},$$

then we consider the next assumption on the functions \(\varphi\) and \(\psi\):

**H1**: There exists \(L_1, L_2 > 0\)

\[ |\varphi(x) - \varphi(y)| \leq L_1 |x - y| \quad \text{and} \quad |\psi(x) - \psi(y)| \leq L_2 |x - y| . \]

**H2**: There exists \(L^1_1, L^1_2, L^2_1\) and \(L^2_2\) non negatives, such that

\[ L^0_1 \leq \varphi(x) \leq L^1_1 \quad \text{and} \quad L^0_2 \leq \psi(x) \leq L^1_2, \quad \forall x, y \in [0, H]. \]

First, we define the set of admissible shape \(\Theta_{ad}\),

\[ \Theta_{ad} = \left\{ (I_1(\varphi), I_2(\psi)) : (\varphi, \psi) \text{ satisfy the assumption } H1 \text{ and } H2 \right\} \]

**Remark 1.** We must assume that \(L^2_1 < L^1_1\) is hold, so that the free layers will not intersect, in order to keep the domain \(D\) in the middle convex. Also to have the ability to apply the domain decomposition technique.

Let the following functional space

\[ U = \left\{ u \in H^1(\Omega) : u = j \text{ on } \Gamma_D \right\}, \quad U_0 = \left\{ u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_D \right\} \]

and

\[ W = \left\{ u \in H^1(\Omega) : \int_D u = 0 \right\} \]

We can see that (5) has supplement boundary conditions. Thus we split problem (5) into two state problems, the first is given by:

\[ -\Delta p = f \text{ in } \Omega, \quad p = j^\delta \text{ on } \Gamma_D \quad \text{and} \quad \nabla \nu p = g^\delta \text{ on } \Gamma_N \]

with \(\Gamma_N = \Gamma_1 \cup \Gamma_3\) and \(\Gamma_D = \Gamma_2 \cup \Gamma_4\), it is associated with the variational form

Find \(p \in U\) satisfying \(A(p, v) = B_1(v)\) for \(v \in U_0\) \hspace{1cm} (7)

and the second state equation is written as:

\[ -\Delta q = f \text{ in } \Omega \quad \text{and} \quad \nabla \nu q = g^\delta \text{ on } \partial \Omega, \]

where its variational form is defined by

Find \(d \in W\) satisfying \(A(q, w) = B_2(w)\) for \(w \in W\) \hspace{1cm} (8)

where

\[ A(u, v) = \int_\Omega \nabla u \nabla v ds, \quad B_1(v) = \int_\Omega f v ds + \int_{\Gamma_N} g^\delta v ds \]

and \(B_2(v) = \int_\Omega f v ds + \int_{\partial \Omega} g^\delta v ds.\)

For any pair \((I_1, I_2)\) in \(\theta_{ad}\), it is trivial to show the continuity of the operator \(A\) and \(B_i, i = 1, 2\). By the Poincaré inequality \(A\) is coercive. Hence the variational problem (7) has a unique solution, and with the Riesz representation theorem it is easy to show the existence of \(q \in W\) solution of the problem (9) we refer to [9]. We recall the following result:

**Proposition 1.** Let be \(p\) and \(q\) solution of (7) and (9) respectively, we have the estimates [9]

\[ \exists M_1, M_2 > 0, \quad \|p\|_U \leq M_1 \quad \text{and} \quad \|q\|_W \leq M_2 \]
To construct the shape optimization problem, first we need to introduce an energy functional, consider then the following functional:

$$J(I_1, I_2, p, q) = \frac{1}{2} \int_{I_1} (p(1, I_2) - q(1, I_2))^2 dx + \frac{1}{2} \int_{I_2} (p(1, I_2) - q(1, I_2))^2 dx$$

where $p(1, I_2)$ solution of (7) for the given pain $(I_1, I_2)$ and $q(1, I_2)$ solution of (9). For the sake of simplicity, we omit the notation $p$ and $q$ in place of $p(1, I_2)$ and $q(1, I_2)$. Since we are trying to solve an inverse problem, we add an regularization term to our functional, in order to ensure the smoothness and the regularity of the identified shape. Thus we consider the new form

$$J(I_1, I_2, p, q) = J(I_1, I_2, p, q) + rP(D)$$

(10)

with $r > 0$ and $P(D)$ is the perimeter of the depletion region. The choice of this regularization using $D$ comes of the fact that the boundary of $D$ contain both free interfaces $I_1$ and $I_2$, which allow to regularize both of them simultaneously.

Now, we can summarize the shape optimization problem as follows:

$$\min_J J(I_1, I_2, p, q) \text{ such that }$$

$$A(p, v) = B_1(v), \text{ for all } v \in U_0$$

$$A(q, w) = B_2(w), \text{ for all } w \in W$$

(11)

with $F$ is a space defined by $F = \Theta_{ad} \times U \times W$

**Theorem 2.1.** Problem (11) has at least a solution in $F$

The proof of this theorem is based on the lower semi-continuity of $J$ and the compactness of $F$. First of all, it is necessary to define some topology on $F$, we consider then the following, for any $(I_1^n, I_2^n, p^n, q^n)$ and $(I_1, I_2, p, q)$ in $F$

$$(I_1^n, I_2^n, p^n, q^n) \xrightarrow{n \to \infty} (I_1, I_2, p, q) \iff \begin{cases} 1_{I_1^n} \xrightarrow{*} 1_{I_1} \\ (p^n, q^n) \xrightarrow{n \to \infty} (p, q) \end{cases}$$

(12)

means that $1_{I_1^n}$ converge weak star to $1_{I_1}$ in $L^\infty(\Omega)$ and the convergence of $(p^n, q^n)$ to $(p, q)$ is weak in $U \times W$.

**Lemma 2.2.** Let $(p^n, q^n)$ be solution sequence of (7)-(9), then there exist $(p, q)$ in $V \times W$ such that $(p^n, q^n)$ converge strongly to $(p, q)$ in $[L^2(\Omega)]^2$. In addition $p$ and $q$ are solutions of (7) and (9) resp.

*Proof.** Let $(p^n, q^n)$ be solution sequence of (7)-(9). Using the estimate (10) we guaranty the existence of $p, q \in H^1(\Omega)$ such that $p_n$ and $q_n$ converge weakly to $p$ and $q$ in $H^1(\Omega)$. By the Rellich theorem we show that $p_n$ and $q_n$ converge strongly in term of subsequences to $p$ and $q$ respectively in $L^2(\Omega)$.

Let us show that $(p, q)$ is a solution of (7)-(9), since we $\nabla p_n$ converge to $\nabla p$ weakly in $L^2(\Omega)$ then

$$A(p, v) = \lim_{n \to \infty} A(p^n, v), \text{ for all } v \in U_0$$

using the fact that $A(p^n, v) = B_1(v)$ thereafter $A(p, v) = B_1(v)$, there after it is easy to conclude that $p$ belongs to $U$.

Similarly we show that $A(q, w) = B_2(w)$ for all $w \in W$, it remains to prove that $q$ belongs to $W$, we have that

$$\int_{\Omega} (q_n - q) dx \leq |\Omega|^{\frac{1}{2}} \|q_n - q\|_{L^2(\Omega)}$$
Using the fact that \( q_n \) converge to \( q \) strongly in \( L^2(\Omega) \) then \[ \int_{\Omega} q_n dx = \int_{\Omega} q dx, \] since \[ \int_{\Omega} q_n dx = 0 \] it follows that \( q \in W \).

**Proposition 2.** \( F \) is compact for the topology defined in 12.

**Proof.** Let \((I^n_1, I^n_2, p^n, q^n)\) a sequence of \( F \). Thanks to the last lemma we have the existence of \((p, q)\) such that \((p^n, q^n)\) converges weakly as a subsequence to \((p, q)\) in \( H^1(\Omega) \). Since \( I^n_1 = I_1(\varphi^n) \) \( I^n_2 = I_2(\psi^n) \), by the Ascoli-Arzela [18], theorem we can derive the existence of \((\varphi, \psi)\) such that \((\varphi^n, \psi^n)\) converges uniformly to \((\varphi, \psi)\) in \([0, H] \). Thereafter we can derive easily that \((I^n_1, I^n_2, p^n, q^n)\) converges to \((I_1, I_2, p, q)\) in term of subsequence. Finally \( F \) is compact.

**Proposition 3.** The functional \( J \) is lower semi-continuous on \( F \)

**Proof.** Let \((I^n_1, I^n_2, p^n, q^n)\) be sequence of \( F \) that converges to \((I_1, I_2, p, q)\). Using the fact that \( p_n \) and \( q_n \) converge strongly to \( p \) and \( q \) in \( L^2(\Omega) \), we can easily show that

\[
\int_{\Omega} (p - q)^2 dx = \lim_{n \to \infty} \int_{\Omega} (p^n - q^n)^2 dx = \lim_{n \to \infty} \int_{\Omega} 11_{\delta} (p^n - q^n)^2 dx
\]

in addition to lower semi-continuity of the perimeter \([22]\)

\[
\mathcal{P}(D) \leq \liminf_{n \to \infty} \mathcal{P}(D_n)
\]

it follows then

\[
J(I_1, I_2, p, q) \leq \liminf_{n \to \infty} J(I^n_1, I^n_2, p^n, q^n)
\]

with conclude the proof.

Let consider \( \Omega^* \) the exact solution of the inverse problem 5.

3. **Discrete shape optimization problem.** Let consider \( \Omega \in \Theta_{ad} \) and \( h > 0 \) a mesh size, \( \mathcal{T}_h \) a family of regular triangulation of \( \Omega \) [1], we note \( \Omega_h = \bigcup_{T \in \mathcal{T}_h} T \).

Consider now the finite element space

\[
P_h = \{ v_h \in C(\bar{\Omega}) : v_h|_T \in \mathbb{P}_1(T), \quad \forall T \in \mathcal{T}_h \}
\]

with \( \mathbb{P}_1 \) is the space of polynomial whose degree does not exceed 1 on \( \mathbb{R}^2 \). Let the following discrete functional space

\[
U_h = U \cap P_h, \quad U_{0,h} = U_0 \cap P_h \quad \text{and} \quad W_h = W \cap P_h.
\]

The first discrete variational formulation is given as follows

Find \( p_h \in U_h \) satisfying \( A_h(p_h, v_h) = B_{1,h}(v_h) \) for \( v_h \in U_{0,h} \), \( (13) \)

similarly, the second variational problem is given by

Find \( q_h \in W_h \) satisfying \( A_h(q_h, w_h) = B_{2,h}(w_h) \) for \( w_h \in W_h \) \( (14) \)

where

\[
A_h(u_h, v_h) = \int_{\Omega_h} \nabla u_h \nabla v_h dx, \quad B_{1,h}(v_h) = \int_{\Omega_h} f_h v_h dx + \int_{\Gamma_{N,h}} \delta g_h v_h ds
\]

and \( B_{2,h}(v_h) = \int_{\Omega_h} f_h v_h dx + \int_{\partial \Omega_h} \delta g_h v_h ds \).
Then, the discrete version of the shape optimization problem (11) is as follows:

\[
\begin{align*}
\min_{\mathcal{F}_h} & \quad J(I_{1,h}, I_{2,h}, p_h, q_h) \\
\text{such that} & \quad A_h(p_h, v_h) = B_1(v_h), \text{ for all } v_h \in U_{0,h} \\
& \quad A(q_h, w_h) = B_2(w_h), \text{ for all } w_h \in W_h
\end{align*}
\]

with \( \mathcal{F}_h \) is a space defined by \( \mathcal{F}_h = \Theta_{ad,h} \times U_h \times W_h \).

Let associate \( U_h, U_{0,h} \), and \( W_h \) respectively with the basis \( \{ \xi_i \}_{1 \leq i \leq N_1}, \{ \eta_i \}_{1 \leq i \leq N_2} \) and \( \{ \varsigma_i \}_{1 \leq i \leq N_3} \), where \( N_1 \), \( N_2 \), and \( N_3 \) being the dimension of \( U_h \), \( U_{0,h} \) and \( W_h \).

Solving (13) and (14) is equivalent to solve the matrix form \( A_h p_h = B_{1,h} \) and \( A_h q_h = B_{2,h} \) respectively, where

\[
\begin{align*}
A_h &= \left( \int_{\Omega_h} \nabla \xi_j \nabla \eta_k dx \right)_{j,k}, \\
B_{1,h} &= \left( \int_{\Omega_h} f_h \eta_k dx + \int_{\Gamma_N,h} g_h^k \eta_k ds \right)_{k},
\end{align*}
\]

and

\[
B_{2,h} = \left( \int_{\Omega_h} f_h \varsigma_k dx + \int_{\partial \Omega_h} g_h^k \varsigma_k ds \right)_{k}.
\]

The matrix form associated to the functional \( J \) is as follows

\[
J_h(I_{1,h}, I_{2,h}, p_h, q_h) = \frac{1}{2} \left( \langle M_{I_1} (p_h - q_h), p_h - q_h \rangle + \langle M_{I_2} (p_h - q_h), p_h - q_h \rangle \right)
\]

with

\[
M_{I_i} = \left( \int_{I_{i,h}} \phi_j \phi_k ds \right)_{j,k},
\]

\( \{ \phi_j \} \) is the basis of \( H^1(\Omega) \cap P_h \). To this end, the matrix form of the discrete shape optimization problem (15) is given by

\[
\begin{align*}
\min_{\mathcal{F}_h} & \quad J(I_{1,h}, I_{2,h}, p_h, q_h) \\
\text{such that} & \quad A_h p_h = B_{1,h} \quad \text{and} \quad A_h q_h = B_{2,h}
\end{align*}
\]

4. Shape gradient. In this part, we explore the computation of the shape gradient. Before that, let us recall some tools in shape calculus, we introduce the fictitious time \( t \) and we define the perturbation mapping

\[
P_t = \text{id} + tV
\]

where \( V \) is a smooth vector field belongs to

\[
\Pi = \left\{ V \in C^{1,1}(\overline{\Omega} \times \mathbb{R}^2) : V|_{\overline{\Omega} \setminus (I_1 \cup I_2)} = 0 \right\}
\]

\( P_t \) is bijective Lipschitz and its inverse is Lipschitz continuous [22], which allows to define the perturbed boundaries

\[
I_{1,t} = P_t(I_1) \quad \text{and} \quad I_{2,t} = P_t(I_2)
\]

Definition 4.1. Let \( K \) be a shape functional. \( K \) is said shape differentiable [7, 22] at \( (I_1, I_2) \in \Theta_{ad} \) if

\[
dK[V] = \lim_{t \to 0} \frac{K(I_{1,t}, I_{2,t}) - K(I_1, I_2)}{t}
\]

exists for all \( V \in \Pi \).
Definition 4.2. The derivative of a state solution $u$ is denoted by $u'$, it is given by the following limit

$$u' = \lim_{t \to 0} \frac{u_t \circ P_t - u}{t}.$$ 

Now we recall the next important result [22].

Lemma 4.3. Let $u \in W^{2,1}(\Omega)$ depending on $(I_1, I_2)$ and $V \in \Pi$, then the functional $K(I_1, I_2) = \int_{I_1 \cup I_2} u ds$ is shape differentiable, and we have

$$dK[V] = \int_{I_1 \cup I_2} \left[ u' + (\nabla \nu \cdot u + \kappa u) \langle V, \nu \rangle \right] ds$$

where $\kappa$ is the mean curvature of the boundary $I_1 \cup I_2$.

The derivative of the state solution $(p, q)$ is given by the pair $(p', q')$ which satisfies the next variational equations

$$\int_{\Omega} \nabla p' \nabla v dx + \int_{I_1 \cup I_2} \nabla p \nabla \langle V, \nu \rangle ds = \int_{I_1 \cup I_2} f \langle V, \nu \rangle ds$$  \hspace{1cm} (18)

$$\int_{\Omega} \nabla q' \nabla w dx + \int_{I_1 \cup I_2} \nabla q \nabla \langle V, \nu \rangle ds = \int_{I_1 \cup I_2} f \langle W, \nu \rangle ds$$  \hspace{1cm} (19)

Let us prove then, the next result

Lemma 4.4. For any $\Omega$ in $\theta_{ad}$, the functional $J$ is shape differentiable and for all $V \in \Pi$ we have

$$dJ[V] = \int_{I_1 \cup I_2} \left[ \nabla p \nabla \lambda + \nabla q \nabla \mu - f(\lambda + \mu) + \nabla \nu ((p - q)^2) + \kappa(p - q)^2 + r \kappa \right] \langle V, \nu \rangle ds$$  \hspace{1cm} (20)

with $(p, q)$ and $(\lambda, \mu)$ are the pair of state and adjoint solutions.

Proof. With lemma 4.3 we differentiate the shape functional $J$ we get

$$dJ[V] = \int_{I_1 \cup I_2} (p' - q')(p - q) + \left[ \nabla \nu ((p - q)^2) + \kappa(p - q)^2 \right] \langle V, \nu \rangle ds$$  \hspace{1cm} (21)

To eliminate the derivative $p'$ and $q'$ we manipulate the adjoint solutions. To do so, we introduce the Lagrangian functional $L$ associated to the cost functional $J$ defined on $\Theta_{ad} \times U \times W \times U_0 \times W$ by the following

$$L(I_1, I_2, p, q, \lambda, \mu) := J(I_1, I_2, p, q) + A(p, \lambda) - B_1(\lambda) + A(q, \mu) - B_1(\mu).$$  \hspace{1cm} (22)

The optimality conditions on $\partial_p L[v]$ and $\partial_q L[w]$ lead to variational equations:

$$\int_{\Omega} \nabla \lambda \nabla v dx = - \int_{I_1 \cup I_2} (p - q) v ds$$  \hspace{1cm} (23)

$$\int_{\Omega} \nabla \mu \nabla w dx = \int_{I_1 \cup I_2} (p - q) w ds$$  \hspace{1cm} (24)

$(\lambda, \mu)$ is the pair of adjoint solution's.
Thereafter, we take $\lambda$ and $\mu$ as test functions in (18) and (19) we get
\[
\int_{\Omega} \nabla p' \nabla \lambda ds + \int_{I_1 \cup I_2} \nabla p \nabla \lambda (V, \nu) ds = \int_{I_1 \cup I_2} f \lambda (V, \nu) ds
\] (25)
\[
\int_{\Omega} \nabla q' \nabla \mu ds + \int_{I_1 \cup I_2} \nabla q \nabla \mu (V, \nu) ds = \int_{I_1 \cup I_2} f \mu (V, \nu) ds
\] (26)
also we take $p'$ and $q'$ as test functions in (23) and (24) respectively we obtain
\[
\int_{\Omega} \nabla \lambda \nabla p' dx = - \int_{I_1 \cup I_2} (p - q)p' ds
\] (27)
\[
\int_{\Omega} \nabla \mu \nabla q' dx = \int_{I_1 \cup I_2} (p - q)q' ds
\] (28)
Then we have
\[
\int_{I_1 \cup I_2} (p' - q')(p - q) ds = - \int_{\Omega} \nabla \lambda \nabla p' dx - \int_{\Omega} \nabla \mu \nabla q' dx
\] (29)
Manipulating the equations (25) and (26) we infer
\[
\int_{I_1 \cup I_2} (p' - q')(p - q) ds = \int_{I_1 \cup I_2} \left[ \nabla p \nabla \lambda + \nabla q \nabla \mu - f(\lambda + \mu) \right] (V, \nu) ds
\] (30)
Substituing the last equality in (21) we infer
\[
d \mathcal{J}[V] = \int_{I_1 \cup I_2} \left[ \nabla p \nabla \lambda + \nabla q \nabla \mu - f(\lambda + \mu) + \nabla \nu ((p - q)^2 + \kappa (p - q)^2) + r \kappa \right] (V, \nu) ds
\]
which conclude this proof.

We will set the following notation
\[
d \mathcal{J}[V] = \int_{I_1 \cup I_2} G(V, \nu) ds = d \mathcal{J}_1 [V] + d \mathcal{J}_2 [V] = \int_{I_1} G(V, \nu) ds + \int_{I_2} G(V, \nu) ds
\]
it will be useful for the next sections.

5. The proposed hybrid method. In this section we describe the used numerical scheme to solve the shape optimization problem (11). The state problems are discretized using the finite element [1], then using the domain decomposition technique[11] we split the solutions on each region. To perform the minimization we combine the conjugate gradient with the heuristic differential evolution method.

5.1. Domain decomposition. The Dirichlet-Neumann decomposition method is used to split problem (3) to a system of three sub problems. Starting with an initial $\lambda^0$ and $\mu^0$ we solve in three fractional steps, in each domain, a subproblem with Dirichlet boundary data $\lambda^0$ on $I_1$ in $C_1$, in $D$ a subproblem with Neumann condition computed by the solution in $C_1$ and $\mu^0$ as Dirichlet data on the interface $I_2$, the last region we solve a subproblem with Neumann boundary data computed by the solution in $D$.
Then we perform an update for $\lambda$ and $\mu$ using a linear combination using the last iterate and the computed solutions, with chosen relaxation parameter $\theta$ and $\varsigma$. 

In the next, we write the split problem (6) as follows:

\[
\begin{aligned}
-\Delta p^{k+1}_1 &= f \quad \text{in } C_1, \\
\nabla_\nu p^{k+1}_1 &= g^\delta \quad \text{on } \Gamma_N \cap \partial \Omega, \\
 p^{k+1}_1 &= j^\delta \quad \text{on } \Gamma_2, \\
 p^{k+1}_1 &= \lambda^k \quad \text{on } I_1 \\
-\Delta p^{k+1}_2 &= f \quad \text{in } D, \\
\nabla_\nu p^{k+1}_2 &= g^\delta \quad \text{on } \partial D \cap \partial \Omega, \\
\nabla_\nu p^{k+1}_2 &= \nabla_\nu p^{k+1}_1 \quad \text{on } I_1 \\
p^{k+1}_2 &= \mu^k \quad \text{on } I_2 \\
-\Delta p^{k+1}_3 &= f \quad \text{in } C_2, \\
\nabla_\nu p^{k+1}_3 &= g^\delta \quad \text{on } \Gamma_N \cap \partial \Omega, \\
p^{k+1}_3 &= j^\delta \quad \text{on } \Gamma_4, \\
\nabla_\nu p^{k+1}_3 &= \nabla_\nu p^{k+1}_2 \quad \text{on } I_2
\end{aligned}
\] (31)

with the update

\[
\lambda^{k+1} = \theta p^{k+1}_2 + (1 - \theta) \lambda^k \quad \text{and} \quad \mu^{k+1} = \nu p^{k+1}_3 + (1 - \nu) \mu^k
\] (34)

We can use another form of the cost functional:

\[
\min J(I_1, I_2, p, q) = \frac{1}{2} \int_{I_1} (p_1 - q_1)^2 dx + \frac{1}{2} \int_{I_2} (p_3 - q_3)^2 dx + r \mathcal{P}(D)
\] (39)

Similarly we decompose the second state equation (8)

\[
\begin{aligned}
-\Delta q^{k+1}_1 &= f \quad \text{in } C_1, \\
\nabla_\nu q^{k+1}_1 &= g^\delta \quad \text{on } \partial C_1 \cap \partial \Omega, \\
 q^{k+1}_1 &= \eta^k \quad \text{on } I_1 \\
-\Delta q^{k+1}_2 &= f \quad \text{in } D, \\
\nabla_\nu q^{k+1}_2 &= g^\delta \quad \text{on } \partial D \cap \partial \Omega, \\
\nabla_\nu q^{k+1}_2 &= \nabla_\nu q^{k+1}_1 \quad \text{on } I_1 \\
 q^{k+1}_2 &= \xi^k \quad \text{on } I_2 \\
-\Delta q^{k+1}_3 &= f \quad \text{in } C_2, \\
\nabla_\nu q^{k+1}_3 &= g^\delta \quad \text{on } \partial C_2 \cap \partial \Omega, \\
\nabla_\nu q^{k+1}_3 &= \nabla_\nu q^{k+1}_2 \quad \text{on } I_2
\end{aligned}
\] (36)

with the update

\[
\eta^{k+1} = \tau q^{k+1}_2 + (1 - \tau) \eta^k \quad \text{and} \quad \xi^{k+1} = \kappa q^{k+1}_3 + (1 - \kappa) \xi^k
\] (38)

This process is summarized in algorithm 1.

In the next subsection, we will describe the conjugate gradient iteration.
5.2. Conjugate gradient method. Let consider the iterations

$$I_1^{n+1} = I_1^n + \beta_1^n d_1^n \quad \text{and} \quad I_2^{n+1} = I_2^n + \beta_2^n d_2^n. \quad (40)$$

with $\beta_i^n$ is the search step size associated to the interface $I_i$, and the directions of descent $d_i^n$ is updated with the relation

$$d_i^n = -dJ_i^n + \gamma_i^n d_i^{n-1}, \quad \text{for} \quad i = 1, 2 \quad (41)$$

where $dJ_i^n = \int_{I_i} G_i(V, \nu)ds$. The conjugate coefficient $\gamma_i^n$ is updated such that $\langle d_i^n, d_i^{n-1} \rangle = 0$, which gives

$$\gamma_i^n = \frac{\langle dJ_i^n, d_i^{n-1} \rangle}{\|d_i^{n-1}\|^2}. \quad (42)$$

Still to explore the update of the step size $\beta_i$ for $i = 1, 2$. For that we manipulate the fact that our cost functional is quadratic, which means that we need to express the shape hessian.

We note that the shape hessian requires some smoothness hypothesis on the interfaces $I_1$ and $I_2$, in the work [14] we get that the hessian exists for domains of class $C^{k+2}$ for $k \geq 0$. Following the same steps in [14] we have that

$$d^2J[V, W] = \int_{I_1 \cup I_2} G'(W)(V, \nu) + (\nabla_\nu G + \kappa G) \langle V, \nu \rangle \langle W, \nu \rangle ds$$

$$- \int_{I_1 \cup I_2} G(V_1 \cdot D_1 \nu W_1 + \nu \cdot D_1 W V_1) ds$$

$$+ \int_{I_1 \cup I_2} G(DV) \langle W, \nu \rangle + GV' \nu ds$$

Let consider the following writing

$$d^2J[V] = \int_{I_1 \cup I_2} H ds = d^2J_1[V] + d^2J_2[V] = \int_{I_1} H ds + \int_{I_2} H ds$$

Thereafter, with Taylor expansion formula we can write

$$\mathcal{J}(I_1^n + \beta_1^n d_1^n, I_2^n) = \mathcal{J}(I_1^n, I_2^n) + \beta_1^n d\mathcal{J}_1[d_1^n] + \frac{(\beta_1^n)^2}{2} d^2\mathcal{J}_1[d_1^n] + o(\|d_1^n\|^2)$$

$$\mathcal{J}(I_1^n, I_2^n + \beta_2^n d_2^n) = \mathcal{J}(I_1^n, I_2^n) + \beta_2^n d\mathcal{J}_2[d_2^n] + \frac{(\beta_2^n)^2}{2} d^2\mathcal{J}_2[d_2^n] + o(\|d_2^n\|^2)$$
Hence the step sizes $\beta_1^n$ and $\beta_2^n$ are updated with the following
\[
\beta_1^n = -\frac{\langle dJ_n^1, d^n_1 \rangle}{\langle d^2J_n^1 d^n_1, d^n_1 \rangle} \quad \text{and} \quad \beta_2^n = -\frac{\langle dJ_n^2, d^n_2 \rangle}{\langle d^2J_n^2 d^n_2, d^n_2 \rangle}
\] (43)

In the next part, we will explore an heuristic method that we use for finding the best initial guess to start the minimization with conjugate gradient method.

5.3. Differential Evolution heuristic method. Differential evolution [19] (DE) in one of the recent metaheuristic methods, was firstly introduced in 1995 by S-torn [20], lately Storn and Price provide the description of DE for continuous optimization problem [17]. Some of the advantages of DE compared to the other heuristic methods are the adequate convergence rate, it need few control parameter. DE is also a population based approach, it uses three operators to create the next new population, mutation, crossover and selection.

Starting with an initial population $P_0$ of size $N$, generated in a given range $[A, B]$. The mutation operator generates a new offspring vector respect to the following formula, for each $i \in \{1, ..., N\}$
\[
Y_{i}^{n+1} = X_{i}^{n} + \rho (X_{j_2}^{n} - X_{j_1}^{n})
\]
n denotes the generation number, the indexes $j_1$, $j_2$ and $j_3$ are generated randomly in $\{1, ..., i-1, i+1, ..., N\}$. $X_i^n$ is a vector from the current population $P_n$, and $\rho$ is the scaling coefficient chosen in the range $[0, 2]$.

The crossover operator is for adding some diversity to the future population, for each $i \in \{1, ..., N\}$ and $j \in \{1, ..., M\}$ with $M$ is the length of $X_i$, generate the vector
\[
Z_{ij}^{n+1} = \begin{cases} 
X_{ij}^{n} & \text{if } d_j > \sigma \\
Y_{ij}^{n+1} & \text{if } d_j \leq \sigma
\end{cases}
\]
with $d_j$ is a random number uniformly taken in $[0, 1]$ for each index $j$. The vector $Y_i^{n+1}$ is the one generated with the mutation operator.

The selection operator is for making the decision which vectors will belongs to the future generation, basing on the comparison of the fitness of $X_i^n$ and $Z_i^{n+1}$, the fittest means the one with small cost will belongs to the future generation $P_{n+1}$.

To solve our shape optimization problem, we generate in the first a random population in the range $[0, H]$, then for each vector, we shall solve the systems (31)-(33) and (35)-(37). At each generation we apply the three operators mutation, crossover and selection, then we extract the fittest individual it is one with the smallest fitness in the current population, that we called the best vector, then we check the stopping criteria, if is satisfied we stop the process if not we repeat the previous steps. In algorithm 2 we have summarized all steps for our proposed numerical scheme.

6. Numerical experiment. In this section, we establish some numerical simulation to prove the validity of the presented method to solve this kind of inverse problem. We call the bézier curve [16] to parameterize the free interfaces, in order to simplify their representation and to reduce the number of variables. Accordingly the individual in this application is a vector of the control points of $I_1$ and $I_2$. For the stopping criterion we can choose a desired precision $\varepsilon$ or a max number of generation. The parameter used for tuning the algorithm 2 are in table 1.
Algorithm 2:

Input: Choose $\varrho$, $\sigma$, $N$, $\varepsilon$, $N_{\text{max}}$ and set $t = 0$.

1. Generate a random population $P(t)$ in the range $[0, H]$ of size $N$.
2. for $i = 1$ to $N$ do
   3. Apply the operator: mutation, crossover and selection
   4. Compute $p^n$ and $q^n$ solution of (7) and (9) with algorithm 1
   5. Evaluate $J_i$ for the current individual
   6. Extract the best individual.
7. if $t \leq N_{\text{max}}$ then
   8. Stop,
   9. else
     10. set $t = t + 1$ and continue to step (2)
   11. while $J(I^n_1, I^n_2) > \varepsilon$ or $n \leq N_{\text{max}}$ do
     12. Find $\lambda^n$ and $\mu^n$ solutions of (23) and (24) with algorithm 1.
     13. Compute the shape gradient $dJ_n$ with (20).
     14. Update the conjugate coefficient $\gamma_n$ using (42).
     15. Update $d^n_1$ and $d^n_2$ according to (41).
     16. Compute the step size $\beta^n_1$ and $\beta^n_2$.
     17. Update the interfaces with (40).
     18. Compute $p^n$ and $q^n$ solution of (7) and (9) with algorithm 1.
     19. Set $n = n + 1$, back to step 2.

Output: The optimal solution $(\Omega, u)$

| Population size | Max generations | Mutation scale $\varrho$ | Crossover ratio $\sigma$ |
|-----------------|-----------------|------------------------|-------------------------|
| 25              | 10              | 0.1                    | 0.75                    |

6.1. Algorithm validation. First of all, we concentrate on proving the validity of the proposed algorithm to solve problem (11). We assume that $\Omega = [0, 6] \times [0, 2]$ and the analytical solution is

$$u(x, y) = e^{x + y}, \quad x, y \in \Omega.$$ 

The functions $f$, $g$ and $h$ are constructed from above expression. $g^p$ and $h^p$ are constructed for different noise level $p$. We study two different examples, the first is when $I_1$ and $I_2$ are given by:

$$I_1 = \left\{ \left( \frac{3}{2} - y, y \right) / y \in [0, 1] \right\} \quad \text{and} \quad I_2 = \left\{ \left( 4 + 2y(1 - y^2), y \right) / y \in [0, 1] \right\},$$

and in the second example, we will try to identify the following

$$I_1 = \left\{ \left( 2 + \frac{1}{2} \sin(\frac{3\pi y}{4}), y \right) / y \in [0, 1] \right\} \quad \text{and} \quad I_2 = \left\{ \left( 2 + 2\sqrt{\frac{1 + y^2}{2}}, y \right) / y \in [0, 1] \right\}.$$

First, we will show why we have proposed this hybridization. To do so, we illustrate the obtained results with the conjugate gradient method only for example 1. The initial guesses used in this experiment are assumed to be $I_1 = \{0\} \times [0, 1]$ and $I_2 = \{0\} \times [0, 1]$. In figure 2 we plot the obtained results
Figure 2. Example 1: the optimal interfaces versus the exact ones

One can see, that the conjugate gradient method did not find a good approximation of the exact boundaries, the first thing comes in mind is to change the initial guesses, for that we assume this time $I_1 = \{1\} \times [0, 1]$ and $I_2 = \{5\} \times [0, 1]$, the new results are illustrated in the next figure.

Figure 3. Example 2: the optimal interfaces versus the exact ones.

This time, the conjugate gradient succeed to recover the exact boundaries, with the cost 0.0216. A simple question to ask, should we each time seek the best initial guess manually or build an automatic search for this initial guess. Here comes the idea behind the hybridization we have proposed, the differential evolution heuristic method will find the initial guess for the conjugate gradient method.

Now, we will show the result obtained with the proposed algorithm. In figure 4 and 5 we illustrate the obtained interfaces after the first stage of the algorithm (DE stage) and the optimal interfaces, all are compared with the exact ones.

It is seen that, the Differential evolution stage did generate a good initial guess, which facilitates the minimization process of conjugate gradient. In both examples,
the optimal interfaces $I_1$ and $I_2$ are near enough to the exact one and are almost identical as figures 4 and 5 show.

In figure 6 and 7 we have represented the optimal interfaces with noisy data, as expect the quality of optimal interfaces decreases, as the noise level increases the cost increases as well, although the optimal interfaces still near to the exact ones. At this stage, the obtained numerical results only means that the proposed hybrid algorithm is efficient to solve such kind of shape optimization problems.

In table 2 we read the optimal cost for examples 1 and 2 with respect to different noise levels.

**Table 2. Comparison of errors.**

| Noise level | 0%     | 1%     | 5%     | 10%    |
|-------------|--------|--------|--------|--------|
| Example 1   | 0.0095 | 0.0184 | 0.0676 | 0.1779 |
| Example 2   | 0.0213 | 0.0243 | 0.0458 | 0.0589 |
6.2. Application to semiconductor equations. Now we will illustrate some numerical test for the depletion region identification. We assume that the pn junction domain is $[0, 6] \times [0, 2]$, the range of the positive and negative electrodes are $[0, 3] \times [0, 2]$ and $[3, 6] \times [0, 2]$ respectively. The working of a pn-junction is governed by two mode known as the forward and the reverse biased mode. The first mode is established when the n-type (resp. n-type) is connected to a negative (resp. positive) terminal, in this mode the pn-junction allows the current flow to cross the depletion region, which means that when the applied voltages increases the depletion region $\Omega$ width’s decreases. In contrast when the pn-junction is under reverse bias, it is when the n-type terminal (resp. p-type) is connected to a positive (resp. negative) terminal, the depletion region $\Omega$ becomes wide, this is natural because the semiconductor blocks the current flow in this mode.

For the cost functional we consider the same form given by (39), but the solution $p$ and $q$ are of the next problems:

$$- \Delta p = 0 \text{ in } C_1 \cup C_2, \quad - \Delta p = \zeta \text{ in } D, \quad \nabla \nu p = 0 \text{ on } \Gamma_N \text{ and } p = V_d \text{ on } \Gamma_D \quad (44)$$
and the second state equation

\[-\Delta q = 0 \text{ in } C_1 \cup C_2, \quad -\Delta q = \zeta \text{ in } D \quad \text{and} \quad \nabla \nu q = 0 \text{ on } \partial \Omega,\]

the system (44)-(45) reads as the split of the problem (3).

Figure 8 and 9 illustrate the optimal depletion layers in the pn-junction for different voltages, under the modes forward and the reverse biased. we can see that as we change the applied voltages the depth of the depletion region changes, in addition the physical proprieties of the pn junction functioning are still hold.

![Figure 8. Forward mode](image)

![Figure 9. Reverse mode](image)

The table 3 we write the obtained cost for different voltages.

**Table 3. Optimal cost for each functioning mode.**

| Depletion mode | Enhancement mode |
|----------------|------------------|
| $V^+$ $V^-$ | cost $V^+$ $V^-$ | cost |
| +0.1V -0.0V | 0.018 | -0.3V +0.3V | 0.029 |
| +0.3V -0.3V | 0.047 | -0.6V +0.6V | 0.063 |
| +0.6V -0.6V | 0.079 | -0.6V +1.2V | 0.085 |

We conclude that the developed algorithm succeeds to solve the general problem with pretty results with and without noisy data. Also it succeed to approximate the depletion region, as it keeps the physical proprieties of the pn junction hold, which show the robustness and the efficiency of the proposed algorithm to solve this kind of inverse problems.
7. Conclusion. In this paper the depletion region identification problem in pn junction semiconductor was considered. The shape optimization problem was established using a cost functional that depended on the free interfaces and the solution of two state equations. Also we have proved the existence of an optimal solution, in addition to the computation of the shape gradient. The presented numerical approach is based on the domain decomposition technique and the differential evolution combined with conjugate gradient method. The obtained numerical results show the efficiency of the presented method to solve the considered problem. As an application, we have applied the developed algorithms to identify the depletion region in pn-junction, for different values of the potentials, under the functioning modes the forward and reverse bias modes.

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