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A Finite Element Method for the 2D Drift-Diffusion Semiconductor Model

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Abstract. Stability and convergence properties are stated for a finite element method for numerically solving the 2D drift-diffusion semiconductor device equations. The method combines a mixed finite element method for the approximation of the electric field and a discontinuous upwinding finite element method for the approximation of the electron and hole concentrations. The mixed method gives an approximate electric field in the precise form needed by the discontinuous method, which is conservative and fully parallelizable.

1. Introduction

In this paper we consider a finite element method for the 2D drift-diffusion semiconductor model

$$u_t - \operatorname{div} J_u = -\lambda^2 \alpha_u \mathcal{R}(u,p), \quad (x,y) \in \Omega, \tag{1.1a}$$

$$p_t + \operatorname{div} J_p = -\lambda^2 \alpha_p \mathcal{R}(u,p), \quad (x,y) \in \Omega, \tag{1.1b}$$

$$u = u_D, \quad (x,y) \in \partial\Omega_D, \tag{1.1c}$$

$$p = p_D, \quad (x,y) \in \partial\Omega_D, \tag{1.1d}$$

$$\partial u/\partial \nu = 0, \quad (x,y) \in \partial\Omega_N, \tag{1.1e}$$

$$\partial p/\partial \nu = 0, \quad (x,y) \in \partial\Omega_N, \tag{1.1f}$$

$$u(0,x,y) = u_{\text{init}}(x,y), \quad (x,y) \in \Omega, \tag{1.1g}$$

$$p(0,x,y) = p_{\text{init}}(x,y), \quad (x,y) \in \Omega, \tag{1.1h}$$

where $t > 0$, $\Omega = (0,1)^2$, $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ with $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ and Ω_N containing the endpoints of its segments, u and p are the (scaled) electron and hole concentrations, $\mathcal{R}$ is the carrier recombination-generation rate, λ is the normed Debye length, α_u and α_p are the lifetime-dependent constants, and J_u and J_p are the current densities

$$J_u = \mu_u(\beta)(\lambda^2 \nabla u - u\beta), \quad t > 0, \quad (x,y) \in \Omega, \tag{1.2a}$$

$$J_p = -\mu_p(\beta)(\lambda^2 \nabla p + p\beta), \quad t > 0, \quad (x,y) \in \Omega, \tag{1.2b}$$

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where β is the (scaled) negative electric field given by

$$-\operatorname{div}\beta = C - u + p, \quad t > 0, \quad (x,y) \in \Omega, \tag{1.3a}$$

$$\beta = \nabla\phi, \quad t > 0, \quad (x,y) \in \Omega, \tag{1.3b}$$

$$\phi = \phi_D, \quad t \geq 0, \quad (x,y) \in \partial\Omega_D, \tag{1.3c}$$

$$\partial\phi/\partial\nu = 0, \quad t \geq 0, \quad (x,y) \in \partial\Omega_N, \tag{1.3d}$$

with C being the (scaled) doping profile and ϕ being the (scaled) potential, and μ_u and μ_p are the field-dependent electron and hole mobilities. The numerical method considered in this paper is an extension of the finite element method introduced in [5, 6, 2, 3] for the 1D case, and combines a mixed method for a piecewise linear approximation of the electric field, $-\beta$, with an explicit upwinding method for piecewise constant approximations of the electron and hole concentrations, u and p. The reason for using the mixed finite element approximation of the electric field is that the electron and hole concentration equations (1.1a–b) depend on the potential only through this field, and the mixed method provides a better approximation of it than more standard Galerkin approaches would give [1, 7]. The motivation for including the discontinuous upwinding finite element method in approximating u and p is that, since the normed Debye length ranges from 10^{-3} to 10^{-5}, the concentration equations, while formally parabolic, are in fact more nearly hyperbolic. Thus, the upwinding method is applied to follow the transport more accurately than the standard finite difference or finite element method does. In particular, this method can capture discontinuities in the solution without producing spurious oscillations [4]. Another computational advantage of the method is its full parallelizability.

2. The Finite Element Method

Let $\{x_{i+1/2}\}_{i=0}^{n_x} \times \{y_{j+1/2}\}_{j=0}^{n_y}$ be a partition of Ω with $x_{1/2} = y_{1/2} = 0$ and $x_{n_x+1/2} = y_{n_y+1/2} = 1$, and let $\{t^n\}_{n=0}^{n_T}$ be a partition of $[0,T]$ with $t^0 = 0$ and $t^{n_T} = T$. Then, set $I_i^x = (x_{i-1/2}, x_{i+1/2})$, $I_j^y = (y_{j-1/2}, y_{j+1/2})$, $\Delta x_i = x_{i+1/2} - x_{i-1/2}$, $\Delta y_j = y_{j+1/2} - y_{j-1/2}$, $J^n = [t^n, t^{n+1})$, and $\Delta t^n = t^{n+1} - t^n$. Associated with these partitions, we introduce the spaces

$$V_h = \{v \in H(\operatorname{div};\Omega) : v|_{I_i^x \times I_j^y} = (a_{i,j}^1 + a_{i,j}^2 x, a_{i,j}^3 + a_{i,j}^4 y), \quad a_{i,j}^k \in \mathbb{R},$$
$$i = 1, \ldots, n_x,\ j = 1, \ldots, n_y, \quad v \cdot \nu|_{\partial\Omega_N} = 0\},$$

$$W_h^\phi = \{w \in L^2(\Omega) : w|_{I_i^x \times I_j^y} \in P^0(I_i^x \times I_j^y), \quad i = 1, \ldots, n_x,\ j = 1, \ldots, n_y\},$$

$$W_h = \{w \in L^\infty(\Omega) : w|_{I_i^x \times I_j^y} \in P^0(I_i^x \times I_j^y), \quad i = 1, \ldots, n_x,\ j = 1, \ldots, n_y\},$$

$$W_{\Delta t} = \{w \text{ right continuous} : w|_{J^n} \in P^0(J^n),\ n = 0, \ldots, n_T - 1\}.$$

If $v \in V_h$, then $v_{i+1/2,j}$ and $v_{i,j+1/2}$ will denote $v(x_{i+1/2}, y_j)$ and $v(x_i, y_{j+1/2})$, respectively. If $w \in W_h$, then $w_{i,j}$ represents the constant value $w(x,y)$, $(x,y) \in I_i^x \times I_j^y$. Finally, w^n will indicate the constant $w(t)$, $t \in J^n$, if $w \in W_{\Delta t}$.

Let P_h and $P_{\Delta t}$ denote the L^2-projections into W_h and $W_{\Delta t}$, respectively, and set

$$u_{\text{init},h} = P_h u_{\text{init}},$$
$$p_{\text{init},h} = P_h p_{\text{init}},$$
$$C_h = P_h C.$$

Then our numerical method is formulated as follows.

i) The electric potential and field: Find $(\beta_h, \phi_h) \in W_{\Delta t} \otimes V_h \times W_{\Delta t} \otimes W_h^{\phi}$ for $n = 0, \ldots, n_T$ such that

$$\begin{aligned} -(\operatorname{div} \beta_h^n, w) &= (C_h - u_h^n + p_h^n, w), \quad \forall w \in W_h^{\phi}, \\ (\beta_h^n, v) + (\phi_h^n, \operatorname{div} v) &= \langle \phi_D^n, v \cdot \nu \rangle_{\partial\Omega_D}, \qquad \forall v \in V_h. \end{aligned}$$

ii) The electron concentration: Find $u_h \in W_{\Delta t} \otimes W_h$ for $n = 0, \ldots, n_T - 1$, $i = 1, \ldots, n_x$, and $j = 1, \ldots, n_y$ such that

$$\begin{aligned} &\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t^n} + \frac{f_{1,i+1/2,j}^n - f_{1,i-1/2,j}^n}{\Delta x_i} + \frac{f_{2,i,j+1/2}^n - f_{2,i,j-1/2}^n}{\Delta y_j} \\ &\quad - \frac{2\lambda^2}{\Delta x_i + \Delta x_{i+1}} \left(\mu_{u,1,i+1,j}^n q_{1,i+1/2,j}^n - \mu_{u,1,i,j}^n q_{1,i-1/2,j}^n \right) \\ &\quad - \frac{2\lambda^2}{\Delta y_j + \Delta y_{j+1}} \left(\mu_{u,2,i,j+1}^n q_{2,i,j+1/2}^n - \mu_{u,2,i,j}^n q_{2,i,j-1/2}^n \right) = -\lambda^2 \alpha_u \mathcal{R}(u_{i,j}^n, p_{i,j}^n), \end{aligned}$$

where

$$\begin{aligned} f_{1,i-1/2,j}^n &= \mu_{u,1,i,j}^n \left(u_{i-1,j}^n \beta_{1,i-1/2,j}^{n^+} + u_{i,j}^n \beta_{1,i-1/2,j}^{n^-} \right), \\ f_{2,i,j-1/2}^n &= \mu_{u,2,i,j} \left(u_{i,j-1}^n \beta_{2,i,j-1/2}^{n^+} + u_{i,j}^n \beta_{2,i,j-1/2}^{n^-} \right), \\ \mu_{u,1,i,j}^n &= \mu_u \left(\beta_{i-1/2,j}^n \right), \\ \mu_{u,2,i,j}^n &= \mu_u \left(\beta_{i,j-1/2}^n \right), \\ \beta_{i-1/2,j}^n &= \left(\beta_{1,i-1/2,j}^n, \left(\beta_{2,i-1,j-1/2}^n + \beta_{2,i-1,j+1/2}^n + \beta_{2,i,j-1/2}^n + \beta_{2,i,j+1/2}^n \right) /4 \right), \\ \beta_{i,j-1/2}^n &= \left(\left(\beta_{1,i-1/2,j-1}^n + \beta_{1,i+1/2,j-1}^n + \beta_{1,i-1/2,j}^n + \beta_{1,i+1/2,j}^n \right) /4, \beta_{2,i,j-1/2} \right), \end{aligned}$$

and the function $q_h = (q_1, q_2) \in W_{\Delta t} \otimes V_{\Delta x}$ is the solution of

$$(q_h(t^n), v_h) = (u_h(t^n), \operatorname{div} v_h) + \langle u_{D,\Delta t}, v_h \cdot \nu \rangle_{\partial\Omega_D}, \quad \forall v_h \in V_h,$$

after the mass matrix has been mass-lumped. In our case, the expression for the degrees of freedom of q_h is taken as follows:

$$\begin{aligned} q_{1,i-1/2,j}^n &= (u_{i,j}^n - u_{i-1,j}^n)/\Delta x_i, \\ q_{2,i,j-1/2}^n &= (u_{i,j}^n - u_{i,j-1}^n)/\Delta y_j. \end{aligned}$$

iii) The hole concentration: Find $p_h \in W_{\Delta t} \otimes W_h$ for $n = 0, \ldots, n_T - 1$, $i = 1, \ldots, n_x$, and $j = 1, \ldots, n_y$ such that

$$\begin{aligned} &\frac{p_{i,j}^{n+1} - p_{i,j}^n}{\Delta t^n} - \frac{g_{1,i+1/2,j}^n - g_{1,i-1/2,j}^n}{\Delta x_i} - \frac{g_{2,i,j+1/2}^n - g_{2,i,j-1/2}^n}{\Delta y_j} \\ &\quad - \frac{2\lambda^2}{\Delta x_i + \Delta x_{i+1}} \left(\mu_{p,1,i+1,j}^n r_{1,i+1/2,j}^n - \mu_{p,1,i,j}^n r_{1,i-1/2,j}^n \right) \\ &\quad - \frac{2\lambda^2}{\Delta y_j + \Delta y_{j+1}} \left(\mu_{p,2,i,j+1}^n r_{2,i,j+1/2}^n - \mu_{p,2,i,j}^n r_{2,i,j-1/2}^n \right) = -\lambda^2 \alpha_p \mathcal{R}(u_{i,j}^n, p_{i,j}^n), \end{aligned}$$

where

$$g^n_{1,i-1/2,j} = \mu_{p,1,i,j}\left(p^n_{i-1,j}\beta^{n^-}_{1,i-1/2,j} + p^n_{i,j}\beta^{n^+}_{1,i-1/2,j}\right),$$
$$g^n_{2,i,j-1/2} = \mu_{p,2,i,j}\left(p^n_{i,j-1}\beta^{n^-}_{2,i,j-1/2} + p^n_{i,j}\beta^{n^+}_{2,i,j-1/2}\right).$$

Similar expressions hold for $\mu_{p,1,i,j}$ and $\mu_{p,2,i,j}$, and the function $r_h = (r_1, r_2) \in W_{\Delta t} \otimes V_{\Delta x}$ is similarly computed (after mass-lumped) in the form

$$r^n_{1,i-1/2,j} = (p^n_{i,j} - p^n_{i-1,j})/\Delta x_i,$$
$$r^n_{2,i,j-1/2} = (p^n_{i,j} - p^n_{i,j-1})/\Delta y_j.$$

iv) The Neumann boundary conditions in (1.1e–f) are imposed by the reflection principle:

$$\pi_{i,j-1} = \pi_{i,j} \quad \text{if } (x_i, y_{j-1}) \text{ or } (x_i, y_j) \in \partial\Omega_N,\ \pi = u, p,$$
$$\pi_{i-1,j} = \pi_{i,j} \quad \text{if } (x_{i-1}, y_j) \text{ or } (x_i, y_j) \in \partial\Omega_N,\ \pi = u, p.$$

On $\partial\Omega_D$, we have

$$\pi_{D,\Delta t,i,j} = P_{\Delta t}\pi_D(x_i, y_j) \quad \text{if } (x_i, y_j) \in \partial\Omega_D,\ \pi = u, p.$$

We remark that it follows from the definition of V_h that the elements in V_h have continuous normal components on interelements edges. Thus, the numerical fluxes $f^n_{1,i-1/2,j}$, $f^n_{2,i,j-1/2}$, $g^n_{1,i-1/2,j}$, and $g^n_{2,i,j-1/2}$ are all well defined.

3. Stability and Convergence

Stability and convergence properties for the numerical method of the previous section will be stated only in case of $\partial\Omega_D = \emptyset$; i.e., we only consider the Neumann boundary conditions. It turns out that the standard approach used in the 1D case [5, 6, 2, 3] cannot be extended to the 2D case if the Dirichlet boundary conditions are included. The reason for this is that the numerical electric field, on which the flux operators in (1.1a–b) depend globally, does not have the required smoothness in the proof of the stability and convergence properties. Thus, new techniques will be needed in the case of Dirichlet boundary conditions. This will be for future work.

It is assumed that C is constant and that

(3.1a) $$u_{\text{init}}(x, y) \in [0, u^\star],\ p_{\text{init}}(x, y) \in [0, p^\star], \quad (x, y) \in \Omega,$$

(3.1b) $$\nabla u_{\text{init}},\ \nabla p_{\text{init}} \in (L^\infty(\Omega))^2.$$

THEOREM 3.1 (STABILITY). *Assume that* (3.1) *and the following hypothesis are satisfied:*

(3.2) $$u^\star = C + p^\star.$$

Then there is a constant $Q_1 = Q_1(u^\star, p^\star, C, \alpha_u, \alpha_p)$ *such that if for* $n = 0, \ldots, n_T - 1$ *the following* CFL *condition is satisfied:*

(3.3) $$\Delta t^n \le Q_1 \left(\frac{1}{\Delta x_i} + \frac{1}{\Delta y_j} + \frac{\lambda^2}{\Delta x_i \Delta y_j}\right)^{-1},$$

we have

$$u_h(t,x,y) \in [0,u^*], \qquad (t,x,y) \in [0,T] \times \Omega, \tag{3.4a}$$

$$p_h(t,x,y) \in [0,p^*], \qquad (t,x,y) \in [0,T] \times \Omega. \tag{3.4b}$$

Moreover, there exists a constant Q_2 independent of h such that

$$||\beta_h||_{L^\infty(0,T;L^\infty(\Omega))} \leq Q_2, \tag{3.5a}$$

$$||\operatorname{div} \beta_h||_{L^\infty(0,T;L^1(\Omega))} \leq Q_2. \tag{3.5b}$$

We denote below by $(v_h, q_h, \sigma_h, \psi_h)$ the approximate solution $(u_h, p_h, \beta_h, \phi_h)$ of (1.1)–(1.3) with u_{init} and p_{init} replaced by v_{init} and q_{init}, respectively.

THEOREM 3.2 (CONTINUITY WITH RESPECT TO THE INITIAL DATA). *Suppose that the hypotheses of Theorem* 3.1 *are satisfied for both sets of data. Then,*

$$||u_h(t) - v_h(t)||_{L^\infty(\Omega)} + ||p_h(t) - q_h(t)||_{L^\infty(\Omega)} \leq Q_3 \left(||u_{\text{init}} - v_{\text{init}}||_{L^\infty(\Omega)} + ||p_{\text{init}} - q_{\text{init}}||_{L^\infty(\Omega)} \right),$$

with Q_3 independent of h.

THEOREM 3.3 (CONVERGENCE). *Assume that the hypotheses of Theorem* 3.1 *are satisfied. Then, the numerical sequence $\{(u_h, p_h, \beta_h, \phi_h)\}_{h>0}$ converges in $L^\infty(0,T;L^\infty(\Omega)) \times L^\infty(0,T;L^\infty(\Omega)) \times L^\infty(0,T;H(\operatorname{div};\Omega)) \times L^\infty(0,T;BV(\Omega))$ to the unique solution of the equations* (1.1)–(1.3).

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