Anisotropic mesh adaptivity via a dual-based a posteriori error estimation for semiconductors *

Stefano Micheletti Simona Perotto

MOX - Modeling and Scientific Computing, Dipartimento di Matematica "F. Brioschi",
Politecnico di Milano, via Bonardi 9,
20133 Milano, Italy.
{stefano.micheletti,simona.perotto}@mate.polimi.it

1 Introduction

The accurate computation of a physically meaningful quantity (the goal quantity) associated with the solution of a given problem is of paramount importance in engineering applications. For example, in micro- or nano-electronics the output current is a fundamental quantity to assess the performance of the device at hand. In particular, we consider the Drift-Diffusion (DD) model for semiconductors describing the charge-transport in a device in terms of the electric potential (ψ), electron (n) and hole (p) concentrations [Sel84]. Thus, the goal quantity can be described by a suitable functional J, either linear or nonlinear, of the variables ψ, n and p. The accurate approximation of J can be dealt with in the framework of the optimal control theory. In particular, we consider an anisotropic a posteriori error estimation relying on the dual-based approach of [BR01, GS02]. We solve an adjoint (dual) linearized problem while employing anisotropic interpolation estimates [FP01, FP03] to bound the approximation error associated with the solution of the dual problem with respect to a suitable finite dimensional space. Thus, the parameters describing the distribution and shaping of the elements of the computational mesh act as control parameters, through which it is possible to approximate the goal quantity as accurate as needed.

The outline of the paper is as follows. In Section 2 the DD model for semiconductors is introduced. In Section 3 we sketch the abstract framework on which the anisotropic analysis is based. In particular, in Section 3.1 we recall some anisotropic interpolation error estimates which are the basic tool linking the dual-based a posteriori analysis of Section 4 to the anisotropic mesh adaptivity procedure. In Section 5 we derive the desired anisotropic a posteriori error estimator, while in Section 6 we address the iterative adaptive procedure used to construct the anisotropic meshes. A numerical validation is carried out on some test cases dealing with a pn-junction diode in Section 7. Finally, some conclusions and open issues are drawn in Section 8.

*This work was partially supported by the INDAM 2003 Project "Modellistica Numerica per il Calcolo Scientifico e Applicazioni Avanzate".

2 The Drift-Diffusion model

In this section we recall the stationary Drift-Diffusion charge transport model (see e.g. [Sel84]), consisting of the conservation laws for charge and for electron and hole concentrations (1)(left)

$$\begin{cases} \quad \mathrm{div}(\epsilon\vec{E}) - \rho = 0, \\ - \quad \mathrm{div}\vec{J}_n + qR = 0, \\ \quad \mathrm{div}\vec{J}_p + qR = 0, \end{cases} \qquad \begin{cases} \vec{E} &= -\nabla\psi, \\ \vec{J}_n &= q(D_n\nabla n - \mu_n\, n\,\nabla\psi), \\ \vec{J}_p &= -q(D_p\nabla p + \mu_p\, p\,\nabla\psi), \\ \rho &= q(p - n + D), \\ D_n &= \mu_n V_{\mathrm{th}}, \\ D_p &= \mu_p V_{\mathrm{th}}. \end{cases} \tag{1}$$

completed by the constitutive relations (1)(right). In (1), ψ, n and p are the unknowns, i.e. the electric potential, and the electron and hole concentrations, while $\vec{J}_n, \vec{J}_p$ are the electron and hole current densities, $\vec{E}$ is the electric field, ρ is the net charge density, D is the given doping profile, R is the recombination/generation rate, D_n, μ_n (D_p, μ_p) are the electron (hole) diffusion coefficient and mobility, V_{th} is the thermal voltage, ϵ is the semiconductor dielectric permittivity, and q is the positive electron charge. As typical expression for R, we consider henceforth the so-called Shockley-Read-Hall form, given by $R = (pn - n_i^2)/[(p + n_i)\tau_n + (n + n_i)\tau_p]$, where n_i is the electron/hole intrinsic concentration, and τ_n and τ_p are suitable relaxation times (see, e.g., [Sel84]). The whole system is completed by suitable boundary conditions, usually of mixed type. For simplicity, we consider the case where the device is made up of a homogeneous semiconductor material, occupying the computational domain Ω, that is we do not deal with metal-semiconductor or metal-oxide-semiconductor structures. Thus, the boundary $\partial\Omega$ of Ω is split into two non-overlapping parts, Γ_{D} and Γ_{N}, where Dirichlet and Neumann boundary conditions are imposed, respectively. For instance, in the case of the pn junction diodes of Fig. 1, we have $\Gamma_{\mathrm{D}} = \overline{\mathrm{AG}} \cup \overline{\mathrm{CD}}$ while $\Gamma_{\mathrm{N}} = \partial\Omega\backslash\Gamma_{\mathrm{D}}$. The boundary conditions characterizing the devices in Fig. 1 are thus given by $\psi = \psi_{\mathrm{D}}$,

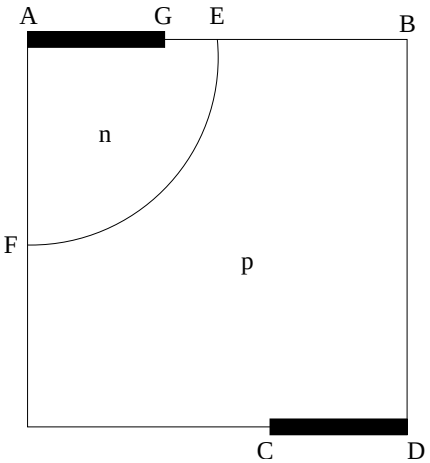

Figure 1: Geometry of a pn junction diode

$n = n_{\mathrm{D}}$ and $p = p_{\mathrm{D}}$ on Γ_{D}, while $\nabla\psi \cdot \vec{n} = \nabla n \cdot \vec{n} = \nabla p \cdot \vec{n} = 0$, on Γ_{N}, where $\vec{n}$ is the

unit outward normal vector to $\partial\Omega$, $\psi_{\rm D} = V_{\rm app} + V_{\rm bi}$, with $V_{\rm app}$ the external applied voltage and $V_{\rm bi} = V_{\rm th}\sinh^{-1}(D/(2n_i))|_{\Gamma_{\rm D}}$, the so-called built-in voltage, while $n_{\rm D} = \big[(D + \sqrt{D^2 + 4n_i^2})/2\big]\Big|_{\Gamma_{\rm D}}$ and $p_{\rm D} = -\big[(D + \sqrt{D^2 + 4n_i^2})/2\big]\Big|_{\Gamma_{\rm D}}$.

3 The anisotropic "tool box"

Let us introduce a conformal partition $\mathcal{T}_h$ of Ω, in the usual sense [Cia78], consisting of triangular elements and let K denote the general triangle. Let $T_K : \widehat{K} \to K$ be the standard affine mapping between the reference triangle $\widehat{K}$ (e.g. the unit equilateral one) and the general one K, with $\vec{x} = (x_1, x_2)^{\rm T} = T_K(\widehat{\vec{x}}) = M_K\widehat{\vec{x}} + \vec{t}_K$. Then let us introduce the polar decomposition of M_K, i.e. $M_K = B_K\, Z_K$, with B_K symmetric positive definite and Z_K orthogonal matrices, respectively. Decomposing B_K in terms of its eigenvectors $\vec{r}_{i,K}$ and eigenvalues $\lambda_{i,K}$, with $i = 1, 2$, yields

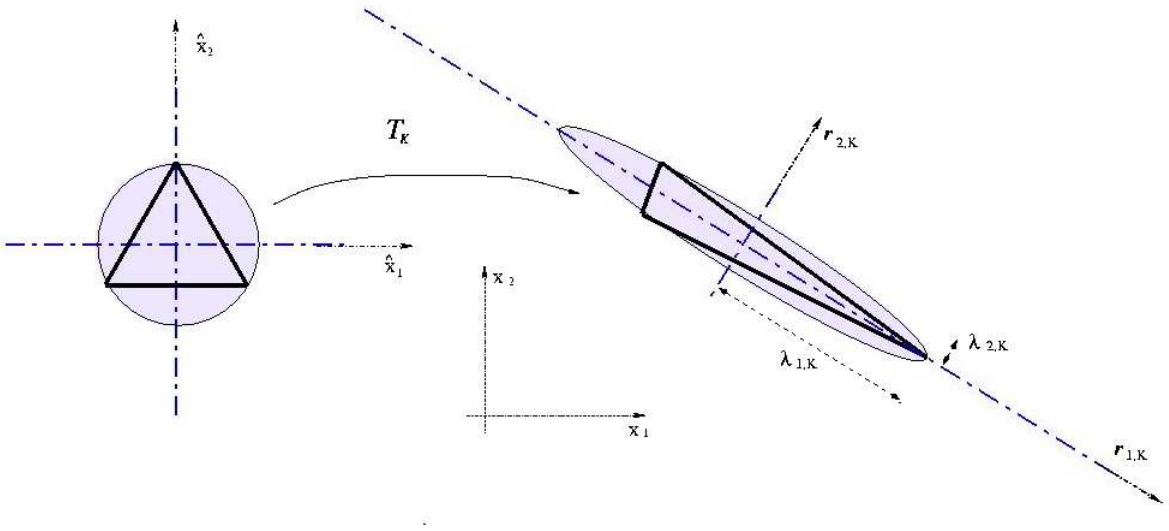

Figure 2: Geometrical quantities related to the affine mapping T_K

$B_K = R_K^{\rm T}\Lambda_K R_K$, where $R_K^{\rm T} = \big[\mathbf{r}_{1,K}, \mathbf{r}_{2,K}\big]$ and $\Lambda_K = {\rm diag}[\lambda_{1,K}, \lambda_{2,K}]$. Throughout we assume $\lambda_{1,K} \geq \lambda_{2,K}$, that is $s_K = \lambda_{1,K}/\lambda_{2,K} \geq 1$, s_K being the so called stretching factor (see Fig. 2 for the geometrical meaning of the quantities $\lambda_{i,K}, \vec{r}_{i,K}$).

3.1 Anisotropic interpolation error estimates

Moving from the above abstract framework, we now recall some anisotropic interpolation error estimates, introduced in [FP01, FP03]. We assume a standard notation for the Lebesgue and Sobolev spaces, see, e.g., [Cia78]. For any function $v \in H^1(\Omega)$, let $G_K(v)$ be the symmetric positive semi-definite matrix with entries $(G_K(v))_{i,\,j} = \int_{\Delta_K} \partial_{x_i} v\, \partial_{x_j} v\, d\vec{x}$, and let $I_K(v) \in \mathbb{P}^1(K)$ be a Clément-like interpolant of v on K, where $\mathbb{P}^1(K)$ is the space of polynomials of degree less than or equal to one on K, Δ_K being a suitable patch of elements surrounding K. Then the following

estimates can be proved:

$$\|v - I_K(v)\|^2_{L^2(K)} \leq C_1 \sum_{i=1}^{2} \lambda^2_{i,K} \left(\vec{r}^{\,\mathrm{T}}_{i,K} G_K(v) \vec{r}_{i,K}\right), \tag{2}$$

$$\|v - I_K(v)\|^2_{L^2(e)} \leq C_2 \frac{1}{\lambda_{2,K}} \sum_{i=1}^{2} \lambda^2_{i,K} \left(\vec{r}^{\,\mathrm{T}}_{i,K} G_K(v) \vec{r}_{i,K}\right), \tag{3}$$

where the edge $e \in \partial K$ and C_1, C_2 suitable constants (see [MPP03] for more details).

4 Dual-based a posteriori analysis

Suppose that we are interested in approximating the goal quantity $J(u)$ by $J(u_h)$ such that $|J(u) - J(u_h)| \leq \tau$, with J a continuous functional, possibly nonlinear, u and u_h the exact and approximate solutions to the problem at hand, and τ a given tolerance. In electronics, J can be, for example, the total current in a device, or in Computational Fluid Dynamics, it can represent the kinetic energy or the vorticity of a fluid, the lift or drag in a flow past a body, while in structural mechanics, it can be the torsion moment, the stress values or the total surface tension.

With this aim we can follow the so-called dual approach in [BR01, GS02]. In a general setting, let $a(u; v)$ and $J(u)$ be semilinear forms, where it is understood that, when more than one argument is present, the forms are linear with respect to all the arguments on the right of the semicolon. The problem at hand can be formulated as the following control problem: find $u \in V$ such that

$$J(u) = \min_{v \in M} J(v) \quad \text{with} \quad M = \{w \in V : a(w; v) = F(v), \quad \forall v \in V\},$$

where F is a linear form and V is a suitable Hilbert space. Let $\mathcal{L}(u; z) = J(u) + F(z) - a(u; z)$, for any $u, z \in V$, be the corresponding Lagrangian. The condition for finding the critical points of $\mathcal{L}$, that is

$$\mathcal{L}'(u, z; \varphi, v) = J'(u; \varphi) + F(v) - a(u; v) - a'(u; \varphi, z) = 0, \qquad \forall \varphi, v \in V,$$

yields the primal problem (P.P.): find $u \in V$ such that

$$a(u; v) = F(v), \qquad \forall v \in V,$$

and the adjoint problem (A.P.): find $z \in V$ such that

$$a'(u; \varphi, z) = J'(u; \varphi), \qquad \forall \varphi \in V,$$

where $a'(u; \varphi, z) = \lim_{\epsilon \to 0} \frac{1}{\epsilon}[a(u + \epsilon\varphi; z) - a(u; z)]$ is the Gâteaux derivative of $a(u; z)$ with respect to its first argument, and likewise for $J'(u; \varphi)$. Then let us consider the Galerkin approximation (G.A.) of (P.P.): find $u_h \in V_h$ such that

$$a(u_h; v_h) = F(v_h), \qquad \forall v_h \in V_h,$$

where V_h is a suitable finite dimensional subspace of V. The problems (P.P.) and (G.A.) are linked by the Galerkin orthogonality (G.O.) condition:

$$a(u; v_h) - a(u_h; v_h) = 0, \qquad \forall v_h \in V_h.$$

In the case when both a and J are linear, from (P.P.), (A.P.) and (G.O.) the following error representation holds: $J(u) - J(u_h) = F(z - \varphi_h) - a(u_h; z - \varphi_h)$, for any $\varphi_h \in V_h$. Otherwise in the more general case when either a or J are nonlinear, it can be proved that

$$J(u) - J(u_h) = F(z - \varphi_h) - a(u_h; z - \varphi_h) + \mathcal{R} \qquad \forall \varphi_h \in V_h, \tag{4}$$

where

$$\mathcal{R} = \int_0^1 [a''(u_h + se; e, e, z) - J''(u_h + se; e, e)] s \, ds,$$

is a remainder term quadratic with respect to $e = u - u_h$ (see Propositions 2.2 and 2.3 in [BR01]). In practice, neglecting $\mathcal{R}$, choosing φ_h as a suitable interpolant of z and integrating by parts over the elements of the mesh, we obtain an estimate of the form

$$|J(u) - J(u_h)| \leq C \sum_{K \in \mathcal{T}_h} \rho_K(u_h) \, \omega_K(z),$$

where $\rho_K(u_h)$ is a residual term depending only on the approximate solution u_h and $\omega_K(z)$ is a weighting term taking into account the dual solution z.

5 Goal-oriented a posteriori analysis for the DD model

In this section we apply the general framework of the previous section to the Drift-Diffusion model (1) (more details can be found in [MP04]). For this purpose, let $U = (\psi, n, p)$ and $Z = (z_1, z_2, z_3)$ be the primal and dual solution triplets, respectively, and let $(u, v) = \int_\Omega u \, v \, d\Omega$ denote the standard $L^2(\Omega)$-scalar product. Then problem (1) can be cast in the abstract framework above by defining

$$\begin{aligned} a(U; Z) &= (\epsilon \nabla \psi, \nabla z_1) - q(p - n + D, z_1) + q(D_n \nabla n - \mu_n n \nabla \psi, \nabla z_2) + q(R, z_2) \\ &+ q(D_p \nabla p + \mu_p p \nabla \psi, \nabla z_3) + q(R, z_3), \end{aligned}$$

while $F(U) = 0$. Thus $\mathcal{L}(U; Z) = J(U) - a(U; Z)$, for any $(U, Z) \in W \times \widetilde{W}$, where W is the affine space of functions in $[H^1(\Omega)]^3$ taking into account the nonhomogeneous Dirichlet boundary conditions, while $\widetilde{W} = [H^1_{\Gamma_D}(\Omega)]^3$. Letting $V = (v_1, v_2, v_3)$, we have

$$\begin{aligned} &a'(U; V, Z) = (\epsilon \nabla v_1, \nabla z_1) - q(v_3 - v_2, z_1) \\ &+ q(D_n \nabla v_2 - \mu_n n \nabla v_1 - \mu_n v_2 \nabla \psi, \nabla z_2) + q(R'_n(U) v_2, z_2) + q(R'_p(U) v_3, z_2) \\ &+ q(D_p \nabla v_3 + \mu_p p \nabla v_1 + \mu_p v_3 \nabla \psi, \nabla z_3) + q(R'_n(U) v_2, z_3) + q(R'_p(U) v_3, z_3), \end{aligned}$$

$R'_n(U), R'_p(U)$ being the derivatives of the recombination/generation term with respect to n and p, respectively. Let $J(U)$ be the quantity we are interested in and let us introduce the Galerkin approximation $U_h = (\psi_h, n_h, p_h) \in W_h$ of the primal solution, such that $a(U_h, V_h) = 0$, for any $V_h \in \widetilde{W}_h$, where W_h and $\widetilde{W}_h$ are finite dimensional subspaces of W and $\widetilde{W}$, respectively. Moving from equality (4) and neglecting the remainder term $\mathcal{R}$, it holds

$$J(U) - J(U_h) \simeq -a(U_h; Z - V_h), \qquad \forall V_h \in \widetilde{W}_h.$$

In more detail, by splitting the integrals over Ω as sums over the elements K of the mesh $\mathcal{T}_h$, we get

$$J(U) - J(U_h) \simeq \sum_{i=1}^{3} \sum_{K \in \mathcal{T}_h} \Big\{ (\rho_K^i, z_i - v_{h,i})_K + \frac{1}{2} (j_e^i, z_i - v_{h,i})_{\partial K} \Big\},$$

where $\rho_K^i = \rho_K^i(\psi_h, n_h, p_h)$ and $j_e^i = j_e^i(\psi_h, n_h, p_h)$, with $i = 1, 2, 3$, are the internal and edge residuals, respectively, defined by

$$\begin{cases} \rho_K^1 = [\,\mathrm{div}(\epsilon \vec{E}_h) - q(p_h - n_h + D)\,]\big|_K, \\ \rho_K^2 = [\,-\mathrm{div}\vec{J}_{n,h} + qR(U_h)\,]\big|_K, \\ \rho_K^3 = [\,\mathrm{div}\vec{J}_{p,h} + qR(U_h)\,]\big|_K, \end{cases} \quad \text{and} \quad j_e^i = \begin{cases} [\vec{j}^i \cdot \vec{n}]_e, & \forall e \in \mathcal{E}_h, \\ 2\vec{j}^i \cdot \vec{n}, & \forall e \in \Gamma_{\mathrm{N}}, \\ 0, & \forall e \in \Gamma_{\mathrm{D}}, \end{cases}$$

where $\vec{j}^1 = -\epsilon \vec{E}_h = \epsilon \nabla \psi_h$, $\vec{j}_h^2 = \vec{J}_{n,h} = q(D_n \nabla n_h - \mu_n n_h \nabla \psi_h)$ and $\vec{j}_h^3 = -\vec{J}_{p,h} = q(D_p \nabla p_h + \mu_p p_h \nabla \psi_h)$ are the discrete displacement, electron and hole current densities, respectively, $R(U_h)$ is the recombination/generation term evaluated at U_h, $\mathcal{E}_h$ is the set of the internal edges of $\mathcal{T}_h$ and $[\,v\,]_e$ denotes the jump of the function v across the edge e. Now choosing $V_h\big|_K = I_K(Z)$, i.e. by identifying the test function V_h with the Clément-like interpolant of the dual solution Z, and thanks to the anisotropic interpolation error estimates (2)-(3), we obtain

$$|J(U) - J(U_h)| \leq C \sum_{i=1}^{3} \sum_{K \in \mathcal{T}_h} \alpha_K \, R_K^i(U_h) \, \omega_K^i(z_i), \tag{5}$$

where $C = C(C_1, C_2)$, $\alpha_K = (\lambda_{1,K}\lambda_{2,K})^{3/2}$, and for $i = 1, 2, 3$,

$$\begin{aligned} R_K^i(U_h) &= \frac{1}{(\lambda_{1,K}\lambda_{2,K})^{1/2}} \Big(\|\rho_K^i\|_{L^2(K)} + \frac{1}{2\lambda_{2,K}^{1/2}} \|j_e^i\|_{L^2(\partial K)} \Big), \\ \omega_K^i(z_i) &= \frac{1}{(\lambda_{1,K}\lambda_{2,K})^{1/2}} \Big[s_K \big(\vec{r}_{1,K}^{\,\mathrm{T}} G_K(z_i) \vec{r}_{1,K} \big) + \frac{1}{s_K} \big(\vec{r}_{2,K}^{\,\mathrm{T}} G_K(z_i) \vec{r}_{2,K} \big) \Big]^{1/2}, \end{aligned}$$

with $R_K^i(U_h)$ and $\omega_K^i(z_i)$ independent of $|K|$, at least asymptotically, i.e. when the mesh is sufficiently fine.

6 Generation of the mesh

The technique used to compute the adapted meshes is a metric-based, adaptive iterative procedure that, starting from a given mesh, $\mathcal{T}_h^{(k)}$, consisting of $N_h^{(k)}$ elements, finds the new mesh $\mathcal{T}_h^{(k+1)}$ by exploiting the error estimator (5). In practice, the anisotropic quantities describing the new mesh $\mathcal{T}_h^{(k+1)}$ are approximated by functions piecewise constant on $\mathcal{T}_h^{(k)}$. Since we are dealing with a vector problem, each of the three terms in (5) yields a contribution to the adaptive procedure, i.e. a corresponding mesh. As the procedure to obtain each mesh is the same for all the three contributions, we detail in the following the general procedure for a given $i \in \{1, 2, 3\}$. For this purpose, let $\eta_K^i = \alpha_K \, R_K^i(U_h) \, \omega_K^i(z_i)$ be the local error estimator. We impose that:

i) $\eta_K^i = \tau / N_h^{(k)}$, for any $K \in \mathcal{T}_h^k$, where τ is the given tolerance (equidistribution criterion);

ii) $|K|$ be as large as possible (mesh elements minimization criterion).

Requirement *ii)* amounts to solving the minimization problem for the quantities at step $k+1$:

find the optimal values $\widetilde{s}_K$ *of* s_K *and* $\widetilde{\vec{r}}_{1,K}$ *of* $\vec{r}_{1,K}$ *such that* $\omega_K^i(z_i)$ *be minimized, subject to the constraints* $s_K \geq 1$, $\vec{r}_{1,K}, \vec{r}_{2,K} \in \mathbb{R}^2$, $\vec{r}_{i,K} \cdot \vec{r}_{j,K} = \delta_{ij}$, *for* $i,j = 1,2$, *with* δ_{ij} *the Kronecker symbol,*

where the dependence on $k+1$ is understood. Let μ_m and μ_M be the (positive) minimum and maximum eigenvalues of $G_K(z_i)/(\lambda_{1,K}^{(k)}\lambda_{2,K}^{(k)})$, respectively. Then the solution of this minimization problem yields $\widetilde{\vec{r}}_{1,K}$ parallel to the eigenvector associated with μ_m and $\widetilde{s}_K = \widetilde{\lambda}_{1,K}/\widetilde{\lambda}_{2,K} = (\mu_M/\mu_m)^{1/2}$. Finally, requirement *i)* allows us to obtain the specific values for $\widetilde{\lambda}_{1,K}$ and $\widetilde{\lambda}_{2,K}$, as

$$\widetilde{\lambda}_{1,K}\widetilde{\lambda}_{2,K} \simeq \left(\frac{\tau}{N_h^{(k)}}\right)^{2/3} \left(R_K^i(U_h)\Big(\widetilde{s}_K\,\mu_m + \frac{1}{\widetilde{s}_K}\,\mu_M\Big)^{1/2}\right)^{-2/3}.$$

The above quantities define in a unique way the size and shape of the elements of the new mesh $\mathcal{T}_h^{i,(k+1)}$. Following the same above procedure, once the three metrics for $\mathcal{T}_h^{1,(k+1)}, \mathcal{T}_h^{2,(k+1)}$ and $\mathcal{T}_h^{3,(k+1)}$ have been obtained, the final mesh $\mathcal{T}_h^{(k+1)}$ may be obtained by computing the intersection of the three metrics, as described in [GB98].

7 Numerical results

We asses the procedure outlined in the previous sections on some test cases. Firstly, let us provide some computational details:

- the Scharfetter-Gummel node-centred box method is used as numerical approximation scheme, thus, only the current densities along the edges are meaningful [BBFS90]. This scheme guarantees a discrete maximum principle for the unknowns;
- the reconstruction of the current densities inside each triangle is carried out by the lowest order edge elements of Nédélec's first family [Ned80];
- the Newton method is used to solve the whole system;
- the stiffness matrix for the dual problem is just the transpose of the Jacobian associated with the non-linear system of the primal problem, so that the overhead of solving the dual problem is approximately the same as that of one further iteration of the Newton method;
- the software BAMG [Hec98] is used to compute all the meshes.

We consider the step-junction diode of Fig. 1, with the following choice for the data: $\Omega = (0,10) \times (0,10)\,\mu$m, symmetric doping, i.e. $D = 10^{17}\,\mathrm{cm}^{-3}$ in the curved polygonal n-region A-G-E-F-A, and $D = -10^{17}\,\mathrm{cm}^{-3}$ in the remaining part, contact length $|\overline{\mathrm{AG}}| = |\overline{\mathrm{CD}}| = 4\,\mu$m, and junction radius $|\overline{\mathrm{AE}}| = |\overline{\mathrm{AF}}| = 5\,\mu$m centred at A, $\tau_n = \tau_p = 10^{-9}\,\mathrm{s}$, $\mu_n = 1300\,\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$, and $\mu_p = 400\,\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$.

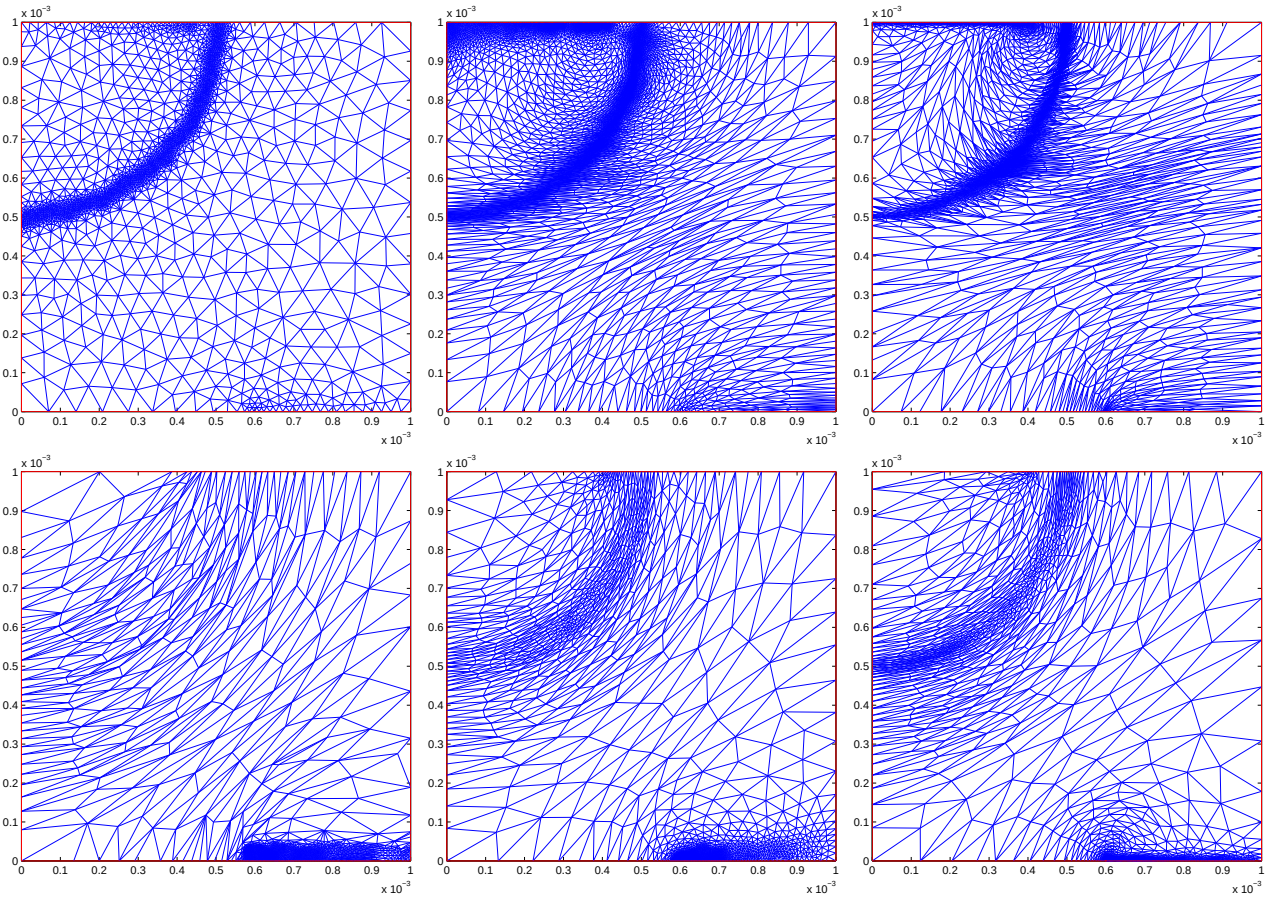

Figure 3: Control of total current: sequence of adapted meshes

7.1 Control of total current

As first choice, we identify the goal functional J with the total current, i.e. with the flux of the total current density $\vec{J} = \vec{J}_n + \vec{J}_p$, either at the n-side contact $\overline{\mathrm{AG}}$, or at the p-side edge $\overline{\mathrm{CD}}$. In the case of the n-side contact, for example, the functional J is computed as $J(U) = \int_{\overline{AG}} \vec{J} \cdot \vec{n}\, ds = \int_{\partial\Omega} \vec{J} \cdot \vec{n}\, \omega\, ds = \int_\Omega \omega\, \mathrm{div}\vec{J}\, d\Omega + \int_\Omega \vec{J} \cdot \nabla\omega\, d\Omega = \int_\Omega \vec{J} \cdot \nabla\omega\, d\Omega$, for any function ω smooth enough, such that $\omega|_{\overline{\mathrm{AG}}} = 1$ and $\omega|_{\overline{\mathrm{CD}}} = 0$. Notice that, we have used the divergence theorem and, from (1), the property that $\mathrm{div}\, \vec{J} = 0$, so that, thanks also to the boundary conditions, the flux of $\vec{J}$ at the two contacts is equal and of opposite sign. This escamotage holds for the weak formulation but it generally fails in the discrete case. It is shown however, to provide rather accurate results in the FEM context (see [BR01, GS02]). In Fig. 3, both rows show the evolution of the meshes at the first three iterates at $V_{\mathrm{app}} = 0.9\,\mathrm{V}$. The top row refers to the control on the n-side and the meshes are those corresponding to the dual variable z_1 only, while the bottom row deals with the control on the p-side contact, respectively, and the meshes are associated with z_3.

7.2 Control of pointwise electron concentration

As second test case, we consider the control of the electron concentration at the point $(4.167, 8.638)\,\mu$m at the two biases corresponding to a forward $V_{\text{app}} = 0.7V$ and a reverse $V_{\text{app}} = -5V$. Figure 4

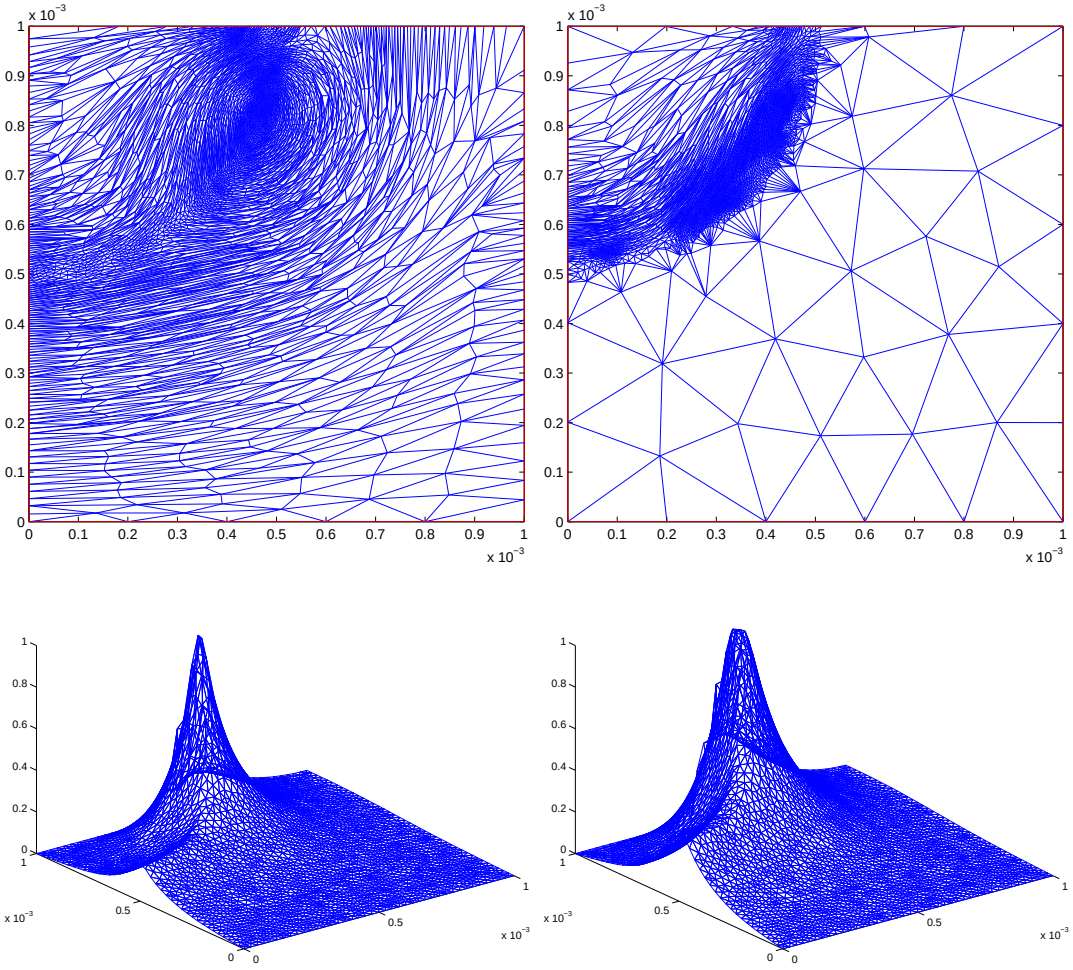

Figure 4: Control of pointwise electron concentration: sequence of meshes for $V_{\text{app}} = 0.7V$ (left) and $V_{\text{app}} = -5V$ (right) at the first iteration

shows the meshes corresponding to the dual variable z_2 at the first iteration (top row) and the corresponding plot of z_2 (bottom row). The left column refers to the forward-bias case while the right column is associated with the reverse-bias polarization.

8 Conclusions

We have dealt with a dual-based anisotropic a posteriori error estimation for the Drift-Diffusion model in semiconductors. This allows us to control suitable goal quantities via the optimal control theory where the controls are essentially the geometrical quantities describing the mesh. By an appropriate distribution and shaping of the elements we can guarantee that the error in the desired

output functional is below a given tolerance. Several open issues are in oder: the validation on other functionals and on other devices; the extension to the time-dependent problem.

References

[BBFS90] Bank, R.E., Bürgler, J.F., Fichtner, W., Smith, R.K.: Some upwinding techniques for finite element approximations of convection-diffusion equations. Numer. Math., **58**, 185–202 (1990)

[BR01] Becker, R., Rannacher, R.: An optimal control approach to a posteriori error estimation in finite element methods. Acta Numer., **10**, 1–102 (2001)

[Cia78] Ciarlet, Ph.: The Finite Element Method for Elliptic Problems. North-Holland Publishing Company, Amsterdam (1978)

[FP01] Formaggia, L., Perotto, S.: New anisotropic a priori error estimates. Numer. Math., **89**, 641–667 (2001)

[FP03] Formaggia, L., Perotto, S.: Anisotropic error estimates for elliptic problems. Numer. Math., **94**, 67–92 (2003)

[GB98] George, P.L., Borouchaki, H.: Delaunay Triangulation and Meshing - Application to Finite Elements. Editions Hermes, Paris (1998)

[GS02] Giles, M.B., Süli, E.: Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality. Acta Numer., **11**, 145–236 (2002)

[Hec98] Hecht, F.: http://www-rocq.inria.fr/gamma/cdrom/www/bamg/eng.htm (1998)

[MP04] Micheletti, S., Perotto, S.: Goal-oriented a posteriori error estimation and anisotropic mesh adaptivity for semiconductors. In preparation.

[MPP03] Micheletti, S., Perotto, S., Picasso, M.: Stabilized finite elements on anisotropic meshes: a priori error estimates for the advection-diffusion and Stokes problems. SIAM J. Numer. Anal., **41** (3), 1131–1162 (2003)

[Ned80] Nédélec, J.C.: Mixed finite elements in $\mathbb{R}^3$. Numer. Math., **35** (3), 315–341 (1980)

[Sel84] Selberherr, S.: Analysis and Simulation of Semiconductor Devices. Springer Verlag, Wien (1984)