CHARACTERISTIC-GALERKIN METHODS FOR CONTAMINANT TRANSPORT WITH NON-EQUILIBRIUM ADSORPTION KINETICS

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Abstract

A procedure based on combining the method of characteristics with a Galerkin finite element method is analyzed for approximating reactive transport in groundwater. In particular, we consider equations modeling contaminant transport with nonlinear, non-equilibrium adsorption reactions. This phenomena gives rise to non-Lipschitz but monotone nonlinearities which complicate the analysis. A physical and mathematical description of the problem under consideration is given, then the numerical method is described and *a priori* error estimates are derived.

Keywords: method of characteristics, Galerkin finite elements, contaminant transport

AMS(MOS) subject classification: 65N15, 65N30

1 Introduction

In this paper, we describe a characteristic-Galerkin finite element method (CGFEM) for modeling contaminant transport with nonlinear, non-equilibrium adsorption kinetics. The CGFEM, also known as the modified method of characteristics, Lagrange-Galerkin, or Euler-Lagrange method, has been used

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extensively in the modeling of linear and nonlinear flows; see, for example, [9,12,13,14]. The method was first analyzed in [3] for advective flow problems in one space dimension, and improvements and extensions of these estimates were derived in [4]. These estimates were proved primarily for linear problems; however, certain types of smooth nonlinearities were also considered.

Here we consider the application of the CGFEM to a nonlinear system of equations which arises in contaminant transport, and derive an *a priori* error estimate. The primary difficulty in these equations is the presence of possibly non-Lipschitz nonlinearities, which require special treatment in the analysis. The presence of such nonlinearities also reduces the regularity of the solution, thus, the expected rates of convergence are possibly suboptimal when approximating by piecewise polynomials.

In the next section, we give some basic notation. In Sections 3 and 4, the physical problem is described, and existence and uniqueness of weak solutions, and regularity of solutions are discussed. In Section 5, we describe the application of the CGFEM method, and in Section 6, the method is analyzed, assuming optimal regularity of the solution.

2 Notation

For Y a measurable space or space-time domain, let $L^p(Y)$, $1 \leq p \leq \infty$, denote the standard Banach space on Y, with norm $||\cdot||_{L^p(Y)}$. For Ω a bounded spatial domain in $\mathbb{R}^d$, $1 \leq d \leq 3$, denote by $W_2^k(\Omega)$ the standard Sobolev space on Ω with norm $||\cdot||_k$. We denote the $L^2(\Omega)$ norm by $||\cdot||$.

Let $[\alpha, \beta] \in [0,T]$ denote a time interval, where $T > 0$ is a fixed constant, and let $X = X(\Omega)$ denote a normed space. Denote by $||\cdot||_{L^p(\alpha,\beta;X)}$ the norm of $X-$ valued functions f with the map $t \longrightarrow ||f(\cdot,t)||_X$ belonging to $L^p(\alpha,\beta)$.

Letting $Q_T = \Omega \times (0,T]$ we denote by $V_2^{1,0}(Q_T)$ the Banach space consisting of elements having a finite norm

$$|u|_{Q_T} = ||u||_{L^\infty(0,T;L^2(\Omega))} + ||\nabla u||_{L^2(0,T;L^2(\Omega))}.$$

We denote by $W_2^{1,1}(Q_T)$ the Hilbert space with scalar product

$$(u,v)_{W_2^{1,1}(Q_T)} = \int_{Q_T} (uv + \nabla u \cdot \nabla v + u_t v_t) dx dt.$$

For $\phi : [0,\infty) \to [0,\infty)$, the notation $\phi \in C^p([0,\infty))$, $p \in (0,1)$ means ϕ is Hölder continuous in its argument with exponent p. We denote by $C^{\alpha,\beta}(Q_T)$, where α and β are nonintegral positive numbers, the standard Hölder space defined on Q_T. Here α represents smoothness in space and β represents smoothness in time.

3 Statement of the Problem

When chemical species are dissolved in groundwater they may undergo adsorption or exchange processes on the surface of the porous skeleton. Knowledge about the influence of these chemical processes on the transport of the solutes when the groundwater is moving is of fundamental importance to understand, for instance, how pollutants spread in space and time through the soil.

Below we present the mathematical formulation for a one-species system in which the chemicals undergo non-equilibrium adsorption reactions. Certain types of two-species systems of binary ion exchange can also be put into this framework. In particular this is the case when a conservation property allows for the reduction to a one-species system. In [7], details of this reduction are given, as well as a fundamental discussion of adsorption processes in porous media and related references.

The domain Ω is occupied by a porous material through which an incompressible fluid, say water, flows. The related specific discharge $\bar{q}(m/s)$, with components $q_i, i = 1, \ldots, d$ and length $|\bar{q}|$, satisfies the equation

$$\frac{\partial \theta}{\partial t} + \nabla \cdot \bar{q} = 0 \ , \tag{3.1}$$

which expresses conservation of fluid volume. In this equation, θ denotes the water content.

In what follows we shall consider θ and $\bar{q}$ as given quantities which are determined independently of the concentration of the dissolved chemicals. Thus, we implicitly assume here that concentrations occur only at tracer levels and hence do not influence the flow.

Let $c(\text{mol}/m^3)$ denote the concentration of adsorbate in solution and $A(\text{mol/kg porous medium})$ the adsorbed concentration. Conservation for the chemical species gives the equation

$$\frac{\partial}{\partial t}(\theta c + \rho A) + \nabla \cdot (\bar{q}c - \theta D \nabla c) = 0 \ , \tag{3.2}$$

in which $\rho = \rho(x)$ (kg porous medium/m^3) denotes the density of the porous medium (bulk density), and $D(m^2/s)$ the hydrodynamic dispersion matrix which incorporates the effects of molecular diffusion and mechanical (velocity-dependent) dispersion. In most transport models for porous media D takes the form, e.g. see [1]

$$\theta D_{ij} = \left\{\theta D_{\text{mol}} + \alpha_T|\bar{q}|\right\} \delta_{ij} + (\alpha_L - \alpha_T)\frac{q_i q_j}{|\bar{q}|} \quad i,j = 1,\ldots,d \ , \tag{3.3}$$

where $D_{\text{mol}}(m^2/s)$ is the molecular diffusivity of the adsorbate in the fluid (incorporating the tortuosity effect) and $\alpha_T(m)$ and $\alpha_L(m)$ are the transversal and longitudinal dispersion lengths, respectively.

Next we turn to the adsorption process. In this paper we assume that the reactions are relatively slow compared to the flow of the fluid. This makes it necessary to consider non-equilibrium adsorption. In addition, the adsorbent surface of the grains may be heterogeneous. Consider a subdivision of a representative grain surface (i.e. rescaled grain surface, e.g. the unit sphere) into m chemically different collections of adsorption sites corresponding to $i \in \{1,\ldots,m\}$; let λ_i be their relative size at the representative grain surface and s_i the corresponding adsorbed concentration. Then

$$\sum_{i=1}^{m} \lambda_i = 1 \qquad (\lambda_i > 0), \tag{3.4}$$

and

$$A = \sum_{i=1}^{m} \lambda_i s_i \ . \tag{3.5}$$

Each component s_i is related to the dissolved concentration c through an adsorption reaction which is described by the first order equation

$$\frac{\partial s_i}{\partial t} = k f_i(c, s_i) \quad \text{with} \quad i \in \{1,\ldots,m\} \ . \tag{3.6}$$

In these equations $k > 0$ $(1/s)$ is the rate constant, which we assume here to be constant (thus independent of space, time, and i), and f_i is the rate function describing the adsorption reactions at sites i. For the rate function in (3.6) we use the explicit form

$$f_i(c, s_i) = \phi_i(c) - s_i, \qquad i \in \{1, \ldots, m\} , \tag{3.7}$$

which, in a heuristic approach, is widely used in contaminant transport models, e.g. see [2]. The functions ϕ_i in (3.7) are called the adsorption isotherms. They are the adsorbed concentrations in the equilibrium, i.e. fast reaction case, as $k \to \infty$. Typical examples are the Langmuir isotherm

$$\phi(c) = \frac{K_1 c}{1 + K_2 c}, \qquad K_1, K_2 > 0, \tag{3.8}$$

and the Freundlich isotherm

$$\phi(c) = K_3 c^p, \qquad K_3 > 0 \, , p > 0 \, . \tag{3.9}$$

In the last example one usually takes $p \in (0, 1]$. For $p < 1$, the nonlinearities are not Lipschitz continuous up to $c = 0$. This results in the finite speed of propagation property for the concentration c as $c \downarrow 0$, and thus gives rise to a free boundary as the boundary of the support of c.

Thus, together with the transport equation (3.2), with A given by (3.5), we have to solve for the m-O.D.E.'s

$$\frac{\partial s_i}{\partial t} = k \left(\phi_i(c) - s_i \right) \quad \text{with} \quad i \in \{1, \ldots, m\} \, . \tag{3.10}$$

We consider (3.1), (3.2), (3.5) and (3.10) in the cylinder $Q_T = \Omega \times (0, T]$.

For all unknowns c and s_i we need to specify initial conditions. Thus

$$c(\cdot\, , 0) = c_0 \quad \text{and} \quad s_i(\cdot\, , 0) = s_{0i} \quad \text{in } \Omega, \tag{3.11}$$

for $i \in \{1, \ldots, m\}$. In addition we prescribe for c conditions along the boundary $\mathcal{S} = \partial\Omega$ of Ω. Letting $\alpha = -\bar{n} \cdot \bar{q}$, we distinguish an inflow boundary S_1 where $\alpha \geq 0$ and an outflow/no flow boundary S_2 where $\alpha \leq 0$. Here $S_1 \cup S_2 = \mathcal{S}$ and $\bar{n}$ denotes the outer unit normal. Then we impose

$$(\theta D \nabla c - \bar{q} c) \cdot \bar{n} = F \quad \text{on} \quad S_{1T} = S_1 \times (0, T] \, , \tag{3.12}$$

$$(\theta D \nabla c) \cdot \bar{n} = 0 \quad \text{on} \quad S_{2T} = S_2 \times (0, T]. \tag{3.13}$$

In (3.12), the function $F = F(x,t)$, with $(x,t) \in S_{1T}$, denotes the flux of solute entering the flow domain across S_1 at time $t > 0$.

Equations (3.1)–(3.13) define the Contaminant Transport Model, which we shall refer to as Problem CTM. In defining a weak solution or a weak formulation for Problem CTM we follow the usual definition for linear problems, e.g. see [11] and [10]. In particular we use the space $V_2^{1,0}(Q_T)$. Then we have the following definition.

Definition 3.1 *The functions $c, s_i : \bar{Q}_T \to [0,\infty)$ for $i \in \{1,\dots,m\}$ form a weak solution of Problem CTM if the following holds:*

(i) $c \in V_2^{1,0}(Q_T)$, $\phi_i(c) \in L^2(Q_T)$ *for* $i \in \{1,\dots,m\}$;

(ii) $s_i, \dfrac{\partial s_i}{\partial t} \in L^2(Q_T)$ *for* $i \in \{1,\dots,m\}$;

(iii)
$$-\int_\Omega (\theta c\eta)(\cdot,0) - \int_{Q_T} \theta c \frac{\partial \eta}{\partial t} + \int_{Q_T} \rho \left(\sum_{i=1}^m \lambda_i \frac{\partial s_i}{\partial t} \right) \eta + \int_{Q_T} (\theta D \nabla c - \bar{q} c) \cdot \nabla \eta = \int_{S_{1T}} F\eta + \int_{S_{2T}} \alpha c \eta \,, \tag{3.14}$$

for all $\eta \in W_2^{1,1}(Q_T)$ *which vanish at* $t = T$;

(iv) $\dfrac{\partial s_i}{\partial t} = k\,\{\phi_i(c) - s_i\}$, $i \in \{1,\dots,m\}$, $(x,t) \in Q_T$;

(v) $c(\cdot\,,0) = c_0$ *and* $s_i(\cdot\,,0) = s_{0i}$, $i \in \{1,\dots,m\}$, $(x,t) \in Q_T$.

Throughout this paper we take $\mathcal{S}$ to be piecewise smooth. With respect to the coefficients and functions appearing in Definition 2.1 we shall assume that the following structural and regularity conditions are satisfied; see also [5] and [10].

(H1a) For each $i \in \{1,\dots,m\}$ the isotherms $\phi_i : [0,\infty) \to [0,\infty)$ are nondecreasing;

(H1b) There are constants $\nu, \mu > 0$ such that for $\xi \in \mathbb{R}^d$, $(x,t) \in Q_T$,

$$\nu|\xi|^2 \le \xi^T(\theta D)(x,t)\xi \le \mu|\xi|^2 \,,$$

the D_{ij} are measurable in Q_T, $\partial_t D_{ij} \in L^\infty(Q_T)$ for $i,j = 1,\dots,d$, θD is symmetric;

(H1c) There exists $\theta_0 > 0$ such that

$$\theta(x,t) \geq \theta_0 \quad \text{for} \quad (x,t) \in Q_T \ ,$$

$\theta, \partial_t\theta \in L^\infty(Q_T)$;

(H1d) $q_i \in L^\infty(Q_T)$ for $i = 1, \ldots, d$, $\nabla \cdot \bar{q} \in L^\infty(Q_T)$, $\bar{q} \cdot \bar{n}$ exists in the sense of trace and $\bar{q} \cdot \bar{n} \in L^\infty(S_T)$, θ and $\bar{q}$ satisfy equation (3.1);

(H1e) $F \in L^\infty(S_{1T})$, $c_0, s_{0i} \geq 0$ and $c_0, s_{0i} \in L^2(\Omega)$ for $i \in \{1, \ldots, m\}$;

(H1f) $\rho \in L^\infty(\Omega)$, $\rho \geq 0$.

4 Some Analytical Observations

Weak solutions of Problem CTM, in the sense of Definition 2.1, were studied in [5] and [10]. The main, and nonstandard, difficulty for this problem lies in the fact that one of the isotherms ϕ_i may be non-smooth at $c = 0$. This happens for instance when it is of Freundlich type, see (3.9). Then a situation may occur where the set $\{c > 0\}$ spreads at finite speed through the flow domain Ω. A free boundary or interface arises as the boundary of the support of c, i.e. $\partial\{c > 0\}$. Across the free boundary c will have limited smoothness, even though the coefficients in (3.2) may be C^∞. The free boundary aspect of the problem was studied for a 1-dimensional flow situation in [5] and further, for the special case of travelling wave solutions, in [6,8].

To prove uniqueness and stability for weak solutions only the monotonicity of the isotherms ϕ_i is required. There are three essential steps needed which we outline briefly below. In a later section about the convergence estimates they will reappear in discrete form.

Let $\zeta = c_1 - c_2$ and $\beta_i = s_{1i} - s_{2i}$, $i \in \{1, \ldots, m\}$, where (c_1, s_{1i}) and (c_2, s_{2i}) are two weak solutions of Problem CTM. First, in (3.14), set

$$\eta(x,t) = \begin{cases} 0, & t \in (\tau, T], \\ \zeta(x,t), & t \in (0, \tau), \end{cases} \tag{4.1}$$

where $\tau \in (0, T)$. This leads to an expression that contains the term

$$\int_{Q_\tau} \rho \sum_{i=1}^{m} \lambda_i \frac{\partial \beta_i}{\partial t} \zeta \ . \tag{4.2}$$

Next, multiplying (3.10) by η defined by (4.1) gives

$$\frac{\partial \beta_i}{\partial t}\,\zeta = k\{\phi_i(c_1) - \phi_i(c_2)\}\zeta - k\beta_i\zeta \geq -k\beta_i\zeta \;, \tag{4.3}$$

where we have used the monotonicity of the isotherms. Then (4.2) can be estimated from below by

$$- k \int_{Q_T} \rho \sum_{i=0}^{m} \lambda_i \beta_i \zeta \;. \tag{4.4}$$

Thirdly, in (3.14), we set

$$\eta(x,t) = \begin{cases} 0, & t \in (\tau, T], \\ -\displaystyle\int_t^{\tau} \zeta(x,s)ds, & t \in (0,\tau). \end{cases} \tag{4.5}$$

This gives an expression which contains a term similar to (4.4). After some technicalities and a Gronwall argument we obtain:

Theorem 4.1 *Let hypothesis (H1) be satisfied. Then Problem CTM has a unique weak solution.*

At the expense of some additional conditions it is possible to extend the uniqueness proof and to obtain a Lipschitz stability result for the difference in the $V_2^{1,0}(Q_T)$ norm. Assume

(H2a) $\quad \bar{q}$ and $\dfrac{\partial \theta}{\partial t}$ are independent of time;

(H2b) $\quad \dfrac{\partial}{\partial t}(\theta D)$ is positive definite a.e. in Q_T and $\frac{\partial}{\partial t}\theta \leq 0$ in Ω.

Then we obtain

Theorem 4.2 *Let (c_1, s_{1i}) and (c_2, s_{2i}), $i \in \{1, \ldots, m\}$ denote the weak solution of Problem CTM corresponding to the data $\{c_{01}, s_{01i}, F_1\}$ and $\{c_{01}, s_{02i}, F_2\}$, respectively. Then there exists a constant $C > 0$ such that*

$$|c_1 - c_2|_{Q_T} \leq C\left\{ \|c_{01} - c_{02}\| + \sum_{i=1}^{m} \|\rho(s_{01i} - s_{02i})\| + \|F_1 - F_2\|_{L^\infty(S_{1T})} \right\} . \tag{4.6}$$

Remark 4.3 *Using expression (3.3) for the hydrodynamic dispersion matrix, hypotheses (H2) are obviously fulfilled for the case of stationary water distribution* (θ) *and flow* ($\bar{q}$).

Existence of weak, stong, and classical solutions was also established in [5] and [10]. Here we make some remarks in the direction of classical solutions. When the isotherms satisfy in addition to the monotonicity (H1a), the conditions (for $i \in \{1, \ldots, m\}$)

$$\phi_i(0) = 0\,, \quad \phi_i(s) > 0 \quad \text{for} \quad s > 0, \tag{4.7}$$

$$\phi_i \in C^p([0,\infty)) \cap C^1_{loc}((0,\infty)) \quad \text{for some} \quad p \in (0,1), \tag{4.8}$$

(such as the Freundlich isotherm (1.9)), and if the coefficients and initial/boundary data in Problem CTM are sufficiently smooth (e.g. $c_0 \in C^{2+p}(\bar{\Omega})$, $s_{0i} \in C^p(\bar{\Omega})$, $F = \alpha c_f$ with $c_f \geq 0$ and $c_f \in L^\infty(S_{1T})$, and other technical conditions), then

$$c \in C^{2+p,1+p/2}(\bar{Q}_T) \quad \text{and} \quad s_i \in C^{p,p+1}(\bar{Q}_T)\,. \tag{4.9}$$

Note that if one of the isotherms is of Freundlich type (3.9), then (4.9) is the optimal global regularity. Even if the coefficients in (3.2) (θ, ϕ, q and D) were C^∞, this would only imply

$$c, s_i \in C^\infty(\{c > 0\} \cap Q_T)\,.$$

4 The CGFEM for Non-Equilibrium Adsorption

In this section we discuss the numerical approximation of solutions to (3.2), (3.10) by the CGFEM. For simplicity, assume $m = 1$ and $s_1 \equiv s$. We will make the following assumptions:

(H3a) The data and coefficients are sufficiently smooth so that (4.9) holds.

(H3b) The isotherm ϕ satisfies (H1a), (4.7), and (4.8).

(H3c) $\mathcal{S} = S_2$, with $D\nabla c \cdot n = 0$ on $\mathcal{S}$.

(H3d) θ and $\bar{q}$ are independent of time.

(H3e) $D = D(\bar{q})$ is symmetric and positive definite.

For convenience, we will assume Problem CTM is Ω–periodic; i.e., we assume all functions involved are spatially Ω–periodic. This assumption is reasonable since the no-flow boundary conditions (H3c) are generally treated by reflection, and we are primarily interested in interior flow patterns and not boundary effects.

Let $0 = t^0 < t^1 < \cdots < t^M = T$ be a given sequence, with $\Delta t^n = t^n - t^{n-1}$. Define $f^n(\cdot) = f(\cdot, t^n)$. Let $h > 0$ and M_h be a finite dimensional subspace of $W_2^1(\Omega)$ consisting of continuous, piecewise polynomials of degree $\leq k$ on a quasi-uniform mesh of diameter less than or equal to h.

In the CGFEM, we approximate $c(x, t^n)$ and $s(x, t^n)$ by functions C^n and S^n in M_h. Writing (3.2) in nondivergence form and applying (3.1), we obtain

$$\theta c_t + \rho A_t + \bar{q} \cdot \nabla c - \nabla \cdot (\theta D \nabla c) = 0 . \tag{4.1}$$

Let τ denote the unit vector in the direction $(\bar{q}, \theta)$ and set

$$\psi = (|\bar{q}|^2 + |\theta|^2)^{\frac{1}{2}} . \tag{4.2}$$

Then

$$\psi c_\tau \equiv \theta c_t + \bar{q} \cdot \nabla c \tag{4.3}$$

and (4.1) can be written as

$$\psi c_\tau - \nabla \cdot (\theta D \nabla c) + \rho A_t = 0 . \tag{4.4}$$

Let

$$\hat{x} = x - \frac{\bar{q}(x)}{\theta(x)} \Delta t , \tag{4.5}$$

and let $\hat{f}(x) \equiv f(\hat{x})$ for a given function f. Approximate ψc_τ by the backward difference

$$\psi c_\tau(x, t^n) \approx \theta(x) \, \frac{c(x, t^n) - c(\hat{x}, t^{n-1})}{\Delta t} . \tag{4.6}$$

Let

$$\sigma^n(x) = \theta(x)\frac{c^n(x) - c(\hat{x}, t^{n-1})}{\Delta t} - \psi(x)c_\tau^n(x), \tag{4.7}$$

and

$$\omega^n(x) = \frac{s^n(x) - s^{n-1}(x)}{\Delta t} - s_t^n(x). \tag{4.8}$$

Then (3.2) can be written

$$\theta\frac{c^n - \hat{c}^{n-1}}{\Delta t} - \nabla\cdot(\theta D\nabla c^n) + \rho\frac{s^n - s^{n-1}}{\Delta t} = \sigma^n + \rho\omega^n\ , \tag{4.9}$$

and (3.10) can be written

$$\rho\frac{s^n - s^{n-1}}{\Delta t} = k\rho(\phi(c^n) - s^n) + \rho\omega^n. \tag{4.10}$$

Initially, set $C^0 = \tilde{C}^0 \in M_h$, where $\tilde{C}(x,t)$ is the $\theta-$weighted L^2-projection defined by

$$(\theta\tilde{C}(\cdot,t),\chi) = (\theta c(\cdot,t),\chi)\ , \quad \chi \in M_h\ . \tag{4.11}$$

Furthermore, set $S^0 = \tilde{S}^0 \in M_h$, where $\tilde{S}(x,t)$ is the $\rho-$weighted L^2-projection

$$(\rho\tilde{S}(\cdot,t),\chi) = (\rho s(\cdot\ ,t),\chi)\ , \quad \chi \in M_h\ . \tag{4.12}$$

For $n = 1, 2, \ldots, M$, define $C^n \in M_h$, $S^n \in M_h$ by

$$\begin{aligned}\left(\theta\,\frac{C^n - \hat{C}^{n-1}}{\Delta t}\ ,\chi\right) + \left(\rho\,\frac{S^n - S^{n-1}}{\Delta t}\ ,\chi\right)& \\ + (\theta D\nabla C^n, \nabla\chi) = 0, \quad \chi \in M_h,&\end{aligned} \tag{4.13}$$

and

$$\left(\rho\frac{S^n - S^{n-1}}{\Delta t}\ ,v\right) \ = \ k(\rho(\phi(C^n) - S^n)\ ,v), \qquad v \in M_h\ . \tag{4.14}$$

Equations (4.13) and (4.14) are obtained by multiplying (4.9) and (4.10) by test functions χ and v in $\mathcal{M}_h$, respectively, integrating (4.9) by parts, and substituting C^n for c^n, and S^n for s^n.

5 Error Estimates

In this section we analyze the method given by (4.11)-(4.14). In the arguments that follow, K will denote a generic positive constant and ϵ a small positive constant, independent of h and Δt. We will also employ the well-known inequality

$$ab \le \frac{1}{2\epsilon}\, a^2 + \frac{\epsilon}{2}\, b^2\,, \quad a, b, \epsilon \in \mathbb{R}\,, \quad \epsilon > 0\,.$$

Let $\zeta = C - \tilde{C}$, $\xi = c - \tilde{C}$, where $\tilde{C}$ is given by (4.11), and let $\beta = S - \tilde{S}$, where $\tilde{S}$ is given by (4.12). Then by (4.9)-(4.14),

$$\begin{aligned}
&\left(\theta\frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \chi\right) + (\theta D\nabla\zeta^n, \nabla\chi) + \left(\rho\frac{\beta^n - \beta^{n-1}}{\Delta t}, \chi\right) \\
&= (\sigma^n, \chi) + \left(\theta\frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \chi\right) + (\theta D\nabla\xi^n, \nabla\chi) \\
&\quad + \left(\theta\frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \chi\right) + (\rho\omega^n, \chi)\,, \qquad \chi \in M_h,
\end{aligned} \tag{5.1}$$

and

$$\left(\rho\frac{\beta^n - \beta^{n-1}}{\Delta t}, v\right) = k(\rho(\phi(C^n) - \phi(c^n) - \beta^n), v) + (\rho\omega^n, v)\,, \quad v \in M_h, \tag{5.2}$$

where σ^n is given by (4.7) and ω^n by (4.8).

Following the uniqueness arguments given in [5], we first set $v = \zeta^n$ in (5.2) and note that by the monotonicity of ϕ:

$$\begin{aligned}
\left(\rho\frac{\beta^n - \beta^{n-1}}{\Delta t}, \zeta^n\right) &= k(\rho(\phi(C^n) - \phi(c^n)), \zeta^n) \\
&\quad - k(\rho\beta^n, \zeta^n) + (\rho\omega^n, \zeta^n) \\
&= k(\rho(\phi(C^n) - \phi(c^n)), C^n - c^n) \\
&\quad - k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) \\
&\quad - k(\rho\beta^n, \zeta^n) + (\rho\omega^n, \zeta^n) \\
&\ge -k(\rho\beta^n, \zeta^n) - k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) \\
&\quad + (\rho\omega^n, \zeta^n).
\end{aligned} \tag{5.3}$$

Setting $\chi = \zeta^n$ in (5.1) and using (5.3), we find

$$\begin{aligned}
&\left(\theta\frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \zeta^n\right) + (\theta D\nabla\zeta^n, \nabla\zeta^n) \\
&\qquad - k(\rho\beta^n, \zeta^n) - k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) + (\rho\omega^n, \zeta^n) \\
&\leq (\sigma^n, \zeta^n) + \left(\theta\frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n\right) \\
&\qquad + (\theta D\nabla\xi^n, \nabla\zeta^n) + \left(\theta\frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \zeta^n\right) + (\rho\omega^n, \zeta^n) . \qquad (5.4)
\end{aligned}$$

We next consider (5.1) with

$$\chi = \sum_{\ell=n}^{M} \zeta^\ell \Delta t , \qquad (5.5)$$

multiply the result by Δt, and sum on n, $n = 1, \ldots, M$. First, we observe

$$\begin{aligned}
&\sum_{n=1}^{M}\left(\theta\frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^{M}\zeta^\ell\Delta t\right)\Delta t \\
&\quad= \sum_{n=1}^{M}\left(\theta\zeta^n, \left[\sum_{\ell=n}^{M}\zeta^\ell + \sum_{\ell=n+1}^{M}\zeta^\ell\right]\right)\Delta t \\
&\quad= \sum_{n=1}^{M}(\theta\zeta^n, \zeta^n)\Delta t , \qquad (5.6)
\end{aligned}$$

by summation by parts and because $\zeta^0 = 0$. Similarly, since $\beta^0 = 0$,

$$\begin{aligned}
&\sum_{n=1}^{M}\left(\rho\frac{\beta^n - \beta^{n-1}}{\Delta t}, \sum_{\ell=n}^{M}\zeta^\ell\Delta t\right)\Delta t \\
&\quad= \sum_{n=1}^{M}(\rho\beta^n, \zeta^n)\Delta t . \qquad (5.7)
\end{aligned}$$

Furthermore,

$$(\nabla\zeta^n) \cdot \sum_{\ell=n}^{M}\nabla\zeta^\ell\Delta t$$

$$= \frac{1}{2}\frac{\left\|\sum_{\ell=n}^{M}\nabla\zeta^{\ell}\Delta t\right\|^{2}-\left\|\sum_{\ell=n+1}^{M}\nabla\zeta^{\ell}\Delta t\right\|^{2}}{\Delta t} + \frac{1}{2}\nabla\zeta^{n}\cdot\nabla\zeta^{n}\Delta t\,.$$

Thus

$$\sum_{n=1}^{M}\left(\theta D\nabla\zeta^{n},\sum_{\ell=n}^{M}\nabla\zeta^{\ell}\Delta t\right)\Delta t$$
$$= \frac{1}{2}\left(\theta D\sum_{n=1}^{M}\nabla\zeta^{n}\Delta t,\sum_{n=1}^{M}\nabla\zeta^{n}\Delta t\right)$$
$$\frac{1}{2}\sum_{n=1}^{M}(\theta D\nabla\zeta^{n},\nabla\zeta^{n})\Delta t^{2}\,. \tag{5.8}$$

Using (5.7) and (5.1) with $\chi=\sum_{n=1}^{M}\nabla\zeta^{n}\Delta t$, (5.6), and (5.8), we obtain

$$-k\sum_{n=1}^{M}(\rho\beta^{n},\zeta^{n})\Delta t$$
$$= k\sum_{n=1}^{M}\left(\rho\frac{\beta^{n}-\beta^{n-1}}{\Delta t},-\sum_{\ell=n}^{M}\zeta^{\ell}\Delta t\right)\Delta t$$
$$= k\sum_{n=1}^{M}\left\{\left(\theta\,\frac{\zeta^{n}-\zeta^{n-1}}{\Delta t},\sum_{\ell=n}^{M}\zeta^{\ell}\Delta t\right)+\left(\theta D\nabla\zeta^{n},\sum_{\ell=n}^{M}\nabla\zeta^{\ell}\Delta t\right)\right.$$
$$+\left(\theta D\nabla\xi^{n},-\sum_{\ell=n}^{M}\nabla\zeta^{\ell}\Delta t\right)$$
$$+\left(\sigma^{n}+\theta\left(\frac{\xi^{n}-\hat{\xi}^{n-1}}{\Delta t}\right)\right.$$
$$\left.\left.+\ \theta\ \left(\frac{\hat{\zeta}^{n-1}-\zeta^{n-1}}{\Delta t}\right)+\rho\omega^{n},-\sum_{\ell=n}^{M}\zeta^{\ell}\Delta t\right)\right\}\Delta t$$
$$= k\sum_{n=1}^{M}\left\{(\theta\zeta^{n},\zeta^{n})+\frac{1}{2}(\theta D\nabla\zeta^{n},\nabla\zeta^{n})\Delta t\right.$$

$$
\begin{aligned}
&+ \left(\theta D \nabla \xi^n, - \sum_{\ell=n}^{M} \nabla \zeta^\ell \Delta t\right) \\
&+ \left(\sigma^n + \theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}\right. \\
&\qquad \left.+ \theta\, \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t} + \rho\omega^n, - \sum_{\ell=n}^{M} \zeta^\ell \Delta t\right)\Bigg\} \Delta t \\
&+ \frac{k}{2}\left(\theta D \sum_{n=1}^{M} \nabla \zeta^n \Delta t, \sum_{n=1}^{M} \nabla \zeta^n \Delta t\right) . \qquad (5.9)
\end{aligned}
$$

Multiplying (5.4) by Δt and summing on n, substituting (5.9) into the result, and using assumption (H1b), we obtain

$$
\begin{aligned}
&\sum_{n=1}^{M} \left\{ \left(\theta\, \frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \zeta^n\right) + (\theta D \nabla \zeta^n, \nabla \zeta^n) \right. \\
&\qquad \left. + k\left[(\theta\, \zeta^n, \zeta^n) + \frac{1}{2}\, (\theta D \nabla \zeta^n, \nabla \zeta^n)\Delta t\right]\right\} \Delta t \\
&\qquad + \frac{k\nu}{2}\left[\left(\sum_{n=1}^{M} \nabla \zeta^n \Delta t, \sum_{n=1}^{M} \nabla \zeta^n \Delta t\right) + \left(\sum_{n=1}^{M} \zeta^n \Delta t, \sum_{n=1}^{M} \zeta^n \Delta t\right)\right] \\
\leq\ &\sum_{n=1}^{M} \{ k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) \\
&\qquad + (\sigma^n, \zeta^n) + \left(\theta\, \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n\right) \\
&\qquad + (\theta D \nabla \xi^n, \nabla \zeta^n) + \left(\theta\, \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \zeta^n\right) \\
&\qquad + k\left[\left(\sigma^n, \sum_{\ell=n}^{M} \zeta^\ell \Delta t\right)\right. \\
&\qquad\qquad + \left(\theta\, \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \sum_{\ell=n}^{M} \zeta^\ell \Delta t\right)
\end{aligned}
$$

$$
\begin{aligned}
&+ \left(\theta D\nabla\xi^n, \sum_{\ell=n}^{M}\nabla\zeta^\ell\Delta t\right) \\
&+ \left(\theta\,\frac{\hat{\zeta}^{n-1}-\zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^{M}\zeta^\ell\Delta t\right) + \left(\rho\omega^n, \sum_{\ell=n}^{M}\zeta^\ell\Delta t\right)\Bigg]\Bigg\}\Delta t \\
&+ \frac{k\nu}{2}\left(\sum_{n=1}^{M}\zeta^n\Delta t, \sum_{n=1}^{M}\zeta^n\Delta t\right) \\
\equiv\ & T_1 + \cdots + T_{11}\ .
\end{aligned} \tag{5.10}
$$

We now estimate the terms T_1 through T_{11}.

By the Hölder continuity of ϕ, and Hölder's inequality

$$
\begin{aligned}
T_1 &= k\sum_{n=1}^{M}(\rho(\phi(C^n)-\phi(c^n)), \xi^n)\Delta t \\
&\le k||\rho||_\infty \sum_{n=1}^{M}||\phi(C^n)-\phi(c^n)||_{L^q(\Omega)}||\xi^n||_{L^r(\Omega)}\Delta t \\
&\le k||\rho||_\infty \sum_{n=1}^{M}\left(\int_\Omega|\zeta^n-\xi^n|^{qp}dx\right)^{\frac{1}{q}}||\xi^n||_{L^r(\Omega)}\Delta t,
\end{aligned}
$$

where

$$
\frac{1}{q}+\frac{1}{r}=1\ .
$$

Choose $q=\frac{2}{p}$, then $r=\dfrac{1}{1-\frac{p}{2}}$, and

$$
\begin{aligned}
T_1 &\le Kh^2\sum_{n=1}^{M}\left(||\xi^n||^2+||\zeta^n||^2\right)^{\frac{2}{q}}\Delta t + Kh^{-2}\sum_{n=1}^{M}||\xi^n||^2_{L^r(\Omega)}\Delta t \\
&\le Kh^2\sum_{n=1}^{M}[||\xi^n||^{2p}+||\zeta^n||^{2p}]\Delta t + Kh^{-2}\sum_{n=1}^{M}||\xi^n||^2_{L^r(\Omega)}\Delta t\ .
\end{aligned}
$$

Applying Hölder's inequality again to the second term, at the expense of a possibly larger constant, we obtain

$$
T_1 \le Kh^2\sum_{n=1}^{M}[||\zeta^n||^{2p}+||\xi^n||^{2p}]\Delta t + Kh^{-2}\sum_{n=1}^{M}||\xi^n||^2\Delta t\ .
$$

Before estimating T_2, we note that, for a spatially periodic, L^2 function g, it is shown in [3] that

$$\begin{aligned}\left\|\frac{\hat{g}-g}{\Delta t}\right\|_{-1} &\equiv \sup_{f\in W_2^1(\Omega)}\left[\frac{1}{||f||_1}\int_\Omega \frac{\hat{g}(x)-g(x)}{\Delta t}f(x)dx\right] \\ &\leq K||g||. \end{aligned} \tag{5.11}$$

Consider

$$\begin{aligned} T_2 &= \sum_{n=1}^{M}(\rho\sigma^n,\zeta^n)\Delta t \\ &= \Delta t\sum_{n=1}^{M}\int_\Omega \rho(x)\left[\theta(x)\frac{c^n(x)-\hat{c}^{n-1}(x)}{\Delta t} - \left(\theta c_t^n + u\cdot\nabla c^n\right)(x)\right]\zeta^n(x)dx \\ &= \Delta t\sum_{n=1}^{M}\left\{\int_\Omega \rho(x)\left[\theta(x)\frac{c^n(x)-\hat{c}^n(x)}{\Delta t} - (u\cdot\nabla c^n)(x)\right]\zeta^n(x)dx\right. \\ &\quad \left. + \int_\Omega \rho(x)\theta(x)\left[\frac{\hat{c}^n(x)-\hat{c}^{n-1}(x)}{\Delta t} - c_t^n(x)\right]\zeta^n(x)dx\right\} \\ &= T_{2,1}+T_{2,2}. \end{aligned}$$

By Taylor expansion,

$$\theta(x)\frac{c^n(x)-\hat{c}^n(x)}{\Delta t} = (u\cdot\nabla c^n)(\bar{x}),$$

where $\bar{x}$ is between x and $\hat{x}$. Thus,

$$\begin{aligned}\theta(x)\frac{c^n(x)-\hat{c}^n(x)}{\Delta t} - (u\cdot\nabla c^n)(x) &= (u\cdot\nabla c^n)(\bar{x}) - (u\cdot\nabla c^n)(x) \\ &= \nabla(u\cdot\nabla c^n)(\tilde{x})\cdot(x-\bar{x}),\end{aligned}$$

where $\tilde{x}$ is between x and $\bar{x}$. Since $|x-\bar{x}| = \mathcal{O}(\Delta t)$,

$$\begin{aligned}|T_{2,1}| &\leq K\Delta t\sum_{n=1}^{M}\left\|\theta\frac{c^n-\hat{c}^n}{\Delta t} - u\cdot\nabla c^n\right\| ||\zeta^n|| \\ &\leq K\Delta t^2\sum_{n=1}^{M}\left(||c^n||_2 + ||u||_1||c^n||_1\right)||\zeta^n||\end{aligned}$$

$$\leq \ K\Delta t^2 + K\sum_{n=1}^{M}||\zeta^n||^2\Delta t.$$

For the second term $T_{2,2}$, we note that

$$T_{2,2} = \Delta t\sum_{n=1}^{M}\int_\Omega \rho\theta\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[\hat{c}_t(x,s) - c_t^n(x)]\,ds\ \zeta^n(x)dx.$$

Consider

$$\begin{aligned}
&\int_\Omega \rho\theta\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[\hat{c}_t(x,s) - c_t^n(x)]\,ds\zeta^n(x)dx \\
&= \int_\Omega \rho\theta\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[\hat{c}_t(x,s) - c_t(x,s) + c_t(x,s) - c_t^n(x)]\,ds\ \zeta^n(x)dx \\
&= \int_\Omega \rho\theta\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[\hat{c}_t(x,s) - c_t(x,s)]\,ds\ \zeta^n(x)dx \\
&\quad + \int_\Omega \rho\theta\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[c_t(x,s) - c_t^n(x)]\,ds\ \zeta^n(x)dx \\
&\equiv T_{2,2,1} + T_{2,2,2}.
\end{aligned}$$

By (5.11), the first term above satisfies

$$\begin{aligned}
|T_{2,2,1}| &\leq \left\|\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}[\hat{c}_t(\cdot,s) - c_t(\cdot,s)]\,ds\right\|_{-1}||\rho\theta\zeta^n||_1 \\
&\leq K\left\|\int_{t^{n-1}}^{t^n}c_t(\cdot,s)ds\right\|||\zeta^n||_1 \\
&\leq K\Delta t||c_t||_{L^\infty(L^2)}||\zeta^n||_1 \\
&\leq K\Delta t^2 + \epsilon||\zeta^n||_1^2.
\end{aligned}$$

For the second term above, by the Hölder continuity of c_t,

$$\begin{aligned}
|T_{2,2,2}| &\leq K\int_\Omega\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}|c_t(x,s) - c_t^n(x)|ds\ |\zeta^n|dx \\
&\leq K\Delta t^{\frac{p}{2}}\int_\Omega|\zeta^n(x)|dx \\
&\leq K\Delta t^p + K||\zeta^n||^2.
\end{aligned}$$

Combining these estimates we find

$$T_2 \leq K(h^2 + \Delta t^2 + \Delta t^p) + K\sum_{n=1}^{M} ||\zeta^n||^2 \Delta t + \epsilon \sum_{n=1}^{M} ||\zeta^n||_1^2 \Delta t.$$

For a function $g(x) \in W_2^1(\Omega)$, we note that

$$||g - \hat{g}|| \leq K \Delta t ||\nabla g||,$$

and using the fact that $(\theta \xi^n, \chi) = 0$ for $\chi \in \mathcal{M}_h$, we obtain

$$\begin{aligned} T_3 &= \sum_{n=1}^{M} \left(\theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &= \sum_{n=1}^{M} \left(\theta \frac{\xi^{n-1} - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &\leq K \sum_{n=1}^{M} ||\nabla \xi^{n-1}||^2 \Delta t + K \sum_{n=1}^{M} ||\zeta^n||^2 \Delta t. \end{aligned}$$

Moreover,

$$\begin{aligned} T_4 &= \sum_{n=1}^{M} (\theta D \nabla \xi^n, \nabla \zeta^n) \Delta t \\ &\leq K \sum_{n=1}^{M} ||\nabla \xi^n||^2 \Delta t + \epsilon \sum_{n=1}^{M} ||\nabla \zeta^n||^2 \Delta t \,. \end{aligned}$$

Similar to the estimate for T_3,

$$\begin{aligned} T_5 &\leq \sum_{n=1}^{M} \left(\theta \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &\leq K \sum_{n=1}^{M} ||\zeta^n||^2 \Delta t + \epsilon \sum_{n=1}^{M} ||\nabla \zeta^{n-1}||^2 \Delta t \,. \end{aligned}$$

Similar to the estimate for T_2,

$$T_6 = k \sum_{n=1}^{M} \left(\sigma^n, \sum_{\ell=n}^{M} \zeta^\ell \Delta t \right) \Delta t$$

$$
\begin{aligned}
&= k \sum_{n=1}^{M} \left(\sigma^n, \sum_{\ell=1}^{M} \zeta^\ell \Delta t - \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right) \Delta t \\
&\leq K(\Delta t^p + h^2) + \epsilon \left\| \sum_{\ell=1}^{M} \zeta^\ell \Delta t \right\|_1^2 \\
&\quad + K \sum_{n=1}^{M} \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|_1^2 \Delta t \,.
\end{aligned}
$$

Similar to the estimates for T_3 and T_4,

$$
\begin{aligned}
T_7 &= \sum_{n=1}^{M} \left(\theta \frac{\xi^{n-1} - \hat{\xi}^{n-1}}{\Delta t}, \sum_{\ell=n}^{M} \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^{M} \|\nabla \xi^{n-1}\|^2 \Delta t + \epsilon \left\| \sum_{\ell=1}^{M} \zeta^\ell \Delta t \right\|^2 \\
&\quad + K \sum_{n=1}^{M} \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|^2 \Delta t \,,
\end{aligned}
$$

and

$$
\begin{aligned}
T_8 &= \sum_{n=1}^{M} \left(\theta D \nabla \xi^n, \sum_{\ell=n}^{M} \nabla \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^{M} \|\nabla \xi^n\|^2 \, \Delta t + \epsilon \left\| \sum_{\ell=1}^{M} \zeta^\ell \Delta t \right\|_1^2 \\
&\quad + K \sum_{n=1}^{M} \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|_1^2 \Delta t.
\end{aligned}
$$

By (5.11),

$$
\begin{aligned}
T_9 &= \sum_{n=1}^{M} \left(\theta \, \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^{M} \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^{M} \left\| \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t} \right\|_{-1} \left\| \sum_{\ell=n}^{M} \zeta^\ell \Delta t \right\|_1 \Delta t
\end{aligned}
$$

$$
\begin{aligned}
&\le K\sum_{n=1}^{M}\|\zeta^{n-1}\|^2\,\Delta t+\epsilon\left\|\sum_{\ell=1}^{M}\zeta^{\ell}\Delta t\right\|_1^2\\
&\qquad+K\sum_{n=1}^{M}\left\|\sum_{\ell=1}^{n-1}\zeta^{\ell}\Delta t\right\|_1^2\Delta t.
\end{aligned}
$$

Moreover,

$$
\begin{aligned}
T_{10} &= \frac{k\nu}{2}\left(\sum_{n=1}^{M}\zeta^n\Delta t,\sum_{n=1}^{M}\zeta^n\Delta t\right)\\
&\le \frac{k\nu}{2}\int_\Omega\left|\sum_{n=1}^{M}\zeta^n\Delta t\right|\,\left|\sum_{n=1}^{M}\zeta^n\Delta t\right|\,dx\\
&\le K\int_\Omega\left[\sum_{n=1}^{M}|\zeta^n|\,\Delta t\right]^2 dx\\
&\qquad+\epsilon\left\|\sum_{n=1}^{M}\zeta^n\Delta t\right\|^2\\
&\le K\left[\sum_{n=1}^{M}\int_\Omega|\zeta^n|^2dx\Delta t\right]\,\left[\sum_{n=1}^{M}\int_\Omega dx\;\Delta t\right]\\
&\qquad+\epsilon\left\|\sum_{n=1}^{M}\zeta^n\Delta t\right\|^2\\
&\le K\sum_{n=1}^{M}\|\zeta^n\|^2\Delta t+\;\epsilon\left\|\sum_{n=1}^{M}\zeta^n\Delta t\right\|_1^2.
\end{aligned}
$$

For the estimate of T_{11}, consider

$$
\begin{aligned}
\omega^n &= s_t(\cdot,t^n)-\frac{s^n-s^{n-1}}{\Delta t}\\
&= \frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}\left[s_t(\cdot,t^n)-s_t(\cdot,t)\right]dt\;.
\end{aligned}
$$

By the Hölder continuity of s_t, we obtain

$$
\frac{1}{\Delta t}\int_{t^{n-1}}^{t^n}\left[s_t(\cdot,t^n)-s_t(\cdot,t)\right]dt
$$

$$
\begin{aligned}
&\le \frac{K}{\Delta t}\int_{t^{n-1}}^{t^n} |t-t^n|^p dt \\
&\le K\Delta t^p\,.
\end{aligned}
$$

Thus,

$$
\begin{aligned}
T_{11} &= \sum_{n=1}^{M}\left(\rho\omega^n, -\sum_{\ell=n}^{M}\zeta^\ell\Delta t\right)\Delta t \\
&\le K\Delta t^{2p} + \epsilon\left\|\sum_{\ell=1}^{M}\zeta^\ell\Delta t\right\|^2 + K\sum_{n=1}^{M}\left\|\sum_{\ell=1}^{n-1}\zeta^\ell\Delta t\right\|^2\Delta t.
\end{aligned}
$$

Combining the estimates for T_1–T_{11} with (5.10), and using the fact that

$$
\sum_{n=1}^{M}\left(\theta\frac{\zeta^n-\zeta^{n-1}}{\Delta t},\zeta^n\right)\Delta t \ge \frac{1}{2}(\theta\zeta^M,\zeta^M)
$$

and the estimate

$$
||\xi(\cdot,t)|| + h||\xi(\cdot,t)||_1 \le Kh^2||c(\cdot,t)||_2,
$$

we find

$$
\begin{aligned}
&\frac{1}{2}(\theta\zeta^M,\zeta^M) \\
&+\sum_{n=1}^{M}\left[(D\nabla\zeta^n,\nabla\zeta^n) + k(\,\theta\zeta^n,\zeta^n) + \frac{1}{2}\,(D\nabla\zeta^n,\nabla\zeta^n)\Delta t\right]\Delta t \\
&+\frac{k\nu}{2}\left[\left(\sum_{n=1}^{M}\nabla\zeta^n\Delta t,\sum_{n=1}^{M}\nabla\zeta^n\Delta t\right)+\left(\sum_{n=1}^{M}\zeta^n\Delta t,\sum_{n=1}^{M}\zeta^n\Delta t\right)\right] \\
&\quad\le Kh^2\sum_{n=1}^{M}||\zeta^n||^{2p}\Delta t + K\sum_{n=1}^{M}||\zeta^n||^2\Delta t + K\,\Delta t^{2p} + K\Delta t^p + Kh^2 \\
&\quad+\epsilon\sum_{n=1}^{M}||\zeta^n||_1^2\Delta t + K\sum_{n=1}^{M}\left\|\sum_{\ell=1}^{n-1}\zeta^\ell\Delta t\right\|_1^2\Delta t \\
&\quad+\epsilon\left\|\sum_{n=1}^{M}\zeta^n\Delta t\right\|_1^2\,. \qquad (5.12)
\end{aligned}
$$

We now hide terms multiplied by ϵ, and define

$$g^n = (\zeta^n, \zeta^n) + \left\| \sum_{\ell=1}^{n} \zeta^\ell \Delta t \right\|_1^2 .$$

The L^2 stability of C^n can be demonstrated using essentially the same arguments given above; i.e., we set χ and $v = C^n$ in (4.13) and (4.14), and use the monotonicity of ϕ. We then set $\chi = \sum_{\ell=n}^{M} C^\ell \Delta t$ in (4.13), multiply the result by Δt and sum on n, and sum by parts. The result is that $\|C^n\| \leq K\|C^0\|$ for each n, where K is independent of h and Δt. Thus, by the L^2 stability of $\tilde{C}$, we have

$$\|\zeta^n\|^{2p} \leq K.$$

Then, (5.12) implies

$$g^M \leq K(h^2 + \Delta t^p) + K \sum_{n=1}^{M} |g^n| \Delta t.$$

Applying Gronwall's Lemma and the triangle inequality, we obtain the following result:

Theorem 5.1 *Assume (H1a)-(H1f), (4.7)-(4.9), and (H3a)-(H3e) hold, then*

$$\max_n \|c^n - C^n\| \leq K(\Delta t^{\frac{p}{2}} + h).$$

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975	**Avner Friedman and Juan J.L. Velázquez**, A time-dependence free boundary problem modeling the visual image in electrophotography	
976	**Richard A. Brualdi, Hyung Chan Jung and William T. Trotter, Jr.**, On the poset of all posets on n elements	
977	**Ricardo D. Fierro and James R. Bunch**, Multicollinearity and total least squares	
978	**Adam W. Bojanczyk, James G. Nagy and Robert J. Plemmons**, Row householder transformations for rank-k Cholesky inverse modifications	
979	**Chaocheng Huang**, An age-dependent population model with nonlinear diffusion in R^n	
980	**Emad Fatemi and Farouk Odeh**, Upwind finite difference solution of Boltzmann equation applied to electron transport in semiconductor devices	
981	**Esmond G. Ng and Barry W. Peyton**, A tight and explicit representation of Q in sparse QR factorization	
982	**Robert J. Plemmons**, A proposal for FFT-based fast recursive least-squares	
983	**Anne Greenbaum and Zdenek Strakos**, Matrices that generate the same Krylov residual spaces	
984	**Alan Edelman and G.W. Stewart**, Scaling for orthogonality	
985	**G.W. Stewart**, Note on a generalized sylvester equation	
986	**G.W. Stewart**, Updating URV decompositions in parallel	
987	**Angelika Bunse-Gerstner, Volker Mehrmann and Nancy K. Nichols**, Numerical methods for the regularization of descriptor systems by output feedback	
988	**Ralph Byers and N.K. Nichols**, On the stability radius of generalized state-space systems	
989	**David C. Dobson**, Designing periodic structures with specified low frequency scattered in far-field data	
990	**C.-T. Pan and Kermit Sigmon**, A bottom-up inductive proof of the singular value decomposition	
991	**Ricardo D. Fierro and James R. Bunch**, Orthogonal projection and total least squares	
992	**Chiou-Ming Huang and Dianne P. O'Leary**, A Krylov multisplitting algorithm for solving linear systems of equations	
993	**A.C.M Ran and L. Rodman**, Factorization of matrix polynomials with symmetries	
994	**Mike Boyle**, Symbolic dynamics and matrices	
995	**A. Novick-Cohen and L.A. Peletier**, Steady states of the one-dimensional Cahn-Hilliard spaces	
996	**Zhangxin Chen**, Large-scale averaging analysis of single phase flow in fractured reservoirs	
997	**Boris Mordukhovich**, Stability theory for parametric generalized equations and variational inequalities via nonsmooth analysis	
998	**Yongzhi Xu**, CW mode structure and constraint beamforming in a waveguide with unknown large inclusions	
999	**R.P. Gilbert and Yongzhi Xu**, Acoustic waves and far-field patterns in two dimensional oceans with porous-elastic seabeds	
1000	**M.A. Herrero and J.J.L. Velázquez**, Some results on blow up for semilinear parabolic problems	
1001	**Pierre-Alain Gremaud**, Numerical analysis of a nonconvex variational problem related to solid-solid phase transitions	
1002	**Izchak Lewkowicz**, Stability robustness of state space systems inter-relations between the continuous and discrete time cases	
1003	**Kenneth R. Driessel and Wasin So**, Linear operators on matrices: Preserving spectrum and displacement structure	

1004 **Carolyn Eschenbach**, Idempotence for sign pattern matrices
1005 **Carolyn Eschenbach, Frank J. Hall and Charles R. Johnson**, Self-inverse sign patterns
1006 **Marc Moonen, Paul Van Dooren and Filiep Vanpoucke**, On the QR algorithm and updating the SVD and URV decomposition in parallel
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1009 **Stephen J. Kirkland and Michael Neumann**, Convexity and concavity of the Perron root and vector of Leslie matrices with applications to a population model
1010 **Stephen J. Kirkland and Bryan L. Shader**, Tournament matrices with extremal spectral properties
1011 **E.G. Kalnins, Willard Miller, Jr. and Sanchita Mukherjee**, Models of q-algebra representations: Matrix Elements of $U_q(su_2)$
1012 **Zhangxin Chen and Bernardo Cockburn**, Error estimates for a finite element method for the drift-diffusion semiconductor device equations
1013 **Chaocheng Huang**, Drying of gelatin asymptotically in photographic film
1014 **Richard E. Ewing and Hong Wang**, Eulerian-Lagrangian localized adjoint methods for reactive transport in groundwater
1015 **Bing-Yu Zhang**, Taylor series expansion for solutions of the Korteweg-de Vries equation with respect to their initial values
1016 **Kenneth R. Driessel**, Some remarks on the geometry of some surfaces of matrices associated with Toeplitz eigenproblems
1017 **C.J. Van Duijn and Peter Knabner**, Flow and reactive transport in porous media induced by well injection: Similarity solution
1018 **Wasin So**, Rank one perturbation and its application to the Laplacian spectrum of a graph
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1020 **T.R. Hoffend Jr.**, Magnetostatic interactions for certain types of stacked, cylindrically symmetric magnetic particles
1021 **IMA Summer Program for Graduate Students**, Mathematical Modeling
1022 **Wayne Barrett, Charles R. Johnson, and Pablo Tarazaga**, The real positive definite completion problem for a simple cycle
1023 **Charles A. McCarthy**, Fourth order accuracy for a cubic spline collocation method
1024 **Martin Hanke, James Nagy, and Robert Plemmons**, Preconditioned iterative regularization for I11-posed problems
1025 **John R. Gilbert, Esmond G. Ng, and Barry W. Peyton**, An efficient algorithm to compute row and column counts for sparse Cholesky factorization
1026 **Xinfu Chen**, Existence and regularity of solutions of a nonlinear nonuniformly elliptic system arising from a thermistor problem
1027 **Xinfu Chen and Weiqing Xie**, Discontinuous solutions of steady state, viscous compressible Navier-Stokes equations
1028 **E.G. Kalnins, Willard Miller, Jr., and Sanchita Mukherjee**, Models of q-algebra representations: Matrix elements of the q-oscillator algebra
1029 **W. Miller, Jr. and Lee A. Rubel**, Functional separation of variables for Laplace equations in two dimensions
1030 **I. Gohberg and I. Koltracht**, Structured condition numbers for linear matrix structures
1031 **Xinfu Chen**, Hele-Shaw problema nd area preserved curve shortening motion
1032 **Zhangxin Chen and Jim Douglas, Jr.** Modelling of compositional flow in naturally fractured reservoirs
1033 **Harald K. Wimmer**, On the existence of a least and negative-semidefinite solution of the discrete-time algebraic Riccati equation
1034 **Harald K. Wimmer**, Monotonicity and parametrization results for continuous-time algebraic Riccati equations and Riccati inequalities
1035 **Bart De Moor, Peter Van Overschee, and Geert Schelfhout**, H_2 model reduction for SISO systems
1036 **Bart De Moor**, Structured total least squares and L_2 approximation problems
1037 **Chjan Lim**, Nonexistence of Lyapunov functions and the instability of the Von Karman vortex streets
1038 **David C. Dobson and Fadil Santosa**, Resolution and stability analysis of an inverse problem in electrical impedance tomography – dependence on the input current patterns
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1041 **Neerchal K. Nagaraj and Wayne A. Fuller**, Least squares estimation of the linear model with autoregressive errors
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