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FINITE ELEMENT SOLUTION OF A NONLINEAR DIFFUSION PROBLEM WITH A MOVING BOUNDARY

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In recent years two-dimensional process simulators for modelling and simulation in the design of VLSI semiconductor devices have appeared (see, e.g., Maldonado [2]). The underlying mathematical problem consists in solving numerically the following boundary value problem:

$$(1)\qquad \frac{\partial u}{\partial t} = \nabla.[D(u)\nabla u] \text{ in } \Omega(t),\ 0 < t < T,$$
$$\Omega(t) = \{(x,y) \mid \varphi(y,t) < x < L_0,\ 0 < y < B\},$$

$$(2)\qquad \frac{\partial u}{\partial n}\Big|_{\partial\Omega(t)-\Gamma(t)} = 0,\ 0 < t < T,\ \Gamma(t) = \{(x,y) \mid x = \varphi(y,t),$$
$$0 < y < B\},$$

$$(3)\qquad D(u)\frac{\partial u}{\partial n} = \gamma\dot{\varphi}_n u \text{ on } \Gamma(t),\ 0 < t < T,$$

$$(4)\qquad u(x,y,0) = u^*(x,y) \text{ in } \Omega(0).$$

Here u is the unknown concentration of an impurity, $D(u)$ is the concentration dependent diffusion coefficient ($0 < d_0 \le D(u) \le d_0^{-1}\ \forall u \ge 0$), $\varphi(y,t)$ is a given function ($0 \le \varphi \le \frac{1}{2}L_0$), $\frac{\partial u}{\partial n}$ is the derivative in the direction of the outward normal, γ is constant, $\dot{\varphi}_n$ is the rate of the motion of $\Gamma(t)$ in the direction of the outward normal and u^* is the given initial concentration.

If u is a sufficiently smooth solution of (1) - (4) (we remark that we do not know any result from which existence of a solution of (1) - (4) follows), then by multiplying (1) by $v \in H^1(\Omega(t))$ and integrating over $\Omega(t)$ we get

$$(5)\qquad \forall t \in (0,T)\ \left(\frac{\partial u}{\partial t}, v\right)_{L^2(\Omega(t))} + a(u,t;u,v) = 0\ \ \forall v \in V(t) \equiv H^1(\Omega(t));$$

here

$$a(w,t;u,v) = \int_{\Omega(t)} D(w)\nabla u.\nabla v\,dxdy - \gamma\int_{\Gamma(t)} \dot{\varphi}_n uv\,dxdy.$$

We use (5) for defining the semidiscrete solution. First we construct a suitable moving triangulation of $\bar{\Omega}(t)$. We consider the one-to-one mapping of the rectangle $\bar{Q} = \langle 0,L_0\rangle \times \langle 0,B\rangle$ on $\bar{\Omega}(t)$:

$$(6)\qquad x = F(\alpha,\beta,t) \equiv \varphi(\beta,t) + \alpha[1-L_0^{-1}\varphi(\beta,t)],\quad y = \beta.$$

We cover $\bar{\Omega}(0)$ by triangles completed along $\Gamma(0)$ by curved elements in a manner described in Zlámal [4]. Let $P_k = (x_k,y_k)$, $k = 1,\ldots,d$, be the nodes of this triangulation and let $Q_k = (\alpha_k, \beta_k)$ be their inverse immages in the mapping (6), i.e.

$$\alpha_k = \frac{x_k - \varphi(\beta_k, 0)}{1 - L_0^{-1}\varphi(\beta_k, 0)}, \quad \beta_k = y_k .$$

The triangulation $T(t)$ of $\bar{\Omega}(t)$ is determined for $t > 0$ by the nodes $P_k(t) = (x_k(t), y_k)$, $x_k(t) = F(\alpha_k, \beta_k, t)$. The elements of $T(t)$ are again triangles or curved elements. As shape functions we use linear polynomials. We denote by $V_h(t) \subset H^1(\Omega(t))$ the set of all trial functions and by $w_k(x,y,t)$, $k = 1,\dots,d$, the basis functions of $V_h(t)$.

The semidiscrete solution is assumed in the form

$$U(x,y,t) = \sum_{k=1}^{d} U_k(t) w_k(x,y,t)$$

and determined by

$$\text{(7)} \qquad \forall t \in (0,T) \ \left(\frac{\partial}{\partial t} U, v\right)_{L^2(\Omega(t))} + a(U,t;U,v) = 0 \quad \forall v \in V_h(t),$$
$$U(x,y,0) = U^*(x,y) .$$

$U^* \in V_h(0)$ is a suitable approximation of u^*.

If we denote by $\underline{U}(t)$ the d-dimensional vector $(U_1(t),\dots, U_d(t))^T$ by $M(t)$, $R(t)$ and $K(U,t)$ the $d \times d$ matrices

$$M(t) = \{(w_j, w_k)_{L^2(\Omega(t))}\}_{j,k=1}^{d}, \quad R(t) = \{(w_j, \frac{\partial w_k}{\partial t})_{L^2(\Omega(t))}\}_{j,k=1}^{d},$$
$$K(U,t) = \{a(U,t;w_j,w_k)\}_{j,k=1}^{d} ,$$

then the matrix form of (7) is

$$\text{(8)} \qquad M(t)\dot{\underline{U}} + [R(t) + K(U,t)]\underline{U} = \underline{0} ,$$
$$\underline{U}(0) = \underline{U}^* .$$

Here $\dot{\underline{U}} = \frac{d}{dt}\underline{U}$ and the matrices M and K are standard mass and stiffness matrices, respectively. The matrix R is unsymmetric.

We discretize (8) in time. For simplicity, we use a uniform partition of $\langle 0,T \rangle$: $t_i = i\Delta t$, $i = 0,1,\dots,q$. In the sequal $\underline{U}^i$, $M^i,\dots$ means $\underline{U}(t_i)$, $M(t_i),\dots$. Now we set $t = t_{i+1}$ in (8), replace $\dot{\underline{U}}^{i+1}$ by $\Delta t^{-1}\Delta\underline{U}^i$, $\Delta\underline{U}^i = \underline{U}^{i+1} - \underline{U}^i$, and linearize the nonlinear term in (8). We get

$$\text{(9)} \qquad M^{i+1}\Delta\underline{U}^i + \Delta t[R^{i+1} + K(\tilde{U}^i, t_{i+1})]\underline{U}^{i+1} = \underline{0}, \quad \tilde{U}^i = \sum_{k=1}^{d} U_k^i w_k^{i+1},$$
$$\underline{U}^0 = \underline{U}^* .$$

For practical computations it is necessary to do one more step: to replace curved elements by triangles and to compute all matrices numerically. Also, we could apply the Crank-Nicholson approach for solving (8) or, more generally, the θ-method. We have restricted ourselves to justify the procedure defined by (9).

We consider a family $\{T_h^0\}$ of triangulations of $\bar{\Omega}^0$ from which a family $\{T_h(t)\}$ of the triangulations of $\bar{\Omega}(t)$ is constructed as described above. Let h_{K0} be the greatest side of an element $K^0 \in T_h^0$ and

$$h = \max_{K^0 \in T_h^0} h_{K0}.$$

We consider a family $\{T_h^0\}$ such that $h \to 0$ and the minimum angle condition is satisfied. We have proved the following main results:

1. Let

$$b(w,t;v,v) \geq 0 \quad \forall v \in V(t),\ t \in (0,T)$$

where

$$b(w,t;u,v) = a(w,t;u,v) - \frac{1}{2} \int_{\Gamma(t)} \dot{\varphi}_n uv d\Gamma .$$

Then for Δt sufficiently small, $\Delta t \leq \Delta t_0$ where Δt_0 does not depend on h and on the index i, the matrices $M^{i+1} + \Delta t(R^{i+1} + K(\tilde{U}^i, t_{i+1})]$, $i = 0,\dots,q-1$, of the systems (9) are regular so that U^i, $i = 1,\dots,q$ are uniquely determined. Furthermore, the scheme (9) is unconditionally stable in the L^2-norm, i.e. for $\Delta t \leq \Delta t_0$ we have

$$(10) \qquad \max_{1 \leq i \leq q} \|U^i\|_{L^2(\Omega^i)} \leq C\|U^0\|_{L^2(\Omega^0)}$$

where C does not depend on Δt and on h.

2. Let the form b be uniformly V(t)-elliptic, i.e.

$$b(w,t;v,v) \geq b_0 \|v\|^2_{H^1(\Omega(t))} \qquad \forall v \in V(t),\ t \in (0,T)$$

and let $\dot{\varphi}_n \leq 0$. Then for Δt sufficiently small, $\Delta t \leq \Delta t_0$ where Δt_0 does not depend on h, there holds

$$(11) \qquad \max_{1 \leq i \leq q} \|u^i - U^i\|_{L^2(\Omega^i)} + \{\Delta t \sum_{i=1}^{q} \|u^i - U^i\|_{H^1(\Omega^i)}\}^{1/2} \leq$$

$$\leq C(\|u^0 - U^0\|_{L^2(\Omega^0)} + h + \Delta t) .$$

The proof starts from the variational formulation

$$(12) \qquad \begin{cases} (U^{i+1} - \tilde{U}^i, v)_{L^2(\Omega^{i+1})} - \Delta t(\frac{\partial U^{i+1}}{\partial x}, G^{i+1}v)_{L^2(\Omega^{i+1})} + \Delta t a(\tilde{U}^i, t_{i+1}; \\ \qquad U^{i+1}, v) = 0 \\ \qquad \forall v \in V_h^{i+1},\ i = 0,\dots,q-1, \\ U^0 = U^* . \end{cases}$$

Here G is a computable function defined on each element by means of the map which maps uniquely this element on the reference one. From (12) the existence and an unconditional stability of the scheme can be proved. The error estimating is based on the Ritz approximation $\zeta \in V_h(t)$ defined by

$$d(u,t;u-\zeta,v) = 0 \quad \forall v \in V_h(t)$$

where $d(w,t;u,v) = b(w,t;u,v) - \frac{1}{2}\int_{\Gamma(t)}\phi_n uv d\Gamma$. $u - \zeta$ is estimated using a technique which in a case that the boundary does not move is essentially that of Wheeler [3], Dupont, Fairweather, Johnson [1] and Zlámal [5]. Instead of estimating $\frac{\partial}{\partial t}(u-\zeta)$ we estimate $D_t(u-\zeta)$ where the operator D_t is defined by $D_t = G\frac{\partial}{\partial x} + \frac{\partial}{\partial t}$. If the boundary does not move, $G = 0$ and $D_t = \frac{\partial}{\partial t}$.

R e f e r e n c e s

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