

Domain Decomposition Modified with Characteristic Finite Element Method for Numerical Simulation of Semiconductor Transient Problem of Heat Conduction

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Abstract

A characteristic finite element algorithm based on domain decomposition is structured in this paper to approximate numerically multi-dimensional semiconductor transient problems of heat conduction. Finite element approximation is presented for the electric field potential equation, and a domain decomposition discretization with characteristic finite element is put forward for the electron concentration equation, hole concentration equation and heat conductor equation. An optimal order error estimate in L^2 norm is derived for the coupled system by using some techniques such as variation, domain decomposition, the method of characteristics, the principle of energy, negative norm estimates, induction hypothesis, prior estimates theory and other techniques of partial differential equations. Finally, experimental data consistent with theoretical convergence rate are shown. This type of numerical method is of high computational efficiency and can successfully solve this international problem.

Keywords: Numerical simulation of semiconductor device, domain decomposition, characteristic finite element, optimal order estimates in L^2 norm, numerical experiments

1. Introduction

Because of the great development of semiconductor device industry described by an initial-boundary value system of diffusion type of nonlinear partial differential equations, numerical simulation must be of high order accuracy and quite efficient, and traditional numerical methods are not considered in actual computation. Then some new modern discretization techniques are introduced to solve multi-dimensional problems with complicated and irregular geometric regions (He & Wei, 1989; Shi, 2002; Yuan, 2009, 2013).

Numerical simulation of semiconductor device begins at the use of the sequence iteration presented Gummel successfully in 1964 (Gummel, 1964). Considering actual computations, Douglas and Yuan put forward a useful finite difference method for simplified one-dimensional and two-dimensional models (constant coefficient, without consideration of temperature) and give the precise theoretical results firstly (Douglas & Yuan, 1987; Yuan, Ding & Yang, 1982). Then Yuan applies the method of characteristics respectively with finite element and mixed finite element to solve two-dimensional problems with variable coefficients and gives optimal order error in H^1 norm and L^2 norm (Yuan, 1991, 1993, 1991). In view of applications, Yuan discusses the effect of heat conduction to semiconductor device and gives the characteristic finite difference and upwind fractional steps finite difference of three dimensional problem on uniform partition and the convergence rate in discrete l^2 norm (Yuan, 1996, 2000, 2005, 2008). In numerical simulation of modern semiconductor device, the computation scale is huge, and the discretization consists of tens of thousand or several millions nodes, so a powerful parallel tool is introduced (He & Wei, 1989; Shi, 2002; Yuan, 2009, 2013). For the simplest parabolic equation, Dawson, Dupont and Du take the lead in discussing Galerkin domain decomposition method and theoretical analysis (Dawson & Dupont,

1992, 1994; Dawson, Du & Dupont, 1991; Dawson & Du, 1990). On the discussion how to simulate three-dimensional semiconductor transient problem of heat conduction efficiently, the authors state a type of domain decomposition with modified characteristic finite element and analyze the convergence and optimal order estimates in l^2 norm by using the techniques such as variation, domain decomposition, characteristics, energy norm, negative norm estimates, mathematical induction hypothesis and prior estimate theory and technique of partial differential equation. Numerical data of experimental example are shown consistent with theoretical convergence rate and by which it illustrates that this procedure is more efficient and applied successfully to solve international famous problems (He & Wei, 1989; Shi, 2002; Yuan, 2009, 2013; Bank, et al., 1985; Jerome, 1994; Seidmann, 1986; Lou, 1995). It is most valuable in model analysis, numerical method, principle research, theory and application of semiconductor device simulation.

This paper is organized as follows. In the first section, mathematical model, physical interpretation and some related research are introduced. Some notations and primary work are given in the second section. In the third section, the authors present the procedures of domain decomposition and modified characteristic finite element. In the fourth section, the authors attempt to give convergence analysis. We examine numerically the accuracy and parallelism of the scheme by an example. Some conclusions and discussions are stated in the last section. In this paper M and ε express general positive constant and general positive small constant, respectively, and they have different meanings at different places.

2. Mathematical Model and Physical Background

The mathematical model of semiconductor transient problem of heat conduction is described by an initial boundary value system of four partial differential equations (Yuan, 1996, 2000, 2005, 2008; Bank, et al., 1985; Jerome, 1994; Seidmann, 1986; Lou, 1995), where the potential is defined by an elliptic equation, the concentrations of electron and hole are defined by convection-diffusion equations and the temperature is defined by a heat conduction equation. Electronic field potential is generated by the intensity in the electron equation, the hole concentration equation and the heat conduction equation, and becomes a system with initial and boundary conditions, which is defined on three variables spatial domain Ω as follows,

$$-\Delta\psi = \alpha(p - e + N(X)), \quad X = (x_1, x_2, x_3)^T \in \Omega, \quad t \in J = (0, \bar{T}], \quad (1)$$

$$\frac{\partial e}{\partial t} = \nabla \cdot (D_e(X)\nabla e - \mu_e(X)\nabla\psi) - R_1(e, p, T), \quad (X, t) \in \Omega \times J, \quad (2)$$

$$\frac{\partial p}{\partial t} = \nabla \cdot (D_p(X)\nabla p + \mu_p(X)p\nabla\psi) - R_2(e, p, T), \quad (X, t) \in \Omega \times J, \quad (3)$$

$$\rho(X)\frac{\partial T}{\partial t} - \Delta T = \{(D_p(X)\nabla p + \mu_p(X)p\nabla\psi) - (D_e(X)\nabla e - \mu_e(X)e\nabla\psi)\} \cdot \nabla\psi, \quad (X, t) \in \Omega \times J, \quad (4)$$

where the electronic field potential ψ , electron concentration e , hole concentration p , and temperature T are unknown functions. All the coefficients of (1)-(4) are greater than a positive number and less than another positive number. The number $\alpha = q/\varepsilon$ denotes the quotient of two positive constants, electronic load q and dielectric coefficient ε . The relation of diffusion coefficient $D_s(X)$ and mobility ratio $\mu_s(X)$ is formulated by $D_s(X) = U_T\mu_s(X)$ ($s = e, p$), where U_T means the quantity of heat (unit: volt). $N(X)$, a given function, is the difference of the donor impurity concentration $N_D(X)$ and the acceptor impurity concentration $N_A(X)$. The values of $N(X)$ vary quickly as X lies nearby semiconductor knot P-N. $R_i(e, p, T)$ ($i = 1, 2$) represents the recombination rate influenced by the electron concentration, the hole concentration and the temperature. $\rho = \rho(X)$ is the coefficient of heat conduction. Let gradient operator and Laplace operator of a function be denoted by $\nabla = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})^T$ and $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$.

Initial-value conditions are stated as follows,

$$e(X, 0) = e_0(X), \quad p(X, 0) = p_0(X), \quad T(X, 0) = T_0(X), \quad X \in \Omega. \quad (5)$$

Boundary-value conditions are defined by

$$\frac{\partial\psi}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial e}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial p}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial T}{\partial\gamma}\Big|_{\partial\Omega} = 0, \quad (X, t) \in \partial\Omega \times J, \quad (6)$$

where $\partial\Omega$ denotes the boundary of Ω , and γ is the outward unit normal vector of $\partial\Omega$.

Neumann boundary value conditions determine a family of electric field potential functions differed by a constant. So an additional condition is supplied to get a unique formulation

$$\int_{\Omega} \psi dX = 0, \quad t \in J, \tag{7a}$$

A compatibility condition is given,

$$\int_{\Omega} (p - e + N) dX = 0, \quad t \in J. \tag{7b}$$

In general, the problem (1)-(7) is supposed to be positive definite,

$$(C) \quad 0 < D_* \leq D_s(X) \leq D^*, \quad 0 < \mu_* \leq \mu_s(X) \leq \mu^*, \quad s = e, p; \quad 0 < \rho_* \leq \rho(X) \leq \rho^*, \tag{8}$$

where $D_*, D^*, \mu_*, \mu^*, \rho_*$ and ρ^* are positive constants. $R_i(e, p, T) (i = 1, 2)$ are Lipschitz continuous in ϵ_0 -neighbor centered by (e, p, T) .

Assume that exact solutions of (1)-(7) are regular,

$$(R) \quad \psi \in L^\infty(J; W^{k+1}(\Omega)), \quad e, p, T \in L^\infty(J; W^{l+1}(\Omega)), \quad \frac{\partial^2 e}{\partial \tau_e^2}, \frac{\partial^2 p}{\partial \tau_p^2}, \frac{\partial^2 T}{\partial t^2} \in L^\infty(J; L^2(\Omega)). \tag{9}$$

3. Notations and Preparations

For simplification, let the computational domain $\Omega = \{(x_1, x_2, x_3) | 0 < x_1 < 1, 0 < x_2 < 1, 0 < x_3 < 1\}$ be decomposed into two cuboids $\Omega_1 = \{(x_1, x_2, x_3) | 0 < x_1 < 1/2, 0 < x_2 < 1, 0 < x_3 < 1\}$, $\Omega_2 = \{(x_1, x_2, x_3) | 1/2 < x_1 < 1, 0 < x_2 < 1, 0 < x_3 < 1\}$, whose interior boundary is $\Gamma = \{(x_1, x_2, x_3) | x_1 = 1/2, 0 < x_2 < 1, 0 < x_3 < 1\}$, as in Fig. 1. We use approximation of derivatives of delta function at several points in this work, and for further

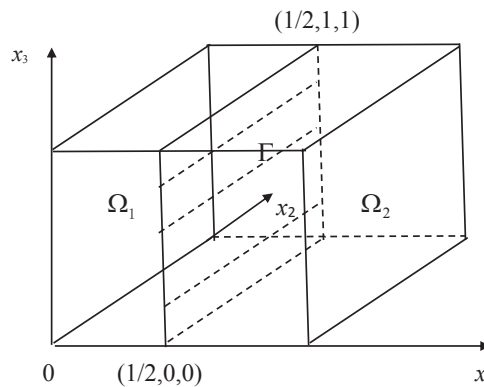


Figure 1. Sketch of domain decomposition partition $\Omega_1, \Omega_2, \Gamma$

reference we define two special functions Φ_2 and Φ_4 as follows (Dawson & Dupont, 1992, 1994; Dawson, Du & Dupont, 1991; Dawson & Du, 1990).

$$\Phi_2(x_1) = \begin{cases} 1 - x_1, & 0 \leq x_1 \leq 1, \\ x_1 + 1, & -1 \leq x_1 \leq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{10a}$$

$$\Phi_4(x_1) = \begin{cases} (x_1 - 2)/12, & 1 \leq x_1 \leq 2, \\ -5x_1/4 + 7/6, & 0 \leq x_1 \leq 1, \\ 5x_1/4 + 7/6, & -1 \leq x_1 \leq 0, \\ -(x_1 + 2)/12, & -2 \leq x_1 \leq -1, \\ 0, & \text{otherwise.} \end{cases} \tag{10b}$$

Note that if $p(x_1)$ is a polynomial of degree at most one, then

$$\int_{-\infty}^{\infty} p(x_1) \Phi_2(x_1) dx_1 = p(0), \tag{11a}$$

and if $p(x_1)$ is a polynomial of degree at most three, then

$$\int_{-\infty}^{\infty} p(x_1)\Phi_4(x_1)dx_1 = p(0). \tag{11b}$$

Definition 1: For any number $H \in (0, \frac{1}{2})$, define a normalized function

$$\Phi(x_1) = \Phi_m((x_1 - 1/2)/H)/H, \quad m = 2, 4. \tag{12}$$

Let $N_{h,j}$ be a finite-dimensional finite element space $H^1(\Omega_j)$ ($j = 1, 2$), and let $N_h(\Omega)$ be a finite-dimensional finite element subspace of l degree of $L^2(\Omega)$. Moreover, if a function v comes from N_h , then $v|_{\Omega_j}$ must belong to $N_{h,j}$. Note that a given function $v \in N_h(\Omega)$ has a well-defined jump $[v]$ on Γ ,

$$[v]_{(\frac{1}{2}, x_2, x_3)} = v(\frac{1}{2} + 0, x_2, x_3) - v(\frac{1}{2} - 0, x_2, x_3). \tag{13}$$

Definition 2: Define a bilinear mapping $\bar{D}_s(u, v)$,

$$\bar{D}_s(u, v) = \int_{\Omega_1 \cup \Omega_2} D_s(X)\nabla u \cdot \nabla v dx_1 dx_2 dx_3 + \lambda_s \int_{\Omega_1 \cup \Omega_2} uv dx_1 dx_2 dx_3, \quad s = e, p, T, \tag{14}$$

where $u, v \in H^1(\Omega_j)$, $j = 1, 2$, and $D_s(X)$ ($s = e, p$) are all positive definite functions, $D_T = 1$, and λ_s is a positive constant.

Definition 3: An integral operator approximating normal derivative at interior boundary is defined as follows

$$B(\psi)(\frac{1}{2}, x_2, x_3) = - \int_0^1 \Phi'(x_1)\psi(x_1, x_2, x_3)dx_1, \tag{15}$$

where Φ formulated by (12) is used.

Let (\cdot, \cdot) denote a product inner in $L^2(\Omega_1 \cup \Omega_2)$, and omit the subscript notation $(\psi, \rho) = (\psi, \rho)_{\Omega}$ as $\Omega_1 \cup \Omega_2 = \Omega$. Consider a function ψ of $H^1(\Omega_1)$ and $H^1(\Omega_2)$, and give a special norm,

$$\|\psi\|_s^2 = \bar{D}_s(\psi, \psi) + H^{-1}\|D_s[\psi]\|_{L^2(\Gamma)}^2, \quad s = e, p, T. \tag{16}$$

Note

$$\begin{aligned} (D(x_1, x_2, x_3)B(\psi), [\psi])_{\Gamma} &= - \int_0^1 \int_0^1 D(\frac{1}{2}, x_2, x_3) \int_0^1 \Phi'(x_1)\psi(x_1, x_2, x_3)dx_1 [\psi](\frac{1}{2}, x_2, x_3)dx_2 dx_3, \\ \int_0^1 \Phi'(x_1)\psi(x_1, x_2, x_3)dx_1 &= \psi(x_1, x_2, x_3)\Phi(x_1)|_0^1 - \int_0^1 \Phi(x_1)\psi_{x_1}(x_1, x_2, x_3)dx_1 \\ &= -\frac{1}{H}[\psi](\frac{1}{2}, x_2, x_3) - \int_0^1 \Phi(x_1)\psi_{x_1}(x_1, x_2, x_3)dx_1, \end{aligned}$$

we have

$$\begin{aligned} (D(x_1, x_2, x_3)B(\psi), [\psi])_{\Gamma} &= \frac{1}{H} \int_0^1 \int_0^1 D(\frac{1}{2}, x_2, x_3)[\psi]^2(\frac{1}{2}, x_2, x_3)dx_2 dx_3 \\ &\quad + \int_0^1 \int_0^1 D(\frac{1}{2}, x_2, x_3) \int_0^1 \Phi(x_1)\psi_{x_1}(x_1, x_2, x_3)dx_1 [\psi](\frac{1}{2}, x_2, x_3)dx_2 dx_3. \end{aligned} \tag{17}$$

The second term is formulated in another expression,

$$\begin{aligned} &\int_0^1 \int_0^1 D^{1/2}(\frac{1}{2}, x_2, x_3) \int_{\frac{1}{2}-H}^{\frac{1}{2}+H} D^{1/2}(\frac{1}{2}, x_2, x_3)\Phi(x_1)\psi_{x_1}(x_1, x_2, x_3)dx_1 [\psi](\frac{1}{2}, x_2, x_3)dx_2 dx_3 \\ &\leq \int_0^1 \int_0^1 D^{1/2}(\frac{1}{2}, x_2, x_3) \left(\int_0^1 \Phi^2(x_1)dx_1 \right)^{1/2} \left(\int_{\frac{1}{2}-H}^{\frac{1}{2}+H} D(\frac{1}{2}, x_2, x_3)\psi_{x_1}^2(x_1, x_2, x_3)dx_1 \right)^{1/2} \\ &\quad \cdot [\psi](\frac{1}{2}, x_2, x_3)dx_2 dx_3 \\ &\leq \left(\frac{2}{3H} \right)^{1/2} \left(\int_0^1 \int_0^1 D(\frac{1}{2}, x_2, x_3)[\psi]^2(\frac{1}{2}, x_2, x_3)dx_2 dx_3 \right)^{1/2} \\ &\quad \cdot \left(\int_0^1 \int_0^1 \int_{\frac{1}{2}-H}^{\frac{1}{2}+H} D(\frac{1}{2}, x_2, x_3)\psi_{x_1}^2(x_1, x_2, x_3)dx_1 dx_2 dx_3 \right)^{1/2}. \end{aligned}$$

Note that the value of $D(x_1, x_2, x_3)$ at $x_1 = 1/2$ is defined by

$$D\left(\frac{1}{2}, x_2, x_3\right) = D(x_1, x_2, x_3) + \left(x_1 - \frac{1}{2}\right) \frac{\partial D}{\partial x_1}(\xi_1(x_1), x_2, x_3),$$

then we have

$$\begin{aligned} & \int_0^1 \int_0^1 \int_{\frac{1}{2}-H}^{\frac{1}{2}+H} D\left(\frac{1}{2}, x_2, x_3\right) \psi_{x_1}^2(x_1, x_2, x_3) dx_1 dx_2 dx_3 \\ &= \int_0^1 \int_0^1 \int_{\frac{1}{2}-H}^{\frac{1}{2}+H} \left[D(x_1, x_2, x_3) + \left(x_1 - \frac{1}{2}\right) \frac{\partial D}{\partial x_1}(\xi_1(x_1), x_2, x_3) \right] \psi_{x_1}^2(x_1, x_2, x_3) dx_1 dx_2 dx_3 \\ &\leq (1 + M^* H) \int_0^1 \int_0^1 \int_{\frac{1}{2}-H}^{\frac{1}{2}+H} D(x_1, x_2, x_3) \psi_{x_1}^2(x_1, x_2, x_3) dx_1 dx_2 dx_3, \end{aligned}$$

where $M^* = \max_{\substack{x_1 \in (\frac{1}{2}-H, \frac{1}{2}+H) \\ (x_2, x_3) \in (0, 1) \times (0, 1)}} \frac{\left| \frac{\partial D}{\partial x_1}(\xi_1(x_1), x_2, x_3) \right|}{D(x_1, x_2, x_3)}$.

Continue to find a positive constant M_0 such that

$$\bar{D}_s(\psi, \psi) + (D_s B(\psi), [\psi])_\Gamma \geq \frac{1}{M_0} \|\psi\|_s^2, \quad s = e, p, T, \tag{18a}$$

or

$$\|\psi\|_s^2 \leq M_0 \left\{ \bar{D}_s(\psi, \psi) + (D_s B(\psi), [\psi])_\Gamma \right\}, \quad s = e, p, T. \tag{18b}$$

Similarly, we have the following estimates for $0 \leq t \leq T$,

$$\|B(\psi)\|_{L^2(\Gamma)}^2 \leq M_1 H^{-3} \|\psi\|_0^2, \tag{19a}$$

$$\|B(\psi)\|_{L^2(\Gamma)} \leq M_2 H^{-1} \|\psi\|_{0,\infty}, \tag{19b}$$

$$\left\| \frac{\partial u(\cdot, t)}{\partial \gamma} - B(u)(\cdot, t) \right\|_{L^2(\Gamma)} \leq M_3 H^m, \tag{19c}$$

where M_1, M_2, M_3 are positive constants, $m = 2, 4$, and $\frac{\partial u}{\partial \gamma}$ denotes the normal derivative of u across interior boundary Γ .

4. Domain Decomposition Scheme Modified with Characteristic Finite Element

The parallel procedures are illustrated in this section, which consists of a finite element scheme for the electric field potential and a domain decomposition scheme modified with characteristics for the electron concentration, hole concentration and temperature. Firstly, rewrite the potential equation (1),

$$(\nabla \psi, \nabla v) = \alpha (p - e + N, v), \quad \forall v \in H^1(\Omega), t \in J, \tag{20a}$$

$$(\psi, 1) = 0. \tag{20b}$$

Secondly, (2)-(4) are reformulated as follows

$$\frac{\partial e}{\partial t} = \nabla \cdot (D_e(X) \nabla e) + \mu_e \underline{u} \cdot \nabla e + \alpha \mu_e e (p - e + N) + e \underline{u} \cdot \nabla \mu_e - R_1(e, p, T), \quad (X, t) \in \Omega \times J, \tag{21a}$$

$$\frac{\partial p}{\partial t} = \nabla \cdot (D_p(X) \nabla p) - \mu_p \underline{u} \cdot \nabla p - \alpha \mu_p p (p - e + N) - p \underline{u} \cdot \nabla \mu_p - R_2(e, p, T), \quad (X, t) \in \Omega \times J, \tag{21b}$$

$$\rho(X) \frac{\partial T}{\partial t} = \nabla \cdot (\nabla T) - \left\{ (D_p(X) \nabla p - \mu_p(X) p \underline{u}) - (D_e(X) \nabla e + \mu_e(X) e \underline{u}) \right\} \cdot \underline{u}, \quad (X, t) \in \Omega \times J, \tag{21c}$$

where $\underline{u} = \nabla \psi$.

Let $W_h = W_{h_\psi}$ denote a finite element space of k degree, and let h_ψ be the partition step, then we have

$$\inf_{v_h \in W_h} \|v - v_h\|_{L^2(\Omega)} \leq M \|v\|_{k+1} h_\psi^{k+1}. \tag{22}$$

Noting that the electric field potential changes very slow with respect to t , we can adopt a large step in its calculations. While in the computations of the electron concentration, hole concentration and temperature small steps are adopted. Some notations are given as follows, Δt_c , time step of the concentration equation, Δt_ψ , time step of the potential equation, $j = \Delta t_\psi / \Delta t_c$, $t^n = n\Delta t_c$, $t_m = m\Delta t_\psi$, $\psi^n = \psi(t^n)$, and $\psi_m = \psi(t_m)$. For a potential function $\psi(X, t)$, define a linear extrapolation $E\psi^n$ of the values at the closest two time levels to t^n ,

$$E\psi^n = \begin{cases} \psi_0, & t^n \leq t_1 \\ (1 + \gamma/j)\psi_m - \gamma/j\psi_{m-1}, & t_m < t^n < t_{m+1}, t^n = t_m + \gamma\Delta t_c. \end{cases}$$

where the subscripts correspond to potential time levels, superscripts to concentration time levels. The extrapolation can be applied for the vector function $\underline{u} = -\nabla\psi$, that is to say $E\underline{u}$ is defined similarly to $E\psi$ and has some same properties.

Electric field potential equation (20) is approximated by the following finite element scheme

$$(\nabla\psi_{h,m}, \nabla v_h) = \alpha(p_{h,m} - e_{h,m} + N_m, v_h), \quad \forall v_h \in W_h, \quad (23a)$$

$$(\psi_{h,m}, 1) = 0. \quad (23b)$$

Then the gradient of potential is computed by $\underline{u}_{h,m} = -\nabla\psi_{h,m}$.

The electron concentration equation (2), hole concentration equation (3) and heat conduction equation (4) are considered. Multiply them by $\omega \in N_h(\Omega)$, apply integration by parts, then we have weak forms of domain decomposition as follows

$$\begin{aligned} & \left(\frac{\partial e}{\partial t}, \omega\right)_\Omega - (\mu_e \underline{u} \cdot \nabla e, \omega)_\Omega + (D_e \nabla e, \nabla \omega)_\Omega + (D_e \frac{\partial e}{\partial \gamma}, [\omega])_\Gamma - (e \underline{u} \cdot \nabla \mu_e, \omega)_\Omega \\ & = \alpha(\mu_e e(p - e + N), \omega)_\Omega - (R_1(e, p, T), \omega)_\Omega, \quad \forall \omega \in N_h(\Omega), \end{aligned} \quad (24a)$$

$$\begin{aligned} & \left(\frac{\partial p}{\partial t}, \omega\right)_\Omega + (\mu_p \underline{u} \cdot \nabla p, \omega)_\Omega + (D_p \nabla p, \nabla \omega)_\Omega + (D_p \frac{\partial p}{\partial \gamma}, [\omega])_\Gamma + (p \underline{u} \cdot \nabla \mu_p, \omega)_\Omega \\ & = -\alpha(\mu_p p(p - e + N), \omega)_\Omega - (R_2(e, p, T), \omega)_\Omega, \quad \forall \omega \in N_h(\Omega), \end{aligned} \quad (24b)$$

$$\begin{aligned} & \left(\rho \frac{\partial T}{\partial t}, \omega\right)_\Omega - (\nabla T, \nabla \omega)_\Omega + \left(\frac{\partial T}{\partial \gamma}, [\omega]\right)_\Gamma \\ & = [(D_p \nabla p + \mu_p p \nabla \psi) - (D_e \nabla e - \mu_e e \nabla \psi)] \cdot \nabla \psi, \omega)_\Omega, \quad \forall \omega \in N_h(\Omega). \end{aligned} \quad (24c)$$

Noting that the flow moves essentially along the characteristics, we apply a modified procedure of characteristics for the first-order hyperbolic part of (2) and (3) to overcome numerical dispersion and oscillation. This kind of method has a high order accuracy and a fine stability in numerical simulation and a large time step can be adopted (Ewing 1983; Ewing, Russell & Wheeler, 1984; Douglas & Russell, 1982; Russell, 1985; Douglas & Yuan, 1986; Ewing, Yuan & Li, 1989). Let $\tau = \tau(X, t)$ denote the unit vector in characteristic direction $(-\mu_e u_1, -\mu_e u_2, -\mu_e u_3, 1)$ and let $\tau_p = \tau_p(X, t)$ be the unit vector in $(\mu_p u_1, \mu_p u_2, \mu_p u_3, 1)$ -direction. Let $\Phi_s = \left[1 + \mu_s^2 |\underline{u}|^2\right]^{1/2}$, $s = e, p$, and compute the characteristic directional derivative by

$$\Phi_e \frac{\partial}{\partial \tau_e} = \frac{\partial}{\partial t} - \mu_e \underline{u} \cdot \nabla, \quad \Phi_p \frac{\partial}{\partial \tau_p} = \frac{\partial}{\partial t} + \mu_p \underline{u} \cdot \nabla.$$

Then (24a) and (24b) are changed into

$$\begin{aligned} & \left(\Phi_e \frac{\partial e}{\partial \tau_e}, \omega\right)_\Omega + (D_e \nabla e, \nabla \omega)_\Omega + (D_e \frac{\partial e}{\partial \gamma}, [\omega])_\Gamma - (e \underline{u} \cdot \nabla \mu_e, \omega)_\Omega \\ & = \alpha(\mu_e e(p - e + N), \omega)_\Omega - (R_1(e, p, T), \omega)_\Omega, \quad \forall \omega \in N_h(\Omega), \end{aligned} \quad (25a)$$

$$\begin{aligned} & \left(\Phi_p \frac{\partial p}{\partial \tau_p}, \omega\right)_\Omega + (D_p \nabla p, \nabla \omega)_\Omega + (D_p \frac{\partial p}{\partial \gamma}, [\omega])_\Gamma + (p \underline{u} \cdot \nabla \mu_p, \omega)_\Omega \\ & = -\alpha(\mu_p p(p - e + N), \omega)_\Omega - (R_2(e, p, T), \omega)_\Omega, \quad \forall \omega \in N_h(\Omega). \end{aligned} \quad (25b)$$

Approximate $\frac{\partial e^{n+1}}{\partial \tau_e} = \frac{\partial e}{\partial \tau_e}(X, t^{n+1})$ by a backward difference quotient in τ_e -direction,

$$\frac{\partial e^{n+1}}{\partial \tau_e}(X) \approx \frac{e^{n+1} - e^n(X + \mu_e \underline{u}^{n+1} \Delta t)}{\Delta t(1 + \mu_e^2 |\underline{u}^{n+1}|^2)^{1/2}},$$

and approximate $\frac{\partial p^{n+1}}{\partial \tau_p}(X)$ in τ_p ,

$$\frac{\partial p^{n+1}}{\partial \tau_p}(X) \approx \frac{p^{n+1} - p^n(X - \mu_p \underline{u}^{n+1} \Delta t)}{\Delta t(1 + \mu_p^2 |\underline{u}^{n+1}|^2)^{1/2}}.$$

Then the procedures of domain decomposition with characteristic finite element are stated as follows to approximate the concentrations (25),

$$\begin{aligned} & \left(\frac{e_h^{n+1} - \hat{e}_h^n}{\Delta t_c}, \omega_h \right)_\Omega + (D_e \nabla e_h^{n+1}, \nabla \omega_h)_\Omega + (D_e B(e_h^n), [\omega_h])_\Gamma \\ & = \alpha(\mu_e e_h^n(\hat{p}_h^n - \hat{e}_h^n + N), \omega_h)_\Omega + (\hat{e}_h^n E \underline{U}_h^{n+1} \cdot \nabla \mu_e, \omega_h)_\Omega - (R_1(\hat{e}_h^n, \hat{p}_h^n, T_h^n), \omega_h)_\Omega, \forall \omega_h \in N_h(\Omega), \end{aligned} \tag{26a}$$

$$\begin{aligned} & \left(\frac{p_h^{n+1} - \hat{p}_h^n}{\Delta t_c}, \omega_h \right)_\Omega + (D_p \nabla p_h^{n+1}, \nabla \omega_h)_\Omega + (D_p B(p_h^n), [\omega_h])_\Gamma \\ & = -\alpha(\mu_p p_h^n(\hat{p}_h^n - \hat{e}_h^n + N), \omega_h)_\Omega - (\hat{p}_h^n E \underline{U}_h^{n+1} \cdot \nabla \mu_p, \omega_h)_\Omega - (R_2(\hat{e}_h^n, \hat{p}_h^n, T_h^n), \omega_h)_\Omega, \forall \omega_h \in N_h(\Omega), \end{aligned} \tag{26b}$$

where $\hat{e}_h^n = e_h^n(\hat{X}_e^n)$, $\hat{X}_e^n = X + \mu_e E \underline{U}_h^{n+1} \Delta t_c$, $\hat{p}_h^n = p_h^n(\hat{X}_p^n)$, $\hat{X}_p^n = X - \mu_p E \underline{U}_h^{n+1} \Delta t_c$, $\underline{U}_{h,m} = -\nabla \psi_{h,m}$, and $\underline{U}_{h,m-1} = -\nabla \psi_{h,m-1}$. Noting that the values of \hat{X}_e^n and \hat{X}_p^n maybe lie outside the boundary $\partial \Omega$, while we can use the reflection of the boundary because of Neumann conditions (6) and define the values of $\hat{e}_h^n(\hat{X}_e^n)$ and $\hat{p}_h^n(\hat{X}_p^n)$ (Douglas & Yuan, 1986; Ewing, Yuan & Li, 1989).

Similarly, the heat conduction equation is discretized by the method of domain decomposition with finite element,

$$\begin{aligned} & \left(\rho \frac{T_h^{n+1} - T_h^n}{\Delta t}, \omega_h \right)_\Omega + (\nabla T_h^{n+1}, \nabla \omega_h)_\Omega + (B(T_h^n), [\omega_h])_\Gamma \\ & = ([(D_p \nabla p_h^n - \mu_p p_h^n E \underline{U}_h^{n+1}) - (D_e \nabla e_h^n + \mu_e e_h^n E \underline{U}_h^{n+1})] \cdot E \underline{U}_h^{n+1}, \omega_h)_\Omega, \forall \omega_h \in N_h(\Omega). \end{aligned} \tag{26c}$$

The program works for a time step as follows. Firstly, given the initial approximation $\{e_h^0, p_h^0, T_h^0\}$, $\{\psi_{h,0}, \underline{U}_{h,0}\}$ is computed by the finite element scheme (23). Secondly, $\{e_h^1, p_h^1, T_h^1\}$, $\{e_h^2, p_h^2, T_h^2\}$, \dots , $\{e_h^j, p_h^j, T_h^j\}$ are computed in parallel by the domain decomposition scheme with finite element (26). It continues to get $\{\psi_{h,1}, \underline{U}_{h,1}\}$ by the values $\{e_h^j, p_h^j, T_h^j\} = \{e_{h,1}, p_{h,1}, T_{h,1}\}$ and (23), and as a result, the solutions $\{e_h^{j+1}, p_h^{j+1}, T_h^{j+1}\}, \dots, \{e_{h,2}, p_{h,2}, T_{h,2}\}$ are obtained in parallel by (26). Finally, numerical solutions can be shown after a series of above computation and they exist and are sole by the positive definite condition (C).

5. Convergence Analysis

Several subsidiary elliptic projections are introduced first in this section, and let $\{\tilde{\psi}\} : J \rightarrow N_h$ be defined on $J = (0, T]$,

$$(\nabla(\psi - \tilde{\psi}), \nabla v_h) = 0, \forall v_h \in W_h, \tag{27a}$$

$$(\psi - \tilde{\psi}, 1) = 0. \tag{27b}$$

Let $\theta = \psi - \tilde{\psi}_h$ and $\eta = \psi_h - \tilde{\psi}_h$ be error functions and they are estimated as follows (Ciarlet, 1978; Wheeler, 1973),

$$\|\theta\|_0 + h_\psi \|\theta\|_1 \leq M \|\psi\|_{k+1} h_\psi^{k+1}, \tag{28a}$$

$$\left\| \frac{\partial \theta}{\partial t} \right\|_0 + h_\psi \left\| \frac{\partial \theta}{\partial t} \right\|_1 \leq M \left\{ \|\psi\|_{k+1} + \left\| \frac{\partial \psi}{\partial t} \right\|_{k+1} \right\} h_\psi^{k+1}. \tag{28b}$$

Define elliptic mapping $\{\tilde{e}, \tilde{p}, \tilde{T}\} : J \rightarrow N_h \times N_h \times N_h$ as follows,

$$\bar{D}_e(e(\cdot, t) - \tilde{e}(\cdot, t), \omega_h) + \lambda_e(e(\cdot, t) - \tilde{e}(\cdot, t), \omega_h) = 0, \forall \omega_h \in N_h, \tag{29a}$$

$$\bar{D}_p(p(\cdot, t) - \tilde{p}(\cdot, t), \omega_h) + \lambda_p(p(\cdot, t) - \tilde{p}(\cdot, t), \omega_h) = 0, \forall \omega_h \in N_h, \tag{29b}$$

$$\bar{D}_T(T(\cdot, t) - \tilde{T}(\cdot, t), \omega_h) + \lambda_T(T(\cdot, t) - \tilde{T}(\cdot, t), \omega_h) = 0, \forall \omega_h \in N_h, \tag{29c}$$

where the elliptic operator is coercive in $H^1(\Omega)$ for sufficiently large constant λ_e, λ_p and λ_T .

Initial approximation is given by

$$e_h^0 = \tilde{e}(0), p_h^0 = \tilde{p}(0), T_h^0 = \tilde{T}(0). \tag{30}$$

Introduce error functions denoted by $\xi_e = e_h - \tilde{e}$, $\zeta_e = e - \tilde{e}$, $\xi_p = p_h - \tilde{p}$, $\zeta_p = p - \tilde{p}$, $\pi = T_h - \tilde{T}$ and $\sigma = T - \tilde{T}$. By Galerkin method (Ciarlet, 1978; Wheeler, 1973),

$$\|\zeta_e\|_0 + h_c \|\zeta_e\|_1 \leq M \|e\|_{l+1} h_c^{l+1}, \tag{31a}$$

$$\|\zeta_p\|_0 + h_c \|\zeta_p\|_1 \leq M \|p\|_{l+1} h_c^{l+1}, \tag{31b}$$

$$\|\sigma\|_0 + h_c \|\sigma\|_1 \leq M \|T\|_{l+1} h_c^{l+1}, \tag{31c}$$

$$\left\| \frac{\partial \zeta_e}{\partial t} \right\|_0 + h_c \left\| \frac{\partial \zeta_e}{\partial t} \right\|_1 \leq M \left\{ \|e\|_{l+1} + \left\| \frac{\partial e}{\partial t} \right\|_{l+1} \right\} h_c^{l+1}, \tag{32a}$$

$$\left\| \frac{\partial \zeta_p}{\partial t} \right\|_0 + h_c \left\| \frac{\partial \zeta_p}{\partial t} \right\|_1 \leq M \left\{ \|p\|_{l+1} + \left\| \frac{\partial p}{\partial t} \right\|_{l+1} \right\} h_c^{l+1}, \tag{32b}$$

$$\left\| \frac{\partial \sigma}{\partial t} \right\|_0 + h_c \left\| \frac{\partial \sigma}{\partial t} \right\|_1 \leq M \left\{ \|T\|_{l+1} + \left\| \frac{\partial T}{\partial t} \right\|_{l+1} \right\} h_c^{l+1}, \tag{32c}$$

where $\Omega = \Omega_1 \cup \Omega_2$, and h_c denotes the spacial step of finite element space $N_h(\Omega)$.

Theorem 1 Suppose that exact solutions of (1)-(7) are suitably regular, $\psi \in L^\infty(J; W^{k+1}(\Omega))$, $e, p, T \in L^\infty(J; W^{l+1}(\Omega))$, $\frac{\partial^2 e}{\partial \tau_e^2}, \frac{\partial^2 p}{\partial \tau_p^2}, \frac{\partial^2 T}{\partial \tau^2} \in L^\infty(J; L^\infty(\Omega))$. Adopt the parallel procedure modified characteristic finite element (23) and (26) on Ω_1 and Ω_2 , and suppose that the relation of partition parameters is

$$\Delta t = O(h_c^2), \quad h_\psi = O(h_c), \quad \Delta t_c \leq M_1^{-1} H^2, \quad h_c^{l+1} = o(H), \tag{33}$$

where M_1 is a positive constant and $k \geq 1$ and $l \geq 1$ are the indexes of finite element space. We have

$$\begin{aligned} & \|\psi - \psi_h\|_{\tilde{L}^\infty(J; W)} + \|e - e_h\|_{\tilde{L}^\infty(J; L^2(\Omega))} + \|p - p_h\|_{\tilde{L}^\infty(J; L^2(\Omega))} + \|T - T_h\|_{\tilde{L}^\infty(J; L^2(\Omega))} \\ & \leq M^* \left\{ \Delta t_c + H^{m+1/2} + h_\psi^k + h_c^{l+1} + H^{-1} h_c^{l+1} \right\}, \end{aligned} \tag{34}$$

where $\|g\|_{\tilde{L}^\infty(J; X)} = \sup_{n\Delta t \leq T} \|g^n\|_X$ and the constant M^* is dependent on ψ, e, p, T and their derivatives.

Proof. The potential function ψ is considered firstly, and $\psi_h - \tilde{\psi}$ is estimated. By (20) ($t = t_m$), (27) ($t = t_m$) and (23), we have

$$\|\nabla \eta_m\|^2 \leq M \left\{ \|\xi_{e,m}\|^2 + \|\xi_{p,m}\|^2 + h_c^{2(l+1)} \right\}. \tag{35}$$

The electron concentration e is discussed secondly. Subtract (26a) from (24a) ($t = t^{n+1}$), and use (29a) ($t = t^{n+1}$),

$$\begin{aligned} & \left(\frac{\xi_e^{n+1} - \xi_e^n}{\Delta t_c}, \omega_h \right) + (D_e \nabla \xi_e^{n+1}, \omega_h) + (D_e B(\xi_e^n), [\omega_h])_\Gamma \\ & = \left(\frac{e^{n+1} - e^n}{\Delta t_c} - \frac{\partial e^{n+1}}{\partial t} - \mu_e E \underline{U}_h^{n+1} \cdot \nabla e^{n+1}, \omega_h \right) + \lambda_e (\xi_e^{n+1}, \omega_h) \\ & + \alpha \left(\mu_e [\hat{e}_h^n (\hat{p}_h^n - \hat{e}_h^n + N) - e^{n+1} (p^{n+1} - e^{n+1} + N)], \omega_h \right) + \left([\hat{e}_h^n E \underline{U}_h^{n+1} - e^{n+1} \underline{u}^{n+1}] \cdot \nabla \mu_e, \omega_h \right) \\ & - (R_1(\hat{e}_h^n, \hat{p}_h^n, T_h^n) - R_1(e^{n+1}, p^{n+1}, T^{n+1}), \omega_h) + (\mu_e (E \underline{U}_h^{n+1} - \underline{u}^{n+1}) \cdot \nabla e^{n+1}, \omega_h) \\ & + \left(\frac{\hat{\xi}_e^n - \xi_e^n}{\Delta t_c}, \omega_h \right) + \left(\frac{\xi_e^{n+1} - \hat{\xi}_e^n}{\Delta t_c}, \omega_h \right) + \left(D_e \left(\frac{\partial e^{n+1}}{\partial \gamma} - B(e_h^n) \right), [\omega_h] \right)_\Gamma, \quad \forall \omega_h \in N_h, \end{aligned} \tag{36}$$

where $\hat{e}^n = e^n(\hat{X}_e^n)$, $\hat{\xi}_e^n = \xi_e^n(\hat{X}_e^n)$, $\hat{\zeta}_e^n = \zeta_e^n(\hat{X}_e^n)$ and $\hat{X}_e^n = X + \mu_e E \underline{U}_h^{n+1} \Delta t_c$.

Take $\omega_h = \xi_e^{n+1}$ as a test function in (36),

$$\begin{aligned} & \left(\frac{\xi_e^{n+1} - \xi_e^n}{\Delta t_c}, \xi_e^{n+1} \right) + (D_e \nabla \xi_e^{n+1}, \xi_e^{n+1}) + \lambda_e (\xi_e^{n+1}, \xi_e^{n+1}) + (D_e B(\xi_e^n), [\xi_e^{n+1}])_\Gamma \\ & = (D_e B(\xi_e^{n+1} - \xi_e^n), [\xi_e^{n+1}])_\Gamma + \left(D_e \left(\frac{\partial e^{n+1}}{\partial \gamma} - \frac{\partial e^n}{\partial \gamma} \right), [\xi_e^{n+1}] \right)_\Gamma + \left(D_e \left(\frac{\partial e^n}{\partial \gamma} - B(e^n) \right), [\xi_e^{n+1}] \right)_\Gamma \\ & + (D_e B(\xi_e^n), [\xi_e^{n+1}])_\Gamma + \left(\frac{e^{n+1} - e^n}{\Delta t_c} - \frac{\partial e^{n+1}}{\partial t} - \mu_e E \underline{U}_h^{n+1} \cdot \nabla e^{n+1}, \xi_e^{n+1} \right) + \left(\frac{\xi_e^{n+1} - \hat{\xi}_e^n}{\Delta t_c}, \xi_e^{n+1} \right) \\ & + \left(\frac{\hat{\xi}_e^n - \xi_e^n}{\Delta t_c}, \xi_e^{n+1} \right) + \lambda_e (\xi_e^{n+1}, \xi_e^{n+1}) + \lambda_e (\xi_e^{n+1}, \xi_e^{n+1}) - (R_1(\hat{e}_h^n, \hat{p}_h^n, T_h^n) \end{aligned}$$

$$\begin{aligned}
 & -R_1(e^{n+1}, p^{n+1}, T^{n+1}), \xi_e^{n+1}) + \alpha \left(\mu_e \left[e_h^n (\hat{p}_h^n - \hat{p}_h^n + N) - e^{n+1} (p^{n+1} - e^{n+1} + N) \right], \xi_e^{n+1} \right) \\
 & + \left(\left[\hat{p}_h^n E \underline{U}_h^{n+1} - e^{n+1} \underline{u}^{n+1} \right] \cdot \nabla \mu_e, \xi_e^{n+1} \right) + \left(\mu_e \left(E \underline{U}_h^{n+1} - \underline{u}^{n+1} \right) \cdot \nabla e^{n+1}, \xi_e^{n+1} \right).
 \end{aligned} \tag{37}$$

The terms on the left-hand side are estimated as follows,

$$\left(\frac{\xi_e^{n+1} - \xi_e^n}{\Delta t_c}, \xi_e^{n+1} \right) = \frac{1}{2\Delta t} \left\{ \|\xi_e^{n+1}\|^2 - \|\xi_e^n\|^2 \right\} + \frac{1}{2\Delta t} \|\xi_e^{n+1} - \xi_e^n\|^2, \tag{38a}$$

$$\left(D_e \nabla \xi_e^{n+1}, \xi_e^{n+1} \right) + \lambda_e \left(\xi_e^{n+1}, \xi_e^{n+1} \right) + \left(D_e B(\xi_e^n), [\xi_e^{n+1}] \right)_\Gamma \geq M_0^{-1} \|\xi_e^{n+1}\|_e^2. \tag{38b}$$

The terms on the right hand side of (37) are estimated later. Using (19), we have for positive constants $M_i (i = 1, 2, 3)$,

$$\begin{aligned}
 & \left(D_e B(\xi_e^{n+1} - \xi_e^n), [\xi_e^{n+1}] \right)_\Gamma \leq M_1 \|B(\xi_e^{n+1} - \xi_e^n)\|_{L^2(\Gamma)} \cdot \|[\xi_e^{n+1}]\|_{L^2(\Gamma)} \\
 & \leq M_1 H^{-3/2} \|\xi_e^{n+1} - \xi_e^n\| \cdot H^{1/2} \|\xi_e^{n+1}\| \leq M_1 H^{-2} \|\xi_e^{n+1} - \xi_e^n\|^2 + \varepsilon \|\xi_e^{n+1}\|^2,
 \end{aligned} \tag{39a}$$

$$\begin{aligned}
 & \left(D_e \left[\frac{\partial e^{n+1}}{\partial \gamma} - \frac{\partial e^n}{\partial \gamma} \right], [\xi_e^{n+1}] \right)_\Gamma \leq M_2 \left\| \frac{\partial e^{n+1}}{\partial \gamma} - \frac{\partial e^n}{\partial \gamma} \right\|_{L^2(\Gamma)} \cdot \|[\xi_e^{n+1}]\|_{L^2(\Gamma)} \\
 & \leq M_2 \Delta t H^{1/2} \|\xi_e^{n+1}\| \leq M_2 (\Delta t_c)^2 H + \varepsilon \|\xi_e^{n+1}\|^2,
 \end{aligned} \tag{39b}$$

$$\left(D_e \left[\frac{\partial e^n}{\partial \gamma} - B(e^n) \right], [\xi_e^{n+1}] \right)_\Gamma \leq M_3 H^{2m+1} + \varepsilon \|\xi_e^{n+1}\|^2, \tag{39c}$$

$$\left(D_e B(\xi_e^n), [\xi_e^{n+1}] \right)_\Gamma \leq M_3 H^{-2} \|\xi_e^n\|^2 + \varepsilon \|\xi_e^{n+1}\|^2 \leq M_3 H^{-2} h_c^{2(l+1)} + \varepsilon \|\xi_e^{n+1}\|^2. \tag{39d}$$

Take Δt_c sufficiently small,

$$2\Delta t \leq M_1^{-1} H^2. \tag{40}$$

Then

$$\frac{1}{2\Delta t} \|\xi_e^{n+1} - \xi_e^n\|^2 \geq M_1 H^{-2} \|\xi_e^{n+1} - \xi_e^n\|^2. \tag{41}$$

An induction hypothesis is given,

$$\sup_{0 \leq m \leq (L-1)/j} \|\nabla \eta_m\|_{0,\infty} \rightarrow 0, \quad \sup_{0 \leq n \leq L} \max \left\{ \|\xi_e^n\|_{0,\infty}, \|\xi_p^n\|_{0,\infty}, \|\pi^n\|_{0,\infty} \right\} \rightarrow 0, \quad h_c \rightarrow 0. \tag{42}$$

Other terms on the right hand side are estimated. Note that

$$\left\| \frac{e^{n+1} - \hat{e}^n}{\Delta t_c} - \frac{\partial e^{n+1}}{\partial t} - \mu_e E \underline{U}_h^{n+1} \cdot \nabla e^{n+1} \right\|_0^2 \leq \Delta t_c \|\Phi_e\|_{0,\infty} \int_\Omega \int_{(\hat{x}, t^n)}^{(X, t^{n+1})} \left| \frac{\partial^2 e}{\partial \tau_e^2} \right| dt dX,$$

and Φ_e is bounded because of (42), we have

$$\left(\frac{e^{n+1} - \hat{e}^n}{\Delta t_c} - \frac{\partial e^{n+1}}{\partial t} - \mu_e E \underline{U}_h^{n+1} \cdot \nabla e^{n+1}, \xi_e^{n+1} \right) \leq M \left\{ \Delta t_c \left\| \frac{\partial^2 e}{\partial \tau_e^2} \right\|_{L^2(J^n; L^2(\Omega))}^2 + \|\xi_e^{n+1}\|_0^2 \right\}, \tag{43}$$

where $J^n = (t^n, t^{n+1}]$.

It follows from negative norm estimate and induction hypothesis (42),

$$\begin{aligned}
 & \left(\frac{\xi_e^{n+1} - \hat{\xi}_e^n}{\Delta t}, \xi_e^{n+1} \right) = \left(\frac{\xi_e^{n+1} - \xi_e^n}{\Delta t}, \xi_e^{n+1} \right) + \left(\frac{\xi_e^n - \hat{\xi}_e^n}{\Delta t}, \xi_e^{n+1} \right) \\
 & \leq M \left\{ (\Delta t)^{-1} \left\| \frac{\partial \xi_e}{\partial t} \right\|_{L^2(J^n; L^2(\Omega))}^2 + \|\xi_e^{n+1}\|^2 + \|\xi_e^n\|^2 \right\} + \varepsilon \|\nabla \xi_e^{n+1}\|^2,
 \end{aligned} \tag{44a}$$

$$\left(\frac{\hat{\xi}_e^n - \xi_e^n}{\Delta t_c}, \xi_e^{n+1} \right) \leq M \|\xi_e^n\|^2 + \varepsilon \|\nabla \xi_e^{n+1}\|^2, \tag{44b}$$

$$\lambda_e \left\{ (\xi_e^{n+1}, \xi_e^{n+1}) + (\xi_e^{n+1}, \xi_e^{n+1}) \right\} \leq M \left\{ h_c^{2(l+1)} + \|\xi_e^{n+1}\|^2 \right\}, \tag{44c}$$

$$\begin{aligned}
 & - \left(R_1(\hat{p}_h^n, \hat{p}_h^n, T_h^n) - R_1(e^{n+1}, p^{n+1}, T^{n+1}), \xi_e^{n+1} \right) \\
 & \leq M \left\{ (\Delta t)^2 + h_\psi^{2k} + h_c^{2(l+1)} + \|\xi_e^{n+1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\pi^n\|^2 \right\},
 \end{aligned} \tag{44d}$$

By (42), we can see that e_h^n , p_h^n and T_h^n are bounded, then we have

$$\begin{aligned} & \alpha \left(\mu_e \left[e_h^n (\hat{p}_h^n - \hat{e}_h^n + N) - e^{n+1} (p^{n+1} - e^{n+1} + N) \right], \xi_e^{n+1} \right) \\ & \leq M \left\{ (\Delta t_c)^2 + h_\psi^{2k} + h_c^{2(l+1)} + \|\xi_e^{n+1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 \right\}, \end{aligned} \tag{44e}$$

$$\begin{aligned} & \left([\hat{e}_h^n E \underline{U}_h^{n+1} - e^{n+1} \underline{u}^{n+1}] \cdot \nabla \mu_e, \xi_e^{n+1} \right) + \left(\mu_e (E \underline{U}_h^{n+1} - \underline{u}^{n+1}) \cdot \nabla e^{n+1}, \xi_e^{n+1} \right) \\ & \leq M \left\{ (\Delta t_c)^2 + h_\psi^{2k} + h_c^{2(l+1)} + \|\xi_e^{n+1}\|^2 + \|\xi_{e,[n/j]}\|^2 + \|\xi_{p,[n/j]}\|^2 \right\}. \end{aligned} \tag{44f}$$

Collecting (38)-(44), we derive

$$\begin{aligned} & \frac{1}{2\Delta t} \left\{ \|\xi_e^{n+1}\|^2 - \|\xi_e^n\|^2 \right\} + \frac{1}{M_0} \|\xi_e^{n+1}\|^2 \\ & \leq M \left\{ (\Delta t_c)^{-1} \left\| \frac{\partial \xi_e}{\partial t} \right\|_{L^2(J^n; L^2(\Omega))}^2 + \Delta t_c \left\| \frac{\partial^2 e}{\partial \tau_e^2} \right\|_{L^2(J^n; L^2(\Omega))}^2 + h_\psi^{2k} + h_c^{2(l+1)} + (\Delta t_c)^2 + (\Delta t_c)^2 H \right. \\ & \quad \left. + H^{-2} h_c^{2(l+1)} + H^{2m+1} + \|\xi_e^{n+1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\pi^n\|^2 + \|\xi_{e,[n/j]}\|^2 + \|\xi_{p,[n/j]}\|^2 \right\} \\ & \quad + \varepsilon \left\{ \|\nabla \xi_e^{n+1}\|^2 + \|\nabla \xi_e^n\|^2 \right\}. \end{aligned} \tag{45}$$

It continues to estimate the hole concentration. Subtract (26b) from (24b) ($t = t^{n+1}$), and use (29b) ($t = t^{n+1}$),

$$\begin{aligned} & \left(\frac{\xi_p^{n+1} - \xi_p^n}{\Delta t_c}, \omega_h \right) + \left(D_p \nabla \xi_p^{n+1}, \omega_h \right) + \left(D_p B(\xi_p^n), [\omega_h] \right)_\Gamma \\ & = \left(\frac{p^{n+1} - p^n}{\Delta t_c} - \frac{\partial p^{n+1}}{\partial t} - \mu_p E \underline{U}_h^{n+1} \cdot \nabla p^{n+1}, \omega_h \right) + \lambda_p \left(\xi_p^{n+1}, \omega_h \right) \\ & \quad - \alpha \left(\mu_p \left[p_h^n (\hat{p}_h^n - \hat{e}_h^n + N) - p^{n+1} (p^{n+1} - e^{n+1} + N) \right], \omega_h \right) - \left([\hat{p}_h^n E \underline{U}_h^{n+1} - p^{n+1} \underline{u}^{n+1}] \cdot \nabla \mu_p, \omega_h \right) \\ & \quad - \left(R_2(\hat{e}_h^n, \hat{p}_h^n, T_h^n) - R_2(e^{n+1}, p^{n+1}, T^{n+1}), \omega_h \right) + \left(\mu_p (E \underline{U}_h^{n+1} - \underline{u}^{n+1}) \cdot \nabla p^{n+1}, \omega_h \right) \\ & \quad + \left(\frac{\hat{e}_p^n - \xi_p^n}{\Delta t_c}, \omega_h \right) + \left(\frac{\xi_p^{n+1} - \hat{e}_p^n}{\Delta t_c}, \omega_h \right) + \left(D_p \left(\frac{\partial p^{n+1}}{\partial \gamma} - B(p_h^n) \right), [\omega_h] \right)_\Gamma, \quad \forall \omega_h \in N_h, \end{aligned} \tag{46}$$

where $\hat{p}^n = p^n(\hat{X}_p^n)$ and $\hat{X}_p^n = X + \mu_p E \underline{U}_h^{n+1} \Delta t_c$. Test function $\omega_h = \xi_p^{n+1}$ is substituted in (46), and it follows from a similar discussion and analysis,

$$\begin{aligned} & \frac{1}{2\Delta t} \left\{ \|\xi_p^{n+1}\|^2 - \|\xi_p^n\|^2 \right\} + \frac{1}{M_0} \|\xi_p^{n+1}\|^2 \\ & \leq M \left\{ (\Delta t_c)^{-1} \left\| \frac{\partial \xi_p}{\partial t} \right\|_{L^2(J^n; L^2(\Omega))}^2 + \Delta t_c \left\| \frac{\partial^2 p}{\partial \tau_p^2} \right\|_{L^2(J^n; L^2(\Omega))}^2 + h_\psi^{2k} + h_c^{2(l+1)} + (\Delta t_c)^2 \right. \\ & \quad \left. + H^{-2} h_c^{2(l+1)} + H^{2m+1} + \|\xi_p^{n+1}\|^2 + \|\xi_p^n\|^2 + \|\xi_e^n\|^2 + \|\pi^n\|^2 + \|\xi_{e,[n/j]}\|^2 + \|\xi_{p,[n/j]}\|^2 \right\} \\ & \quad + \varepsilon \left\{ \|\nabla \xi_p^{n+1}\|^2 + \|\nabla \xi_p^n\|^2 \right\}. \end{aligned} \tag{47}$$

Finally, error equation of temperature is derived from (4),

$$\begin{aligned} & \left(\rho \frac{\pi^{n+1} - \pi^n}{\Delta t_c}, \omega_h \right) + \left(\nabla \pi^{n+1}, \omega_h \right) + \left(B(\pi^n), [\omega_h] \right)_\Gamma \\ & = \left(\rho \left[\frac{T^{n+1} - T^n}{\Delta t_c} - \frac{\partial T^{n+1}}{\partial t} \right], \omega_h \right) + \lambda_T \left(\sigma^{n+1}, \omega_h \right) - \left((D_p \nabla p_h^n - \mu_p p_h^n E \underline{U}_h^{n+1} - D_e \nabla e_h^n \right. \\ & \quad \left. + \mu_e e_h^n E \underline{U}_h^{n+1}) \cdot E \underline{U}_h^{n+1} - (D_p \nabla p^{n+1} - \mu_p p^{n+1} \underline{u}^{n+1} - D_e \nabla e^{n+1} + \mu_e e^{n+1} \underline{u}^{n+1}) \cdot \underline{u}^{n+1}, \omega_h \right) \\ & \quad + \left(\rho \frac{\sigma^{n+1} - \sigma^n}{\Delta t_c}, \omega_h \right) + \left(\frac{\partial T^{n+1}}{\partial \gamma} - B(T_h^n), [\omega_h] \right)_\Gamma, \quad \forall \omega_h \in N_h. \end{aligned} \tag{48}$$

Take $\omega_h = \pi^{n+1}$ as test function in (48),

$$\begin{aligned} & \frac{1}{2\Delta t} \left\{ \|\pi^{n+1}\|^2 - \|\pi^n\|^2 \right\} + \frac{1}{M_0} \|\|\pi^{n+1}\|\|^2 \\ & \leq M \left\{ (\Delta t_c)^{-1} \left\| \frac{\partial \sigma}{\partial t} \right\|_{L^2(J^n; L^2(\Omega))}^2 + \Delta t_c \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(J^n; L^2(\Omega))}^2 + h_\psi^{2k} + h_c^{2(l+1)} + (\Delta t_c)^2 \right. \\ & \quad \left. + H^{-2} h_c^{2(l+1)} + H^{2m+1} + \|\pi^{n+1}\|^2 + \|\xi_p^n\|^2 + \|\xi_e^n\|^2 + \|\xi_{e,[n/j]}\|^2 + \|\xi_{p,[n/j]}\|^2 \right\}. \end{aligned} \tag{49}$$

Collecting (45), (47) and (49), multiplying both sides of the resulting equation by $2\Delta t_c$, summing on n ($0 \leq n \leq L - 1$), and noting that $\xi_e^0 = \xi_p^0 = \pi^0 = 0$, we have

$$\begin{aligned} & \|\xi_e^L\|^2 + \|\xi_p^L\|^2 + \|\pi^L\|^2 + \sum_{n=0}^{L-1} \left\{ \|\|\xi_e^{n+1}\|\|^2 + \|\|\xi_p^{n+1}\|\|^2 + \|\|\pi^{n+1}\|\|^2 \right\} \Delta t_c \\ & \leq M \left\{ \left\| \frac{\partial \zeta_e}{\partial t} \right\|_{L^2(J; L^2(\Omega))}^2 + \left\| \frac{\partial \zeta_p}{\partial t} \right\|_{L^2(J; L^2(\Omega))}^2 + \left\| \frac{\partial \sigma}{\partial t} \right\|_{L^2(J; L^2(\Omega))}^2 + \sum_{n=0}^{L-1} \left[\|\pi^{n+1}\|^2 + \|\xi_p^n\|^2 \right. \right. \\ & \quad \left. \left. + \|\xi_e^n\|^2 + \|\xi_{e,[n/j]}\|^2 + \|\xi_{p,[n/j]}\|^2 \right] \Delta t_c + (\Delta t_c)^2 \left[\left\| \frac{\partial^2 e}{\partial \tau_e^2} \right\|_{L^2(J; L^2(\Omega))}^2 + \left\| \frac{\partial^2 p}{\partial \tau_p^2} \right\|_{L^2(J; L^2(\Omega))}^2 \right. \right. \\ & \quad \left. \left. + \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(J; L^2(\Omega))}^2 \right] + (\Delta t_c)^2 + h_\psi^{2k} + h_c^{2(l+1)} + H^{-2} h_c^{2(l+1)} + H^{2m+1} \right\}. \end{aligned} \tag{50}$$

Using Gronwall Lemma,

$$\begin{aligned} & \|\xi_e^L\|^2 + \|\xi_p^L\|^2 + \|\pi^L\|^2 + \sum_{n=0}^{L-1} \left\{ \|\|\xi_e^{n+1}\|\|^2 + \|\|\xi_p^{n+1}\|\|^2 + \|\|\pi^{n+1}\|\|^2 \right\} \Delta t_c \\ & \leq M \left\{ (\Delta t_c)^2 + h_\psi^{2k} + h_c^{2(l+1)} + H^{-2} h_c^{2(l+1)} + H^{2m+1} \right\}. \end{aligned} \tag{51}$$

Therefore, it follows from (35) and (51),

$$\|\psi_{h,m} - \tilde{\psi}_m\| \leq M \left\{ \Delta t_c + h_\psi^k + h_c^{l+1} + H^{-1} h_c^{l+1} + H^{m+1/2} \right\}. \tag{52}$$

It remains to testify the induction hypothesis (42). It is right as n is equal to 0 because of $\xi_e^0 = \xi_p^0 = \pi^0 = 0$. Assume (42) holds for any positive integer n between 1 and a given positive integer $L - 1$. By (51) (52) and the restriction (40), it is easy to see that (42) holds for $n = L$. Based on the resulting estimates (51) and (52), and (31), Theorem 1 is proved.

The method discussed in this paper can be extended to three-dimensional case, such as Mespert model (see Fig.2) (He & Wei,1989). The technique of domain decomposition is very important in numerical simulation of actual applications, as shown in Fig.2, where computational region Ω is divided into five subdomains, $\Omega = \bigcup_{i=1}^5 \Omega_i$ (He & Wei, 1989; Shi, 2002; Yuan, 2009, 2013).

6. Numerical Example

In this section one numerical example is presented to testify the efficiency of the parallel algorithm discussed above. Consider the following model problem,

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} \left(D(x, t) \frac{\partial c}{\partial x} \right) = f(c, x, t), \quad 0 < x < 1, 0 < t < T, \tag{53a}$$

$$c(x, 0) = \cos(2\pi x), \quad 0 \leq x \leq 1, \tag{53b}$$

$$\frac{\partial c}{\partial x}(0, t) = \frac{\partial c}{\partial x}(1, t) = 0, \quad 0 \leq t \leq T. \tag{53c}$$

Some related functions and partition parameters are given as follows, $u = xe^t$, $D(x, t) = 0.01x^2e^{2t}$, $c = e^t \cos(2\pi x)$, $f = e^t \cos(2\pi x) - 2\pi e^{2t} x \sin(2\pi x) + 0.04\pi e^{3t} x (\sin(2\pi x) + \pi x \cos(2\pi x))$, $H = 4h$, $\Delta t = \frac{1}{12}h^2$ and $T = 0.25$.

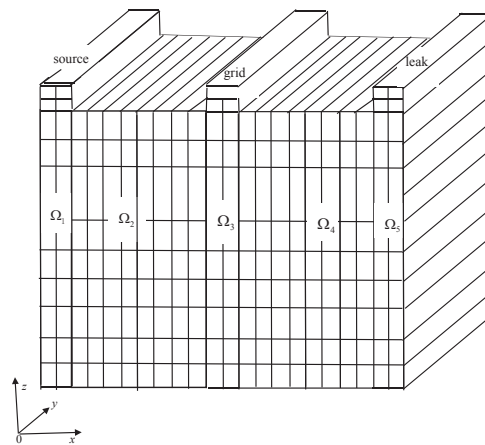


Figure 2. Decomposition of computational domain of three-dimensional Mespet model, $\Omega = \bigcup_{i=1}^5 \Omega_i$

The computational interval is decomposed into two subintervals, $[0, 1] = [0, 0.5] \cup [0.5, 1]$, and interior boundary is $\Gamma = 0.5$. Absolute errors of numerical data are shown in Table 1.

Table 1. Absolute Errors

	$x = 0.05$	$x = 0.25$	$x = 0.45$	$x = 0.55$	$x = 0.75$	$x = 0.95$
$h = 1/40$	$65.1989E - 3$	$1.3641E - 3$	$65.2575E - 3$	$65.1989E - 3$	$1.3641E - 3$	$65.2575E - 3$
$h = 1/80$	$15.3215E - 3$	$0.0829E - 3$	$15.3597E - 3$	$15.3215E - 3$	$0.0829E - 3$	$15.3597E - 3$
$h = 1/160$	$3.7531E - 3$	$0.0051E - 3$	$3.8745E - 3$	$3.7531E - 3$	$0.0051E - 3$	$3.8745E - 3$

Numerical data are consistent with theoretical analysis from Table 1, and error results of approximation to normal derivative at inner boundary, $\frac{\partial c}{\partial x}(0.5) = e^T \sin \pi = 0$ are shown in Table 2.

Table 2. Error results of approximation to norma derivative at interior boundary

B	
$h = 1/40$	$6.2728E - 16$
$h = 1/80$	$5.1736E - 15$
$h = 1/160$	$7.8249E - 14$

Time costs (unit: second) in numerical computation of domain decomposition method (DDM) are illustrated in Table 3 comparing with another computation strategy, non-domain decomposition method (NDDM).

Table 3. Time costs comparison (unit: second)

	DDM	NDDM
$h = 1/40$	0.4530	0.9220
$h = 1/80$	1.0075	2.2500
$h = 1/160$	3.9450	16.5940
$h = 1/320$	88.6170	346.3590

From Table 3, it is easy to conclude that domain decomposition becomes more and more efficient as the partition becomes more refined and the system of algebraic equations becomes larger and larger.

7. Conclusion and Discussion

In this paper a domain decomposition of finite element is discussed to simulate semiconductor transient problems of heat conductor. Mathematical model, physical basic and international research are introduced in the first section. In the second section some primary elliptic projections, notations and basic properties are stated. Then the

procedures of domain decomposition modified with characteristic finite element are structured in the third section. Theoretical analysis is shown and an optimal order estimate in L^2 norm is derived in the fourth section. In the last section a numerical experiment is illustrated to testify the theoretical result and some advantages of this method are concluded as follows. Firstly, this method can be applied in large-scaled numerical computation of three-dimensional problem with complicated domain. Secondly, industrial software is made easily on this method. Thirdly, the algorithm works on modern parallel computers and gives numerical computation of high order accuracy and high efficiency in parallel for semiconductor transient problems. Finally, this paper is an expansive argument of my early research (Yuan, 2012), and a mixed element method combined with domain decomposition is argued firstly in the reference (Yuan, 2012) to solve the problem of semiconductor device. In this paper the optimal error estimate in L^2 norm is derived in theoretical analysis but not obtained in the previous work.

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