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SIMULATION OF THE TRANSIENT BEHAVIOR OF A ONE-DIMENSIONAL SEMICONDUCTOR DEVICE

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ABSTRACT: *A numerical method based on treating the potential by mixed finite elements and the electron and hole density equations by a finite element version of a modification of the method of characteristics is introduced to simulate the transient behavior of a semiconductor device. Error estimates are derived for a single space variable model.*

KEY WORDS: Semiconductor simulation • mixed finite elements • modified method of characteristics

RESUMO: *Para simular o comportamento de um semicondutor não estacionário, apresenta-se um método numérico, no qual o potencial é tratado via um método dos elementos finitos mistos e as concentrações de electrons e "holes" via uma modificação do método das características. Estimativas de erros são deduzidas para o modelo unidimensional.*

PALAVRAS-CHAVE: Simulação de semicondutores • elementos finitos mistos • método modificado das características

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1. INTRODUCTION

A model [1,5,6,7,10] for the transient behavior of a semiconductor device occupying a region $\Omega \subset \mathbf{R}^n$ consists of three quasilinear partial differential equations, one formally of elliptic type for the electric potential and two formally of parabolic type arising from the conservation of electron and hole concentrations, along with relevant initial and boundary data. The equation for the potential ψ is the Maxwell equation,

$$\nabla\cdot\tilde{q} = -\nabla\cdot(\epsilon\nabla\psi) = \rho \ , \tag{1.a}$$

relating the total space charge ρ to the divergence of the electric field

$$\tilde{q} = -\epsilon\nabla\psi \ . \tag{1.b}$$

The function ρ is given by

$$\rho = Q(e-p-c) \quad , \tag{2}$$

where Q is the electric charge, to be assumed constant in this paper, e and p are, respectively, the electron and hole concentrations or densities, and c is the total electric active net impurity concentration (i.e. the doping).

The electric field $\tilde{q}$ and the carrier densities are related through the current densities J_e and J_p, which are given by

$$J_e = Q\mu_e e\tilde{q} + QD_e\nabla e \quad , \tag{3.a}$$

$$J_p = Q\mu_p p\tilde{q} - QD_p\nabla p \quad , \tag{3.b}$$

where μ_e and μ_p are the electron and hole mobilities and D_e and D_p corresponding diffusion coefficients. Conservation of electrons and holes then gives the equations

$$\partial e/\partial t - \nabla\cdot J_e = R(e,p) \quad , \tag{4.a}$$

$$\partial p/\partial t + \nabla\cdot J_p = R(e,p) \quad , \tag{4.b}$$

where R(e,p) is the recombination rate.

In this paper we shall consider ϵ, μ_e, μ_p, D_e, and D_p to be constants. We shall also assume that the diffusion coefficients are related to the mobilities through the Einstein relations

$$D_s = U_T\mu_s \ , \quad s = e \text{ or } p \quad , \tag{5}$$

where U_T is the thermal voltage.

It is helpful to normalize the equations (1) and (4) into dimensionless form. Let [6,7,10]

$$\psi = U_T\tilde{\psi}, \quad e = n_i\tilde{e}, \quad p = n_i\tilde{p}, \quad c = n_i\tilde{c} \quad ,$$

$$x_j = L\tilde{x}_j \ (j=1,\ldots n), \quad t = \tau\tilde{t} \quad .$$

The characteristic length $L = \operatorname{diam}(\Omega)$ is about 5×10^{-4} cm, the intrinsic density n_i is about 10^{10} cm^{-3}, and τ is about 10^{-8} sec. If the equations are first written in terms of the barred quantities and then the bar dropped, the equations take the form

$$\nabla\cdot\tilde{q} = -\Delta\psi = z(e-p-c) \ , \tag{6.a}$$

$$\partial e/\partial t - D_e\tilde{q}\cdot\nabla e - D_e\Delta e - zD_e e(e-p-c) = R(e,p) \ , \tag{6.b}$$

$$\partial p/\partial t + D_p\tilde{q}\cdot\nabla p - D_p\Delta p + zD_p p(e-p-c) = R(e,p) \ , \tag{6.c}$$

where z is a constant.

Note that (6.b) and (6.c) depend explicitly on the field $\tilde{q}$, but not on the potential ψ. This suggests the selection of a numerical method for (6.a) that gives a direct approximation of $\tilde{q}$, such as a mixed finite element method. The equations for e and p, while formally parabolic, are in fact dominated by the convection terms, and it is well known that standard finite difference or Galerkin methods are not effective choices for such equations. Systems having quite analogous properties occur in the simulation of miscible displacement techniques in petroleum reservoirs, and our choice of a numerical method for (6) will be based on research by Douglas, Ewing, Russell, and Wheeler on that problem.

A mixed finite element method will be employed to approximate $\tilde{q}$ and ψ, while a Galerkin form of a modified method of characteristics will be used to approximate e and p. See Douglas and Russell [3] for a discussion of the modified method of characteristics procedure and Douglas [2], Ewing, Russell, and Wheeler [4], and Russell [8] for treatments of the miscible displacement problem by the combination of these techniques.

In this paper we shall confine ourselves to the single space variable problem and to Dirichlet boundary conditions. Let $\Omega = [0,1]$, and let

$$\psi(0,t) = r_0(t), \quad \psi(1,t) = r_1(t) , \tag{7.a}$$

$$e(0,t) = f_0(t), \quad e(1,t) = f_1(t) , \tag{7.b}$$

$$p(0,t) = g_0(t), \quad p(1,t) = g_1(t) , \tag{7.c}$$

and

$$e(x,0) = e^0(t), \quad p(x,0) = p^0(t) . \tag{7.d}$$

In Section 2 we define a modified method of characteristics procedure for e and p. In Section 3 a mixed finite element method is introduced for $\tilde{q}$ and ψ, and certain estimates relating the errors in $\tilde{q}$ and ψ to those in e and p will be derived. In Section 4 L^2 estimates will be carried out for the errors in the electron and hole densities, along with the completion of the analysis of the approximation of the field.

Singularities in the solution of the differential equations that arise in two or three space variables as a result of the shape of the domain or the changing of form of the boundary conditions from Dirichlet to Neumann are avoided in the single space variable case. Clearly, this reduction in dimension leads to a limitation to the generality of the practicality of the analysis of the numerical method, but the primary purpose of the paper is to introduce the method in a relatively simple situation and to justify it there. Higher dimensional work will be reported elsewhere.

Throughout this paper the solution of (6)-(7) will be assumed smooth, so that optimal order accuracy is possible. The precise regularity needed will be clear from the convergence arguments.

2. A MODIFIED METHOD OF CHARACTERISTICS APPROXIMATION FOR THE ELECTRON AND HOLE DENSITIES

The modified method of characteristics procedure [3,8] has as its basic idea the interpretation of the first order parts of (6.b) and (6.c) as directional derivatives. Various spatial and time discretizations can be applied to the resulting equations; we shall discretize in space by a Galerkin method and in time by backward differencing.

Let $\tau_e = \tau_e(x,t)$ be the unit vector in the direction $(-D_e q,1)$ and τ_p the unit vector in the direction $(D_p q,1)$. Set $\phi_\alpha = [1 + D_\alpha{}^2 q^2]^{1/2}$ for $\alpha = e$ or p. Then the characteristic derivatives in the τ_α directions are given by

$$\phi_e \partial/\partial\tau_e = \partial/\partial t - D_e q\, \partial/\partial x , \tag{8.a}$$

$$\phi_p \partial/\partial\tau_p = \partial/\partial t + D_p q\, \partial/\partial x , \tag{8.b}$$

so that (6) can be written in the form

$$\partial q/\partial x = -\partial^2\psi/\partial x^2 = z(e-p-c) , \tag{9.a}$$

$$\phi_e \partial e/\partial\tau_e - D_e \partial^2 e/\partial x^2 - zD_e e(e-p-c) = R(e,p) , \tag{9.b}$$

$$\phi_p \partial p/\partial\tau_p - D_p \partial^2 p/\partial x^2 + zD_p p(e-p-c) = R(e,p) , \tag{9.c}$$

for $x \in \Omega = [0,1]$ and $t \in J = [0,T]$. The weak forms of (9.b) and (9.c) that we employ in our Galerkin scheme are given by testing the equations against $H_0{}^1(\Omega)$. Thus, we begin from

$$(\phi_e \partial e/\partial\tau_e, \zeta) + (D_e \partial e/\partial x, \partial\zeta/\partial x) - (zD_e e(e-p-c), \zeta) = (R,\zeta) , \tag{10.a}$$

$$(\phi_p \partial p/\partial\tau_p, \zeta) + (D_p \partial p/\partial x, \partial\zeta/\partial x) + (zD_p p(e-p-c), \zeta) = (R,\zeta) , \tag{10.b}$$

for $\zeta \in H_0{}^1(\Omega)$.

Partition J into subintervals $[t^{m-1},t^m], t^m = m\Delta t,\ \Delta t = T/N$. Partition Ω into subintervals $[x_{i-1},x_i]$, $0 = x_0 < x_1 < \ldots < x_k = 1$, with $\max(x_i - x_{i-1}) = h_d$. Let $P_j(E)$ indicate the class of restrictions of polynomials of degree not greater than j to the set E. Then, let

$$Z_h = \{\zeta \in C^0(\Omega):\zeta|_{[x_{i-1},x_i]} \in P_1([x_{i-1},x_i])\} . \tag{11}$$

We shall seek approximations e_h^m and p_h^m in Z_h to $e^m = e(\cdot,t^m)$ and p^m, $m = 0,\ldots,N$. We shall denote the approximations to q^m and ψ^m by q_h^m and ψ_h^m; they will lie in different spaces, to be discussed in the next section.

Consider the approximation of $\phi_e \partial e/\partial\tau_e$, which we make by backward differencing along the tangent to the τ_e-characteristic at (x,t^m). Follow this tangent back in time until it intersects $(\Omega\times\{t^{m-1}\}) \cup (\partial\Omega\times[t^{m-1},t^m])$ at a point $(\tilde{x}_e^m(x),t^m - \tilde{\Delta t}_e^m(x))$, so that

$$\tilde{x}_e^m = \tilde{x}_e^m(x) = x + D_e q(x,t^m)\tilde{\Delta t}_e^m(x) , \tag{12.a}$$

where

$$\tilde{\Delta t}_e^m = \tilde{\Delta t}_e^m(x) = \begin{cases} -x/D_e q(x,t^m), & \text{if } x + D_e q(x,t^m)\Delta t < 0 , \\ (1-x)/D_e q(x,t^m), & \text{if } x + D_e q(x,t^m)\Delta t > 1 , \\ \Delta t & , \text{otherwise} . \end{cases} \tag{12.b}$$

Then,

$$(\phi_e \partial e/\partial\tau_e)(x,t^m) \tag{12.c}$$

$$\approx \phi_e(x,t^m)[e(x,t^m) - e(\tilde{x}_e^m,t^m - \tilde{\Delta t}_e^m)]/[(x-\tilde{x}_e^m)^2 + (\tilde{\Delta t}_e^m)^2]^{1/2}$$

$$= [e(x,t^m) - e(\tilde{x}_e^m,t^m - \tilde{\Delta t}_e^m)]/\tilde{\Delta t}_e^m .$$

Note that, if $\tilde{\Delta t}_e^m < \Delta t$, then $(\tilde{x}_e^m,t^m - \tilde{\Delta t}_e^m)$ lies on $\partial\Omega$ and $e(\tilde{x}_e^m,t^m-\tilde{\Delta t}_e^m)$ is evaluated using the boundary value specification.

Similarly, let

$$\tilde{x}_p^m = x - D_p q(x,t^m)\tilde{\Delta t}_p^m , \tag{13.a}$$

$$\tilde{\Delta t}_p^m = \begin{cases} x/D_p q(x,t^m), & \text{if } x - D_p q(x,t^m)\Delta t < 0 , \\ (x-1)/D_p q(x,t^m), & \text{if } x - D_p q(x,t^m)\Delta t > 1 , \\ \Delta t & , \text{otherwise} \end{cases} \tag{13.b}$$

$$(\phi_p \partial p/\partial\tau_p)(x,t^m) \approx [p(x,t^m) - p(\tilde{x}_p^m,t^m - \tilde{\Delta t}_p^m)]/\tilde{\Delta t}_p^m . \tag{13.c}$$

Since the function $q(x,t^m)$ will have to be approximated, we cannot evaluate $\tilde{x}_e^m$ and $\tilde{x}_p^m$. So, let $\hat{x}_e^m$, $\hat{\Delta t}_e^m$, $\hat{x}_p^m$, and $\hat{\Delta t}_p^m$ be defined by the corresponding relations when $q(x,t^m)$ is replaced by $q_h^{m-1}(x)$; note that the time level has been moved back to a level at which q_h will already have been computed.

Let e_h^0 and p_h^0 lie in Z_h and approximate $e(x,0)$ and $p(x,0)$, respectively. Then, for $m \geq 1$, let $\hat{e}_h^{m-1}(x) = e_h(\hat{x}_e^m(x),t^m - \hat{\Delta t}_e^m)$ and $\hat{p}_h^{m-1}(x) = p_h(\hat{x}_p^m(x),t^m - \hat{\Delta t}_p^m)$, and let

$$([e_h^m - \hat{e}_h^{m-1}]/\hat{\Delta t}_e^m,\zeta) + (D_e \partial e_h^m/\partial x,\partial\zeta/\partial x) \tag{14.a}$$

$$-(zD_e e_h^m(\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m),\zeta) = (\hat{R}^{m-1},\zeta), \quad \zeta \in Z_h ;$$

$$([p_h^m - \hat{p}_h^{m-1}]/\hat{\Delta t}_p^m,\zeta) + (D_p \partial p_h^m/\partial x,\partial\zeta/\partial x) \tag{14.b}$$

$$+(zD_p p_h^m(\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m),\zeta) = (\hat{R}^{m-1},\zeta), \quad \zeta \in Z_h ,$$

where $\hat{R}^{m-1} = R(\hat{e}_h^{m-1},\hat{p}_h^{m-1})$. The boundary values (7) must be imposed on e_h and p_h on $\partial\Omega$; this affects both the values of e_h^m and p_h^m on $\partial\Omega$ and those of $\hat{e}_h^{m-1}$ and $\hat{p}_h^{m-1}$ at the points for which $\hat{x}_e^m$ or $\hat{x}_p^m$ lies on $\partial\Omega$.

For later convenience, let

$$\phi_{e,h}\ \partial e^m/\partial\tau_{e,h} = \partial e^m/\partial t - D_e q_h^{m-1}\partial e^m/\partial x ,$$

$$\phi_{p,h}\ \partial p^m/\partial\tau_{p,h} = \partial p^m/\partial t + D_p q_h^{m-1}\partial p^m/\partial x .$$

3. A MIXED METHOD APPROXIMATION OF THE POTENTIAL

Mixed finite element methods are known to be very effective techniques for approximating the vector fields associated with the scalar solutions of elliptic problems. We shall use a rather simple technique here to approximate q and ψ simultaneously. Write (9.a) in the form

$$q + \psi' = 0 , \qquad x \in \Omega , \; t \in J , \tag{15.a}$$

$$q' = z(e-p-c) , \quad x \in \Omega , \; t \in J , \tag{15.b}$$

$$\psi = r , \qquad x \in \partial\Omega, \; t \in J . \tag{15.c}$$

Then, if (15.c) is tested against a function in $H^1(\Omega)$ and (15.b) against one in $L^2(\Omega)$, we find the mixed weak form

$$(q,v) - (v',\psi) = -rv\big|_0^1 , \qquad v \in H^1(\Omega) , \tag{16.a}$$

$$(q',w) = (z(e-p-c),w) , \quad w \in L^2(\Omega) . \tag{16.b}$$

Let Ω be partitioned into subintervals $[y_{i-1},y_i]$, $0 = y_0 < y_1 < \dots < y_L = 1$, with $\max(y_i - y_{i-1}) = h_q$. Let

$$V_h = \{v \in C^0(\Omega): v\big|_{[y_{i-1},y_i]} \in P_1([y_{i-1},y_i])\} , \tag{17.a}$$

$$W_h = \{w: w\big|_{[y_{i-1},y_i]} \in P_0([y_{i-1},y_i])\} . \tag{17.b}$$

Then for $m = 0,\dots,N$, find $\{q_h,\psi_h\} \in V_h \times W_h$ such that

$$(q_h^m,v) - (v',\psi_h^m) = r_0^m\, v(0) - r_1^m\, v(1), \; v \in V_h , \tag{18.a}$$

$$((q_h^m)',w) = (z\,(e_h^m - p_h^m - c^m),w) , \quad w \in W_h . \tag{18.b}$$

Let us note that our computational algorithm is now complete. First, e_h^0 and p_h^0 can be taken either as e^0 and p^0 or as their piecewise-linear interpolant. Then, given $\{e_h^m,p_h^m\}$, (18) can be used to evaluate $\{q_h^m,\psi_h^m\}$. Then, (14) can be used to advance e_h and p_h to time level t^{m+1}.

The error in the approximation of q and ψ can be considered to come from two sources. Let $\{Q_h^m,\Psi_h^m\} \in V_h \times W_h$ satisfy

$$(Q_h^m,v) - (v',\Psi_h^m) = r_0^m\, v(0) - r_1^m\, v(1), \quad v \in V_h, \tag{19.a}$$

$$((Q_h^m)',w) = (z(e^m - p^m - c^m),w), \qquad w \in W_h, \tag{19.b}$$

i.e., $\{Q_h^m,\Psi_h^m\}$ is the mixed method approximation for the exact right hand side. Then,

$$((q_h^m - Q_h^m)',w) = (z[(e_h^m - e^m) - (p_h^m - p^m)],w), \quad w \in W_h . \tag{20}$$

Three estimates are useful. First, if $w = (q_h^m - Q_h^m)'$, then we see that

$$\| (q_h^m - Q_h^m)'\|_0 \le z[\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0] . \tag{21}$$

Next, let $\max\{(q_h^m - Q_h^m)'\} = \pm(q_h^m - Q_h^m)'([y_{i-1},y_i])$. Then, choose $w = \mathrm{sgn}(q_h^m - Q_h^m)'$ on $[y_{i-1},y_i]$ and equal to zero elsewhere. Then, it follows easily that

$$\| (q_h^m - Q_h^m)'\|_{0,\infty} \le z(y_i - y_{i-1})^{-1/2}[\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0] \tag{22}$$

$$\le Mzh_q^{-1/2}[\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0] ,$$

provided that the partition $\{y_i\}$ is quasi-regular:

$$\min(y_i - y_{i-1}) \ge \text{const. } h_q . \tag{23}$$

Finally, if (18.a) and (19.a) are differenced and the test function v is taken to be identically one, it follows that the mean value of $q_h^m - Q_h^m$ is zero, so that (21) implies that

$$\| q_h^m - Q_h^m\|_{0,\infty} \le z[\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0] . \tag{24}$$

Now, consider $q^m - Q_h^m$. Let $\Pi_h : H^1(\Omega) \to V_h$ denote piecewise-linear interpolation; i.e., $(q - \Pi_h q)(y_i) = 0$, $i = 0,\dots,L$. Note that

$$((q - \Pi_h q)',w) = 0, \quad w \in W_h , \tag{25}$$

and recall that

$$\| q - \Pi_h q \|_{0,p} \le M \| q \|_{2,p} h_q^2 \tag{26}$$

Since

$$(\Pi_h q, v) - (v', P_h\psi) = -rv|_0^1 + (\Pi_h q - q, v), \quad v \in V_h , \tag{27.a}$$

$$((\Pi_h q)', w) = (z[e-p-c], w) , \quad w \in W_h , \tag{27.b}$$

it follows that (with the time level t^m understood)

$$(Q_h - \Pi_h q, v) - (v', \Psi_h - P_h\psi) = (q - \Pi_h q, v) , \quad v \in V_h , \tag{28.a}$$

$$((Q_h - \Pi_h q)', w) = 0 , \quad w \in W_h . \tag{28.b}$$

An immediate consequence of (28.b) is that

$$(Q_h - \Pi_h q)' \equiv 0 \text{ or } Q_h - \Pi_h q \equiv \delta, \text{ a constant} . \tag{29}$$

If we then select $v = Q_h - \Pi_h q$ and $w = \Psi_h - P_h\psi$, we see that

$$\| Q_h - \Pi_h q\|_0 \le \| q - \Pi_h q\|_0 \le M\| q\|_2 h_q^2 , \tag{30}$$

so that

$$\delta = \| Q_h - \Pi_h q\|_{0,\infty} = \| Q_h - \Pi_h q\|_0 \le M\| q\|_2 h_q^2. \tag{31}$$

Thus,

$$\| q - Q_h \|_{0,\infty} \le \| q - \Pi_h q\|_{0,\infty} + \| \Pi_h q - Q_h\|_{0,\infty} \le M \| q\|_{2,\infty} h_q^2 . \tag{32}$$

Also, from (29),

$$\| (q - Q_h)' \|_{0,\infty} \le \| (q - \Pi_h q)' \|_{0,\infty} \le M\| q\|_{2,\infty} h_q . \tag{33}$$

If we combine (24) and (32) and then (22) and (33), we find that

$$\| q^m - q_h^m\|_{0,\infty} \le z\{\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0 \} + M\| q^m\|_{2,\infty} h_q^2 , \tag{34.a}$$

$$\| (q^m - q_h^m)'\|_{0,\infty} \le Mzh_q^{-1/2}\{\| e^m - e_h^m\|_0 + \| p^m - p_h^m\|_0\} + M\| q^m\|_{2,\infty} h_q . \tag{34.b}$$

An error estimate for $\psi - \psi_h$ can be derived in terms of $e - e_h$ and $p - p_h$ in like manner; since it will not enter into the consideration of the errors in the electron and hole densities, we shall omit this estimate.

The estimate (34.a) is a stronger form of an estimate of Ewing and Wheeler that played a critical role in their analysis of a Galerkin method for approximating the solution of a model of miscible displacement; every succeeding analysis of a numerical method for miscible displacement has used some form of this result. In more than a single space variable the L^∞ bound is usually replaced by one in L^2.

4. ANALYSIS OF THE CONVERGENCE OF THE APPROXIMATION OF THE DENSITIES

Introduce [9] the projection $E \times P : J \to Z_h \times Z_h$ of the solution (e,p) defined by

$$(D_e \partial(e - E)/\partial x , d\zeta/dx) = 0, \ \zeta \in Z_h , \tag{35.a}$$

$$(D_p \partial(p - P)/\partial x , d\zeta/dx) = 0, \ \zeta \in Z_h . \tag{35.b}$$

In our case of constant D_e and D_p, E and P are the piecewise-linear interpolations over $\{x_i\}$ of e and p, respectively. Standard results give us the bounds

$$\| \partial^k\eta_\alpha/\partial t^k\|_{0,s} + h_d\| \partial^k\eta_\alpha/\partial t^k\|_{1,s} \le \| \partial^k\alpha/\partial t^k\|_{2,s} h_d^2 , \ t \in J , \tag{36}$$

for α = e or p, $k \ge 0$, $1 \le s \le \infty$, and

$$\eta_e = e - E, \quad \sigma_e = e_h - E \ ,$$

$$\eta_p = p - P, \quad \sigma_p = p_h - P \ .$$

As a consequence of (36), it suffices to estimate σ_α, and since the argument for handling σ_p is quite the same as that for σ_e, we shall concentrate on the derivation of an evolution inequality for σ_e. Combining (10.a),(14.a), and (35.a) leads to the error equation

$$((\sigma_e^m - \hat{\sigma}_e^{m-1})/\hat{\Delta}t_e^m, \zeta) + (D_e \partial\sigma_e^m/\partial x, d\zeta/dx) \tag{37}$$

$$= (\phi_e \partial e^m/\partial\tau_e - (e^m - \hat{e}^{m-1})/\hat{\Delta}t_e^m, \zeta) + (\hat{R}^{m-1} - R^m, \zeta)$$

$$+ ((\eta_e^m - \hat{\eta}_e^{m-1})/\hat{\Delta}t_e^m, \zeta)$$

$$+ (zD_e\{e_h^m(\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m) - e^m(e^m - p^m - c^m)\}, \zeta)$$

for $\zeta \in Z_h$. Set

$$\Omega_1^m = \{x \in \Omega : \hat{\Delta}t_e^m = \Delta t\}, \quad \Omega_2^m = \Omega \backslash \Omega_1^m \ .$$

Choose the test function $\zeta = \sigma_e^m$. Note that, since σ_e^m vanishes on $\partial\Omega$, $\hat{\sigma}_e^{m-1} = 0$ on Ω_2^m. Hence,

$$((\sigma_e^m - \hat{\sigma}_e^{m-1})/\hat{\Delta}t_e^m \ , \ \sigma_e^m) = ((\sigma_e^m - \sigma_e^{m-1})/\Delta t \ , \ \sigma_e^m)_{\Omega_1^m} \tag{38}$$

$$+ (\sigma_e^m/\hat{\Delta}t_e^m, \sigma_e^m)_{\Omega_2^m} + ((\sigma_e^{m-1} - \hat{\sigma}_e^{m-1})/\Delta t, \sigma_e^m)_{\Omega_1^m}$$

$$\geq (2\Delta t)^{-1}[\| \sigma_e^m \|_0^2 - \| \sigma_e^{m-1} \|_0^2] + ((\sigma_e^{m-1} - \hat{\sigma}_e^{m-1})/\Delta t, \sigma_e^m)_{\Omega_1^m} \ .$$

In order to facilitate the treatment of the last term above and the right hand side of (37), we impose an induction hypothesis. Assume that

$$\| q_h \|_{L^\infty(\Omega\times\{t^m\})} + \| q_h' \|_{L^\infty(\Omega\times\{t^m\})} \leq K \ ; \tag{39}$$

this relation is valid as $h = (h_d, h_q) \to 0$ for t^0 for K larger than $\| q^0 \|_{0,\infty} + \| (q^0)' \|_{0,\infty}$ and, if e_h and p_h converge sufficiently rapidly, will follow from (34). In order to assure that q_h' remains bounded, we assume that

$$(\Delta t + h_d^2 + h_q^2)[\min(h_d, h_q)]^{-1/2} \to 0 \quad \text{as} \quad h \to 0 \ . \tag{40}$$

The validity of (39) will be established as a part of the convergence proof. It should be noted that in practice h_q would probably be chosen to be $O(\Delta t)$, so that no serious constraint is imposed by (40).

Consider first the last term in (38). Now, for $x \in \Omega_1^m$, $\hat{\Delta}t_e(x) = \Delta t$ and since

$$\sigma_e^{m-1}(x) - \hat{\sigma}_e^{m-1}(x) = \int_{x+D_e q_h^{m-1}\Delta t}^{x} \partial\sigma_e^{m-1}/\partial x \, dy \ , \tag{41}$$

a calculation shows that

$$\| \sigma_e^{m-1} - \hat{\sigma}_e^{m-1} \|_{0,\Omega_1^m} \leq D_e K \, \Delta t \| \sigma_e^{m-1} \|_1 \ . \tag{42}$$

Hence,

$$|((\sigma_e^{m-1} - \hat{\sigma}_e^{m-1})/\Delta t, \sigma_e^m)_{\Omega_1^m}| \leq M \| \sigma_e^{m-1} \|_1 \| \sigma_e^m \|_0 \ . \tag{43}$$

Next,

$$\phi_e \partial e^m/\partial\tau_e - (e^m - \hat{e}^{m-1})/\hat{\Delta}t_e^m$$

$$= [\phi_e \partial e^m/\partial\tau_e - \phi_{e,h}\partial e^m/\partial\tau_{e,h}] + [\phi_{e,h}\partial e^m/\partial\tau_{e,h} - (e^m - \hat{e}^{m-1})/\hat{\Delta}t_e^m]$$

$$= [(q^m - q^{m-1}) + (q^{m-1} - q_h^{m-1})]\partial e^m/\partial x$$

$$+ \frac{1}{2} \phi_{e,h} \partial^2 e/\partial\tau_{e,h}^2 [(x - \hat{x}_e^m)^2 + (\hat{\Delta}t_e^m)^2]^{1/2} \ ,$$

where $\partial^2 e/\partial\tau_{e,h}^2$ is evaluated at some point on the segment between (x, t^m) and $(\hat{x}_e^m, t - \hat{\Delta}t_e^m)$. Thus,

$$|(\phi_e \partial e^m/\partial\tau_e - (e^m - \hat{e}^{m-1})/\hat{\Delta}t_e^m, \sigma_e^m)| \tag{44}$$

$$\leq M \{\| q^{m-1} - q_h^{m-1} \|_{0,\infty} + \Delta t\} \| \sigma_e^m \|_0 \ ,$$

where $M = M(K, \| e \|_{2,\infty,\Omega\times J})$.

Note that η vanishes on $\partial\Omega$. Hence,

$$|((\eta_e^m - \hat{\eta}_e^{m-1})/\hat{\Delta}t_e^m, \sigma_e^m)|$$

$$\leq |((\eta_e^m - \hat{\eta}_e^{m-1})/\Delta t, \sigma_e^m)_{\Omega_1^m}| + |(\eta_e^m/\hat{\Delta}t_e^m, \sigma_e^m)_{\Omega_2^m}| .$$

The argument leading to (43) could be applied to the first term; however, the introduction of the $H^1(\Omega)$-norm of η_e^m would lead to a loss in predicted accuracy. The estimate below modifies an argument of Douglas and Russell [3,8]. Let

$$y = F(x) = x + D_e q_h^{m-1}\Delta t, \quad x \in \Omega_1^m .$$

By the induction hypothesis (39), F is invertible for small Δt and

$$|dy/dx - 1| \leq M_1\Delta t \quad \text{as} \quad \Delta t \to 0 .$$

Set $\Omega_1^* = F(\Omega_1^m)$, and note that

$$(\Omega\setminus\Omega_1^m) \cup (\Omega\setminus\Omega_1^*) \subset [0, M_2\Delta t] \cup [1 - M_2\Delta t, 1] .$$

Then,

$$(\eta_e^m - \hat{\eta}_e^{m-1}, \sigma_e^m)_{\Omega_1^m} = (\eta_e^m - \eta_e^{m-1}, \sigma_e^m)_{\Omega_1^m}$$

$$+ (\eta_e^{m-1} - \hat{\eta}_e^{m-1}, \sigma_e^m)_{\Omega_1^m} .$$

The first term can be bounded in the following form:

$$|(\eta_e^m - \hat{\eta}_e^{m-1}, \sigma_e^m)_{\Omega_1^m}| \leq (\Delta t)^{1/2} \| \partial\eta_e/\partial t\|_{L^2(t^{m-1}, t^m; \Omega)} \|\sigma_e^m\|_0 .$$

Write the second term in the following form (dropping momentarily the indices m-1, m, and e):

$$\int_{\Omega_1} [\eta(x) - \eta(x + D_e q_h \Delta t)]\sigma(x)dx = \int_{\Omega_1^* \cap \Omega_1} \eta(y)[\sigma(y) - \sigma(F^{-1}(y))]dy \tag{45}$$

$$- \int_{\Omega_1^* \cap \Omega_1} \eta(y)\sigma(F^{-1}(y))(dx/dy - 1)dy + \int_{\Omega_1\setminus\Omega_1^*} \eta\sigma dx$$

$$- \int_{\Omega_1^*\setminus\Omega_1} \eta(y)\sigma(F^{-1}(y))(dx/dy)dy .$$

Now, apply the argument leading to (43) to the first right hand side term to see that

$$\left| \int_{\Omega_1^* \cap \Omega_1} \eta(y)[\sigma(y) - \sigma(F^{-1}(y))]dy \right| \leq M \|\eta\|_0 \|\sigma\|_1 \Delta t .$$

Next,

$$\left| \int_{\Omega_1^* \cap \Omega_1} \eta(y)\sigma(F^{-1}(y))(dx/dy - 1)dy \right| \leq M \|\eta\|_0 \|\sigma\|_0 \Delta t .$$

Then, let $\Omega_3 = (\Omega_1\setminus\Omega_1^*) \cap [0, M_2\Delta t]$ and recall that $\sigma(0) = 0$. Thus,

$$\left| \int_{\Omega_3} \eta dx \right| \leq \left| \int_{\Omega_3} \eta(x) \int_0^x (\partial\sigma/\partial x)dy\, dx \right| \leq \|\eta\|_{0,\infty} \int_{\Omega_3} x\|\sigma\|_1 dx$$

$$\leq M(\Delta t)^2 \|\eta\|_{0,\infty} \|\sigma\|_1 .$$

Similarly, if $\Omega_4 = (\Omega_1\setminus\Omega_1^*) \cap [1 - M_2\Delta t, 1]$, then

$$\left| \int_{\Omega_4} \eta\sigma dx \right| \leq M(\Delta t)^2 \|\eta\|_{0,\infty} \|\sigma\|_1 ,$$

so that the last two terms in (45) are bounded by the last quantity. If we collect these results, we see that

$$|((\eta_e^m - \hat{\eta}_e^{m-1})/\Delta t, \sigma_e^m)_{\Omega_1^m}|$$

$$\leq M [\|\eta_e^{m-1}\|_0 + \|\eta_e^{m-1}\|_{0,\infty}\Delta t] \|\sigma_e^m\|_1$$

$$+ (\Delta t)^{-1/2} \|\sigma_e^m\|_0 \|\partial\eta_e/\partial t\|_{L^2(t^{m-1}, t^m; \Omega)} .$$

Next, if $\Omega_5 = \Omega_2^m \cap [0, M_2\Delta t]$,

$$\left| \int_{\Omega_5} (1/\hat{\Delta}t_e^m(x))\eta_e^m(x)\sigma_e^m(x)dx \right|$$

$$= \left| \int_{\Omega_5} \eta_e^m(x)(1/\hat{\Delta}t_e^m(x)) \int_0^x (\partial\sigma_e^m/\partial x)dy\, dx \right|$$

$$\leq \|\eta_e^m\|_{0,\infty} \int_{\Omega_5} (x/\hat{\Delta}t_e^m(x)) \|\sigma_e^m\|_1 dx$$

$$\leq M_2 D_e K\, \Delta t\, \| \eta_e^m \|_{0,\infty} \| \sigma_e^m \|_1 \, .$$

Consequently,

$$\left| \left((\eta_e^m - \hat{\eta}_e^{m-1}) / \hat{\Delta t}_e^m , \sigma_e^m \right) \right| \tag{46}$$

$$\leq M \left[\| \eta_e^{m-1} \|_0 + \left(\| \eta_e^m \|_{0,\infty} + \| \eta_e^{m-1} \|_{0,\infty} \right) \Delta t \right] \| \sigma_e^m \|_1$$

$$+ (\Delta t)^{-1/2} \| \sigma_e^m \|_0 \, \| \partial \eta_e / \partial t \|_{L^2(t^{m-1}, t^m; \Omega)}$$

In order to estimate the term involving

$$\gamma = e_h^m (\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m) - e^m (e^m - p^m - c^m)$$

$$= \sigma_e^m (\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m) - \eta_e^m (e^m - p^m - c^m)$$

$$+ E^m \left((\hat{e}_h^{m-1} - e^m) - (\hat{p}_h^{m-1} - p^m) \right) ,$$

it is convenient to introduce an additional induction hypothesis that

$$\| e_h^m \|_{0,\infty} + \| p_h^m \|_{0,\infty} \leq K, \; m \geq 0 \; ; \tag{47}$$

clearly, any reasonable assignment of e_h^0 and p_h^0 will satisfy such a bound. It will be necessary to verify that (47) remains valid as h and Δt tend to zero, assuming that K is fixed at a value exceeding the corresponding bound for e and p. That E^m is bounded in L^∞ follows easily from its form as a piecewise-linear interpolant of e. Note also that

$$e^m - \hat{e}_h^{m-1} = (e^m - \hat{e}^{m-1}) + \hat{\eta}_e^{m-1} - \hat{\sigma}_e^{m-1} \quad ,$$

so that

$$\| e^m - \hat{e}_h^{m-1} \|_0 \leq M \Delta t \| e \|_{1,\infty,\Omega\times J} + M \left(\| \eta_e^{m-1} \|_0 + \| \sigma_e^{m-1} \|_0 \right) \quad ,$$

using the assumed boundedness of q_h^{m-1}. Thus,

$$\left| (z D_e \gamma, \sigma_e^m) \right| \leq M \left[\| e \|_{1,\infty,\Omega\times J} \Delta t + \| p \|_{1,\infty,\Omega\times J} \Delta t \right. \tag{48}$$

$$+ \| \sigma_e^m \|_0 + \| \sigma_e^{m-1} \|_0 + \| \sigma_p^{m-1} \|_0$$

$$\left. + \| \eta_e^m \|_0 + \| \eta_e^{m-1} \|_0 + \| \eta_p^{m-1} \|_0 \right] \| \sigma_e^m \|_0 \, .$$

Finally a very similar calculation shows that

$$\left| (\hat{R}^{m-1} - R^m, \sigma_e^m) \right| \leq M \left[\left(\| e \|_{1,\infty,\Omega\times J} + \| p \|_{1,\infty,\Omega\times J} \right) \Delta t \right. \tag{49}$$

$$+ \| \sigma_e^{m-1} \|_0 + \| \sigma_p^{m-1} \|_0$$

$$\left. + \| \eta_e^{m-1} \|_0 + \| \eta_p^{m-1} \|_0 \right] \| \sigma_e^m \|_0 \, .$$

Let F indicate a generic constant that can depend on K and the $W^{2,\infty}(\Omega\times J)$ norms of q, e, and p:

$$F \leq F\left(K, \| q \|_{2,\infty,\Omega\times J}, \| e \|_{2,\infty,\Omega\times J}, \| p \|_{2,\infty,\Omega\times J}\right) \, . \tag{50}$$

Collect the implications of (38),(43),(44),(46),(48) and (49) and then apply (34.a) and (36). Then, if $D = \min(D_e, D_p)$,

$$(2\Delta t)^{-1} \left[\| \sigma_e^m \|_0^2 - \| \sigma_e^{m-1} \|_0^2 \right] + D \| \sigma_e^m \|_1^2$$

$$\leq F \left\{ \| \sigma_e^{m-1} \|_1 \| \sigma_e^m \|_0 + \left(\| q^{m-1} - q_h^{m-1} \|_{0,\infty} + \Delta t \right) \| \sigma_e^m \|_0 \right.$$

$$+ \left(\| \eta_e^{m-1} \|_0 + \left(\| \eta_e^{m-1} \|_{0,\infty} + \| \eta_e^m \|_{0,\infty} \right) \Delta t \right) \| \sigma_e^m \|_1$$

$$+ (\Delta t)^{-1/2} \| \partial \eta_e / \partial t \|_{L^2(t^{m-1}, t^m; L^2(\Omega))} \| \sigma_e^m \|_0$$

$$+ \left(\Delta t + \| \sigma_e^m \|_0 + \| \sigma_e^{m-1} \|_0 + \| \sigma_p^{m-1} \|_0 + \| \eta_e^m \|_0 \right.$$

$$\left. \left. + \| \eta_e^{m-1} \|_0 + \| \eta_p^{m-1} \|_0 \right) \| \sigma_e^m \|_0 \right\} ,$$

so that

$$1/\Delta t\,[\|\sigma_e^m\|_0^2 - \|\sigma_e^{m-1}\|_0^2] + D\,\|\sigma_e^m\|_1^2 - D/2\,\|\sigma_e^{m-1}\|_1^2 \tag{51}$$

$$\le F\,\{\|\sigma_e^m\|_0^2 + \|\sigma_e^{m-1}\|_0^2 + \|\sigma_p^{m-1}\|_0^2 + (\Delta t)^2 + h_d^4 + h_q^4\}\,.$$

An estimate with the subscripts e and p interchanged can be derived in like manner. Set

$$\|\sigma\|_j^2 = \|\sigma_e\|_j^2 + \|\sigma_p\|_j^2\,,\quad j = 0 \text{ or } 1\,,$$

and add (51) and its analogue. Then,

$$1/\Delta t\,[\|\sigma^m\|_0^2 - \|\sigma^{m-1}\|_0^2] + D\,\|\sigma^m\|_1^2 - D/2\,\|\sigma^{m-1}\|_1^2 \tag{52}$$

$$\le F\,\{\|\sigma^m\|_0^2 + \|\sigma^{m-1}\|_0^2 + (\Delta t)^2 + h_d^4 + h_q^4\}\,.$$

First, multiply by Δt and sum on m from $m = 1$ to $m = n$, and then apply the Gronwall lemma:

$$\max_{1\le m\le n}\|\sigma^m\|_0^2 + \sum_{m=1}^{n}\|\sigma^m\|_1^2\,\Delta t \tag{53}$$

$$\le F\,\{\|\sigma^0\|_0^2 + \|\sigma^0\|_1^2\,\Delta t + (\Delta t)^2 + h_d^4 + h_q^4\}\,,$$

provided that the two induction hypothesis (39) and (47) hold for $0\le m\le n-1$.

First, choose

$$e_h^0 = E^0\,,\quad p_h^0 = P^0\,; \tag{54}$$

i.e., the piecewise-linear interpolant of e(x,0) and p(x,0), respectively. Then, $\sigma_e^0 = \sigma_p^0 = 0$, so that

$$\max_{1\le m\le n}\|\sigma^m\|_0 + \Big(\sum_{m=1}^{n}\|\sigma^m\|_1^2\,\Delta t\Big)^{1/2} \le F\,\{\Delta t + h_d^2 + h_q^2\}\,, \tag{55}$$

if (39) and (47) hold for $1\le m\le n-1$.

We have seen that (39) and (47) hold for $n = 1$; assume it valid for n. Then, (55) and (34.a) imply that

$$\|q^n - q_h^n\|_{0,\infty} \le F\,(\Delta t + h_d^2 + h_q^2)\,, \tag{56}$$

so that

$$\|q_h^n\|_{0,\infty} \le \|q\|_{0,\infty} + F(\Delta t + h_d^2 + h_q^2)\,.$$

Moreover, by (55) and (34.b),

$$\|(q_h^n)'\|_{0,\infty} \le \|(q^n)'\|_{0,\infty} + F\,((\Delta t + h_d^2)\,h_q^{-1/2} + h_q)\,,$$

so that the restriction (40) forces the satisfaction of (39) for small h_q when n is replaced by $n+1$.

Next, again by (40)

$$\|e_h^n\|_{0,\infty} \le \|e^n\|_{0,\infty} + F\,((\Delta t + h_q^2)h_q^{-1/2} + h_d^{3/2})\,,$$

so that (47) also holds inductively.

We have proved the following theorem.

<u>Theorem</u>. Let q, e, and p lie in $C^2(\Omega\times J)$. Let

$$(\Delta t + h_d^2 + h_q^2)h_i^{-1/2} \to 0 \quad \text{as} \quad h_i \to 0,\quad i = d \text{ or } q\,.$$

Then,

$$\max_n\,\{\|e^n - e_h^n\|_0 + \|p^n - p_h^n\|_0 + \|q^n - q_h^n\|_{0,\infty}\} \le F\,\{\Delta t + h_d^2 + h_q^2\}\,.$$

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