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A Numerical Approximation Structured by Mixed Finite Element and Upwind Fractional Step Difference for Semiconductor Device with Heat Conduction and Its Numerical Analysis

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Abstract. A coupled mathematical system of four quasi-linear partial differential equations and the initial-boundary value conditions is presented to interpret transient behavior of three dimensional semiconductor device with heat conduction. The electric potential is defined by an elliptic equation, the electron and hole concentrations are determined by convection-dominated diffusion equations and the temperature is interpreted by a heat conduction equation. A mixed finite element approximation is used to get the electric field potential and one order of computational accuracy is improved. Two concentration equations and the heat conduction equation are solved by a fractional step scheme modified by a second-order upwind difference method, which can overcome numerical oscillation, dispersion and computational complexity. This changes the computation of a three dimensional problem into three successive computations of one-dimensional problem where the method of speedup is used and the computational work is greatly shortened. An optimal second-order error estimate in L^2 norm is derived by prior estimate theory and other special techniques of partial differential equations. This type of parallel method is important in numerical analysis and is most valuable in numerical application of semiconductor device and it can successfully solve this international famous problem.

AMS subject classifications: 65M015; 65M60; 65N30; 82D37
Key words: Three dimensional transient behavior of heat conduction problem, numerical simulation computation, mixed finite element, modified upwind fractional step difference, second-order error estimates in L^2 norm.

1. Introduction

Traditional numerical methods are generally invalid for modern simulation of semiconductor device, since semiconductor device develops greatly and its mathematical model, an

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initial-boundary value diffusion system of nonlinear partial differential equations is solved in consideration of multi-dimensional problem, complicated geometric domains and high order of accuracy. Therefore, modern numerical simulation techniques are introduced to find its discrete solutions [13, 18, 35, 36].

The mathematical model of transient behavior problem of three-dimensional semiconductor device of heat conduction is formulated by four nonlinear partial differential Eqs. [2, 8, 13, 14, 18, 29, 31, 35, 36]. The first equation is elliptic for describing the electric potential, the second and third equations are of convection-diffusion for finding the electron concentration and hole concentration and the fourth equation is of heat conduction for finding the temperature. The electric potential governs the concentrations and the temperature by its electric field intensity. Combined with corresponding boundary value conditions and initial value conditions, a whole system follows on a three-dimensional domain Ω [2, 8, 13, 14, 18, 29, 31, 35, 36].

$$-\Delta\psi = \nabla\cdot\underline{u} = \alpha(p-e+N(X)), \quad X=(x_1,x_2,x_3)^T\in\Omega, \ \ t\in J=(0,\hat{T}], \tag{1.1a}$$

$$\frac{\partial e}{\partial t} = \nabla\cdot\Big[D_e(X)\nabla e+\mu_e(X)e\underline{u}\Big]-R_e(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t} = \nabla\cdot\Big[D_p(X)\nabla p-\mu_p(X)p\underline{u}\Big]-R_p(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1c}$$

$$\rho\frac{\partial T}{\partial t}-\Delta T = \Big\{(D_e(X)\nabla e+\mu_e(X)e\underline{u})-(D_p(X)\nabla p-\mu_p(X)p\underline{u})\Big\}\cdot\underline{u}, \qquad (X,t)\in\Omega\times J. \tag{1.1d}$$

In the above expressions, the electric potential ψ, the electron concentration e, the hole concentration p and the temperature T, the electric field intensity $\underline{u}=-\nabla\psi$ are unknown functions. The electric field potential is generated by the electric field intensity in the concentration equations and the heat conduction equation, and governs the above three equations. $\alpha=q/\varepsilon$ is defined by the quotient of two positive constants, the electronic load q and the dielectric coefficient ε. All coefficients in (1.1b)-(1.1d) have a positive upper bound and a positive lower bound. The diffusion coefficients $D_s(X)$, $s=e$ or p, are equal to $U_T\mu_s(X)$, a product of the mobility $\mu_s(X)$ and the heat U_T. A given function $N(X)$ is defined by $N_D(X)-N_A(X)$, the difference of impurity concentrations of the donor and the acceptor, whose values change rapidly as X approaches closely the semiconductor P-N junction. The symbols $R_e(e,p,T)$ and $R_p(e,p,T)$ denote generation-recombination rates of the electron, the hole and the temperature. The coefficient of heat conduction $\rho(X)$ is positive definite.

Initial value conditions are given by

$$e(X,0)=e_0(X), \quad p(X,0)=p_0(X), \quad T(X,0)=T_0(X), \quad X\in\Omega. \tag{1.2}$$

where positive functions $e_0(X), p_0(X)$ and $T_0(X)$ are known.

Boundary value conditions of Dirichlet type are given by

$$\psi(X,t)\big|_{\partial\Omega}=0, \qquad e(X,t)|_{\partial\Omega}=\bar{e}(X,t), \tag{1.3a}$$

$$p(X,t)\big|_{\partial\Omega}=\bar{p}(X,t), \qquad T(X,t)|_{\partial\Omega}=\bar{T}(X,t), \ t\in J. \tag{1.3b}$$

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Gummel puts forward a sequence of iterations in 1964 and uses this new numerical method to solve semiconductor device [12]. Considering actual applications, Douglas and Yuan present a kind of applicable difference method for one-dimensional and two-dimensional simple models regardless of temperature effect, and show the theoretical analysis for constant coefficient case firstly [8,25]. Then Yuan discusses a finite element method and a mixed finite element method with the characteristics for multi-dimensional problems with variable coefficients and derives optimal order error estimates in H^1 norm and L^2 norm [26, 28, 29]. In modern numerical computation of three-dimensional semiconductor simulation, the heat conduction affects transient behavior, so the factor of the temperature should be considered. Otherwise, numerical simulation will be distorted [16,19,31,35,36]. Successively, Yuan gives two kinds of fractional step methods modified by characteristic differences and upwind differences and discusses error estimates of second order in L^2 norm [32–34]. Some physical properties such as conservation of mass should be considered in structuring numerical computational algorithms, and a type of mixed finite element-characteristic mixed finite element method is put forward where the electric field potential is solved by low-degree standard mixed finite element approximation and the concentration equations of convection-dominated type are discretized by characteristic mixed finite element essentially keeping the global conservation of mass [20, 22–24]. The method of characteristics is introduced to overcome numerical oscillation and dispersion, while extra interpolations are added to compute the values at the points along the characteristics. It is necessary to testify whether the points along the characteristics direction locate inside the computational domain, then the values at the points outside the domain are calculated with special process and time step corrections. Extra work for finding the points of intersection of the mesh and the characteristic lines and extra calculations for the values of grid functions are considered in structuring computational programs, so actual computations are complicated [31,35,36]. For parabolic problems, Ewing, Lazarov and other researchers present upwind difference schemes to overcome numerical oscillation [11, 15], and Douglas and Peaceman use this type of method to simulate two-phase incompressible displacement problems [10] without theoretical justifications [4, 5]. In this paper a new mixed finite element-fractional step method modified by upwind differences is argued for the system of semiconductor device. The electric field potential is computed by a mixed finite element method, and the computation is improved one order accuracy [7,8]. The electron concentration, the hole concentration and the heat conduction equation are computed by upwind difference fractional step method by decomposing a multi-dimensional problem into three successive one-dimensional subproblems solved by the method of speedup, and this can decrease computational scale and can improve actual computation accuracy by refining space and time partitions. Using a combination of coarse grids and refined grids, calculus of variations, multiplicative operators commutation rule of differential type, induction hypothesis, and prior estimates and other special techniques of differential equations, the authors present optimal order error estimates in l^2 norm of the applicable, parallel algorithm. It is most valuable in model analysis, numerical method, principle research, theory and application of semiconductor device simulation [2, 8, 12–14, 18, 25, 35, 36].

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In general, the problem (1.1a)-(1.3) is supposed to be positive definite,

$$\text{(C)}\quad 0<D_*\le D_s(X)\le D^*,\qquad 0<\mu_*\le\mu_s(X)\le\mu^*, \tag{1.4a}$$

$$s=p,e,\qquad 0<\rho_*\le\rho(X)\le\rho^*, \tag{1.4b}$$

where D_*, D^*, μ_*, μ^*, ρ_* and ρ^* are positive constants.

Suppose exact solutions are suitably regular,

$$\text{(R)}\quad \psi\in L^\infty(J;W^{1,\infty})\cap L^\infty(J;H^{k+3}), \tag{1.5a}$$

$$e,p,T\in L^\infty(W^{4,\infty}),\qquad \frac{\partial^2 e}{\partial t^2},\frac{\partial^2 p}{\partial t^2},\frac{\partial^2 T}{\partial t^2}\in L^\infty(L^\infty). \tag{1.5b}$$

And suppose that $R_e(e,p,T)$ and $R_p(e,p,T)$ are Lipschitz continuous in the ε_0-neighbor centered by (e,p,T), that is to say there exists a positive number M such that for $|\varepsilon_i|\le\varepsilon_0$ $(1\le i\le 6)$,

$$\begin{aligned}&\Big|R_s(e(X,t)+\varepsilon_1,p(X,t)+\varepsilon_2,T(X,t)+\varepsilon_3)\\&\quad -R_s(e(X,t)+\varepsilon_4,p(X,t)+\varepsilon_5,T(X,t)+\varepsilon_6)\Big|\\&\le M\left(|\varepsilon_1-\varepsilon_4|+|\varepsilon_2-\varepsilon_5|+|\varepsilon_3-\varepsilon_6|\right),\quad (X,t)\in\Omega\times J,\quad s=e,p.\end{aligned} \tag{1.6}$$

This assumption is reasonable in physics science [1, 13, 14, 18]. In this paper M and ε denote general positive constant and general positive small constant, respectively, and they have different meanings at different places.

2. A coupled procedure of a mixed finite element scheme and an upwind difference fractional step scheme

A mixed finite element argument is given for (1.1a). Let $V=\{\underline{v}\in H(\mathrm{div};\Omega)\}$, $W=L^2(\Omega)$, and give the saddle point weak form as follows,

$$\left(\underline{u},\underline{v}\right)-\left(\nabla\cdot\underline{v},\psi\right)=0,\qquad \forall\underline{v}\in V, \tag{2.1a}$$

$$\left(\nabla\cdot\underline{u},\varphi\right)=\alpha\left(p-e+N,\varphi\right),\qquad \forall\varphi\in W. \tag{2.1b}$$

Let $V_h\times W_h$ denote a k-degree Raviart-Thomas space [7,8,17,21]. h_ψ denotes the partition parameter, and the following approximations hold,

$$\inf_{\underline{v}_h\in V_h}\left|\left|\underline{v}-\underline{v}_h\right|\right|_{L^2(\Omega)}\le M\left|\left|\underline{v}\right|\right|_{k+1}h_\psi^{k+1}, \tag{2.2a}$$

$$\inf_{\underline{v}_h\in V_h}\left|\left|\nabla\cdot(\underline{v}-\underline{v}_h)\right|\right|_0\le M\left(\left|\left|\underline{v}\right|\right|_{k+1}+\left|\left|\nabla\cdot\underline{v}\right|\right|_{k+1}\right)h_\psi^{k+1}, \tag{2.2b}$$

$$\inf_{w_h\in W_h}\left|\left|w-w_h\right|\right|_0\le M\left|\left|w\right|\right|_{k+1}h_\psi^{k+1}. \tag{2.2c}$$

Let Ω be replaced by Ω_h (an actual engineering computation model "Mespet" as shown in Fig. 1 [13]) and discuss the difference algorithms for the electron concentration, the hole

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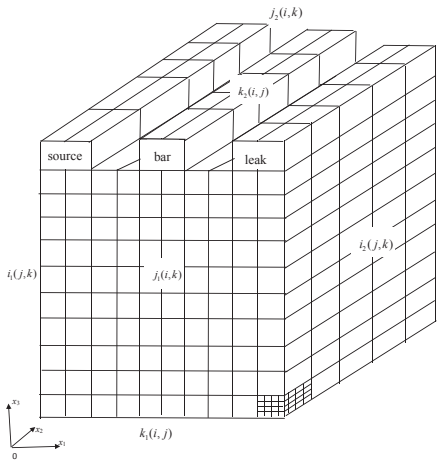


Figure 1: Partition illustration of three-dimensional Mespet Model.

concentration and the heat conduction equation. The partition consists of three different steps h_1, h_2 and h_3 and their grids $X = (x_1, x_2, x_3)^T$ are defined by $X_{1i} = ih_1$, $X_{2j} = jh_2$, $X_{3k} = kh_3$.

$$\Omega_h = \left\{ (x_{1i}, x_{2j}, x_{3k})^T \;\middle|\; \begin{array}{l} i_1(j,k) < i < i_2(j,k) \\ j_1(i,k) < j < j_2(i,k) \\ k_1(i,j) < k < k_2(i,j) \end{array} \right\}$$

Let $\partial\Omega_h$ denote the boundary of Ω_h, and let the grid be denoted by $X_{ijk} = (ih_1, jh_2, kh_3)^T$. Since the electric field potential changes very slowly with respect to t, so a large time step denoted by Δt_ψ is adopted but a small step Δt_c for the concentration equations. Let

$$\begin{aligned} &j = \Delta_\psi / \Delta t_c, \qquad t^n = n\Delta t_s, \qquad t_m = m\Delta t_\psi, \\ &\psi^n = \psi(t^n), \qquad \psi_m = \psi(t_m), \\ &E\psi^n = \begin{cases} \psi_0, & t^n \le t_1, \\ (1 + r/j)\psi_m - (r/j)\psi_{m-1}, & t_m < t^n < t_{m+1}, \\ & t^n = t_m + r\Delta t_c \ \ (r = 1, \cdots, j), \end{cases} \end{aligned} \tag{2.3}$$

where the subscripts and superscripts correspond to potential time layers and concentration time layers, respectively. The extrapolation $E\psi^n$ is obtained at t^n by a linear extrapolation of the values of ψ at the nearest two time layers.

The partition elements in k-degree Raviart-Thomas space should be matched with the grids in Ω_h. Given a cuboid element $[3, 17, 21]$, three measures in different directions denoted by h_1^ψ, h_2^ψ and h_3^ψ are equal to three integers respectively times the length h_1, width h_2 and height h_3 of many embedded small elements of the concentration equations. Let $h = [\sum_{s=1}^3 h_s^2]^{1/2}$ and a whole composite partition is given as in Fig. 2.

The electric field potential and the intensity are approximated by the following mixed

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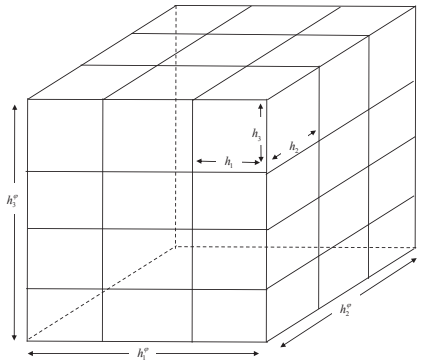


Figure 2: Fig. 2: Composite partition ($h_1^{\psi}=3h_1, h_2^{\psi}=3h_2, h_3^{\psi}=4h_3$).

finite element scheme,

$$\left(\underline{U}_{h,m},\underline{v}\right)-\left(\nabla\cdot\underline{v},\psi_{h,m}\right)=0, \qquad \forall\underline{v}\in V_h, \tag{2.4a}$$

$$\left(\nabla\cdot\underline{U}_{h,m},\varphi\right)=\alpha\left(p_{h,m}-e_{h,m}+N,\varphi\right), \quad \forall\varphi\in W_h. \tag{2.4b}$$

Let

$$D_{i+1/2,jk}=\frac{1}{2}\left[D(X_{ijk})+D(X_{i+1,jk})\right], \qquad D_{i,j+1/2,k}=\frac{1}{2}\left[D(X_{ijk})+D(X_{i,j+1,k})\right],$$

$$D_{ij,k+1/2}=\frac{1}{2}\left[D(X_{ijk})+D(X_{ij,k+1})\right], \qquad D_{i-1/2,jk}=\frac{1}{2}\left[D(X_{ijk})+D(X_{i-1,jk})\right],$$

$$D_{i,j-1/2,k}=\frac{1}{2}\left[D(X_{ijk})+D(X_{i,j-1,k})\right], \qquad D_{ij,k-1/2}=\frac{1}{2}\left[D(X_{ijk})+D(X_{ij,k-1})\right],$$

and let

$$\delta_{\bar{x}_1}\left(D\delta_{x_1}W\right)^n_{ijk}=h_1^{-2}\left[D_{i+1/2,jk}(W^n_{i+1,jk}-W^n_{ijk})-D_{i-1/2,jk}(W^n_{ijk}-W^n_{i-1,jk})\right],$$

$$\delta_{\bar{x}_2}\left(D\delta_{x_2}W\right)^n_{ijk}=h_2^{-2}\left[D_{i,j+1/2,k}(W^n_{i,j+1,k}-W^n_{ijk})-D_{i,j-1/2,k}(W^n_{ijk}-W^n_{i,j-1,k})\right],$$

$$\delta_{\bar{x}_3}\left(D\delta_{x_3}W\right)^n_{ijk}=h_3^{-2}\left[D_{ij,k+1/2}(W^n_{ij,k+1}-W^n_{ijk})-D_{ij,k-1/2}(W^n_{ijk}-W^n_{ij,k-1})\right],$$

$$\nabla_h(D\nabla_h W)^n_{ijk}=\sum_{s=1}^{3}\delta_{\bar{x}_s}\left(D\delta_{x_s}W\right)^n_{ijk}.$$

Note that (1.1b) and (1.1c) can be rewritten as

$$\begin{aligned}&\frac{\partial e}{\partial t}-\mu_e(X)\underline{u}\cdot\nabla e-\nabla\cdot(D_e\nabla e)-\alpha\mu_e(X)e(p-e+N(X))-e\underline{u}\cdot\nabla\mu_e\\&=-R_e(e,p,T),\ X\in\Omega,\ t\in J,\end{aligned} \tag{2.5a}$$

$$\begin{aligned}&\frac{\partial p}{\partial t}+\mu_p(X)\underline{u}\cdot\nabla p-\nabla\cdot(D_p\nabla p)+\alpha\mu_p(X)p(p-e+N(X))+p\underline{u}\cdot\nabla\mu_p\\&=-R_p(e,p,T),\ X\in\Omega,\ t\in J,\end{aligned} \tag{2.5b}$$

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then, the concentrations are computed by the upwind difference fractional step procedures as follows.

$$\Big(1-\Delta t_c\big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\big)_{ijk}^{-1}\delta_{\bar{x}_1}(D_e\delta_{x_1})-\Delta t_c\delta_{EU_{h,1}^{n+1}}\Big)e_{h,ijk}^{n+1/3}$$
$$=e_{h,ijk}^{n}+\Delta t_c\Big\{\big(\alpha\mu_e e_h^n(p_h^n-e_h^n+N)\big)_{ijk}+\big(e_h^n E\underline{U}_h^{n+1}\cdot\nabla\mu_e\big)_{ijk}-R_e(e_h^n,p_h^n,T_h^n)_{ijk}\Big\},$$
$$i_1(j,k)+1<i<i_2(j,k)-1,\quad e_{h,ijk}^{n+1/3}=\bar{e}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h, \tag{2.6a}$$
$$\Big(1-\Delta t_c\big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\big)_{ijk}^{-1}\delta_{\bar{x}_2}(D_e\delta_{x_2})-\Delta t_c\delta_{EU_{h,2}^{n+1}}\Big)e_{h,ijk}^{n+2/3}=e_{h,ijk}^{n+1/3},$$
$$j_1(i,k)+1<j<j_2(i,k)-1,\quad e_{h,ijk}^{n+2/3}=\bar{e}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h, \tag{2.6b}$$
$$\Big(1-\Delta t_c\big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\big)_{ijk}^{-1}\delta_{\bar{x}_3}(D_e\delta_{x_3})-\Delta t_c\delta_{EU_{h,3}^{n+1}}\Big)e_{h,ijk}^{n+1}=e_{h,ijk}^{n+2/3},$$
$$k_1(i,j)+1<k<k_2(i,j)-1,\quad e_{h,ijk}^{n+1}=\bar{e}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h, \tag{2.6c}$$

where

$$\delta_{EU_{h,1}^{n+1}}e_{h,ijk}=\Big(\mu_e EU_{h,1}^{n+1}\Big)_{ijk}\Big\{H(U_{h,1,ijk}^{n+1})D_{e,ijk}^{-1}D_{e,i-1/2,jk}\delta_{\bar{x}_1}e_{h,ijk}$$
$$+(1-H(U_{h,1,ijk}^{n+1}))D_{e,ijk}^{-1}D_{e,i+1/2,jk}\delta_{x_1}e_{h,ijk}\Big\},$$
$$\delta_{EU_{h,2}^{n+1}}e_{h,ijk}=\Big(\mu_e EU_{h,2}^{n+1}\Big)_{ijk}\Big\{H(U_{h,2,ijk}^{n+1})D_{e,ijk}^{-1}D_{e,i,j-1/2,k}\delta_{\bar{x}_2}e_{h,ijk}$$
$$+(1-H(U_{h,2,ijk}^{n+1}))D_{e,ijk}^{-1}D_{e,i,j+1/2,k}\delta_{x_2}e_{h,ijk}\Big\},$$
$$\delta_{EU_{h,3}^{n+1}}e_{h,ijk}=\Big(\mu_e EU_{h,3}^{n+1}\Big)_{ijk}\Big\{H(U_{h,3,ijk}^{n+1})D_{e,ijk}^{-1}D_{e,ij,k-1/2}\delta_{\bar{x}_3}e_{h,ijk}$$
$$+(1-H(U_{h,3,ijk}^{n+1}))D_{e,ijk}^{-1}D_{e,ij,k+1/2}\delta_{x_3}e_{h,ijk}\Big\},$$
$$H(z)=1,\quad z\geq 0,\quad H(z)=0,\quad z<0.$$

Morever, we have

$$\left(1-\Delta t_c\left(1+\frac{h_1}{2}\mu_p\left|EU_{h,1}^{n+1}\right|D_p^{-1}\right)_{ijk}^{-1}\delta_{\bar{x}_1}(D_e\delta_{x_1})+\Delta t_c\delta_{EU_{h,1}^{n+1}}\right)p_{h,ijk}^{n+1/3}$$
$$=p_{h,ijk}^{n}-\Delta t_c\Big\{\big(\alpha\mu_p p_h^n(p_h^n-e_h^n+N)\big)_{ijk}+\big(p_h^n E\underline{U}_h^{n+1}\cdot\nabla\mu_p\big)_{ijk}+R_p(e_h^n,p_h^n,T_h^n)_{ijk}\Big\},$$
$$i_1(j,k)+1<i<i_2(j,k)-1,\quad p_{h,ijk}^{n+1/3}=\bar{p}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h. \tag{2.7a}$$
$$\left(1-\Delta t_c\left(1+\frac{h_2}{2}\mu_p\left|EU_{h,2}^{n+1}\right|D_p^{-1}\right)_{ijk}^{-1}\delta_{\bar{x}_2}(D_p\delta_{x_2})+\Delta t_c\delta_{EU_{h,2}^{n+1}}\right)p_{h,ijk}^{n+2/3}=p_{h,ijk}^{n+1/3},$$
$$j_1(i,k)+1<j<j_2(i,k)-1,\quad p_{h,ijk}^{n+2/3}=\bar{p}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h. \tag{2.7b}$$
$$\left(1-\Delta t_c\left(1+\frac{h_3}{2}\mu_p\left|EU_{h,3}^{n+1}\right|D_p^{-1}\right)_{ijk}^{-1}\delta_{\bar{x}_3}(D_p\delta_{x_3})+\Delta t_c\delta_{EU_{h,3}^{n+1}}\right)p_{h,ijk}^{n+1}=p_{h,ijk}^{n+2/3},$$
$$k_1(i,j)+1<k<k_2(i,j)-1,\quad p_{h,ijk}^{n+1}=\bar{p}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h. \tag{2.7c}$$

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where the symbols $\delta_{EU_{h,s}^{n+1}p_{h,ijk}}$ $(s=1,2,3)$ are defined similarly to $\delta_{EU_{h,s}^{n+1}e_{h,ijk}}$ by replacing μ_e and D_e by μ_p and D_p.

For the heat conduction Eq. (1.1d), the fractional step difference scheme is formulated by

$$\begin{aligned}
&\left(1-\Delta t_c\delta_{\bar{x}_1}(\delta_{x_1})\right)T_{h,ijk}^{n+1/3}\\
=&T_{h,ijk}^{n}+\Delta t_c\rho_{ijk}^{-1}\left\{\left[D_e\nabla_h e_h^n+\mu_e e_h^n E\underline{U}_h^{n+1}\right]-\left[D_p\nabla_h p_h^n-\mu_p p_h^n E\underline{U}_h^{n+1}\right]\right\}_{ijk}E\underline{U}_{h,ijk}^{n+1},\\
&\qquad i_1(j,k)+1<i<i_2(j,k)-1,\quad T_{h,ijk}^{n+1/3}=\bar{T}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h, \qquad (2.8a)\\
&\left(1-\Delta t_c\delta_{\bar{x}_2}(\delta_{x_2})\right)T_{h,ijk}^{n+2/3}=T_{h,ijk}^{n+1/3},\\
&\qquad j_1(i,k)+1<j<j_2(i,k)-1,\quad T_{h,ijk}^{n+2/3}=\bar{T}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h, \qquad (2.8b)\\
&\left(1-\Delta t_c\delta_{\bar{x}_3}(\delta_{x_3})\right)T_{h,ijk}^{n+1}=T_{h,ijk}^{n+2/3},\\
&\qquad k_1(i,j)+1<k<k_2(i,j)-1,\quad T_{h,ijk}^{n+1}=\bar{T}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h. \qquad (2.8c)
\end{aligned}$$

Initial approximation is defined by

$$\begin{aligned}
&e_{h,ijk}^0=e_0(X_{ijk}),\qquad p_{h,ijk}^0=p_0(X_{ijk}), \qquad (2.9a)\\
&T_{h,ijk}^0=T_0(X_{ijk}),\qquad X_{ijk}\in\bar{\Omega}_h=\Omega\cup\partial\Omega. \qquad (2.9b)
\end{aligned}$$

The parallel program works a time step as follows. Firstly, using the initial approximation (2.9) and mixed finite element algorithm (2.4) with $m=0$ we get the initial values of electric field potential and intensity $\{\underline{U}_{h,0},\psi_{h,0}\}$. Secondly, we use the method of speedup and the upwind difference fractional step algorithm (2.6)-(2.8) to get the values of $\{e_h^1,p_h^1,T_h^1\}$, $\{e_h^2,p_h^2,T_h^2\}$, $\cdots$, $\{e_h^j,p_h^j,T_h^j\}$ in parallel. Then combining (2.4) with $\{e_h^j,p_h^j,T_h^j\}=\{e_{h,1},p_{h,1},T_{h,1}\}$ and using the method of conjugate gradient, we obtain the approximations of mixed finite element $\{\underline{U}_{h,1},\psi_{h,1}\}$. Next, from the difference scheme (2.6)-(2.8) we have $\{e_h^{j+1},p_h^{j+1},T_h^{j+1}\}$, $\{e_h^{j+2},p_h^{j+2},T_h^{j+2}\}$, $\cdots$, $\{e_{h,2},p_{h,2},T_{h,2}\}$. After a series of repeated computations, all the numerical solutions are obtained, where they exist and are sole by the positive definite condition (C).

3. Convergence analysis

For convenience to discuss the convergence analysis of electric field potential, a pair of supplementary elliptic projections $\{\tilde{\underline{u}},\tilde{\psi}\}:\ J\to N_h\times W_h$ is introduced by

$$\begin{aligned}
&\left(\tilde{\underline{u}},\underline{v}\right)-\left(\nabla\cdot\underline{v},\tilde{\psi}\right)=0,\qquad \forall\underline{v}\in V_h, \qquad (3.1a)\\
&\left(\nabla\cdot\tilde{\underline{u}},\varphi\right)=\alpha\left(p-e+N,\varphi\right),\quad \forall\varphi\in W_h. \qquad (3.1b)
\end{aligned}$$

Error estimates follow from Brezzi Theorem [8, 17],

$$||\underline{u}-\tilde{\underline{u}}||_V+||\psi-\tilde{\psi}_h||_W\le M||\psi||_{L^\infty(J;H^{k+3}(\Omega))}h_\psi^{k+1}. \qquad (3.2)$$

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Now $\underline{U}_{h,m+1}-\underline{\tilde{u}}_{m+1}$ and $\psi_{m+1}-\tilde{\psi}_{m+1}$ are estimated. Subtract (3.1a) ($t=t_{m+1}$) and (3.1b) ($t=t_{m+1}$) from (2.4a) and (2.4b),

$$\left(\underline{U}_{h,m+1}-\underline{\tilde{u}}_{m+1},\underline{v}\right)-\left(\nabla\cdot\underline{v},\psi_{h,m+1}-\tilde{\psi}_{m+1}\right)=0,\qquad \forall\underline{v}\in V_h, \tag{3.3a}$$

$$\begin{aligned}&\left(\nabla\cdot\left(\underline{U}_{h,m+1}-\underline{\tilde{u}}_{m+1}\right),\varphi\right)\\ =&\alpha\left(p_{h,m+1}-p_{m+1}-e_{h,m+1}+e_{m+1},\varphi\right),\qquad \forall\varphi\in W_h.\end{aligned} \tag{3.3b}$$

Then, it follows [2,8]

$$\begin{aligned}&||\underline{U}_{h,m+1}-\underline{\tilde{u}}_{m+1}||_V+||\psi_{h,m+1}-\tilde{\psi}_{m+1}||_W\\ \le& M\left(||e_{m+1}-e_{h,m+1}||+||p_{m+1}-p_{h,m+1}||\right).\end{aligned} \tag{3.4}$$

Let error functions be denoted by

$$\begin{aligned}&\underline{\rho}=\underline{u}-\underline{\tilde{u}},\quad \underline{\sigma}=\underline{\tilde{u}}-\underline{U}_h,\quad \eta=\psi-\tilde{\psi},\quad \pi=\tilde{\psi}-\psi_h,\\ &\xi=e-e_h,\quad \zeta=p-p_h,\quad \chi=T-T_h,\end{aligned}$$

where $\psi,\underline{u},e,p$ and T are exact solutions, $\{\underline{U}_h,\psi_h\}$ denote mixed finite element solutions and $\{e_h,p_h,T_h\}$ mean difference solutions. The partition $\bar{\Omega}$, a composite partition consisting of cuboid elements, of computational domain Ω is defined by the product of three one-dimensional partitions,

$$\bar{\Omega}_h=\Omega_h\cup\partial\Omega_h=\bar{\omega}_1\times\bar{\omega}_2\times\bar{\omega}_3,$$

where $\bar{\omega}_1=\left\{x_{1i}\middle|i=0,1,\cdots,M_1\right\}$, $\bar{\omega}_2=\left\{x_{2j}\middle|j=0,1,\cdots,M_2\right\}$, $\bar{\omega}_3=\left\{x_{3k}\middle|k=0,1,\cdots,M_3\right\}$. Let $\omega_1^+=\left\{x_{1i}\middle|i=1,2,\cdots,M_1\right\}$, $\omega_2^+=\left\{x_{2j}\middle|j=1,2,\cdots,M_2\right\}$, $\omega_3^+=\left\{x_{3k}\middle|k=1,2,\cdots,M_3\right\}$, where M_1, M_2 and M_3 are positive integers. $|f|_0=\langle f,f\rangle^{1/2}$ denotes a norm of the discrete space corresponding to $L^2(\Omega)$, and

$$\langle f,g\rangle=\sum_{\bar{\omega}_1}h_{1i}\sum_{\bar{\omega}_2}h_{2j}\sum_{\bar{\omega}_3}h_{3k}f(X_{ijk})g(X_{ijk}), \tag{3.5}$$

denotes the inner product, where

$$\begin{aligned}&h_{1i}=h_1,\qquad 1\le i\le M_1-1;\qquad h_{10}=h_{1M_1}=h_1/2,\\ &h_{2j}=h_2,\qquad 1\le j\le M_2-1;\qquad h_{20}=h_{2M_2}=h_2/2,\\ &h_{3k}=h_3,\qquad 1\le k\le M_3-1;\qquad h_{30}=h_{3M_3}=h_3/2.\end{aligned}$$

And $\langle D\nabla_h f,\nabla_h f\rangle$ denotes the square of a weighted semi-norm in discrete space $h^1(\Omega)$ corresponding to $H^1(\Omega)=W^{1,2}(\Omega)$ where $D(X)$ is a positive definite function,

$$\begin{aligned}\langle D\nabla_h f,\nabla_h f\rangle=&\sum_{\bar{\omega}_2}\sum_{\bar{\omega}_3}h_{2j}h_{3k}\sum_{\omega_1^+}h_{1i}\left(D(X)[\delta_{\bar{x}_1}f(X)]^2\right)+\sum_{\bar{\omega}_3}\sum_{\bar{\omega}_1}h_{3k}h_{1i}\sum_{\omega_2^+}h_{2j}\\ &\cdot\left(D(X)[\delta_{\bar{x}_2}f(X)]^2\right)+\sum_{\bar{\omega}_1}\sum_{\bar{\omega}_2}h_{1i}h_{2j}\sum_{\omega_3^+}h_{3k}\left(D(X)[\delta_{\bar{x}_3}f(X)]^2\right).\end{aligned}$$

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Next the electron and hole concentrations are estimated. We can change the electron concentration Eqs. (2.6a)-(2.6c) into an equivalent form by canceling $e_h^{n+1/3}$ and $e_h^{n+2/3}$,

$$\begin{aligned}
&\Big(1-\Delta t_c\big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\big)^{-1}\delta_{\bar{x}_1}(D_e\delta_{x_1})-\Delta t_c\delta_{EU_{h,1}^{n+1}}\Big)\\
&\quad\times\Big(1-\Delta t_c\big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\big)^{-1}\delta_{\bar{x}_2}(D_e\delta_{x_2})-\Delta t_c\delta_{EU_{h,2}^{n+1}}\Big)\\
&\quad\times\Big(1-\Delta t_c\big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\big)^{-1}\delta_{\bar{x}_3}(D_e\delta_{x_3})-\Delta t_c\delta_{EU_{h,3}^{n+1}}\Big)e_{h,ijk}^{n+1}\\
&=e_{h,ijk}^n+\Delta t_c\left\{\alpha\mu_e e_h^n\left(p_h^n-e_h^n+N(X)\right)+e_h^n\underline{EU}_h^{n+1}\cdot\nabla\mu_e-R_e(e_h^n,p_h^n,T_h^n)\right\}_{ijk},\\
&\quad X_{ijk}\in\Omega_h,\quad e_{h,ijk}^{n+1}=\bar{e}_{ijk}^{n+1},\quad X_{ijk}\in\partial\Omega_h.
\end{aligned}\tag{3.6}$$

An expansion of (3.6) is given by

$$\begin{aligned}
&\frac{e_{h,ijk}^{n+1}-e_{h,ijk}^n}{\Delta t_c}-\sum_{s=1}^{3}\Big(1+\frac{h_s}{2}\mu_e\Big|EU_{h,s}^{n+1}\Big|D_e^{-1}\Big)_{ijk}^{-1}\delta_{\bar{x}_s}\left(D_e\delta_{x_s}e_h^{n+1}\right)_{ijk}-\sum_{s=1}^{3}\delta_{EU_{h,s}^{n+1}}e_{h,ijk}^n\\
&+\Delta t_c\Big\{\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{\bar{x}_2}(D_e\delta_{x_2})\Big)+\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{\bar{x}_3}(D_e\delta_{x_3})\Big)+\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}\Big(D_e\delta_{x_2}\Big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{\bar{x}_3}(D_e\delta_{x_3})\Big)\Big\}e_{h,ijk}^{n+1}-(\Delta t_c)^2\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\\
&\cdot\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{\bar{x}_2}\Big(D_e\delta_{x_2}\big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\big)^{-1}\delta_{\bar{x}_3}(D_e\delta_{x_3}e_h^{n+1})\big)\Big)\Big)_{ijk}\\
&+\Delta t_c\Big\{\delta_{EU_{h,1}^{n+1}}(\delta_{EU_{h,2}^{n+1}})+\delta_{EU_{h,1}^{n+1}}(\delta_{EU_{h,3}^{n+1}})+\delta_{EU_{h,2}^{n+1}}(\delta_{EU_{h,3}^{n+1}})\Big\}e_{h,ijk}^{n+1}\\
&-(\Delta t_c)^2\delta_{EU_{h,1}^{n+1}}\Big(\delta_{EU_{h,2}^{n+1}}(\delta_{EU_{h,3}^{n+1}}e_h^{n+1})\Big)_{ijk}\\
&+\Delta t_c\left\{\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\big(D_e\delta_{x_1}\Big(\delta_{EU_{h,2}^{n+1}}\Big)\big)+\cdots\right\}e_{h,ijk}^{n+1}\\
&-(\Delta t_c)^2\left\{\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}(\delta_{EU_{h,2}^{n+1}}(\delta_{EU_{h,3}^{n+1}}))\Big)+\cdots\right.\\
&\left.+\delta_{EU_{h,1}^{n+1}}\Big(\delta_{EU_{h,2}^{n+1}}\Big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_3}(D_e\delta_{x_3})\Big)\right\}e_{h,ijk}^{n+1}\\
&=\left\{\alpha\mu_e e_h^n\left(p_h^n-e_h^n+N(X)\right)+e_h^n\underline{EU}_h^{n+1}\cdot\nabla\mu_e-R_e(e_h^n,p_h^n,T_h^n)\right\}_{ijk},\quad X_{ijk}\in\Omega_h,
\end{aligned}\tag{3.7a}$$

$$e_{h,ijk}^{n+1}=\bar{e}_{ijk}^{n+1},\qquad X_{ijk}\in\partial\Omega_h.\tag{3.7b}$$

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Error equation is derived from (2.5a) ($t = t^{n+1}$) and (3.7),

$$\begin{aligned}
&\frac{\xi_{ijk}^{n+1}-\xi_{ijk}^{n}}{\Delta t_c}-\sum_{s=1}^{3}\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)_{ijk}^{-1}\delta_{\bar{x}_s}\left(D_e\delta_{x_s}\xi^{n+1}\right)_{ijk}\\
&=\sum_{s=1}^{3}\delta_{EU_{h,s}^{n+1}}\xi_{ijk}^{n+1}-\Delta t_c\Big\{\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1\\
&\quad+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_2}\left(D_e\delta_{x_2}\xi^{n+1}\right)\Big)_{ijk}+\cdots\\
&\quad+\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_2}\Big(D_e\delta_{x_2}\Big(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\Big)^{-1}\\
&\quad\cdot\delta_{\bar{x}_3}\left(D_e\delta_{x_3}\xi^{n+1}\right)\Big)_{ijk}\Big\}+(\Delta t_c)^2\Big(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\Big)^{-1}\\
&\quad\cdot\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}\\
&\quad\cdot\Big(D_e\delta_{x_2}\Big(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_3}\left(D_e\delta_{x_3}\xi^{n+1}\right)\Big)\Big)_{ijk}\\
&\quad+\sum_{s=1}^{3}\left\{\delta_{u_s^{n+1}e^{n+1}}-\delta_{EU_{h,s}^{n+1}e^{n+1}}\right\}_{ijk}+\sum_{s=1}^{3}\Big\{\Big[\Big(1+\frac{h_s}{2}\mu_e\left|u_s^{n+1}\right|D_e^{-1}\Big)^{-1}\\
&\quad-\Big(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\Big)^{-1}\Big]\delta_{\bar{x}_s}\left(D_e\delta_{x_s}e^{n+1}\right)\Big\}_{ijk}\\
&\quad-\Delta t_c\Big\{\Big[\Big(1+\frac{h_1}{2}\mu_e\left|u_1^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\left|u_2^{n+1}\right|D_e^{-1}\Big)^{-1}\Big)\\
&\quad-\Big(1\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\Big)^{-1}\Big)\Big]\\
&\quad\cdot\delta_{\bar{x}_2}\left(D_e\delta_{x_2}e^{n+1}\right)_{ijk}+\cdots\Big\}+(\Delta t_c)^2\Big\{\Big[\Big(1+\frac{h_1}{2}\mu_e\left|u_1^{n+1}\right|D_e^{-1}\Big)^{-1}\\
&\quad\cdot\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\left|u_2^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_3}\Big(D_e\delta_{x_3}\Big(1+\frac{h_3}{2}\mu_e\left|u_3^{n+1}\right|D_e^{-1}\Big)^{-1}\Big)\Big)\\
&\quad-\Big(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\Big)^{-1}\\
&\quad\cdot\delta_{\bar{x}_3}\Big(D_e\delta_{x_3}\Big(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\Big)^{-1}\Big)\Big)\Big]\cdot\delta_{\bar{x}_3}\left(D_e\delta_{x_3}e^{n+1}\right)\Big\}_{ijk}\\
&\quad+\cdots+\varepsilon_e\left(X_{ijk},t^{n+1}\right),\qquad X_{ijk}\in\Omega_h \qquad (3.8a)\\
&\xi_{ijk}^{n+1}=0,\qquad X_{ijk}\in\partial\Omega_h. \qquad (3.8b)
\end{aligned}$$

where $\left|\varepsilon_e(X_{ijk},t^{n+1})\right|\le M\{\Delta t_c+h^2\}$.

A restriction of the parameters on time and space partition is given by

$$\Delta t_c=\mathcal{O}(h^2),\quad h^2=o(h_\psi^{3/2}). \qquad (3.9)$$

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And an induction hypothesis is introduced as follows

$$\sup_{0\le n\le L}\left\{|\xi^n|_\infty,|\zeta^n|_\infty,\left|\chi^n\right|_\infty\right\}\to 0, \tag{3.10a}$$

$$\sup_{0\le n\le L\ (m=[n/j])}\left|\left|\underline{\sigma}_m\right|\right|_{0,\infty}\to 0,\ (h,h_\psi,\Delta t_c)\to 0. \tag{3.10b}$$

Multiply both sides of (3.8) by $\xi_{ijk}^{n+1}\Delta t_c$, make inner products and use the summation by parts,

$$\begin{aligned}
&\left\langle \xi^{n+1}-\xi^n,\xi^{n+1}\right\rangle+\Delta t_c\sum_{s=1}^{3}\left\langle D_e\delta_{x_s}\xi^{n+1},\delta_{x_s}\left[\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\xi^{n+1}\right]\right\rangle\\
=&\Delta t_c\sum_{s=1}^{3}\left\langle\delta_{EU_{h,s}^{n+1}}\xi^{n+1},\xi^{n+1}\right\rangle-(\Delta t_c)^2\Big\{\Big\langle\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\\
&\cdot\delta_{\bar{x}_1}\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_2}(D_e\delta_{x_2}\xi^{n+1})\right),\xi^{n+1}\Big\rangle+\cdots\\
&+\Big\langle\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_2}\left(D_e\delta_{x_2}\left(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\right)^{-1}\\
&\cdot\delta_{\bar{x}_3}(D_e\delta_{x_3}\xi^{n+1})\right),\xi^{n+1}\Big\rangle\Big\}+(\Delta t_c)^3\Big\langle\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\\
&\cdot\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\cdot\delta_{\bar{x}_2}\left(D_e\delta_{x_2}\left(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_3}\right.\right.\\
&\left.\left.\cdot\left(D_e\delta_{x_3}\xi^{n+1}\right)\right)\right),\xi^{n+1}\Big\rangle+\Delta t_c\sum_{s=1}^{3}\left\langle\delta_{u_s^{n+1}}e^{n+1}-\delta_{EU_{h,s}^{n+1}}e^{n+1},\xi^{n+1}\right\rangle\\
&+\Delta t_c\sum_{s=1}^{3}\Big\langle\Big[\left(1+\frac{h_s}{2}\mu_e\left|u_s^{n+1}\right|D_e^{-1}\right)^{-1}-\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\Big]\\
&\cdot\delta_{\bar{x}_s}(D_e\delta_{x_s}e^{n+1}),\xi^{n+1}\Big\rangle-(\Delta t_c)^2\Big\{\Big\langle\Big[\left(1+\frac{h_1}{2}\mu_e\left|u_1^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\\
&\cdot\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|u_2^{n+1}\right|D_e^{-1}\right)^{-1}\right)-\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\\
&\cdot\delta_{\bar{x}_1}\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\right)\Big]\delta_{\bar{x}_2}(D_e\delta_{x_2}e^{n+1}),\xi^{n+1}\Big\rangle+\cdots\Big\}\\
&+(\Delta t_c)^3\Big\langle\Big[\left(1+\frac{h_1}{2}\mu_e\left|u_1^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|u_2^{n+1}\right|D_e^{-1}\right)^{-1}\right.\\
&\left.\cdot\delta_{\bar{x}_3}\left(D_e\delta_{x_3}\left(1+\frac{h_3}{2}\mu_e\left|u_3^{n+1}\right|D_e^{-1}\right)^{-1}\right)\right)-\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\\
&\cdot\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_3}\left(D_e\delta_{x_3}\left(1+\frac{h_3}{2}\mu_e\left|EU_{h,3}^{n+1}\right|D_e^{-1}\right)^{-1}\right)\right)\Big]\\
&\cdot\delta_{\bar{x}_3}(D_e\delta_{x_3}e^{n+1}),\xi^{n+1}\Big\rangle+\cdots+\Delta t_c\left\langle\varepsilon_e^{n+1},\xi^{n+1}\right\rangle.
\end{aligned}\tag{3.11}$$

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The terms on the left-hand side of (3.11) are estimated as follows,

$$\begin{aligned}
&\left\langle \xi^{n+1}-\xi^{n},\xi^{n+1}\right\rangle+\Delta t_c\sum_{s=1}^{3}\left\langle D_e\delta_{x_s}\xi^{n+1},\delta_{x_s}\left[\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\xi^{n+1}\right]\right\rangle\\
\geq&\frac{1}{2}\left\{\left|\xi^{n+1}\right|_0^2-\left|\xi^{n}\right|_0^2\right\}+\Delta t_c\sum_{s=1}^{3}\left\{\left\langle D_e\delta_{x_s}\xi^{n+1},\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\right.\right.\\
&\left.\left.\cdot\,\delta_{x_s}\xi^{n+1}\right\rangle+\left\langle D_e\delta_{x_s}\xi^{n+1},\delta_{x_s}\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\cdot\xi^{n+1}\right\rangle\right\}\\
\geq&\frac{1}{2}\left\{\left|\xi^{n+1}\right|_0^2-\left|\xi^{n}\right|_0^2\right\}+\Delta t_c\sum_{s=1}^{3}\left\langle D_e\delta_{x_s}\xi^{n+1},\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\right.\\
&\left.\cdot\,\delta_{x_s}\xi^{n+1}\right\rangle-\varepsilon\left|\nabla_h\xi^{n+1}\right|^2\Delta t_c-M\left|\xi^{n+1}\right|_0^2\Delta t_c\\
\geq&\frac{1}{2}\left\{\left|\xi^{n+1}\right|_0^2-\left|\xi^{n}\right|_0^2\right\}+D_0\Delta t_c\sum_{s=1}^{3}\left|\delta_{x_s}\xi^{n+1}\right|_0^2\\
&-\varepsilon\left|\nabla_h\xi^{n+1}\right|^2\Delta t_c-M\left|\xi^{n+1}\right|_0^2\Delta t_c,
\end{aligned}\tag{3.12}$$

where D_0 is a positive constant and the relation

$$\begin{aligned}
&\delta_{x_s}\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-1}\\
=&\left(1+\frac{h_s}{2}\mu_e\left|EU_{h,s}^{n+1}\right|D_e^{-1}\right)^{-2}\cdot\frac{h_s}{2}\mu_e\frac{EU_{h,s}^{n+1}}{\left|EU_{h,s}^{n+1}\right|}\cdot\delta_{x_s}\left(U_{h,s}^{n+1}\right),
\end{aligned}$$

and the induction hypothesis (3.10), error estimates (3.2) and (3.4) are used.

The terms on the right-hand side of (3.11) are estimated later. From (3.10), (3.2) and (3.4), we have that $\left|EU_h^{n+1}\right|_\infty$ is bounded, then we obtain

$$\Delta t_c\sum_{s=1}^{3}\left\langle\delta_{EU_{h,s}^{n+1}}\xi^{n+1},\xi^{n+1}\right\rangle\leq M\left\{\left|\xi^{n+1}\right|_0^2+\left|\nabla_h\xi^{n+1}\right|_0^2\right\}\Delta t_c.\tag{3.13}$$

Though the discrete operators $-\delta_{\bar{x}_1}(D_e\delta_{x_1})$, $-\delta_{\bar{x}_2}(D_e\delta_{x_2})$ and $-\delta_{\bar{x}_3}(D_e\delta_{x_3})$ are self-conjugate, positive definite and bounded, and the partition element is cuboid, their products are not interchangeable. Noticing $\delta_{x_1}\delta_{x_2}=\delta_{x_2}\delta_{x_1}$, $\delta_{\bar{x}_1}\delta_{x_2}=\delta_{x_2}\delta_{\bar{x}_1}$, $\cdots$, for the second term on the right-hand side of (3.11), we have

$$\begin{aligned}
&-(\Delta t_c)^2\left\langle\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_1}\left(D_e\delta_{x_1}\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\right.\right.\\
&\left.\left.\cdot\,\delta_{\bar{x}_2}\left(D_e\delta_{x_2}\xi^{n+1}\right)\right),\xi^{n+1}\right\rangle\\
=&(\Delta t_c)^2\left\langle D_e\delta_{x_1}\left(\left(1+\frac{h_2}{2}\mu_e\left|EU_{h,2}^{n+1}\right|D_e^{-1}\right)^{-1}\delta_{\bar{x}_2}\left(D_e\delta_{x_2}\xi^{n+1}\right)\right),\right.\\
&\left.\delta_{x_1}\left[\left(1+\frac{h_1}{2}\mu_e\left|EU_{h,1}^{n+1}\right|D_e^{-1}\right)^{-1}\xi^{n+1}\right]\right\rangle
\end{aligned}$$

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$$
\begin{aligned}
=&(\Delta t_c)^2\Big\langle D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}\delta_{x_1}(D_e\delta_{x_2}\xi^{n+1})+D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\\
&\cdot\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}(D_e\delta_{x_2}\xi^{n+1}),\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{x_1}\xi^{n+1}\\
&+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big\rangle\\
=&(\Delta t_c)^2\Big\{\Big\langle D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}\delta_{x_1}(D_e\delta_{x_2}\xi^{n+1}),\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|\\
&\cdot D_e^{-1}\Big)^{-1}\delta_{x_1}\xi^{n+1}+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big\rangle\\
&+\Big\langle D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}(D_e\delta_{x_2}\xi^{n+1}),\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{x_1}\xi^{n+1}+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big\rangle\Big\}\\
=&-(\Delta t_c)^2\Big\{\Big\langle\delta_{x_1}(D_e\delta_{x_2}\xi^{n+1}),\delta_{x_2}\Big[D_e(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1})^{-1}\cdot\Big(D_e(1+\frac{h_1}{2}\mu_e\\
&\cdot\Big|EU_{h,1}^{n+1}\Big|D_e^{-1})^{-1}\delta_{x_1}\xi^{n+1}+\delta_{x_1}(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1})^{-1}\cdot\xi^{n+1}\Big)\Big]\Big\rangle\\
&+\Big\langle D_e\delta_{x_2}\xi^{n+1},\delta_{x_2}\Big[D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(D_e\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{x_1}\xi^{n+1}+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big)\Big]\Big\rangle\Big\}\\
=&-(\Delta t_c)^2\Big\{\Big\langle D_e\delta_{x_1}\delta_{x_2}\xi^{n+1}+\delta_{x_1}D_e\cdot\delta_{x_2}\xi^{n+1},D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{x_1}\delta_{x_2}\xi^{n+1}+\delta_{x_2}\Big[D_e(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1})^{-1}\\
&\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\delta_{x_1}\xi^{n+1}+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_2}\xi^{n+1}\\
&+\delta_{x_1}\delta_{x_2}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big\rangle+\Big\langle D_e\delta_{x_2}\xi^{n+1},D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|\\
&\cdot D_e^{-1}\Big)^{-1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_1}\delta_{x_2}\xi^{n+1}+\delta_{x_2}\Big[D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|\\
&\cdot D_e^{-1}\Big)^{-1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\delta_{x_1}\xi^{n+1}+D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_2}\xi^{n+1}+\delta_{x_2}\Big[D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\xi^{n+1}\Big\rangle\Big\}\\
=&-(\Delta t_c)^2\Big\{\Big\langle D_e\delta_{x_1}\delta_{x_2}\xi^{n+1},D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{x_1}\delta_{x_2}\xi^{n+1}\Big\rangle+\Big\langle\delta_{x_1}D_e\cdot\delta_{x_2}\xi^{n+1},D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|
\end{aligned}
$$

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$$\cdot D_e^{-1}\Big)^{-1}\delta_{x_1}\delta_{x_2}\xi^{n+1}\Big\rangle+\Big\langle D_e\delta_{x_1}\delta_{x_2}\xi^{n+1},\delta_{x_2}\Big[D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}$$
$$\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\delta_{x_1}\xi^{n+1}+\delta_{x_1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}$$
$$\cdot\delta_{x_2}\xi^{n+1}+\delta_{x_1}\delta_{x_2}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\xi^{n+1}\Big\rangle+\Big\langle D_e\delta_{x_2}\xi^{n+1},$$
$$D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_1}\delta_{x_2}\xi^{n+1}\Big\rangle$$
$$+\Big\langle D_e\delta_{x_2}\xi^{n+1},\delta_{x_2}\Big[D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]$$
$$\cdot\delta_{x_1}\xi^{n+1}+D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_2}\xi^{n+1}$$
$$+\delta_{x_2}\Big[D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\xi^{n+1}\Big\rangle\Big\}. \tag{3.14}$$

For the first term on the right-hand side of (3.14), by the positive definite conditions $0<D_*\le D_e(X)\le D^*$ and $0<\mu_*\le\mu(X)\le\mu^*$, the induction hypothesis (3.10) and Cauchy inequality, we cancel high-order difference quotient parts $\delta_{x_1}\delta_{x_2}\xi^{n+1}$, and have for sufficiently small h and a positive constant D_0

$$\begin{aligned}&-(\Delta t_c)^2\Big\langle D_e\delta_{x_1}\delta_{x_2}\xi^{n+1},D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\&\quad\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\delta_{x_1}\delta_{x_2}\xi^{n+1}\Big\rangle\\&\le-(\Delta t_c)^2D_0\left|\delta_{x_1}\delta_{x_2}\xi^{n+1}\right|_0^2.\end{aligned}\tag{3.15}$$

Considering other terms on the right-hand side of (3.14),

$$\begin{aligned}&-(\Delta t_c)^2\Big\{\Big\langle\delta_{x_1}D_e\cdot\delta_{x_2}\xi^{n+1},D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\&\quad\cdot\delta_{x_1}\delta_{x_2}\xi^{n+1}\Big\rangle+\Big\langle D_e\delta_{x_1}\delta_{x_2}\xi^{n+1},\delta_{x_2}\Big[D_e\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\&\quad\cdot\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\Big]\cdot\delta_{x_1}\xi^{n+1}+\cdots\Big\rangle+\cdots\Big\}\\&\le\frac{1}{2}(\Delta t_c)^2D_0\left|\delta_{x_1}\delta_{x_2}\xi^{n+1}\right|_0^2+M\left\{\left|\nabla_h\xi^{n+1}\right|_0^2+\left|\xi^{n+1}\right|_0^2\right\}(\Delta t_c)^2.\end{aligned}\tag{3.16}$$

Collecting (3.14), (3.15) and (3.16), we have

$$\begin{aligned}&-(\Delta t_c)^2\Big\langle\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\&\quad\cdot\delta_{\bar{x}_2}\big(D_e\delta_{x_2}\xi^{n+1}\big)\Big),\xi^{n+1}\Big\rangle\\&\le\frac{1}{2}D_0(\Delta t_c)^2\left|\delta_{x_1}\delta_{x_2}\xi^{n+1}\right|_0^2+M\left\{\left|\nabla_h\xi^{n+1}\right|_0^2+\left|\xi^{n+1}\right|_0^2\right\}(\Delta t_c)^2.\end{aligned}\tag{3.17}$$

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Similar analysis for the other terms,

$$
\begin{aligned}
&-(\Delta t_c)^2\Big\{\Big\langle\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{\bar{x}_2}\big(D_e\delta_{x_2}\xi^{n+1}\big)\Big),\xi^{n+1}\Big\rangle+\cdots+\Big\langle\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_2}\\
&\cdot\Big(D_e\delta_{x_2}\Big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_3}\big(D_e\delta_{x_3}\xi^{n+1}\big)\Big),\xi^{n+1}\Big\rangle\Big\}\\
\le&\frac{1}{2}D_0(\Delta t_c)^2\Big(\big|\delta_{x_1}\delta_{x_2}\xi^{n+1}\big|_0^2+\big|\delta_{x_1}\delta_{x_3}\xi^{n+1}\big|_0^2+\big|\delta_{x_2}\delta_{x_3}\xi^{n+1}\big|_0^2\Big)\\
&+M\Big(\big|\nabla_h\xi^{n+1}\big|_0^2+\big|\xi^{n+1}\big|_0^2\Big)(\Delta t_c)^2.
\end{aligned}
\tag{3.18}
$$

For the third term on the right-hand side of (3.11), similar to the second term, using the positive definite condition (C) and the induction hypothesis, and cancelling high-order term $\delta_{x_1}\delta_{x_2}\delta_{x_3}\xi^{n+1}$, we have for sufficiently small h,

$$
\begin{aligned}
&(\Delta t_c)^3\Big\langle\Big(1+\frac{h_1}{2}\mu_e\Big|EU_{h,1}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_1}\Big(D_e\delta_{x_1}\Big(1+\frac{h_2}{2}\mu_e\Big|EU_{h,2}^{n+1}\Big|D_e^{-1}\Big)^{-1}\\
&\cdot\delta_{\bar{x}_2}\Big(D_e\delta_{x_2}\Big(1+\frac{h_3}{2}\mu_e\Big|EU_{h,3}^{n+1}\Big|D_e^{-1}\Big)^{-1}\delta_{\bar{x}_3}\big(D_e\delta_{x_3}\xi^{n+1}\big)\Big)\Big),\xi^{n+1}\Big\rangle\\
\le&-\frac{D_0}{2}(\Delta t_c)^3\big|\delta_{x_1}\delta_{x_2}\delta_{x_3}\xi^{n+1}\big|_0^2+\varepsilon(\Delta t_c)^2\Big(\big|\delta_{x_1}\delta_{x_2}\xi^{n+1}\big|_0^2+\big|\delta_{x_1}\delta_{x_3}\xi^{n+1}\big|_0^2\\
&+\big|\delta_{x_2}\delta_{x_3}\xi^{n+1}\big|_0^2\Big)+M\Big(\big|\nabla_h\xi^{n+1}\big|_0^2+\big|\xi^{n+1}\big|_0^2\Big)(\Delta t_c)^2.
\end{aligned}
\tag{3.19}
$$

For the fourth term on the right-hand side of (3.11), we have

$$
\begin{aligned}
&\Delta t_c\sum_{s=1}^{3}\Big\langle\delta_{u_s^{n+1}e^{n+1}}-\delta_{EU_{h,s}^{n+1}e^{n+1}},\xi^{n+1}\Big\rangle\\
\le&M\Big((\Delta t_c)^2+h^4+h_\psi^{2(k+1)}+h_\psi^4+\big|\xi^{n+1}\big|_0^2+|\xi^n|_0^2+\big|\xi_m\big|_0^2+\big|\xi_{m-1}\big|_0^2\\
&+\big|\zeta_m\big|_0^2+\big|\zeta_{m-1}\big|_0^2\Big)\Delta t_c,
\end{aligned}
\tag{3.20}
$$

by using the following inequality derived from (3.2) and (3.4),

$$
\big|\underline{u}-\underline{U}_h\big|_0^2\le M\Big(|\xi|_0^2+|\zeta|_0^2+h_\psi^{2(k+1)}+h_\psi^4\Big). \tag{3.21}
$$

Because $\underline{u}-\underline{U}$ is measured by $l^2(\Omega)$ norm replacing $L^2(\Omega)$ norm, the last term on the right-hand side is generated as $k>1$ and disappears as $k=1$ or $k=0$ [6, 28, 29] in the above expression. In actual applications, the computation runs in Raviart-Thomas spaces with $k=1$ or $k=0$ consisting of regular elements such as cubes or tetrahedrons. For the last term of (3.11), we have

$$
\Big|\Big\langle\varepsilon_e^{n+1},\xi^{n+1}\Big\rangle\Delta t_c\Big|\le M\Big((\Delta t_c)^2+h^4+\big|\xi^{n+1}\big|_0^2\Big)\Delta t_c. \tag{3.22}
$$

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Then we have the estimate result of (3.11) by using (3.12), (3.13), (3.18)–(3.20) and (3.22), and summing on

$$0 \le n \le L,$$

for sufficiently small Δt_c,

$$\begin{aligned}
&\left|\xi^{L+1}\right|_0^2 + \sum_{n=0}^{L} \left|\nabla_h \xi^{n+1}\right|_0^2 \Delta t_c \\
\le& M\Big(\sum_{n=0}^{L} \Big[\left|\xi^{n+1}\right|_0^2 + \left|\zeta^{n+1}\right|_0^2 + \left|\chi^{n+1}\right|_0^2 \Big] \Delta t_c + (\Delta t_c)^2 + h^4 + h_\psi^{2(k+1)} + h_\psi^4 \Big). \qquad (3.23)
\end{aligned}$$

Similarly, we can obtain the estimates of the hole concentration equation and the heat conduction equation,

$$\begin{aligned}
&\left|\zeta^{L+1}\right|_0^2 + \sum_{n=0}^{L} \left|\nabla_h \zeta^{n+1}\right|_0^2 \Delta t_c \\
\le& M\Big(\sum_{n=0}^{L} \Big[\left|\xi^{n+1}\right|_0^2 + \left|\zeta^{n+1}\right|_0^2 + \left|\chi^{n+1}\right|_0^2 \Big] \Delta t_c + (\Delta t_c)^2 + h^4 + h_\psi^{2(k+1)} + h_\psi^4 \Big), \qquad (3.24a) \\
&\left|\chi^{L+1}\right|_0^2 + \sum_{n=0}^{L} \left|\nabla_h \chi^{n+1}\right|_0^2 \Delta t_c \\
\le& M\Big(\sum_{n=0}^{L} \Big[\left|\chi^{n+1}\right|_0^2 + \left|\xi^{n+1}\right|_0^2 + \left|\zeta^{n+1}\right|_0^2 \Big] \Delta t_c + (\Delta t_c)^2 + h^4 + h_\psi^{2(k+1)} + h_\psi^4 \Big). \qquad (3.24b)
\end{aligned}$$

Considering all the resulting estimates (3.23)-(3.24b),

$$\begin{aligned}
&\left|\xi^{L+1}\right|_0^2 + \left|\zeta^{L+1}\right|_0^2 + \left|\chi^{L+1}\right|_0^2 + \sum_{n=0}^{L} \Big[\left|\nabla_h \xi^{n+1}\right|_0^2 + \left|\nabla_h \zeta^{n+1}\right|_0^2 + \left|\nabla_h \chi^{n+1}\right|_0^2 \Big] \Delta t_c \\
\le& M\Big(\sum_{n=0}^{L} \Big[\left|\xi^{n+1}\right|_0^2 + \left|\zeta^{n+1}\right|_0^2 + \left|\chi^{n+1}\right|_0^2 \Big] \Delta t_c + (\Delta t_c)^2 + h^4 + h_\psi^{2(k+1)} + h_\psi^4 \Big). \qquad (3.25)
\end{aligned}$$

Using discrete Gronwall Lemma, we have

$$\begin{aligned}
&\left|\xi^{L+1}\right|_0^2 + \left|\zeta^{L+1}\right|_0^2 + \left|\chi^{L+1}\right|_0^2 + \sum_{n=0}^{L} \Big[\left|\nabla_h \xi^{n+1}\right|_0^2 + \left|\nabla_h \zeta^{n+1}\right|_0^2 + \left|\nabla_h \chi^{n+1}\right|_0^2 \Big] \Delta t_c \\
\le& M\left((\Delta t_c)^2 + h^4 + h_\psi^{2(k+1)} + h_\psi^4 \right). \qquad (3.26)
\end{aligned}$$

It remains to testify the induction hypothesis (3.10). For $n = 0$ because of

$$\xi^0 = \zeta^0 = \chi^0 = 0, \qquad \underline{\sigma}_0 = 0$$

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is derived from (3.4), then (3.10) is right. Assume (3.10) holds for any positive integer n between 1 and a given positive integer L. By (3.26) and the restriction (3.9), it is easy to see that for $k \geq 1$

$$\left|\xi^{L+1}\right|_\infty + \left|\zeta^{L+1}\right|_\infty + \left|\chi^{L+1}\right|_\infty \leq Mh^{-3/2}\left(h^2 + h_\psi^{k+1} + h_\psi^2 + \Delta t_c\right) \leq Mh^{1/2} \to 0, \quad (3.27a)$$

$$\left|\left|\underline{\sigma}_{[(L+1)/j]}\right|\right|_{0,\infty} \leq Mh_\psi^{-3/2}\left(h^2 + h_\psi^{k+1} + h_\psi^2 + \Delta t_c\right) \leq Mh_\psi^{1/2} \to 0. \quad (3.27b)$$

Therefore, (3.10) is right for $n = L + 1$ and the induction hypothesis is proved completely.

Theorem 3.1. *Suppose that exact solutions of* (1.1)-(1.3) are suitably regular (R) and the problem is positive definite (C). Adopt mixed finite element-modified upwind difference fractional step scheme (2.6)-(2.9) and obtain numerical solutions layer by layer in parallel by simple computations of the method of speedup. Then we get the following error result for the degree of mixed finite element space $k \geq 1$ and the restriction (3.9)

$$\begin{aligned}
&\left|\left|e - e_h\right|\right|_{\bar{L}^\infty((0,\hat{T}],l^2)} + \left|\left|p - p_h\right|\right|_{\bar{L}^\infty((0,\hat{T}],l^2)} + \left|\left|T - T_h\right|\right|_{\bar{L}^\infty((0,\hat{T}],l^2)} \\
&\quad + \left|\left|e - e_h\right|\right|_{\bar{L}_2((0,\hat{T}],h^1)} + \left|\left|p - p_h\right|\right|_{\bar{L}_2((0,\hat{T}],h^1)} + \left|\left|T - T_h\right|\right|_{\bar{L}_2((0,\hat{T}],h^1)} \\
&\quad + \left|\left|\psi - \psi_h\right|\right|_{\bar{L}^\infty((0,\hat{T}],W)} + \left|\left|\underline{u} - \underline{U}_h\right|\right|_{\bar{L}^\infty((0,\hat{T}],V)} \\
\leq & M^*\left(\Delta t_c + h^2 + h_\psi^{k+1} + h_\psi^2\right), \qquad (3.28)
\end{aligned}$$

where

$$\left|\left|g\right|\right|_{\bar{L}^\infty(J;X)} = \sup_{n\Delta t \leq T}\left|\left|g^n\right|\right|_X, \quad \left|\left|g\right|\right|_{\bar{L}_2(J;X)} = \sup_{L\Delta t \leq T}\left\{\sum_{n=0}^{L}\left|\left|g^n\right|\right|_X \Delta t\right\},$$

and the constant M^* is dependent on ψ, e, p, T and their derivatives.

4. Conclusions and discussions

In this paper a composite algorithm of a mixed-finite element scheme and a modified upwind difference fractional step scheme is structured for numerical simulation of transient behavior of semiconductor device with heat conduction. In §1, mathematical model, physical background and some related research are introduced. In §2, the partition of computational domain is given, then a mixed finite element scheme, a high-order accuracy approximation, is used to compute the electric field intensity. A fractional step scheme modified by upwind difference is formulated for the concentrations and heat, which is carried out by changing a three-dimensional problem into three successive one-dimensional computations, and this parallel algorithm can shorten the computation scale greatly. Finally, a theoretical convergence analysis in l^2 norm is shown in §3. In particular, for some problems without consideration of high order accuracy, we can present another composite algorithm of a mixed-finite element scheme and an upwind difference (first-order) fractional step scheme and discuss a similar analysis to derive a first-order estimate in l^2 norm. In this research there serval interesting results are stated as follows:

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- The effect of the heat is considered in structuring procedures for transient behavior problems, so numerical approximation of this type can reflect physical natures very well.
- This method can be applied in large-scaled numerical computation of three-dimensio -nal problem with complicated geometric domain.
- A mixed finite element method is adopted and this can improve computation accuracy of one order in computing electric field intensity. It is very important to understand numerical simulation of semiconductor device.
- The fractional step algorithm modified by upwind difference is adopted to compute the concentrations and the heat which works on modern parallel computers and gives numerical computation of second-order accuracy and high efficiency in parallel for transient behavior problems.

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References

[1] R. E. Bank, W. M. Fichtner and D. J. Rose, *Transient simulation of sillcon devices and circuits*, IEEE Computer-Aided Design, 6 (1985), pp. 436–451.
[2] F. Brezzi, *On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers*, RATRO., Anal. Numer., 2 (1974), pp. 129–151.
[3] P. G. Ciariet, *The finite element methods for elliptic problem*, North-Holland, Amsterdam, 1978.
[4] J. Douglas Jr, J. E. Gunn, *Two order correct difference analogues for the equation of multidimensional heat flow*, Math. Comp., 17 (1963), pp. 71–80.
[5] J. Douglas Jr and J. E. Gunn, *A general formulation of alternating direction methods, Part I. Parabolic and hyperbolic problems*, Numer. Math., 6(5) (1964), pp. 428–453.
[6] J. Douglas Jr., *Simulation of miscible displacement in porous media by a modified method of characteristics procedure*, In Numerical Analysis, Dundee, 1981, Lecture Note in Mathematics 912, Springer-Verlag, Berlin, 1982.
[7] J. Douglas Jr., R. E. Ewing, M. F. Wheeler, *Approximation of the pressure by a mixed method in the simulation of miscible displacement*, RAIRO Anal. Numer., 17(1) (1983), pp. 17–33.
[8] J. Douglas Jr., Y. R. Yuan, *Numerical simulation of immiscible flow in porous media based on combining the method of characteristics with mixed finite element procedure*, Numerical Simulation in Oil Recovery, Springer-Verlag, New York, (1986), pp. 119–132.
[9] J. Douglas Jr., Y. R. Yuan, *Finite difference methods for transient behavior of a semiconductor device*, Mat. Apli. Comp., 6(1) (1987), pp. 25–38.
[10] R. E. Ewing, *The Mathematics of reservoir simulation*, SIAM, Philadelphia, 1983.

https://doi.org/10.4208/nmtma.2017.y15013 Published online by Cambridge University Press

[11] R. E. Ewing, R. D. Lazarov, A. T. Vassilev, *Finite difference scheme for parabolic problems on a composite grids with refinement in time and space*, SIAM J. Numer. Anal., 31(6) (1994), pp. 1605–1622.
[12] H. K. Gummel, *A self-consistent iterative scheme for one-dimensional steady-state transistor calculation*, IEEE Trans: Electron Device, 11(10) (1964), pp. 455–465.
[13] Y. He, T. F. Wei, *Computer simulation method for semiconductor device*, Scicence Press, Beijing, 1989 (in Chinese).
[14] J. W. Jerome, *Mathematical Theory and Approximation of Semiconductor Models*, SIAM, Philadelphia 1994.
[15] R. D. Lazarov, I. D. Mischev, P. S. Vassilevski, *Finite volume methods for convection-diffusion problems*, SIAM J. Numer. Anal., 33(1) (1996), pp. 31–55.
[16] Y. Lou, *On basic semiconductor equation with heat conduction*, J. Partial. Diff. Eqs., 8(1) (1995), pp. 43ÍC-54.
[17] R. A. Raviart, J. M. Thomas, *A mixed finite element method for second order elliptic problems*, Lecture Notes in Math., 606, Springer-Verlag, Berlin, 1977, pp. 292–315.
[18] M. Shi, *Physics of modern semiconductor device*, Science Press, Beijing, 2002 (in Chinese).
[19] C. W. Sun, Q. S. Lu, Z. X. Fan, *Laser irradiation effect*, National Defence Industry Press, Beijing, 2002 (in Chinese).
[20] T. J. Sun, Y. R. Yuan, *An approximation of incompressible miscible displacment in porous media by mixed finite element method and characteristics-mixed finite element method*, J. Comp. Appl. Math., 228(2009), pp. 391–411.
[21] J. M. Thomas, *SurL'analyse numerique des methods d'elements finis hybrides et mixtes*, These. Universite Pierre et Marie Curie, 1977.
[22] Q. Yang, Y. R. Yuan, *An approximation of semiconductor device of heat conduction by mixed finite element method characteristics-mixed finite element method*, Appl. Numer. Math., 70(2013), pp. 42–57.
[23] Q. Yang, Y. R. Yuan, *An approximation of semiconductor device by mixed finite element method and characteristics-mixed finite element method*, Appl. Math. Comput., 225(2013), pp. 407–424.
[24] Q. Yang, Y. R. Yuan, *An approximation of three-dimensional semiconductor device by mixed finite element method and characteristics-mixed finite element method*, Numer. Math-Theory. ME., to appear.
[25] Y. R. Yuan, L. Y. Ding, H. A. Yang, *A new method and theoretical analysis of numerical analog of semiconductor*, Chin. Sci. Bull., 27(7) (1982), pp. 790–795.
[26] Y. R. Yuan, *Characteristics method with mixed finite element for transient behavior of semiconductor device*, Chin. Sci. Bull., 36(17) (1991), pp. 1356–1357.
[27] Y. R. Yuan, *The approximation of the electronic potential by a mixed method in the simulation of semiconductor*, J. Systems Sci. Math. Sci., 11(2) (1991), pp. 117–120.
[28] Y. R. Yuan, *Time stepping along characteristics for the finite element approximation of compressible miscible displacement in porous media*, Math. Numer. Sinica, 14(4) (1992), pp. 386–406.
[29] Y. R. Yuan, *Finite element method and analysis of numerical simulation of semiconductor device*, Acta Math. Sci., 13(3) (1993), pp. 241–251.
[30] Y. R. Yuan, *Finite difference methods for a compressible miscible displacement problem in porous media*, Math. Numer. Sinica, 15(1) (1993), pp. 16–28.
[31] Y. R. Yuan, *Finite difference method and analysis for three-dimensional semiconductor device of heat conduction*, Sci. China Math., 39(11) (1996), pp. 1140–1151.
[32] Y. R. Yuan, *Characteristic finite difference fractional step methods for three-dimensional semiconductor device of heat conduction*, Chin. Sci. Bull., 45(2) (2000), pp. 123–131.

https://doi.org/10.4208/nmtma.2017.y15013 Published online by Cambridge University Press

[33] Y. R. YUAN, *Finite difference fractional step method for transient behavior of a semiconductor device*, Acta. Math. Sci. (Ser. B), 25(3) (2005), pp. 427–438.
[34] Y. R. Yuan, *Modification of upwind finite difference fractional step methods by the transient state of the semiconductor device*, Numer. Meth. Part. D. E., 24(2) (2008), pp. 400–417.
[35] Y. R. YUAN, *Recent progress in numerical methods for semiconductor devices*, Chinese J. Computational Physics, 26(3) (2009), pp. 317–324.
[36] Y. R. YUAN, *Theory and application of reservoir numerical simulation*, Chapter 7, *numercial method of transient behavior of semiconductor device*, Science Press, Beijing, 2013 (in Chinese).

https://doi.org/10.4208/nmtma.2017.y15013 Published online by Cambridge University Press