# A $P^1-P^1$ FINITE ELEMENT METHOD FOR A PHASE RELAXATION MODEL. PART I: QUASI-UNIFORM MESH*

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**Abstract.** We study a simple model of phase relaxation which consists of a parabolic PDE for temperature $\theta$ and an ODE with a small parameter $\varepsilon$ and double obstacles for phase variable $\chi$. The model replaces sharp by diffuse interfaces and gives rise to superheating effects. A semi-explicit time discretization with uniform time-step $\tau$ is combined with continuous piecewise linear finite elements for both $\theta$ and $\chi$, over a fixed quasi-uniform mesh of size $h$. At each time step, an inexpensive nodewise algebraic correction is performed to update $\chi$, followed by the solution of a linear positive definite symmetric system for $\theta$ by a preconditioned conjugate gradient method. A priori estimates for both $\theta$ and $\chi$ are derived in $L^2$-based Sobolev spaces provided the stability constraint $\tau \leq \varepsilon$ is enforced. Asymptotic behavior of the fully discrete model is examined as $\varepsilon, \tau, h \downarrow 0$ independently, which leads to a rate of convergence of order $\mathcal{O}((\tau + h)\varepsilon^{-1/2})$, provided a natural compatibility condition on the initial data is satisfied. Numerical experiments illustrate the performance of the proposed method for the natural choice $h \approx \tau \leq \varepsilon$.

**Key words.** phase relaxation, diffuse interface, piecewise linear finite elements, numerical integration, double obstacles

**AMS(MOS) subject classifications.** 65N15, 65N30, 35R35

## 1. Introduction.

We study the following simple model of phase relaxation

$$\partial_t \theta + \partial_t \chi - \Delta \theta = f, \tag{1.1}$$

$$\varepsilon \partial_t \chi + \Lambda(\chi) \ni \theta, \tag{1.2}$$

proposed by Visintin [23,24], with Neumann boundary condition $\frac{\partial \theta}{\partial \nu} = g$, where $\nu$ is the unit outer normal vector. Hereafter $\theta$ is the temperature of a substance that occupies a domain $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$ and undergoes solidification, $\chi$ is the phase variable (or order parameter), $u = \theta + \chi$ is the enthalpy (or energy density), $\varepsilon > 0$ is a small relaxation parameter, and $\Lambda$ is the inverse of the sign function, namely, the following maximal monotone graph

$$\Lambda(s) := \begin{cases} [-\infty, 0] & s = -1, \\ 0 & -1 < s < 1, \\ [0, \infty] & s = 1. \end{cases}$$

The constitutive relation $\theta \in \Lambda(\chi)$, typical of the Stefan problem, is thus replaced by the dynamic condition (1.2) but the double obstacle constraint $|\chi| \leq 1$ is still enforced. Sharp interfaces are diffused into transition layers of thickness $\mathcal{O}(\sqrt{\varepsilon})$ and superheating effects, without surface tension, take place; note that $\mathrm{Int}\{\chi = 1\} \subset \{\theta > 0\}$ and $\mathrm{Int}\{\chi = -1\} \subset \{\theta < 0\}$, but equalities may not hold. Existence and uniqueness are discussed in [24], along with modifications relevant in polymer crystallization; this connection is further explored in [10,12]. In [22] the Stefan problem is shown to be

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the singular limit of (1.1) and (1.2) as $\varepsilon \downarrow 0$, and a suboptimal rate of convergence of order $\mathcal{O}(\varepsilon^{1/4})$ is derived; an optimal order $\mathcal{O}(\varepsilon^{1/2})$ is obtained in [14]. Therefore, the above model is intermediate between the Stefan problem and the phase field model for which (1.2) is replaced by the singularly perturbed parabolic PDE

$$\varepsilon\partial_t\chi - \varepsilon\Delta\chi + \tfrac{1}{\varepsilon}\psi(\chi) = \theta, \tag{1.3}$$

where $\psi(s) = \Lambda(s) - s$ [2] or $\psi(s) = s(s^2-1)$ [3] are no longer monotone. The regularizing effect of phase relaxation is fully characterized in 1D [18], and is further exploited in our analysis [8].

Our interest in (1.1)-(1.2) is twofold: first its connection with classical solidification, including polymers, and second its relative simple structure that allows a precise design and analysis of adaptive procedures. These techniques are indispensable for the efficient solution of (1.1) and (1.3) because of their stiff character. Fast interpolation is essential to transfer information between consecutive meshes and dictates the success of adaptivity for evolution problems, most notably for incompatible meshes [15,16,17]. Bearing this in mind, we consider a finite element method that can be applied to the models in [2,3] and handles fast interpolation, and we investigate its stability and convergence over a fixed quasi-uniform mesh. We extend this analysis in [9] to adaptively graded meshes that are highly refined near the transition layers and are totally regenerated from time to time in accordance with certain admissibility tests. Our fully discrete method combines the semi-explicit time discretization of (1.2) due to Verdi and Visintin [21,22]

$$\tfrac{\varepsilon}{\tau}(X^n - X^{n-1}) + \Lambda(X^n) \ni \Theta^{n-1}, \tag{1.4}$$

and the implicit time discretization of (1.1)

$$\tfrac{1}{\tau}(\Theta^n - \Theta^{n-1}) + \tfrac{1}{\tau}(X^n - X^{n-1}) - \Delta\Theta^n = f^{n-1}, \tag{1.5}$$

with continuous piecewise linear finite elements for space discretization of both $\Theta^n$ and $X^n$. Each time step consists of an inexpensive nodewise algebraic correction for $X^n$, which arises from (1.4), followed by the solution of a *linear* positive definite symmetric system for $\Theta^n$, which results from (1.5), by a preconditioned conjugate gradient method. A similar method over a fixed mesh is proposed in [4] but no error analysis is given.

In this paper we continue our stability and convergence analyses of [8], but just for a fully discrete version of (1.4) and (1.5); the extrapolation scheme of [8] deserves further research. Scheme (1.4)-(1.5) is stable, provided $\tau \le \varepsilon$, and convergent with an optimal rate $\mathcal{O}(\tau\varepsilon^{-1/2})$, provided a *compatibility* condition on the initial data holds [8]. Under slightly stronger conditions, we derive here stability bounds and error estimates of order $\mathcal{O}\big((\tau+h)\varepsilon^{-1/2}\big)$ in the usual Sobolev norms. We stress that this rate is linear and thus *optimal* for $\varepsilon$ fixed, as expected from approximation theory, but deteriorates as $\varepsilon \downarrow 0$ as predicted by the semidiscrete traveling waves of [18]; whether $\mathcal{O}(h\varepsilon^{-1/2})$ is the correct asymptotics if both $h, \varepsilon \downarrow 0$ is an intriguing open question. In any event, our estimate improves substantially upon that in [22], not only in view of the previous rate of convergence $\mathcal{O}\big(h^{1/2}+\tau^{1/4}+\varepsilon^{1/2}\big)$ but also in terms of the asymptotic behavior for $\varepsilon$ fixed. Instead, in [21] a rate $\mathcal{O}(h+\tau^{1/2})$, with exponential dependence on $\varepsilon$, is derived for the more general constitutive relation

$$\varepsilon\partial_t\chi + \Lambda(\chi) \ni \gamma(\theta,\chi),$$

with a Lipschitz nonlinearity $\gamma(\theta,\chi)$ on the right-hand side. Piecewise constant elements are used for $\chi$ in both [21,22], which is inconvenient for fast interpolation on incompatible meshes. An optimal rate $\mathcal{O}(h+\tau)$ for a $P^1-P^0$ approximation of a related model of polymer crystallization with $\varepsilon=1$ is derived in [10].

This paper is organized as follows. In §2, we briefly state the weak form of the semidiscrete problem and recall some useful results from [8] without proofs. In §3 we formulate the fully discrete method, which will be compared next with the semidiscrete problem of [8]. We derive stability estimates in various $L^2$-based Sobolev norms in §4, and applied them in §5 to obtain error estimates. Numerical results are discussed in §6, which illustrate the performance and potentials of the method for $h\approx\tau\le\varepsilon$.

**2. Semidiscrete Problem.** Let $\Omega$ be a convex polyhedron of $\mathbb{R}^d$ $(d\ge 1)$ with boundary $\Gamma$, and set $Q:=\Omega\times(0,T)$ with $0<T<+\infty$ fixed. Let the initial functions $\theta_0$ and $\chi_0$ satisfy $\theta_0\in W^{2,\infty}(\Omega)$ and $\chi_0\in W^{1,\infty}(\Omega;[-1,1])$. The study of semidiscrete traveling waves of [18] reveals that violation of $\theta\in\Lambda(\chi)$ may take place only within the transition region $\{|\chi(\cdot,t)|<1\}$, which is a thin layer of thickness $\mathcal{O}(\sqrt{\varepsilon})$ where $|\nabla\chi(\cdot,t)|\le C\varepsilon^{-1/2}$ and $|\theta(\cdot,t)|\le C\varepsilon^{1/2}$. Hereafter $C$ denotes a positive constant which may vary at the various occurrences but will always be independent of the relevant parameters involved, namely $\varepsilon, h$ and $\tau$. It is thus quite reasonable to assume

$$\|\nabla\theta_0\|_{L^\infty(\Omega)},\ \varepsilon^{1/2}\|\nabla\chi_0\|_{L^\infty(\Omega)}\le C, \tag{2.1}$$

along with the *compatibility* condition

$$\|\theta_0-z_0\|_{L^\infty(\Omega)}\le A\varepsilon^{1/2}, \tag{2.2}$$

where $z_0\in\Lambda(\chi_0)$ is defined by

$$z_0:=\begin{cases}\min(\theta_0,0), & \text{if } \chi_0=-1\\ 0, & \text{if } -1<\chi_0<1\\ \max(\theta_0,0), & \text{if } \chi_0=1.\end{cases} \tag{2.3}$$

We remark that (2.2) is stronger than the compatibility condition of [8], namely $\|\theta_0-z_0\|_{L^2(\Omega)}\le A\varepsilon^{1/2}$, and that $z_0$ may be discontinuous.

We now formulate the semi-explicit method (1.4)-(1.5) in weak form. Let $\tau:=T/N>0$ be the time step, $N$ be a positive integer, $t^n:=n\tau$, and $I^n:=(t^{n-1},t^n]$ for $1\le n\le N$. For any given sequence $\{z^n\}_{n=0}^N$, we set $\partial z^n:=(z^n-z^{n-1})/\tau$. *Given $\Theta^0=\theta_0$ and $X^0=\chi_0$, for any $1\le n\le N$, we seek $\Theta^n\in H^1(\Omega), |X^n|\le 1$ and $Z^n\in\Lambda(X^n)$ a.e. in $\Omega$ such that*

$$\langle\partial\Theta^n,\phi\rangle+\langle\partial X^n,\phi\rangle+\langle\nabla\Theta^n,\nabla\phi\rangle=0 \qquad \forall\ \phi\in H^1(\Omega), \tag{2.4}$$

$$\varepsilon\langle\partial X^n,\varphi\rangle+\langle Z^n,\varphi\rangle=\langle\Theta^{n-1},\varphi\rangle \qquad \forall\ \varphi\in L^2(\Omega). \tag{2.5}$$

We note that (2.4) corresponds to a vanishing Neumann boundary condition, and that $f=0$ for simplicity. Our results are valid also for Dirichlet boundary conditions, provided the phase transition $\{|\chi|<1\}$ occurs in the interior of $\Omega$, as well as $f^{n-1}=$

$f(\Theta^{n-1})$. The following *strong* stability estimate holds provided $\tau \le \varepsilon$ [8]

$$\begin{aligned}\sum_{n=1}^{N} \tau \|\partial\Theta^n\|^2_{L^2(\Omega)} + \max_{1\le n\le N} \|\nabla\Theta^n\|^2_{L^2(\Omega)}\\ + \varepsilon \max_{1\le n\le N} \|\partial X^n\|^2_{L^2(\Omega)} + \sum_{n=1}^{N} \tau \langle \partial X^n, \partial Z^n\rangle \le C(A^2 + \|\nabla\theta_0\|^2_{L^2(\Omega)}).\end{aligned} \tag{2.6}$$

Upon adding (2.4) on $n$, and invoking elliptic regularity theory, we easily derive

$$\|\sum_{n=1}^{N} \tau\Theta^n\|^2_{H^2(\Omega)} + \varepsilon \sum_{n=1}^{N} \tau \|\Theta^n\|^2_{H^2(\Omega)} \le C(A^2 + \|\nabla\theta_0\|^2_{L^2(\Omega)}), \tag{2.7}$$

because $\Omega$ is convex. In addition, there exists $C > 0$, depending on $\|\nabla\theta_0\|_{L^2(\Omega)}$ and $A$ but independent of $m \le N$, such that the following *optimal* error estimate is valid

$$\begin{aligned}\|u(t^m) - U^m\|_{H^1(\Omega)^*} + \sqrt{\varepsilon}\|\chi(t^m) - X^m\|_{L^2(\Omega)}\\ + \Big(\sum_{n=1}^{m} \int_{I^n} \tau\varepsilon \|\partial_t\chi - \partial X^n\|^2_{L^2(\Omega)}\, dt\Big)^{\frac{1}{2}}\\ + \Big(\sum_{n=1}^{m} \int_{I^n} \big(\|\theta - \Theta^n\|^2_{L^2(\Omega)} + \tau\|\theta - \Theta^n\|^2_{H^1(\Omega)}\big)\, dt\Big)^{\frac{1}{2}} \le C\frac{\tau}{\sqrt{\varepsilon}},\end{aligned} \tag{2.8}$$

provided $U^n = \Theta^n + X^n$ and $\tau \le \varepsilon$ [8]. Proofs of (2.6) and (2.8) are given in [8] for zero Dirichlet boundary condition, but they easily extend to Neumann boundary condition. These results will play a prominent role below.

**3. Fully Discrete Problem.** We now introduce continuous piecewise linear finite elements to discretize $\Theta^n$, $X^n$, $U^n$ and $Z^n$. Let $\{\mathcal{M}_h\}_h$ be a family of regular and quasi-uniform partitions of $\Omega$ into simplices and $h > 0$ stand for the meshsize [5]. The finite element subspace $\mathbb{V}_h^1 \subset H^1(\Omega)$ satisfies $\mathbb{V}_h^1|_S = P^1(S)$ for all $S \in \mathcal{M}_h$, where $P^1(S)$ indicates the space of polynomials of degree not greater than 1 restricted to $S$. Let $\{x_j\}_{j=1}^J$ be the set of nodes of $\mathcal{M}_h$ and $\{\phi_j\}_{j=1}^J$ be the canonical basis of $\mathbb{V}_h^1$. We introduce the Ritz projection operator $\mathbf{R}_h : H^1(\Omega) \to \mathbb{V}_h^1$ defined by

$$\langle \nabla(\mathbf{R}_h\phi - \phi), \nabla\psi\rangle + \langle \mathbf{R}_h\phi - \phi, \psi\rangle = 0 \quad \forall\psi \in \mathbb{V}_h^1. \tag{3.1}$$

The following approximation properties are valid because $\Omega$ is convex [5]:

$$\|\mathbf{R}_h\phi - \phi\|_{L^2(\Omega)} \le Ch\|\phi\|_{H^1(\Omega)} \quad \forall\phi \in H^1(\Omega), \tag{3.2}$$

$$\|\mathbf{R}_h\phi - \phi\|_{H^1(\Omega)} \le Ch\|\phi\|_{H^2(\Omega)} \quad \forall\phi \in H^2(\Omega). \tag{3.3}$$

We suppose that $\{\phi_j\}_{j=1}^J$ satisfy

$$k_{ij} := \int_\Omega \nabla\phi_i \nabla\phi_j \, dx \le 0 \qquad \forall\ 1 \le i \ne j \le J, \tag{3.4}$$

which implies that $(k_{ij})_{i,j=1}^J$ is an M-matrix. A sufficient condition for (3.4) in 2D is that $\mathcal{M}_h$ is *weakly acute*: for all interelement sides $S$ and corresponding pair of adjacent triangles, the sum of the angles opposite to $S$ does not exceed $\pi$. This condition can be enforced in practice even with automatic mesh generators and is therefore not too restrictive [20]. Validity of the Discrete Maximum Principle (DMP) is then guaranteed, which in turn is crucial in our stability and error analysis. Let

$\Pi_h^1 : C^0(\bar\Omega) \to \mathbb{V}_h^1$ be the usual piecewise linear Lagrange interpolation operator defined by $(\Pi_h^1\phi)(x_j) = \phi(x_j)$ for $1 \le j \le J$.

We define a discrete inner product and corresponding norm in $\mathbb{V}_h^1$ by

$$\langle \psi, \phi\rangle_h := \int_\Omega \Pi_h^1(\psi\phi)\,dx, \qquad \|\phi\|_h := \big(\langle\phi,\phi\rangle_h\big)^{1/2}.$$

They can be evaluated easily by means of the vertex quadrature rule, which is exact for piecewise linear functions [5]. It is well known that $\langle\cdot,\cdot\rangle_h$ satisfies

$$\|\phi\|_{L^2(\Omega)}^2 \le \langle\phi,\phi\rangle_h \le C\|\phi\|_{L^2(\Omega)}^2, \tag{3.5}$$

and the following estimate holds:

$$\begin{aligned} |\langle\psi,\phi\rangle - \langle\psi,\phi\rangle_h| &\le Ch^2\|\nabla\psi\|_{L^2(\Omega)}\|\nabla\phi\|_{L^2(\Omega)} \\ &\le Ch\|\psi\|_{L^2(\Omega)}\|\nabla\phi\|_{L^2(\Omega)} \quad \forall\ \psi,\phi\in\mathbb{V}_h^1. \end{aligned} \tag{3.6}$$

For $\Theta_h^0 := \Pi_h^1\theta_0$, $X_h^0 := \Pi_h^1\chi_0$ and $Z_h^0 := \Pi_h^1 z_0$, the fully discrete problem reads: *for $1\le n\le N$, we seek $\Theta_h^n, X_h^n, Z_h^n \in \mathbb{V}_h^1$ such that*

$$\langle\partial\Theta_h^n,\varphi\rangle_h + \langle\partial X_h^n,\varphi\rangle_h + \langle\nabla\Theta_h^n,\nabla\varphi\rangle = 0, \qquad \forall\varphi\in\mathbb{V}_h^1, \tag{3.7}$$

$$\varepsilon\partial X_h^n + Z_h^n = \Theta_h^{n-1}, \quad Z_h^n(x_j)\in\Lambda(X_h^n(x_j)) \quad j=1,\cdots,J. \tag{3.8}$$

Sometimes it will be more suggestive to write $\Pi_h^1[\Lambda(X_h^n)]$ instead of $Z_h^n$. Even though $z_0\in\Lambda(\chi_0)$ is discontinuous, it makes sense to evaluate it at every node $x_j$ and so $Z_h^0$ is well defined with $Z_h^0(x_j)\in\Lambda(X_h^0(x_j))$ for $1\le j\le J$.

Note that (3.8) is a simple and inexpensive nodewise algebraic correction which computes $X_h^n$ in terms of $\Theta_h^{n-1}$ and $X_h^{n-1}$. In fact (3.8) can be rewritten explicitly as

$$X_h^n(x_j) = (I-\beta)\big(\tfrac{\tau}{\varepsilon}\Theta_h^{n-1} + X_h^{n-1}\big)(x_j), \tag{3.9}$$

where $\beta(s) := \min(s+1,0)+\max(s-1,0)$ and $I$ is the identity. When $\tau=\varepsilon$, (3.9) coincides with the algebraic correction of the nonlinear Chernoff formula of [1,11,14,17]. The stability constraint $\tau\le\varepsilon$ must be enforced to account for the presence of $\Theta_h^{n-1}$ instead of $\Theta_h^n$ in (3.8) [8,21,22]. On the other hand, (3.7) can be written equivalently as

$$\langle\Theta_h^n,\varphi\rangle_h + \tau\langle\nabla\Theta_h^n,\nabla\varphi\rangle = \langle\Theta_h^{n-1} - X_h^n + X_h^{n-1},\varphi\rangle_h, \qquad \forall\varphi\in\mathbb{V}_h^1. \tag{3.10}$$

This is a linear positive definite symmetric system in the unknown $\Theta_h^n$, which can be solved efficiently with an iterative solver. We resort to the conjugate gradient method preconditioned with an incomplete Cholesky factorization, as in [17].

We now discuss properties of the discrete initial data. In view of (2.1) we have

$$\|\nabla X_h^0\|_{L^2(\Omega)} \le C\|\nabla\chi_0\|_{L^\infty(\Omega)} \le C\varepsilon^{-1/2}. \tag{3.11}$$

This, in conjunction with $\theta_0\in W^{1,\infty}(\Omega)$, yields

$$\|\Theta_h^0 - \theta_0\|_{L^2(\Omega)} \le Ch\|\nabla\theta_0\|_{L^\infty(\Omega)} \le Ch, \tag{3.12}$$

$$\|X_h^0 - \chi(0)\|_{L^2(\Omega)} \le C\tfrac{h}{\sqrt{\varepsilon}}, \tag{3.13}$$

whence

$$\|U_h^0 - u(0)\|_{H^1(\Omega)^*} \le C\|\Theta_h^0 - \theta(0)\|_{L^2(\Omega)} + C\|X_h^0-\chi(0)\|_{L^2(\Omega)} \le C\tfrac{h}{\sqrt{\varepsilon}}. \tag{3.14}$$

It will be helpful in §4 to set $\Theta_h^{-1} := \Theta_h^0$ and choose $X_h^{-1} \in \mathbb{V}_h^1$ such that

$$\tfrac{\varepsilon}{\tau}(X_h^0 - X_h^{-1}) + Z_h^0 = \Theta_h^{-1}. \tag{3.15}$$

Consequently,

$$\varepsilon \partial X_h^n + Z_h^n = \Theta_h^{n-1}, \quad Z_h^n \in \Pi_h^1[\Lambda(X_h^n)] \qquad \forall\, n \geq 0, \tag{3.16}$$

and, with the aid of (2.2),

$$\sqrt{\varepsilon}\|X_h^0 - X_h^{-1}\|_{L^2(\Omega)} = \tfrac{\tau}{\sqrt{\varepsilon}}\|\Pi_h^1(\theta_0 - z_0)\|_{L^2(\Omega)} \leq C\tfrac{\tau}{\sqrt{\varepsilon}}\|\theta_0 - z_0\|_{L^\infty(\Omega)} \leq CA\tau. \tag{3.17}$$

The global relation (3.16) is inconvenient because of the bad behavior of $\nabla Z_h^n$. We thus resort to an idea stemming from *co-volume methods* that leads to yet another equivalent form of (3.8). We decompose the reference simplex $\hat{S}$, with vertices $\hat{x}_i$ and barycentric coordinates $\hat{\lambda}_i$, into $d+1$ polyhedra $\hat{S}_i$ as follows:

$$\hat{S}_i := \{x \in \hat{S} : \hat{\lambda}_i(x) \geq \hat{\lambda}_j(x),\ j \neq i\}.$$

This induces a decomposition of each simplex $S \in \mathcal{M}_h$ and a corresponding dual mesh $\mathcal{D}_h = \{D_j\}_{j=1}^J$, where $D_j$ is the union of all polyhedra associated with node $x_j$. We denote by $\mathbb{V}_h^0$ the space of piecewise constant elements over $\mathcal{D}_h$, and define the Lagrange interpolation operator $\Pi_h^0 : C^0(\bar{\Omega}) \to \mathbb{V}_h^0$ by $(\Pi_h^0\phi)(x_j) = \phi(x_j)$ for $1 \leq j \leq J$. From now on, we use the notation

$$\tilde{V} = \Pi_h^0 V \qquad \forall\, V \in \mathbb{V}_h^1, \tag{3.18}$$

and note that $\|\tilde{V}\|_{L^2(\Omega)}^2 = \|V\|_h^2$. We then extend (3.16) by the global relation

$$\varepsilon \partial \tilde{X}_h^n + \tilde{Z}_h^n = \tilde{\Theta}_h^{n-1}, \quad \tilde{Z}_h^n \in \Lambda(\tilde{X}_h^n) \qquad \forall\, n \geq 0. \tag{3.19}$$

We finish this section by stating three elementary identities to be used below, which are valid for all $a_n,\, b_n \in \mathbb{R}^k$ $(k \geq 1)$:

$$2\sum_{n=1}^m a_n(a_n - a_{n-1}) = |a_m|^2 - |a_0|^2 + \sum_{n=1}^m |a_n - a_{n-1}|^2, \tag{3.20}$$

$$2\sum_{n=1}^m a_n \sum_{i=1}^n a_i = \Big|\sum_{n=1}^m a_n\Big|^2 + \sum_{n=1}^m |a_n|^2, \tag{3.21}$$

$$\sum_{n=1}^m a_n(b_n - b_{n-1}) = a_m b_m - a_0 b_0 - \sum_{n=1}^m (a_n - a_{n-1}) b_{n-1}. \tag{3.22}$$

Identity (3.21) is a consequence of (3.20) applied to $A_n = \sum_{i=1}^n a_i$. Identity (3.22) is usually called the discrete integration (or summation) by parts formula.

**4. Stability.** We derive several a priori estimates for the fully discrete scheme (3.7)-(3.8), which will play a major role later on in the error analysis of §5. We first state a new *strong* a priori estimate — the fully discrete analogue of (2.6). Its proof is identical to that of (2.6) given in [8], and is thus omitted. To account for the definition of $\Theta_h^0 = \mathbf{P}_h^1\theta_0$, which entails direct nodal evaluation of $\theta_0$ without averaging, $\|\nabla\Theta_h^0\|_{L^2(\Omega)}$ has been replaced by $\|\nabla\theta_0\|_{L^\infty(\Omega)}$.

LEMMA 4.1. *The following a priori estimates hold provided* $\tau \leq \varepsilon$

$$\tau\sum_{n=1}^{N}\|\partial\Theta_h^n\|_h^2 + \sum_{n=1}^{N}\|\nabla(\Theta_h^n - \Theta_h^{n-1})\|_{L^2(\Omega)}^2 + \max_{1\leq n\leq N}\|\nabla\Theta_h^n\|_{L^2(\Omega)}^2$$
$$+\varepsilon\sum_{n=1}^{N}\|\partial(X_h^n - X_h^{n-1})\|_h^2 + \varepsilon\max_{1\leq n\leq N}\|\partial X_h^n\|_h^2 \leq C(A^2+\|\nabla\theta_0\|_{L^\infty(\Omega)}^2).$$

The second and fourth terms represent the (discrete) intermediate Sobolev norms of $H^{1/2}(H^1)$ and $H^{3/2}(L^2)$ respectively. In contrast to next result, Lemma 4.1 does not rely on (3.4) and hence is valid for general regular and quasi-uniform meshes. We point out that it is here where we need a Neumann condition.

LEMMA 4.2. *There exists* $C > 0$*, depending on* $A$ *and* $\|\nabla\theta_0\|_{L^\infty(\Omega)}$*, such that for* $\tau \leq \varepsilon$ *the following a priori estimates hold*

$$\max_{1\leq n\leq N}\|\nabla X_h^n\|_{L^2(\Omega)}^2 + \sum_{n=1}^{N}\|\nabla(X_h^n - X_h^{n-1})\|_{L^2(\Omega)}^2 \leq \tfrac{C}{\varepsilon}. \tag{4.1}$$

*Proof.* We differentiate (3.16) and add the resulting expression to (3.7) to obtain

$$\langle\partial X_h^n,\varphi\rangle_h+\langle\partial\Theta_h^n,\varphi\rangle_h + \langle\nabla(\Theta_h^n - \Theta_h^{n-1}),\nabla\varphi\rangle$$
$$+\tfrac{\varepsilon}{\tau}\langle\nabla(X_h^n - X_h^{n-1}),\nabla\varphi\rangle + \langle\nabla Z_h^n,\nabla\varphi\rangle = 0, \quad \forall\varphi\in\mathbb{V}_h^1.$$

Take $\varphi := \tau X_h^n \in \mathbb{V}_h^1$ as a test function and sum over $n$ from 1 to $m \leq N$. We get

$$\begin{aligned} 0 &= \sum_{n=1}^{m}\langle X_h^n - X_h^{n-1}, X_h^n\rangle_h + \sum_{n=1}^{m}\tau\langle\partial\Theta_h^n, X_h^n\rangle_h \\ &+\tau\sum_{n=1}^{m}\langle\nabla(\Theta_h^n - \Theta_h^{n-1}),\nabla X_h^n\rangle + \varepsilon\sum_{n=1}^{m}\langle\nabla(X_h^n - X_h^{n-1}),\nabla X_h^n\rangle \\ &+\tau\sum_{n=1}^{m}\langle\nabla Z_h^n,\nabla X_h^n\rangle =: \mathrm{I}+\mathrm{II}+\mathrm{III}+\mathrm{IV}+\mathrm{V}. \end{aligned} \tag{4.2}$$

We make use of (3.20) and property $|X_h^n| \leq 1$ to deduce

$$\mathrm{I} = \tfrac12\|X_h^m\|_h^2 - \tfrac12\|X_h^0\|_h^2 + \tfrac12\sum_{n=1}^{m}\|X_h^n - X_h^{n-1}\|_h^2 \geq -C,$$

and

$$\mathrm{IV} = \tfrac{\varepsilon}{2}\|\nabla X_h^m\|_{L^2(\Omega)}^2 - \tfrac{\varepsilon}{2}\|\nabla X_h^0\|_{L^2(\Omega)}^2 + \tfrac{\varepsilon}{2}\sum_{n=1}^{m}\|\nabla(X_h^n - X_h^{n-1})\|_{L^2(\Omega)}^2.$$

By virtue of Lemma 4.1 and $|X_h^n| \leq 1$ again, terms II and III can be estimated as follows:

$$|\mathrm{II}| \leq \Big(\sum_{n=1}^{m}\tau\|\partial\Theta_h^n\|_h^2\Big)^{\frac12}\Big(\sum_{n=1}^{m}\tau\|X_h^n\|_h^2\Big)^{\frac12} \leq C,$$

and $(\tau \le \varepsilon)$

$$\begin{aligned}|\mathrm{III}| &\le \tfrac{\tau}{2\varepsilon}\textstyle\sum_{n=1}^m \|\nabla(\Theta_h^n - \Theta_h^{n-1})\|_{L^2(\Omega)}^2 + \tfrac{\varepsilon}{2}\textstyle\sum_{n=1}^m \tau\|\nabla X_h^n\|_{L^2(\Omega)}^2\\ &\le C + \tfrac{\varepsilon}{2}\sum_{n=1}^m \tau\|\nabla X_h^n\|_{L^2(\Omega)}^2.\end{aligned}$$

To estimate term V we exploit (3.4). In fact, it easily follows that (see [15, p. S6])

$$\langle \nabla Z_h^n, \nabla X_h^n\rangle = \sum_{i=1}^J \Big(\sum_{j\ne i} \tfrac12 (Z_i^n - Z_j^n)(X_j^n - X_i^n)k_{ij} + Z_i^n X_i^n \big(k_{ii} + \sum_{j\ne i} k_{ij}\big)\Big) \ge 0,$$

because the nodal values $X_i^n$ and $Z_i^n$ satisfy $Z_i^n \in \Lambda(X_i^n)$, $\Lambda$ is monotone, and $0 \in \Lambda(0)$. Combining the above estimates with (3.11) we obtain

$$\|\nabla X_h^m\|_{L^2(\Omega)}^2 + \sum_{n=1}^m \|\nabla(X_h^n - X_h^{n-1})\|_{L^2(\Omega)}^2 \le \tfrac{C}{\varepsilon} + \sum_{n=1}^m \tau\|\nabla X_h^n\|_{L^2(\Omega)}^2.$$

Invoking the discrete Gronwall inequality, the above inequality implies (4.1). □

**5. Error Analysis.** We derive linear energy error estimates for the three variables $\theta, \chi$ and $u = \theta + \chi$. We will only compare the fully discrete and semidiscrete solutions and use (2.8) to bridge the gap. For $v = \theta, \chi, u$ we will use the symbol $e_v^n := V^n - V_h^n$ to indicate the error between the semidiscrete and fully discrete approximations of $v$.

THEOREM 5.1. *There exists $C > 0$, depending on $A$ and $\|\nabla\theta_0\|_{L^\infty(\Omega)}$ only, such that the following linear error estimates hold for all $1 \le m \le N$*

$$\varepsilon\|e_\chi^m\|_{L^2(\Omega)}^2 + \sum_{n=1}^m \tau\|e_\theta^n\|_{L^2(\Omega)}^2 + \|\sum_{n=1}^m \tau\nabla e_\theta^n\|_{L^2(\Omega)}^2 + \tau\sum_{n=1}^m \tau\|\nabla e_\theta^n\|_{L^2(\Omega)}^2 \le C\tfrac{h^2+\tau^2}{\varepsilon}.$$

*Proof.* From (2.4) and (3.7) we have for all $\varphi \in \mathbb{V}_h^1$

$$\langle \Theta^n, \varphi\rangle + \langle X^n, \varphi\rangle + \tau\langle \nabla\sum_{i=1}^n \Theta^i, \nabla\varphi\rangle = \langle u_0, \varphi\rangle, \tag{5.1}$$

$$\langle \Theta_h^n, \varphi\rangle_h + \langle X_h^n, \varphi\rangle_h + \tau\langle \nabla\sum_{i=1}^n \Theta_h^i, \nabla\varphi\rangle = \langle U_h^0, \varphi\rangle_h. \tag{5.2}$$

We now subtract (5.2) from (5.1), take $\varphi = \varphi^n := \mathbf{R}_h\Theta^n - \Theta_h^n \in \mathbb{V}_h^1$ with $\mathbf{R}_h$ defined in (3.1) and finally sum on $n$ from 1 to $m$ to arrive at

$$\begin{aligned}\sum_{n=1}^m \tau\langle e_\theta^n + e_\chi^n, \varphi^n\rangle + \sum_{n=1}^m \tau\langle \sum_{i=1}^n \tau\nabla e_\theta^i, \nabla\varphi^n\rangle &=: \mathrm{I} + \mathrm{II}\\ &= \sum_{n=1}^m \tau\big(\langle \Theta_h^n - \Theta_h^0, \varphi^n\rangle_h - \langle \Theta_h^n - \Theta_h^0, \varphi^n\rangle\big)\\ &\quad + \sum_{n=1}^m \tau\big(\langle X_h^n - X_h^0, \varphi^n\rangle_h - \langle X_h^n - X_h^0, \varphi^n\rangle\big)\\ &\quad + \langle e_u(0), \sum_{n=1}^m \tau\varphi^n\rangle =: \mathrm{III} + \mathrm{IV} + \mathrm{V}.\end{aligned}\tag{5.3}$$

On the other hand, subtracting (3.19) from (2.5), and then multiplying by $X^n - \tilde{X}_h^n$, we get

$$\varepsilon\partial\big(X^n - \tilde{X}_h^n\big)(X^n - \tilde{X}_h^n) + \big(Z^n - \tilde{Z}_h^n\big)(X^n - \tilde{X}_h^n) = (\Theta^{n-1} - \tilde{\Theta}_h^{n-1})(X^n - \tilde{X}_h^n). \tag{5.4}$$

Noticing that the second term on the left hand side of (5.4) is nonnegative almost everywhere because of the monotonicity of $\Lambda$, we can integrate (5.4) over $\Omega$ and sum on $n$ from 1 to $m$ to deduce

$$\mathrm{VI} := \varepsilon\sum_{n=1}^{m}\tau\langle\partial(X^n - \tilde{X}_h^n), X^n - \tilde{X}_h^n\rangle \le \sum_{n=1}^{m}\tau\langle\Theta^{n-1} - \tilde{\Theta}_h^{n-1}, X^n - \tilde{X}_h^n\rangle =: \mathrm{VII}. \tag{5.5}$$

To derive our main result we add (5.3) and (5.5) and analyze terms I through VII separately. We first point out that

$$\mathrm{I} = \sum_{n=1}^{m}\tau\Big(\langle e_\theta^n, e_\theta^n\rangle + \langle e_\chi^n, e_\theta^n\rangle + \langle e_\theta^n + e_\chi^n, \mathbf{R}_h\Theta^n - \Theta^n\rangle\Big).$$

From (2.6) and (3.2), it follows that $\|(\mathbf{R}_h - \mathbf{I})\Theta^n\|_{L^2(\Omega)} \le Ch$. By Cauchy-Schwarz and Young inequalities, we readily get

$$\begin{aligned}\mathrm{I} &\ge \tfrac{1}{2}\sum_{n=1}^{m}\tau\|e_\theta^n\|_{L^2(\Omega)}^2 + \sum_{n=1}^{m}\tau\langle e_\chi^n, e_\theta^n\rangle\\ &\quad -\varepsilon\sum_{n=1}^{m}\tau\|e_\chi^n\|_{L^2(\Omega)}^2 - \tfrac{C}{\varepsilon}\sum_{n=1}^{m}\tau\|(\mathbf{R}_h - \mathbf{I})\Theta^n\|_{L^2(\Omega)}^2\\ &\ge \tfrac{1}{2}\sum_{n=1}^{m}\tau\|e_\theta^n\|_{L^2(\Omega)}^2 + \sum_{n=1}^{m}\tau\langle e_\theta^n, e_\chi^n\rangle - \varepsilon\sum_{n=1}^{m}\tau\|e_\chi^n\|_{L^2(\Omega)}^2 - C\tfrac{h^2}{\varepsilon}.\end{aligned} \tag{5.6}$$

Hereafter, $\eta$ denotes an arbitrary fixed positive number which will be selected later, and $C$ is a generic constant that may depend on $\eta$, $\|\nabla\theta_0\|_{L^\infty(\Omega)}$ and $A$. In light of (3.1) and (3.21), together with the fact that $\varphi^i = \mathbf{R}_h e_\theta^i$, term II can be equivalently written as follows:

$$\begin{aligned}\mathrm{II} &= \tau^2\sum_{n=1}^{m}\langle\sum_{i=1}^{n}\nabla\mathbf{R}_h e_\theta^i, \nabla\varphi^n\rangle + \tau^2\sum_{n=1}^{m}\langle\sum_{i=1}^{n}(\mathbf{R}_h e_\theta^i - e_\theta^i), \varphi^n\rangle\\ &= \tau^2\sum_{n=1}^{m}\langle\sum_{i=1}^{n}\nabla\varphi^i, \nabla\varphi^n\rangle + \tau\sum_{n=1}^{m}\langle(\mathbf{R}_h - \mathbf{I})\sum_{i=1}^{n}\tau\Theta^i, \varphi^n\rangle.\end{aligned}$$

Consequently, (2.6), (2.7), and (3.2) yield

$$\begin{aligned}\mathrm{II} &\ge \tfrac{1}{2}\|\tau\sum_{n=1}^{m}\nabla\varphi^n\|_{L^2(\Omega)}^2 + \tfrac{\tau}{2}\sum_{n=1}^{m}\tau\|\nabla\varphi^n\|_{L^2(\Omega)}^2\\ &\quad -\eta\tau\sum_{n=1}^{m}\|\varphi^n\|_{L^2(\Omega)}^2 - C\tau\sum_{n=1}^{m}\|(\mathbf{R}_h - \mathbf{I})\Theta^n\|_{L^2(\Omega)}^2\\ &\ge \tfrac{1}{4}\|\tau\sum_{n=1}^{m}\nabla e_\theta^n\|_{L^2(\Omega)}^2 + \tfrac{\tau}{4}\sum_{n=1}^{m}\tau\|\nabla e_\theta^n\|_{L^2(\Omega)}^2 - 2\eta\tau\sum_{n=1}^{m}\|e_\theta^n\|_{L^2(\Omega)}^2 - Ch^2.\end{aligned}$$

With the aid of (3.6) and Lemma 4.1 the estimation of III proceeds as follows:

$$
\begin{aligned}
|\mathrm{III}| &\le \tau\sum_{n=1}^{m}\Big|\langle\Theta_h^n-\Theta_h^0,\varphi^n\rangle_h-\langle\Theta_h^n-\Theta_h^0,\varphi^n\rangle\Big| \\
&\le Ch\sum_{n=1}^{m}\tau\big(\|\nabla\Theta_h^n\|_{L^2(\Omega)}+\|\nabla\Theta_h^0\|_{L^2(\Omega)}\big)\|\varphi^n\|_{L^2(\Omega)} \\
&\le Ch^2\sum_{n=1}^{m}\tau\big(\|\nabla\Theta_h^n\|^2_{L^2(\Omega)}+\|\nabla\Theta_h^0\|^2_{L^2(\Omega)}\big)+\eta\sum_{n=1}^{m}\tau\|\varphi^n\|^2_{L^2(\Omega)} \\
&\le Ch^2+2\eta\sum_{n=1}^{m}\tau\|e_\theta^n\|^2_{L^2(\Omega)}.
\end{aligned}
$$

Similarly, but this time using (3.11) and Lemma 4.2, we obtain

$$
|\mathrm{IV}|\le\tau\sum_{n=1}^{m}\Big|\langle X_h^n-X_h^0,\varphi^n\rangle_h-\langle X_h^n-X_h^0,\varphi^n\rangle\Big|\le C\tfrac{h^2}{\varepsilon}+2\eta\sum_{n=1}^{m}\tau\|e_\theta^n\|^2_{L^2(\Omega)}.
$$

For V, we exploit Young's inequality, together with (2.6), (2.7) and (3.14), to get

$$
|\mathrm{V}|\le\|e_u(0)\|_{H^1(\Omega)^*}\|\sum_{n=1}^{m}\tau\varphi^n\|_{H^1(\Omega)}\le C\tfrac{h^2}{\varepsilon}+\eta\sum_{n=1}^{m}\tau\|e_\theta^n\|_0^2+\eta\|\sum_{n=1}^{m}\tau\nabla e_\theta^n\|^2_{L^2(\Omega)}.
$$

Now we consider the terms coming from the constitutive relations. We first observe that Lemmas 4.1 and 4.2 imply

$$
\begin{aligned}
\|X_h^n-\tilde X_h^n\|_{L^2(\Omega)}&\le Ch\|\nabla X_h^n\|_{L^2(\Omega)}\le C\tfrac{h}{\sqrt{\varepsilon}},\\
\|\Theta_h^n-\tilde\Theta_h^n\|_{L^2(\Omega)}&\le Ch\|\nabla\Theta_h^n\|_{L^2(\Omega)}\le Ch.
\end{aligned}
\tag{5.7}
$$

For VI we use (3.20), in conjunction with (2.1) and (5.7), to arrive at

$$
\begin{aligned}
2\mathrm{VI}&=\varepsilon\|X^m-\tilde X_h^m\|_0^2-\varepsilon\|X^0-\tilde X_h^0\|_0^2+\varepsilon\sum_{n=1}^{m}\|X^n-\tilde X_h^n\|_0^2\\
&\ge\tfrac{\varepsilon}{2}\|e_\chi^m\|_0^2-\varepsilon\|X_h^m-\tilde X_h^m\|_0^2-\varepsilon\|\chi_0-\tilde X_h^0\|_0^2\ge\tfrac{\varepsilon}{2}\|e_\chi^m\|_0^2-Ch^2.
\end{aligned}
$$

We now further split VII into eight terms:

$$
\begin{aligned}
\mathrm{VII}=&\sum_{n=1}^{m}\tau\langle\Theta^n-\Theta_h^n,X^n-X_h^n\rangle+\sum_{n=1}^{m}\tau\langle\Theta^n-\Theta_h^n,X_h^n-\tilde X_h^n\rangle\\
&+\sum_{n=1}^{m}\tau\langle\Theta^{n-1}-\Theta^n,X^n-X_h^n\rangle+\sum_{n=1}^{m}\tau\langle\Theta^{n-1}-\Theta^n,X_h^n-\tilde X_h^n\rangle\\
&+\sum_{n=1}^{m}\tau\langle\Theta_h^n-\Theta_h^{n-1},X^n-X_h^n\rangle+\sum_{n=1}^{m}\tau\langle\Theta_h^n-\Theta_h^{n-1},X_h^n-\tilde X_h^n\rangle\\
&+\sum_{n=1}^{m}\tau\langle\Theta_h^{n-1}-\tilde\Theta_h^{n-1},X^n-X_h^n\rangle+\sum_{n=1}^{m}\tau\langle\Theta_h^{n-1}-\tilde\Theta_h^{n-1},X_h^n-\tilde X_h^n\rangle\\
=:&\mathrm{VII}_1+\mathrm{VII}_2+\cdots+\mathrm{VII}_8.
\end{aligned}
$$

Term $\mathrm{VII}_1$ coincides with $\sum_{n=1}^m \tau\langle e_\theta^n, e_\chi^n\rangle$ in (5.6). The rest of the seven terms are estimated as follows via Young's inequality, (2.6), (2.7) Lemma 4.1 and (5.7):

$$\mathrm{VII}_2 \le \eta\sum_{n=1}^m \tau\|e_\theta^n\|^2_{L^2(\Omega)} + \tfrac{C}{\eta}\sum_{n=1}^m \tau\|X_h^n - \tilde X_h^n\|^2_{L^2(\Omega)} \le \eta\sum_{n=1}^m \tau\|e_\theta^n\|^2_{L^2(\Omega)} + C\tfrac{h^2}{\varepsilon};$$

$$\mathrm{VII}_3 \le C\tfrac{\tau^2}{\varepsilon}\sum_{n=1}^m \tau\|\partial\Theta^n\|^2_{L^2(\Omega)} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)} \le C\tfrac{\tau^2}{\varepsilon} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)};$$

$$\mathrm{VII}_4 \le \tau^2\sum_{n=1}^m \tau\|\partial\Theta^n\|^2_{L^2(\Omega)} + \sum_{n=1}^m \tau\|X_h^n - \tilde X_h^n\|^2_{L^2(\Omega)} \le C\tau^2 + C\tfrac{h^2}{\varepsilon};$$

$$\mathrm{VII}_5 \le C\tfrac{\tau^2}{\varepsilon}\sum_{n=1}^m \tau\|\partial\Theta_h^n\|^2_{L^2(\Omega)} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)} \le C\tfrac{\tau^2}{\varepsilon} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)};$$

$$\mathrm{VII}_6 \le \tau^2\sum_{n=1}^m \tau\|\partial\Theta_h^n\|^2_{L^2(\Omega)} + \sum_{n=1}^m \tau\|X_h^n - \tilde X_h^n\|^2_{L^2(\Omega)} \le C\tau^2 + C\tfrac{h^2}{\varepsilon};$$

$$\mathrm{VII}_7 \le \tfrac{\tau}{\varepsilon}\sum_{n=1}^m \|\Theta_h^{n-1} - \tilde\Theta_h^{n-1}\|^2_{L^2(\Omega)} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)} \le C\tfrac{h^2}{\varepsilon} + \varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)};$$

$$\mathrm{VII}_8 \le \sum_{n=1}^m \tau\|\Theta_h^{n-1} - \tilde\Theta_h^{n-1}\|^2_{L^2(\Omega)} + \sum_{n=1}^m \tau\|X_h^n - \tilde X_h^n\|^2_{L^2(\Omega)} \le Ch^2 + C\tfrac{h^2}{\varepsilon} \le C\tfrac{h^2}{\varepsilon}.$$

Thus

$$\mathrm{VII} \le \sum_{n=1}^m \tau\langle e_\theta^n, e_\chi^n\rangle + 3\varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)} + \eta\sum_{n=1}^m \tau\|e_\theta^n\|^2_{L^2(\Omega)} + C\tfrac{h^2+\tau^2}{\varepsilon}.$$

We finally collect the above estimates and insert them into (5.3) and (5.5). Upon choosing $\eta$ sufficiently small we end up with

$$\begin{aligned}\varepsilon\|e_\chi^m\|^2_{L^2(\Omega)} &+ \sum_{n=1}^m \tau\|e_\theta^n\|^2_{L^2(\Omega)} + \|\sum_{n=1}^m \tau\nabla e_\theta^n\|^2_{L^2(\Omega)} \\ &+ \tau\sum_{n=1}^m \tau\|\nabla e_\theta^n\|^2_{L^2(\Omega)} \le C\tfrac{h^2+\tau^2}{\varepsilon} + C\varepsilon\sum_{n=1}^m \tau\|e_\chi^n\|^2_{L^2(\Omega)}.\end{aligned}$$

The discrete Gronwall inequality finally yields the asserted estimate. ∎

COROLLARY 5.2. $\max_{1\le n\le N}\|e_u^n\|_{H^1(\Omega)^*} \le C\frac{h+\tau}{\sqrt{\varepsilon}}$.

*Proof.* Given an arbitrary $\phi \in H^1(\Omega)$, we take $\varphi := \mathbf{R}_h\phi \in \mathbb{V}_h^1$ as a test function into the difference of (5.1) and (5.2), which then reads

$$\begin{aligned}\langle e_u^m, \phi\rangle = &-\langle\sum_{n=1}^m \tau\nabla(\mathbf{R}_h\Theta^n - \Theta_h^n), \nabla\mathbf{R}_h\phi\rangle \\ &+ \langle e_u^m, (\mathbf{I}-\mathbf{R}_h)\phi\rangle + \langle e_u^0, \mathbf{R}_h\phi\rangle + \langle U_h^0 - U_h^m, \mathbf{R}_h\phi\rangle - \langle U_h^0 - U_h^m, \mathbf{R}_h\phi\rangle_h.\end{aligned}$$

We now combine the following by-product of the above proof

$$\max_{1\le n\le m}\|\sum_{n=1}^m \tau\nabla(\mathbf{R}_h\Theta^n - \Theta_h^n)\|_{L^2(\Omega)} \le C\tfrac{h+\tau}{\sqrt{\varepsilon}}$$

with $\|\mathbf{R}_h\phi\|_{H^1(\Omega)} \le \|\phi\|_{H^1(\Omega)}$ and $\|e_u^m\|_{L^2(\Omega)} \le C$, to obtain the asserted estimate. ∎

**6. Numerical Experiments.** We present two examples which illustrate the implementation and performance of our finite element method. Let $\mathbf{M}$ and $\mathbf{K}$ be the mass and stiffness matrices, namely,

$$\mathbf{M} := \left(\langle\phi_i, \phi_j\rangle_h\right)_{i,j=1}^J, \quad \mathbf{K} := \left(\langle\nabla\phi_i, \nabla\phi_j\rangle\right)_{i,j=1}^J. \tag{6.1}$$

The integrals can be computed via the vertex quadrature rule, which gives rise to a diagonal $\mathbf{M}$. Then the linear algebraic system for $\Theta_h^n$ becomes

$$\mathbf{M}\Theta_h^n + \tau\mathbf{K}\Theta_h^n = \mathbf{M}(\Theta_h^{n-1} + X_h^{n-1} - X_h^n),$$

or equivalently

$$\Theta_h^n + \mathbf{A}\Theta_h^n = \Theta_h^{n-1} + X_h^{n-1} - X_h^n, \tag{6.2}$$

where $\mathbf{A} := \tau(\mathbf{M})^{-1}\mathbf{K}$ is easy to compute. This symmetric positive definite system is actually solved by a Preconditioned Conjugate Gradient Method (PCG) with an incomplete Cholesky factorization as a preconditioner. The finite element code, called AM, is written in C-language on a SunOS 5.4 (SPARC), because of the need to avoid very large static memory space allocations and to use data structures such as quadtrees. The meshes are generated by the 2D automatic mesh generator of [20].

**Example 6.1: Modified Traveling Wave**. This is an example with exact solution based on the traveling waves of [18]. Even though all functions exhibit radial symmetry, this is a true 2D test because symmetry is not exploited by the code. Let $\delta_{12}^+ := V/2$, $\delta_{12}^- := \sqrt{1/\varepsilon + V^2/4}$. A 1D traveling wave $\theta(x,t) = \theta_0(x+Vt)$, $\chi(x,t) = \chi_0(x+Vt)$ is given by

$$\theta_0(x) := \begin{cases} \frac{\gamma}{V}(\mathrm{e}^{Vx} - 1), & \text{if } x \le 0 \\ \frac{\gamma}{\delta_{12}^-}\mathrm{e}^{\delta_{12}^+ x}\sinh(\delta_{12}^- x), & \text{if } 0 < x \le x_\varepsilon \\ \frac{\theta_0'(x_\varepsilon)}{V}(\mathrm{e}^{V(x-x_\varepsilon)} - 1) + \frac{\gamma}{\delta_{12}^-}\mathrm{e}^{\delta_{12}^+ x_\varepsilon}\sinh(\delta_{12}^- x_\varepsilon), & \text{if } x > x_\varepsilon, \end{cases}$$

$$\chi_0(x) := \begin{cases} 0, & \text{if } x \le 0 \\ \frac{\gamma}{2\delta_{12}^- V\varepsilon}\left(\frac{\mathrm{e}^{(\delta_{12}^+ + \delta_{12}^-)x} - 1}{\delta_{12}^+ + \delta_{12}^-} - \frac{\mathrm{e}^{(\delta_{12}^+ - \delta_{12}^-)x} - 1}{\delta_{12}^+ - \delta_{12}^-}\right), & \text{if } 0 < x < x_\varepsilon \\ 1, & \text{if } x \ge x_\varepsilon, \end{cases}$$

where $\gamma$ is a parameter, $V$ represents the traveling wave velocity and $x_\varepsilon$, the transition region thickness, satisfies $\int_0^{x_\varepsilon}\theta_0(s)ds = V\varepsilon$ [18]. Note that $\chi_0$ does not take values between $-1$ and 1 but rather between 0 and 1 as in [18]. We take $\gamma = 0.5$, $V = 1$ and $\varepsilon = 0.003$ to perform our experiments, which gives $x_\varepsilon = 0.09526$.

We now consider a planar annulus transition region moving toward its center in the $x$-$y$ plane. The exact solution is constructed as follows. Let $p(s)$ be a polynomial of degree 4 such that $p'(1) = p''(1) = 0$ and $p(1.5) = \theta_0(-0.5)$, $p'(1.5) = \theta_0'(-0.5)$, $p''(1.5) = \theta_0''(-0.5)$. We take $r := \sqrt{x^2+y^2} + Vt$,

$$\theta(x,y,t) := \begin{cases} p(1), & \text{if } r \le 1 \\ p(r), & \text{if } 1 < r \le 1.5 \\ \theta_0(r-2), & \text{if } 1.5 < r \le 2 + x_\varepsilon \\ \theta_0'(x_\varepsilon)(r - 2 - x_\varepsilon) + \theta_0(x_\varepsilon), & \text{otherwise}, \end{cases}$$

$$\chi(x,y,t) := \begin{cases} 0, & \text{if } r \le 2 \\ \chi_0(r-2), & \text{otherwise}, \end{cases}$$

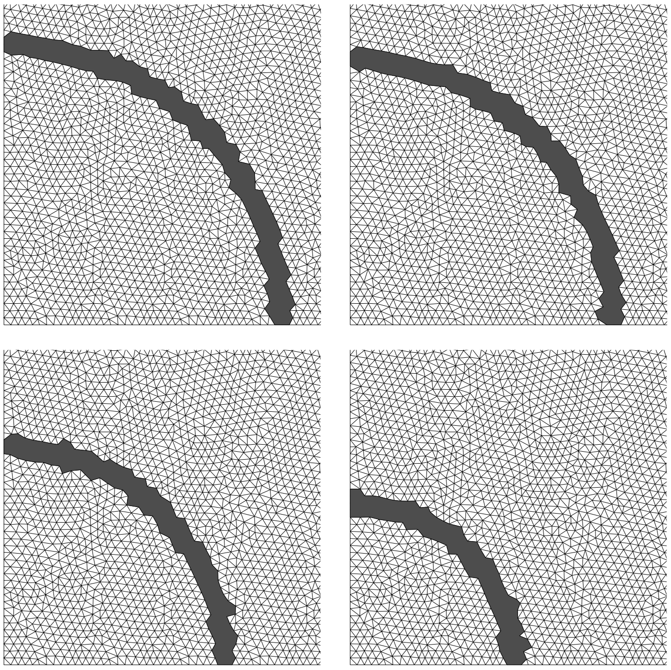

FIGURE 6.1. **Example 6.1: Modified Traveling Wave**
Zoom of Transition Regions ($n = 10,\ 20,\ 50,\ 90$) with $N = 100, h = 0.05$.

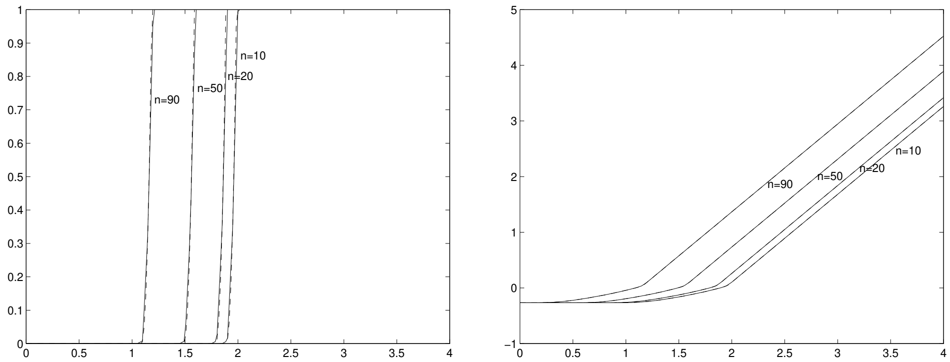


FIGURE 6.2. **Example 6.1: Modified Traveling Wave**
Profiles of $X_h^n$, $\Theta_h^n$ (dashed lines) and $\chi^n$, $\theta^n$ (solid lines) at $n = 10,\ 20,\ 50,\ 90$ along the $x$-axis

$f$ is defined in such a way that (1.1) holds and $\Omega := [0,4] \times [0,4]$, $T := 1$. We impose Dirichlet boundary conditions on $\{x = 4\}$ and $\{y = 4\}$ and Neumann boundary conditions on $\{x = 0\}$ and $\{y = 0\}$. We have $\|\theta\|_{L^2(Q)} \approx 11.59$, $\|\theta\|_{L^\infty(Q)} \approx 7.16$, $\|u\|_{L^\infty(0,T;L^2(\Omega))} \approx 17.63$, $\|u\|_{L^2(Q)} \approx 14.4$ and $\sqrt{\varepsilon}\|\chi\|_{L^\infty(0,T;L^2(\Omega))} \approx 0.21$. The results are shown in TABLE 6.1 for $\tau = h/5$. We have employed the following notation:

**N** := number of (uniform) time steps,
**J** := degrees of freedom (dimension of linear system),
**I** := average number of **PCG** iterations,
**t** := total CPU time in seconds (without graphics),
$E_v^{p,q} := \|e_v\|_{L^p(0,T;L^q(\Omega))}$ and $E_{\chi,\varepsilon}^{\infty,2} := \sqrt{\varepsilon}\|e_\chi\|_{L^\infty(0,T;L^2(\Omega))}$.

Note that we have also included the errors $||e_u||_{L^2(Q)}$ and $||\theta||_{L^\infty(Q)}$ which are not studied in the theory.

TABLE 6.1: Example 6.1 ($\varepsilon = 0.003, \tau = h/5 = 1/\mathbf{N}$ (errors scaled by $10^2$))

| **N** | **J** | **I** | $\mathbf{E}_\theta^{2,2}$ | $\mathbf{E}_u^{\infty,2}$ | $\mathbf{E}_{\chi,\varepsilon}^{\infty,2}$ | $\mathbf{E}_u^{2,2}$ | $\mathbf{E}_\theta^{\infty,\infty}$ | **t** |
|---|---|---|---|---|---|---|---|---|
| 100 | 5070 | 4.00 | 0.5914 | 2.3185 | 0.1128 | 1.9383 | 2.7974 | 97 |
| 200 | 20630 | 6.20 | 0.2464 | 1.0037 | 0.0498 | 0.8780 | 1.1729 | 953 |
| 300 | 46400 | 10.64 | 0.1494 | 1.6358 | 0.0314 | 0.5721 | 0.6090 | 4373 |
| 400 | 83081 | 10.13 | 0.1178 | 0.4636 | 0.0233 | 0.4245 | 0.4161 | 9806 |

Numerical results confirm the linear rate of §5 and also show that the total CPU time increases drastically as $h$ decreases. FIGURE 6.1 shows four transition regions $\{0 < X_h^n < 1\}$ for $\varepsilon = 0.003$, $N = 100$ and $h = 0.05$. FIGURE 6.2 illustrates the rapid variation of $X_h^n$ and $\partial_x \Theta_h^n$ within such regions, which in the limit $\tau \approx h \downarrow 0$ become annuli of thickness $x_\varepsilon = 0.09526$. To obtain better resolved discrete transition regions, we have to reduce $h$ and $\tau$ at the expense of larger CPU time and static space memory allocations. We will show in [9] how to cope with this difficulty via locally refined meshes.

**Example 6.2: Cusp Formation**. This is Example III of [16], whose exact solution is unknown but exhibits a cusp singularity in the $x$-axis. We have taken $\Omega = (-2, 4) \times (0, 5)$, $T = 1$, $N = 480$, $h = 0.02$, $\tau = 0.0208$ and $\varepsilon = 0.0021$. We supply zero Neumann boundary conditon along x-axis and Dirichlet boundary condition along other sides. FIGURE 6.3 contains the transition regions for $n = 17,\ 140,\ 200,\ 228,\ 315$ and 414. They shrink until disappearance at $n = 415$. We stress that the number of interior and Neumann nodes is 61103, and so the CPU time is very high. We shall

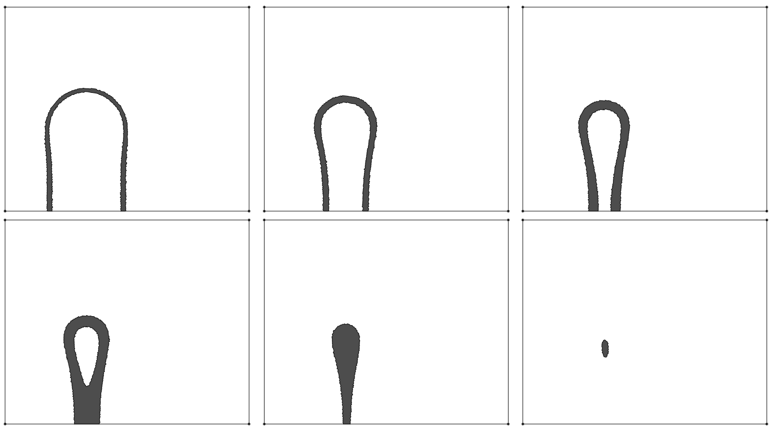

FIGURE 6.3. **Example 6.2: Cusp Formation**
Transition Regions at $n = 17,\ 140,\ 200,\ 228,\ 315,\ 414$.

show in Part II how to reduce the computational work for a desired accuracy via adaptivity.

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