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BY

JIM DOUGLAS, JR.

AND

YIRANG YUAN

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INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS

UNIVERSITY OF MINNESOTA

514 Vincent Hall

206 Church Street S.E.

Minneapolis, Minnesota 55455

FINITE DIFFERENCE METHODS FOR THE TRANSIENT BEHAVIOR OF A SEMICONDUCTOR DEVICE

Jim DOUGLAS, Jr.[+] and YUAN Yirang[++]

Dedicated to Professor Luiz Adauto Medeiros on the occasion of his sixtieth birthday

Abstract. The transient behavior of a semiconductor device is described by a system of three quasilinear partial differential equations, one elliptic in form for the electric potential and two parabolic in form for the conservation of electron and hole concentrations. The electric potential equation is discretized by a standard five-point difference method. The electron and hole density equations are treated by an implicit finite difference method that applies a variant of the method of characteristics to the transport terms. A convergence analysis is given for the method.

1. Introduction. A model of the transient behavior of a semiconductor device 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 [1], [6], [7]:

(1.a) $$\nabla\cdot q = -\Delta\psi = Z(e-p-c),$$

(1.b) $$\frac{\partial e}{\partial t} - D_e q\cdot\nabla e - D_e\Delta e - ZD_e e(e-p-c) = R_1(e,p),$$

(1.c) $$\frac{\partial p}{\partial t} + D_p q\cdot\nabla p - D_p\Delta p + ZD_p p(e-p-c) = R_2(e,p).$$

The unknowns are the electrostatic potential ψ and the electron and hole densities e and p. The function c is the total electric active net impurity

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+ Department of Mathematics, University of Chicago, Chicago, Illinois 60637, and Institute for Mathematics and its Applications, University of Minnesota

++ Department of Mathematics, University of Shandong, Jinan, Shandong, China, and Institute for Mathematics, University of Minnesota

concentration or "doping"; D_e and D_p are the diffusion coefficients. D_e, D_p and Z are assumed to be constants. $R_1(e,p)$ and $R_2(e,p)$ are the recombination rates.

In this paper we study a two-dimensional problem on the domain $\Omega = [0,1] \times [0,1]$. We denote by $\partial\Omega$ the boundary of Ω. Let $J = [0,T]$.

Assume nonhomogeneous Dirichlet boundary conditions:

(2 a) $\quad \psi(x,t)|_{\partial\Omega} = \gamma(x,t) \quad , \quad x \in \partial\Omega, \quad t \in J$,

(2 b) $\quad e(x,t)|_{\partial\Omega} = f(x,t) \quad , \quad x \in \partial\Omega, \quad t \in J$,

(2 c) $\quad p(x,t)|_{\partial\Omega} = g(x,t) \quad , \quad x \in \partial\Omega, \quad t \in J$.

In addition, we have the initial conditions

(3) $\quad e(x,0) = e^0(x), \ p(x,0) = p^0(x) \quad , \quad x \in \Omega$.

The object of this paper is to formulate a finite difference analogue of the mixed finite element - characteristic procedure for the transient behavior of a semiconductor device introduced by Douglas, Martínez-Gamba, and Squeff [4] for a one-dimensional problem. Clearly, the motivation for including the method of characteristics in approximating e and p is to follow the transport more accurately than the standard finite difference or finite element method do [8],[9]. In particular, reduced time-truncation errors were indicated in [5], so that this method should be able to use longer time steps with no loss of accuracy than with more commonly used methods.

The finite difference procedure will be defined in the next section. A convergence analysis will be given in the third section.

In this paper the solution of (1)-(3) is assumed to be smooth, so that optimal order accuracy is possible. The precise regularity needed will be clear from the convergence arguments. Throughout, the symbols M and ε will denote, respectively, a generic constant and a generic small positive constant.

2. **The Finite Difference Procedure.** The modified method for characteristics procedure has as its basic idea the interpretation of the first order parts of (1b) and (1c) as directional derivatives. Various spatial and time discretizations can be applied to the resulting equations; here we shall discretize by finite difference methods.

Let $q(x,t) = (q_1, q_2)^T$,and let $\tau_e = \tau_e(x,t)$ be the unit vector in the direction $(-D_e q_1, -D_e q_2, 1)$ and $\tau_p = \tau_p(x,t)$ the unit vector in the direction $(D_p q_1, D_p q_2, 1)$. Set $\phi_\alpha = [1+ D_\alpha^2(q_1^2 + q_2^2)]^{1/2}$ for $\alpha = e$ or p. Then the characteristic derivatives in the τ_α directions are given by

(4a) $$\phi_e \frac{\partial}{\partial \tau_e} = \frac{\partial}{\partial t} - D_e q \cdot \nabla ,$$

(4b) $$\phi_p \frac{\partial}{\partial \tau_p} = \frac{\partial}{\partial t} + D_p q \cdot \nabla ,$$

so that (1) can be written in the form

(5a) $$\nabla \cdot q = - \Delta\psi = Z(e-p-c),$$

(5b) $$\phi_e \frac{\partial e}{\partial \tau_e} - D_e \Delta e - Z D_e e(e-p-c) = R_1(e,p) ,$$

(5c) $$\phi_p \frac{\partial p}{\partial \tau_p} - D_p \Delta p + Z D_p p(e-p-c) = R_2(e,p) .$$

Let $h = N^{-1}$, $x_{ij} = (ih,jh)$, $\Delta t = > 0$, $t^m = m\Delta t$, and $w(x_{ij},t^m) = w_{ij}^m$. Consider the approximation of $\phi_e \frac{\partial e}{\partial \tau_e}$, which we make by backward differencing along the tangent to the τ_e - characteristic at (x_{ij},t^m). Follow this tangent back in time until it intersects $(\Omega x \{t^{m-1}\}) \cup (\partial\Omega \times [t^{m-1}, t^m])$ at a point

$(\tilde{x}_e^m(x_{ij}), t^m - \tilde{\Delta t}_e^m (x_{ij}))$, so that

(6) $$\tilde{x}_e^m(x_{ij}) = x_{ij} + D_e q(x_{ij}, t^m)\tilde{\Delta t}_e^m(x_{ij}) ,$$

where

(7a) $$\tilde{\Delta t}_e^m(x_{ij}) = -ih/D_e q_1(x_{ij},t^m) , \quad \text{if} \quad ih + D_e q_1(x_{ij}, t^m)\,\Delta t < 0$$
$$\text{and} \quad 0 < jh + D_e q_1(x_{ij},t^m)\,\Delta t < 1 ,$$

(7b) $$\tilde{\Delta t}_e^m(x_{ij}) = -jh/D_e q_2(x_{ij},t^m, \quad \text{if} \quad 0 < ih + D_e q_1(x_{ij},t^m)\,\Delta t < 1$$
$$\text{and} \quad jh + D_e q_2(x_{ij},t^m)\,\Delta t < 0 ,$$

(7c) $$\tilde{\Delta t}_e^m(x_{ij}) = (1-ih)/D_e q_1(x_{ij},t^m), \quad \text{if} \quad ih + D_e q_1(x_{ij},t^m)\,\Delta t > 1$$
$$\text{and} \quad 0 < jh + D_e q_2(x_{ij},t^m)\,\Delta t < 1 ,$$

(7d) $$\tilde{\Delta t}_e^m(x_{ij}) = (1-jh)/D_e q_2(x_{ij},t^m), \quad \text{if} \quad 0 < ih + D_e q_1(x_{ij},t^m)\,\Delta t < 1$$
$$\text{and} \quad jh + D_e q_2(x_{ij},t^m)\,\Delta t > 1 ,$$

(7e) $$\tilde{\Delta t}_e^m(x_{ij}) = \min\,\{-ih/D_e q_1(x_{ij},t^m),\ (1-jh)/D_e q_2(x_{ij},t^m)\}$$
$$\text{if} \quad ih + D_e q_1(x_{ij},t^m)\,\Delta t < 0 \quad \text{and} \quad jh + D_e q_2(x_{ij},t^m)\,\Delta t > 1 ,$$

(7f) $$\tilde{\Delta t}_e^m(x_{ij}) = \min\,\{-ih/D_e q_1(x_{ij},t^m),\ -jh/D_e q_2(x_{ij},t^m)\}$$
$$\text{if} \quad ih + D_e q_1(x_{ij},t^m)\,\Delta t < 0 \quad \text{and} \quad jh + D_e q_2(x_{ij},t^m)\,\Delta t < 0 ,$$

(7g) $$\tilde{\Delta t}_e^m(x_{ij}) = \min\,\{(1-ih)/D_e q_1(x_{ij},t^m),\ -jh/D_e q_2(x_{ij},t^m)\}$$
$$\text{if} \quad ih + D_e q_1(x_{ij},t^m)\,\Delta t > 1 \quad \text{and} \quad jh + D_2 q_2(x_{ij},t^m)\,\Delta t < 0 ,$$

(7h) $$\tilde{\Delta t}_e^m(x_{ij}) = \min\,\{(1-ih)/D_e q_1(x_{ij},t^m) ,\ (1-jh)/D_e q_2(x_{ij},t^m)\}$$
$$\text{if} \quad ih + D_e q_1(x_{ij},t^m)\,\Delta t > 1 \quad \text{and} \quad jh + D_e q_2(x_{ij},t^m)\,\Delta t > 1 ,$$

(7i) $$\tilde{\Delta t}_e^m(x_{ij}) = \Delta t , \quad \text{otherwise.}$$

Then,

(8) $$(\phi_e \frac{\partial e}{\partial \tau_e})(x_{ij},t^m) = \phi_e(x_{ij},t^m)[e(x_{ij},t^m) - e(\tilde{x}_e^m(x_{ij}), t^m - \tilde{\Delta t}_e^m(x_{ij}))]$$

$$/[(x_{ij} - \tilde{x}_e^m(x_{ij}))^2 + (\tilde{\Delta t}_e^m(x_{ij}))^2]^{1/2} + 0(|\frac{\partial^2 e}{\partial \tau_e^2}| \Delta\tau_e)$$

$$= [e(x_{ij},t^m) - e(\tilde{x}_e^m(x_{ij}),t^m - \tilde{\Delta t}_e^m(x_{ij}))] / \tilde{\Delta t}_e^m(x_{ij}) + 0(|\frac{\partial^2 e}{\partial \tau_e^2}| \Delta\tau_e) ,$$

where $\Delta\tau_e = [(x_{ij} - \tilde{x}_e^m(x_{ij}))^2 + (\tilde{\Delta t}_e^m(x_{ij}))^2]^{1/2}$.

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

Similarly, let

(9) $$\tilde{x}_p^m(x_{ij}) = x_{ij} - D_p q(x_{ij},t^m)\tilde{\Delta t}_p^m(x_{ij})$$

where $\tilde{\Delta t}_p^m(x_{i,})$ is determined analogously to $\tilde{\Delta t}_e^m(x_{ij})$, so that

(10) $$(\phi_p \frac{\partial p}{\partial \tau_p})(x_{ij},t^m) = [p(x_{ij},t^m) - p(\tilde{x}_p^m(x_{ij}),t^m - \tilde{\Delta t}_p^m(x_{ij}))]/\tilde{\Delta t}_p^m(x_{ij}) +$$

$$+ 0(|\frac{\partial^2 p}{\partial \tau_p^2}| \Delta\tau_p) ,$$

where $\Delta\tau_p = [(\tilde{x}_p^m(x_{ij}) - x_{ij})^2 + (\tilde{\Delta t}_p^m(x_{ij}))^2]^{1/2}$.

Since the function $q(x,t^m)$ will have to be approximated, we cannot evaluate $\tilde{x}_e^m(x_{ij})$ and $\tilde{x}_p^m(x_{ij})$. So, let $\hat{x}_e^m(x_{ij})$, $\hat{\Delta t}_e^m(x_{ij})$, $\hat{x}_p^m(x_{ij})$ and $\hat{\Delta t}_p^m(x_{ij})$ be defined by the corresponding relations when $q(x_{ij}, t^m)$ is replaced by $q_h^{m-1}(x_{ij})$, where $q_h^{m-1}(x_{ij}) = q_{h,ij}^{m-1}$ is the finite difference solution at time level t^{m-1}, at which time q_h will already have been computed.

Extend the grid values $e_{h,ij}^{m-1}$ and $p_{h,ij}^{m-1}$ to functions e_h^{m-1} and p_h^{m-1} defined on Ω by piecewise-bilinear interpolation; practical semiconductor devices can be asumed to be unions of grid rectangles, with possibly some triangles near the boundary, so that this interpolation, modified to be piecewise-linear on any boundary triangles, would suffice on a more general domain. The functions e_h^o and p_h^o are corresponding interpolations of the initial values for e and p.

Let $\hat{e}_h^{m-1}(x_{ij}) = e_h(\hat{x}_e^m(x_{ij}), t^m - \hat{\Delta t}_e^m(x_{ij})) = \hat{e}_{h,ij}^{m-1}$, and $\hat{p}_h^{m-1}(x_{ij}) = p_h(\hat{x}_p^m(x_{ij}), t^m - \hat{\Delta t}_p^m(x_{ij})) = \hat{p}_{h,ij}^{m-1}$, $m > 1$. Then, the basic finite difference method is given by the equations

$$\text{(11a)} \qquad \frac{e_{h,ij}^m - \hat{e}_{h,ij}^{m-1}}{\hat{\Delta t}_e^m(x_{ij})} - D_e \Delta_h e_{h,ij}^m - ZD_e\, e_{h,ij}^m(\hat{e}_{h,ij}^{m-1} - \hat{p}_{h,ij}^{m-1} - c_{ij}^m) =$$

$$= R_1(\hat{e}_{h,ij}^{m-1}, \hat{p}_{h,ij}^{m-1}), \quad 1 < i,j < N-1 ,$$

$$\text{(11b)} \qquad \frac{p_{h,ij}^m - \hat{p}_{h,ij}^{m-1}}{\hat{\Delta t}_p^m(x_{ij})} - D_p \Delta_h p_{h,ij}^m + ZD_p p_{h,ij}^m (\hat{e}_{h,ij}^{m-1} - \hat{p}_{h,ij}^{m-1} - c_{ij}^m) =$$

$$= R_2(\hat{e}_{h,ij}^{m-1}, \hat{p}_{h,ij}^{m-1}), \quad 1 < i,j < N-1 ,$$

where $\Delta_h e_{h,ij} = \frac{1}{h^2}\{[e_{h,i+1,j} - 2e_{h,ij} + e_{h,i,j}] + [e_{h,i,j+1} - 2e_{h,ij} + e_{h,i,j-1}]\}$. The boundary values (1.2) 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 $\hat{x}_e^m(x_{ij})$ or $\hat{x}_p^m(x_{ij})$ lies on $\partial\Omega$.

For the electric potential equation (1a) the basic finite difference method is given by the equation

(12a) $$-\Delta_h \psi_{h,ij}^{m-1} = Z(e_{h,ij}^{m-1} - p_{h,ij}^{m-1} - C_{ij}^{m-1}) , \quad 1 < i,j < N-1 .$$

Let

(12b) $$q_{h,ij}^{m-1} = -(\nabla_h \psi_h)_{ij}^{m-1} = -\left(\frac{\psi_{h,i+1,j}^{m-1} - \psi_{h,i-1,j}^{m-1}}{2h} , \frac{\psi_{h,i,j+1}^{m-1} - \psi_{h,i,j-1}^{m-1}}{2h}\right) , \ 1 < i,j < N-1 .$$

The algorithm for a time step is as follows. Assume known the approximate solution $\{e_h^{m-1} , p_h^{m-1}\}$ at time t^{m-1}. Then by (12), we can obtain $\{q_h^{m-1}, \psi_h^{m-1}\}$. Finally, from (11) we find $\{e_h^m , p_h^m\}$ at $t = t^m$, so that a complete time step can be taken.

3. Convergence Analysis. Let

(13) $\Pi = \psi - \psi_h, \quad \xi = e - e_h, \quad \eta = p - p_h$,

where from here on the subscripts i and j will be omitted where no confusion will result. For the electric potential equation (1a) we have

(14) $$-\Delta_h \psi^{m-1} = Z(e^{m-1} - p^{m-1} - c^{m-1} + \delta^{m-1}, \quad 1 < i,j < N-1 ,$$

where

(15) $$|\delta_{ij}^{m-1}| < Mh^2 .$$

for a smooth solution. The norms $\|\cdot\|_{\ell,p}$ are those for the Sobolev space $W^{\ell,p}(\Omega)$. The notation

$$\|\alpha\| = < \alpha, \alpha >^{1/2} ,$$

$$< \alpha, \beta > = \sum_{1<i,j<N-1} \alpha_{ij} \beta_{ij} h^2 + \frac{1}{2} \sum_{1<i,j<N-1} \{\alpha_{oj} \beta_{oj} + \alpha_{Nj} \beta_{Nj} + \alpha_{io}\beta_{io} +$$

$$+ \alpha_{iN} \beta_{iN}\}h^2 + \frac{1}{4} \{\alpha_{oo} \beta_{oo} + \alpha_{oN} \beta_{oN} + \alpha_{No} \beta_{No} + \alpha_{NN} \beta_{NN}\}h^2 ,$$

will denote the norm on the discrete space $\ell^2(\Omega)$. Also, $< \nabla_h \alpha , \nabla_h \alpha >$ denotes the square of the weighted semi-norm on the discrete space $h^1(\Omega)$ corresponding to $H^1(\Omega) = W^{1,2}(\Omega)$.

Subtract (12a) from (14a) to obtain the relation

(16) $$-\Delta_h \Pi^{m-1} = Z(\xi^{m-1} - \eta^{m-1}) + \delta^{m-1} , \quad 1 < i,j < N-1 .$$

Test (3.4) against Π^{m-1}, noting that $\Pi_{ij}^{m-1} = 0$ for $x_{ij} \subset \partial\Omega$. Sum by parts:

$$(17) \qquad \langle \nabla_h \Pi^{m-1}, \nabla_h \Pi^{m-1} \rangle = \langle \delta^{m-1}, \Pi^{m-1} \rangle + \langle Z(\xi^{m-1} - \eta^{m-1}), \Pi^{m-1}) .$$

Hence by (15) and an application of the discrete Poincare inequality we have

$$(18) \qquad \|\nabla_h \Pi^{m-1}\| \leq M\{\|\xi^{m-1}\| + \|\eta^{m-1}\| + h^2\} .$$

Consider the error equation for the concentration of electrons. First, note that for smooth solutions (with the subsripts i and j suppressed)

$$(19) \qquad \frac{\partial e^m}{\partial t} - D_e q^m \cdot \nabla e^m = \frac{\partial e^m}{\partial t} - D_e q_h^{m-1} \cdot \nabla e^m - D_e(q^m - q_h^{m-1}) \cdot \nabla e^m$$

$$= \frac{e^m - \hat{e}^{m-1}}{\Delta \hat{t}_e^m} - \frac{e(x_e, t^m - \Delta \hat{t}_e^m) - \hat{e}^{m-1}}{\Delta \hat{t}_e^m}$$

$$- D_e(q^{m-1} - q_h^{m-1}) \cdot \nabla e^m + O(\Delta t),$$

where $\hat{e}^{m-1}$ denotes the bilinear interplant of e^{m-1} on Ω and boundary values on $\partial\Omega$. Then, it follows from (1b), (5b), (11a), and (19) that

$$(20) \qquad \frac{\xi^m - \hat{\xi}^{m-1}}{\Delta \hat{t}_e^m} - D_e \Delta_h \xi^m$$

$$= \frac{e(\hat{x}_e^m, t^m - \Delta \hat{t}_e^m) - e^{m-1}}{\Delta \hat{t}_e^m} + D_e(q^{m-1} - q_h^{m-1}) \cdot \nabla e^m$$

$$+ ZD_e[e^m(e^m - p^m - c^m) - e_h^m (\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m)]$$

$$+ R_1(e^m, p^m) - R_1(\hat{c}_h^{m-1}, \hat{p}_h^{m-1}) + O(\Delta t + h^2).$$

Test (20) against ξ^m and consider the terms one at a time, beginning with the right-hand side. First, if $\hat{x}_e^m \subset \partial\Omega$, $e(\hat{x}_e^m, t^m - \hat{\Delta t}_e^m) - \hat{e}^{m-1} = 0$; if $\hat{x}_e^m \subset \Omega$, then $\Delta\hat{t}_e^m = \Delta t$ and $e(\hat{x}_e^m, t^m - \Delta t) - \hat{e}^{m-1} = O(h^2)$.

Thus,

$$(21) \qquad \left| \left< \frac{e(\hat{x}_e^m, t^m - \hat{\Delta t}_e^m) - \hat{e}^{m-1}}{\hat{\Delta t}_e^m}, \xi^m \right> \right| \le Mh^2(\Delta t)^{-1} \|\xi^m\|$$

$$\le Mh \|\xi^m\| ,$$

under the assumption that

$$(22) \qquad M_1 h \le \Delta t \le M_2 h.$$

Next, $q^{m-1} - q_h^{m-1} = - \nabla_h(\psi^{m-1} - \psi_h^{m-1}) + O(h^2) = -\nabla_h \pi^{m-1} + O(h^2)$, so that

$$(23) \qquad | < D_e(q^{m-1} - q_h^{m-1}) \cdot \nabla e^m, \xi^m > |$$

$$\le M \{ \|\nabla_h \pi^{m-1}\| + h^2\} \|\xi^m\|$$

$$\le M\{ \|^{m-1}\| + \|\eta^{m-1}\| + h^2\} \|\xi^m\|.$$

hr order to estimate the term involving

$$(24) \qquad \delta^m = e^m(e^m - p^m - c^m) - e_h^m(\hat{e}_h^{m-1} - \hat{p}_h^{m-1} - c^m)$$

$$= (e^m - p^m - c^m)\xi^m + e_h^m (\hat{\xi}^{m-1} - \hat{\eta}^{m-1}) +$$

$$+ e_h^m (e^m - \hat{e}^{m-1} - p^m + \hat{p}^{m-1})$$

$$= (e^m - p^m - c^m)\xi^m + e_h^m(\hat{\xi}^{m-1} - \hat{\eta}^{m-1}) + O(\Delta t)e_h^m ,$$

we shall introduce the induction hypothesis that

(25a) $$\|e_h\|_{0,\infty} + \|p_h\|_{0,\infty} \le K ,$$

(25b) $$\|q_h\|_{0,\infty} \le K,$$

where $\|e_h\|_{0,\infty} = \max_{ijm}|e^m_{h,ij}|$. For $m=0$, the assignment of e_h^o and p_h^o through interpolation will satisfy such a bound. This will imply the bound on q_h^o. It will be necessary to verify that (25) remains valid as h and Δt tend to zero whenver K is chosen to exceed the corresponding bounds for e, p, and q. Then,

$$| < ZE_e \gamma^m, \xi^m > | \le M(\|\xi^m\|^2 + [\|\hat{\xi}^{m-1}\| + \|\hat{\eta}^{m-1}\|]\|\xi^m\| + \|\xi^m\|\Delta t).$$

It follows from (25b) that

$$\|\hat{f}\| \le M\|f\|$$

for any mesh function f ; hence,

(26) $$| < ZD_e \gamma^m, \xi^m > | \le M(\|\xi^m\|^2 + \|\xi^{m-1}\|^2 + \|\eta^{m-1}\|^2 + (\Delta t)^2).$$

Similarly,

$$(27)\quad |\langle R_1(e^m,p^m)-R_1(\hat{e}_h{}^{m-1},\hat{p}_h{}^{m-1})\rangle| \le M(\|\xi^m\|^2+\|\xi^{m-1}\|^2+\|\eta^{m-1}\|^2+(\Delta t)^2).$$

Finally,

$$(28)\quad |\langle O(\Delta t+h^2),\xi^m\rangle| \le M(\|\xi^m\|^2 + (\Delta t)^2).$$

The h^1-term on the left-hand side is given by $\langle D_e\nabla_h\xi^m,\nabla_h\xi^m\rangle$. The remaining term can be treated as in [4] by decomposing Ω_h, the set of grid points in Ω, into

$$\Omega_1{}^m = \{x_{ij} \in \Omega_h : \hat{\Delta}t_e{}^m(x_{ij}) = \Delta t\}$$

and

$$\Omega_2{}^m = \Omega_h \setminus \Omega_1{}^m.$$

Denote the inner product restricted to $\Omega_i{}^m$ by $\langle\cdot\,,\,\cdot\rangle_{i,m}$. Then, as $\hat{\xi}_{ij}{}^{m-1} = 0$ if $x_{ij} \in \partial\Omega$,

$$\begin{aligned}(29)\quad \langle(\xi^m-\hat{\xi}^{m-1})/\hat{\Delta}t_e{}^m,\xi^m\rangle &= \langle(\xi^m-\xi^{m-1})/\Delta t,\xi^m\rangle_{1,m}+\langle\xi^m/\hat{\Delta}t_e{}^m,\xi^m\rangle_{2,m} \\ &\quad + \langle(\xi^{m-1}-\hat{\xi}^{m-1})/\Delta t,\xi^m\rangle_{1,m} \\ &\ge (2\Delta t)^{-1}[\|\xi^m\|^2 - \|\xi^{m-1}\|^2] + \langle(\xi^{m-1}-\hat{\xi}^{m-1})/\Delta t,\xi^m\rangle_{1,m}.\end{aligned}$$

Let us estimate the final term above. Note that for $x_{ij} \in \Omega_1{}^m$

$$\begin{aligned}(30)\quad \hat{\xi}_{ij}{}^{m-1} - \xi_{ij}{}^{m-1} &= \xi^{m-1}(x_{ij}+D_eq_{h,ij}{}^{m-1}\Delta t) - \xi^{m-1}(x_{ij}) \\ &= \int_{x_{ij}}^{x_{ij}+D_eq_{h,ij}{}^{m-1}\Delta t} \nabla\xi^{m-1}(x_{ij}+\sigma D_eq_{h,ij}{}^{m-1}\Delta t)q_{h,ij}{}^{m-1}|q_{h,ij}{}^{m-1}|^{-1}d\sigma.\end{aligned}$$

Thus, we have

$$(31)\quad |\hat{\xi}_{ij}{}^{m-1}-\xi_{ij}{}^{m-1}| \le D_e|q_{h,ij}{}^{m-1}|\Delta t\cdot\max\{|\nabla_h\xi_{pq}{}^{m-1}| : |x_{pq}-x_{ij}|\le h+D_e|q_{h,ij}{}^{m-1}|\Delta t\}.$$

By the induction hypothesis (25b) we see that

$$(32)\quad \|\xi^{m-1}-\hat{\xi}^{m-1}\|^2 \le M(\Delta t)^2\sum_{ij}\max\{|\nabla_h\xi_{pq}{}^{m-1}|^2 : |x_{pq}-x_{ij}|\le h+D_eK\Delta t\}h^2 \le M(\Delta t)^2\|\nabla_h\xi^{m-1}\|^2,$$

assuming that the time step constraint (22) holds. Thus,

$$(33)\quad |\langle(\hat{\xi}^{m-1}-\xi^{m-1})/\Delta t,\xi^m\rangle_{1,m}| \le M\|\xi^m\|^2 + \epsilon\|\nabla_h\xi^{m-1}\|^2.$$

By (21)-(33), with $D = \min(D_e,D_p)$ and $\epsilon = .5D$, we have shown that

$$(34)\quad (2\Delta t)^{-1}[\|\xi^m\|^2 - \|\xi^{m-1}\|^2] + D\|\nabla_h\xi^m\|^2 - .5D\|\nabla_h\xi^{m-1}\|^2 \le M\{\|\xi^m\|^2 + \|\xi^{m-1}\|^2 + \|\eta^{m-1}\|^2 + (\Delta t)^2\}.$$

An analogous inequality holds for the error in the hole concentration. Let

$$\|\sigma\|^2 = \|\xi\|^2 + \|\eta\|^2, \quad \|\nabla_h\sigma\|^2 = \|\nabla_h\xi\|^2 + \|\nabla_h\eta\|^2.$$

Then,

$$(35)\quad (2\Delta t)^{-1}[\|\sigma^m\|^2 - \|\sigma^{m-1}\|^2] + D\|\nabla_h\sigma^m\|^2 - .5D\|\nabla_h\sigma^{m-1}\|^2 \le M\{\|\sigma^m\|^2 + \|\sigma^{m-1}\|^2 + (\Delta t)^2\}.$$

To bound σ, first multiply (35) by $2\Delta t$ and then sum on m from m=1 to m-n and apply the discrete Gronwall inequality:

$$\max_{1\le m\le n}\|\sigma^m\|^2 + \sum_{m=1}^{n}\|\nabla_h\sigma^m\|^2\Delta t \le M\{\|\sigma^0\|^2+\|\nabla_h\sigma^0\|^2\Delta t+(\Delta t)^2\} \le M(\Delta t)^2,$$

so that

$$\text{(36)}\quad \max_{1\le m\le n}\|\sigma^m\| + \Big(\sum_{m=1}^{n}\|\nabla_h\sigma^m\|^2\Delta t\Big)^{1/2} \le M\Delta t,$$

where the constant M depends on the constant K in the induction hypotheses and the smoothness of the solution of (1).

Convergence at a rate $O(\Delta t) = O(h)$ will take place if the induction hypotheses can be demonstrated. First, note that (with $|v|_\infty = \max_{ij}|v_{ij}|$)

$$|q_h^{m-1}|_\infty = |\nabla_h\psi_h^{m-1}|_\infty \le |\nabla_h\psi^{m-1}|_\infty + |\nabla_h\pi^{m-1}|_\infty.$$

Bramble [2] has shown that $|v|_\infty \le M\|\nabla_h v\|(\log h^{-1})^{-1/2}$ for any grid function vanishing on the boundary $\partial\Omega_h$. Consequently,

$$|\nabla_h\pi^{m-1}|_\infty \le M\|\pi^{m-1}\|_{2,h}(\log h^{-1})^{1/2},$$

where $\|\cdot\|_{2,h}$ denotes the discrete analogue of the $H^2(\Omega)$-norm. It is well-known that (16) implies that

$$\|\pi^{m-1}\|_{2,h} \le M(\|\sigma^{m-1}\| + h^2),$$

so that, by induction on m,

$$|q_h^{m-1}|_\infty \le \|\psi\|_{1,\infty,\Omega\times[0,T]} + M\Delta t \le K$$

for Δt sufficiently small; i. e., (25b) holds. A similar argument demonstrates (25a), so that the convergence proof is finished and the following theorem is valid.

<u>Theorem</u>. Let h and Δt satisfy (22), and let e_h^0 and p_h^0 be the piece-wise-linear interpolants of e^0 and p^0, respectively. Then, there exists a unique solution of the finite difference equations (11)-(12), and for a smooth solution of (1)

$$\max_m\{\|e^m-e_h^m\| + \|p^m-p_h^m\| + \|\psi^m-\psi_h^m\|\}$$

$$+ [\sum (\|\nabla_h(e^m-e_h^m)\|^2 + \|\nabla_h(p^m-p_h^m)\|^2)\Delta t\ ]^{1/2}$$

$$\le M\Delta t.$$

The demonstration given above of this theorem has relied on ideas developed earlier in [3], [4], and [5] to treat somewhat different problems.

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