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A SECOND ORDER APPROXIMATION FOR QUASILINEAR NON-FICKIAN DIFFUSION MODELS

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Abstract: In this paper initial boundary value problems, defined using quasilinear diffusion equations of Volterra type, are considered. These equations arise for instance to describe diffusion processes in viscoelastic media whose behaviour is represented by a Voigt-Kelvin model or a Maxwell model. We propose a finite difference discretization defined on a general nonuniform grid and we show second convergence order. The analysis does not follows the usual splitting of the global error using the solution of an elliptic equation induced by the integro-differential equation. The new approach enables us to reduce the smoothness required to the theoretical solution when the usual split technique is used. Numerical simulations which shows the effectiveness of the method are included.

Key words: Quasilinear Volterra equation, finite difference methods, supraconvergence

Mathematics Subject Classification (2000): 65M06, 65M20, 65M15

1. Introduction

In this paper we consider the class of quasilinear integro-differential equations of Volterra type

$$\begin{aligned}\frac{\partial c}{\partial t} &= \frac{\partial}{\partial x}\Big(a(c)\frac{\partial c}{\partial x}\Big) + \int_0^t k_{er}(t-s)\frac{\partial}{\partial x}\Big(d(c(s))\frac{\partial c}{\partial x}(s)\Big)\,ds \\ &\quad + f \text{ in } (0,1)\times(0,T],\end{aligned} \tag{1}$$

where k_{er} is a kernel function. In (1) $a(c)$ stands for the diffusion coefficient, $d(c)$ for a viscoelastic diffusion coefficient and f represents a reaction term. Equation (1) is completed with Dirichlet boundary conditions

$$c(0,t) = c_{in}, \quad \text{for } t \in (0,T], \tag{2}$$

$$c(1,t) = c_{out}, \quad \text{for } t \in (0,T], \tag{3}$$

and initial condition

$$c(x,0) = c_0(x), \ x \in (0,1). \tag{4}$$

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Equation (1) is usually used to replace the classical diffusion-reaction equation

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\Big(e(c)\frac{\partial c}{\partial x}\Big) + f \text{ in } (0,1)\times(0,T], \tag{5}$$

when Fick's law for the mass flux J_F,

$$J_F = -e(c)\frac{\partial c}{\partial x} \tag{6}$$

does not hold. In this case the mass flux is split into a Fickian contribution and a non Fickian one that is

$$J = J_F + J_{nF},$$

with J_F given by (6), $e(c)$ replaced by $a(c)$ and

$$J_{nF}(t) = -\int_0^t k_{er}(t-s)d(c(s))\frac{\partial c}{\partial x}(s)\,ds. \tag{7}$$

Integro-differential equation (1) arises in a huge number applications. Without being exhaustive we mention diffusion in polymers ([7], [8], [9], [10] and [28]), diffusion in live tissues ([15], [16], [21], [23] and [25]) and diffusion in porous media ([22], [24] and [26]). The linear version of (1) has been previously studied for instance in [1], [2], [6], [18] and [19].

Our aim is to generalize the results obtained in [4] and [20] for the linear version of the quasilinear equation (1) avoiding the use of an elliptic auxiliary problem induced by this equation. The paper is organized as follows. In Section 2 we introduce the spatial discretization using the piecewise linear finite element method. Its convergence is analysed in Section 3. In the main result of this paper, Theorem 1, we prove that a discrete L^2 norm of the spatial discretization error and of its discrete gradient are of second order. We point out that the convergence analysis presented here does not use the approach introduced by Wheeler in [27] and largely followed in the literature. This approach is essentially based on the splitting of the spatial discretization error considering an elliptic problem induced by (1). In Section 4 we present a numerical illustration of our main convergence result. Finally, some conclusions are included in Section 5.

2. Finite Difference Method

The finite difference method is introduced in what follows considering a variational problem associated with the the integro-differential equation (1). Without loss of generality we will consider homogenous Dirichlet boundary

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followed in the literature and which was introduced by Wheeler in [27]. Our approach allows the weakening of the smoothness conditions usually required when Wheeler's technique is used, namely we replace $c \in H^1(0,T,H^3(0,1)) \cap L^2(0,T,H^3(0,1) \cap H_0^1(0,1))$ by $c \in H^1(0,T,H^2(0,1)) \cap L^2(0,T,H^3(0,1) \cap H_0^1(0,1))$.

For the sake of simplicity only the one dimensional case was studied, but the techniques here presented can be used to extend the analysis for two dimensional problems. Moreover, this technique can be adapted to get error bounds to the error induced by the fully discrete IMEX method considered in the numerical simulation.

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conditions. By $L^2(0,1)$ and $H_0^1(0,1)$ we represent the usual Sobolev spaces where we consider the usual inner products $(.,.)$ and $(.,.)_1$, respectively. By $\|.\|$ and $\|.\|_1$ we denote the correspondent norms. Let V be a Banach space, by $L^2(0,T;V)$, we denote the space of functions $v:\ (0,T) \mapsto V$ such that

$$\|v\|^2_{L^2(0,T;V)} = \int_0^T \|v(t)\|_V^2\, dt < \infty\ .$$

We consider the following space

$$\mathcal{W}(0,T) = \{g \in L^2(0,T,H_0^1(0,1)):\ g' \in L^2(0,T,H^{-1}(0,1))\},$$

where $H^{-1}(0,1)$ denotes the dual space of $H^1(0,1)$. Thus we replace IBVP (1)-(4) by the following variational problem (**VP**): find $c \in \mathcal{W}(0,T)$ such that

$$\begin{aligned}(\frac{dc}{dt}(t),w) + (a(c(t))\frac{\partial c}{\partial x}(t),w') \ &= -\int_0^t k_{er}(t-s)(d(c(s))\frac{\partial c}{\partial x}(s),w')\,ds \\ &\quad +(f(t),w),\ \text{a. e. in } (0,T),\end{aligned} \tag{8}$$

$\forall w \in H_0^1(0,1)$, where

$$c(0) = c_0. \tag{9}$$

Let $h = (h_1,\ldots,\ h_N)$, with $h_i > 0$, for $i = 1,\ldots,\ N$, be such that $\sum_{i=1}^{N} h_i = 1$. We define in $I = [0,1]$ the nonuniform grid

$$I_h = \{x_i, i = 0,\ldots,N, x_i = x_{i-1} + h_i, i = 1,\ldots,\ N,\ x_0 = 0\}$$

and we use the notations $I_h' = I_h - \{0,1\}$ and $\partial I_h = \{0,1\}$.

By $\mathbb{W}_h$ we represent the space of grid functions defined in I_h and by P_h the piecewise linear interpolation operator defined in $\mathbb{W}_h$. By $\mathbb{W}_{h,0}$ we represent the subspace of $\mathbb{W}_h$ of the grid functions null on ∂I_h. The piecewise linear approximation $\hat{c}_h(t) = P_h c_h(t)$ for the concentration $c(t)$ is a solution of the following equation

$$\begin{aligned}&(\frac{d\hat{c}_h}{dt}(t),P_h w_h) + (a(\hat{c}_h(t))\frac{\partial \hat{c}_h}{\partial x}(t),P_h w_h') \\ &= -\int_0^t k_{er}(t-s)(d(\hat{c}_h(s))\frac{\partial}{\partial x}\hat{c}_h h(s),P_h w_h')\,ds + (f(t),P_h w_h),\ \ \forall w_h \in \mathbb{W}_{h,0}\end{aligned} \tag{10}$$

with

$$\hat{c}_h(0) = P_h R_h c_0, \tag{11}$$

where R_h denotes the restriction operator.

Let $h_{i+\frac{1}{2}} = \frac{1}{2}(h_i + h_{i+1})$, $i = 1, \ldots, N-1$, $x_{i\pm\frac{1}{2}} = \frac{1}{2}(x_{i\pm1} + x_i)$. To define the semi-discrete approximation we introduce the following definitions:

$$\begin{cases} g_h(x_i) = \dfrac{1}{h_{i+\frac{1}{2}}} \displaystyle\int_{x_i-\frac{1}{2}}^{x_i+\frac{1}{2}} g(x)\,dx, \ i = 1, \ldots, N-1, \\ g_h(x_0) = \dfrac{2}{h_1} \displaystyle\int_0^{x_{\frac{1}{2}}} g(x)dx, \\ g_h(x_N) = \dfrac{2}{h_N} \displaystyle\int_{x_{N-\frac{1}{2}}}^1 g(x)\,dx, \end{cases} \tag{12}$$

and

$$\begin{array}{l} M_h v_h(x_i) = \frac{1}{2}(v_h(x_{i-1}) + v_h(x_i)), \ i = 1, \ldots, N \\ M_h v_h(x_0) = 0, \ \ v_h \in \mathbb{W}_{h,0}. \end{array} \tag{13}$$

In $\mathbb{W}_{h,0}$ we consider the discrete inner product

$$(v_h, w_h)_h = \sum_{i=1}^{N-1} h_{i+\frac{1}{2}} v_h(x_i) w_h(x_i), \ v_h, w_h \in \mathbb{W}_{h,0}, \tag{14}$$

and by $\|.\|_h$ we represent the norm induced by the previous discrete inner product.

In what follows we use the notations

$$(v_h, w_h)_{h,+} = \sum_{i=1}^{N} h_i v_h(x_i) w_h(x_i), \ v_h, w_h \in \mathbb{W}_h,$$

and

$$\|v_h\|_{h,+} = (v_h, v_h)_{h,+}^{1/2}.$$

In the space $\mathbb{W}_h$ we introduce the norm $\|.\|_{1,h}$ defined by

$$\|u_h\|_{1,h}^2 = \|v_h\|_h^2 + \|D_{-x} v_h\|_{h,+}^2,$$

where D_{-x} represent the usual backward finite difference operator.

Let $\mathcal{W}_h(0,T)$ be defined by

$$\mathcal{W}_h(0,T) = \{g \in L^2(0,T,\mathbb{W}_{h,0}) : g' \in L^2(0,T,\mathbb{W}_h^{-1})\},$$

where $\mathbb{W}_h^{-1}$ denotes the dual space of $\mathbb{W}_h$.

In Table 1 we present the error

$$\mathbb{E}_{r_p} = \max_n \left(\|e_h^n\|_{h_p}^2 + \Delta t \sum_{s=1}^{n} \|e_h^s\|_{1,h_p}^2 \right)^{\frac{1}{2}}. \tag{47}$$

where $e_h^s(x_j) = c(x_j, t_s) - c_h^s(x_j), j = 1, 1dots, N-1, e_h^s(x_0) = e_h^s(x_N) = 0$, and the rate R_p defined by

$$R_p = \frac{\ln(\mathbb{E}_{r_p}/\mathbb{E}_{r_{p+1}})}{\ln(h_{p_{max}}/h_{p+1_{max}})}. \tag{48}$$

N_p	$h_{p_{max}}$	$\mathbb{E}_p$	R_p
23	4.7619×10^{-2}	3.3469×10^{-4}	-
46	2.3810×10^{-2}	9.0189×10^{-5}	1.8918
92	1.1905×10^{-2}	2.2983×10^{-5}	1.9724
184	5.9524×10^{-3}	5.7475×10^{-6}	1.9996
368	2.9762×10^{-3}	1.4302×10^{-6}	2.0067
736	1.4881×10^{-3}	3.5509×10^{-7}	2.0099
1472	7.4405×10^{-4}	8.7942×10^{-8}	2.0136

Table 1: Convergence orders

We note that the rates presented in Table 1 are in agrement with the error bound established in Theorem 1, that is $\mathbb{E}_r = O(h_{max}^2)$.

5. Conclusions

In this paper we propose a finite difference method to solve numerically the IBVP defined by the quasi-linear integro-differential equation (1) of Volterra type with Dirichlet boundary conditions. We point out that the non Fickian equation (1) can be used, as previously mentioned, to model a large number of physical situations where Fick's law is not appropriate to describe the mass flux and a delay effect is needed. The finite difference method (17) can be seen as a fully discrete in space piecewise linear finite element method. Methods of this class were studied for elliptic equations for instance in [3] , [11], [12] and [17].

In the main theorem of this paper - Theorem 1, we prove that a discrete L^2 norm of the spatial discretization error and of its discrete gradient are second order convergent while the spatial truncation error is only of first order with respect to infinity norm. The approach used to prove this result was introduced in [20] for a linear version of (17) and differs from the one usually

4. Numerical Simulations

The aim of this section is to illustrate the main result of the paper - Theorem 1, when the smoothness assumptions assumed for the coefficient functions a and d are weakened.

To integrate in time an IMEX (implicit-explicit) method will be used. In $[0,T]$ we consider a time grid $J_{\Delta t} = \{t_n,\ n = 0,1,2,...,M\}$ with $t_0 = 0,\ t_M = T$ and $t_n - t_{n-1} = \Delta t$. We use the rectangular rule to approximate the integral in (1) and the backward finite-difference operator D_{-t} to approximate the first partial derivative with respect to t. Then the fully discrete approximation for c at (x_j,t_n), $c_h^n(x_j)$, is defined by the following set of equations

$$\begin{aligned} D_{-t}c_h^n(x_j) &= D_x^*\left(a(M_h c_h^{n-1}(x_j))D_{-x}c_h^n(x_j)\right) + f(x_j,t_n) \\ &\quad +\Delta t\sum_{s=0}^{n-1} k_{er}(t_n - t_s)D_x^*\left(d(M_h c_h^s(x_j))D_{-x}c_h^s(x_j)\right), \quad (40) \\ &\quad j = 1,\ldots,\ N-1, \quad (41) \end{aligned}$$

with boundary conditions

$$\begin{aligned} c_h^n(x_0) &= c_{in}, \quad \text{for } n = 1,\ldots,\ M, \quad (42) \\ c_h^n(x_N) &= c_{out}, \quad \text{for } n = 1,\ldots,\ M, \quad (43) \end{aligned}$$

and the initial condition

$$c_h^0(x_j) = c_0,\ \text{for } j = 1,\ldots,\ N-1. \quad (44)$$

Let us consider in (1)-(4)

$$a(c) = c+1,\ d(c) = 5c,\ k_{er} = e^{-\frac{1}{2}t}, \quad (45)$$

and let f, the initial and the boundary conditions be defined such that the IBVP has the following solution

$$c(x,t) = e^t(1 - cos(2\pi x)),\ x \in [0,1],\ t \in [0,T]. \quad (46)$$

The numerical approximation c_h^n was obtained with method (40)-(44) with nonuniform grids in the spatial domain and with an uniform grid in the time domain with $T = 0.1$ and $\Delta t = 1 \times 10^{-6}$. The initial spatial grid I_h was arbitrary and the successively refined grids I_h were obtained introducing in $[x_j, x_{j+1}]$ the midpoint.

The semi-discrete approximation for the solution of the variational problem (10) and (11) is computed using the following discrete variational problem: find $c_h \in \mathcal{W}_h(0,T)$ such that

$$\begin{aligned} &(\frac{dc_h}{dt}(t), w_h)_h + (a(M_h c_h(t))D_{-x}c_h(t), D_{-x}w_h)_{h,+} \\ &\quad = -\int_0^t k_{er}(t-s)(d(M_h c_h(s))D_{-x}c_h(s), D_{-x}w_h)_{h,+}\,ds + (f_h(t), w_h)_h, \quad (15) \end{aligned}$$

$\forall w_h \in \mathbb{W}_{h,0}$, and

$$c_h(0) = R_h c_0, \quad (16)$$

where f_h is defined by (12) with g replaced by $f(t)$. It is easy to show that c_h is solution of the initial value problem (15), (16) if and only if c_h satisfies

$$\begin{aligned} &\frac{dc_h}{dt}(t) - D_x^*\left(a(M_h c_h(t))D_{-x}c_h(t)\right) = \int_0^t k_{er}(t-s)D_x^*\left(d(M_h c_h(s))D_{-x}c_h(s)\right)ds \\ &\qquad +f_h(t)\ \text{ in } I_h', \\ &c_h(t) = 0\ \text{ on } \partial I_h, \end{aligned} \quad (17)$$

and (16).

In (17) D_x^* denotes the following finite difference operator

$$D_x^* v_h(x_i) = \frac{v_h(x_{i+1}) - v_h(x_i)}{h_{i+\frac{1}{2}}},\ i = 1,\ldots,\ N-1,\ v_h \in \mathbb{W}_h.$$

3. Convergence Analysis

Let Λ be a sequence of vectors $h = (h_1,\ldots,h_N)$,$h_i > 0, i = 1,\ldots,N$, $\sum_{i=1}^{N} h_i = 1$, and $h_{max} = \max_{i=1,\ldots,N} h_i \to 0$. For $h \in \Lambda$, let $e_h(t) = R_h c(t) - c_h(t)$ be the semi-discretization error induced by (15) and (16) or equivalently (17) and (16). In this section we prove that $\|e_h(t)\|_h = O(h_{max}^2)$, and $\|D_{-x}e_h(t)\|_{h,+} = O(h_{max}^2)$. In the convergence analysis we require some smoothness to the solution c for(**VP**) that we specify in what follows.

By $H^1(0,T;V)$ we denote the space of functions $v:\ (0,T) \mapsto V$ such that

$$\|v\|^2_{H^1(0,T;V)} = \sum_{i=0}^{1}\int_0^T \left\|v^{(i)}(t)\right\|_V^2 dt < \infty\ .$$

We represent by $W^{1,\infty}(0,1)$ the space of functions $v:(0,1)\to\mathbb{R}$ such that

$$\|v\|_{1,\infty}=\sum_{i=0}^{1} ess\ sup_{(0,1)}|v^{(i)}|<\infty, \tag{18}$$

The space of functions $v:(0,T)\to W^{1,\infty}(0,1)$ such that

$$\|v\|_{L^\infty(W^{1,\infty}(0,1))}=ess\ sup_{(0,T)}\|v(t)\|_{1,\infty}<\infty$$

is denoted as $L^\infty(0,T;W^{1,\infty}(0,1))$.

We assume that the solution of (**VP**), c, satisfies

$$c\in H^1(0,T;H^2(0,1))\bigcap L^2(0,T;H^3(0,1)\cap H_0^1(0,1)) \tag{19}$$

For the kernel function $k_{er}(t)$ we impose the existence of a positive constant k satisfying

$$\int_0^t k_{er}^2(t-s)ds\le k, \tag{20}$$

for $t\in[0,T]$. The discrete Poincaré-Friedrich's inequality

$$\|v_h\|_h^2\le\|D_{-x}v_h\|_{h,+}^2,\ v_h\in\mathbb{W}_{h,0}, \tag{21}$$

will be used in the proof of Theorem 1. By $\mathcal{C}_B^1(\mathbb{R})$ we represent the space of bounded continuous real functions with bounded first order derivative.

Theorem 1. *Let c be a solution of (**VP**), such that c satisfies* (19)*,and let c_h be the approximation defined by* (15)*. If $a,d\in\mathcal{C}_B^1(\mathbb{R})$, $0<a_0\le a$, and k_{er} satisfies* (20)*, then there exist positive constants C_1 and C_2 depending on the coefficient functions a, d and on the kernel k_{er} such that*

$$\|e_h(t)\|_h^2+\int_0^t\|D_{-x}e_h(s)\|_{h,+}^2ds\le C_2h_{max}^4e^{C_1(1+\|c\|^2_{L^\infty(W^{1,\infty}(0,1))})t}\int_0^t T(s)\,ds, \tag{22}$$

where

$$\begin{aligned}T(t)\ &=\|\frac{\partial c}{\partial t}(t)\|_{H^2(0,1)}^2+(1+\|c(t)\|^2_{W^{1,\infty}(0,1)})\|c(t)\|^2_{H^3(0,1)}\\&+k(1+\|c\|^2_{L^\infty W^{1,\infty}(0,1)})\int_0^t\|c(s)\|^2_{H^3(0,1)}ds\end{aligned} \tag{23}$$

where $T(t)$ is defined by (23) and C_T is given by

$$C_T=\max\{C_{Z_1}^2,a_b^2C_{Z_{2,1}}^2,(a_b')^2C_{Z_{2,2}}^2,d_b^2C_{Z_{3,1}}^2,(d_b')^2C_{Z_{3,2}}^2\}.$$

Inequality (36) leads to

$$\begin{aligned}\|e_h(t)\|_h^2\ &+2(a_0-8\epsilon^2)\int_0^t\|D_{-x}e_h(s)\|_{h,+}^2ds\le\frac{1}{2\epsilon^2}\int_0^t\|c(s)\|^2_{W^{1,\infty}(0,1)}\|e_h(s)\|_h^2ds\\&+\frac{1}{2\epsilon^2}k\big(d_b^2+(d_b')^2\|c\|^2_{L^\infty W^{1,\infty}(0,1)}\big)\int_0^t\int_0^s\|D_{-x}e_h(\mu)\|_{h,+}^2d\mu\,ds\\&+h_{max}^4\frac{1}{2\epsilon^2}C_T\int_0^t T(s)\,ds\end{aligned}$$

that implies

$$\begin{aligned}\|e_h(t)\|_h^2\ &+\int_0^t\|D_{-x}e_h(s)\|_{h,+}^2ds\le h_{max}^4\frac{1}{2\epsilon^2\min\{1,2(a_0-8\epsilon^2)\}}C_T\int_0^t T(s)\,ds\\&+\frac{k\big(d_b^2+(d_b')^2\|c\|^2_{L^\infty(W^{1,\infty}(0,1))}\big)}{2\epsilon^2\min\{1,2(a_0-8\epsilon^2)\}}\int_0^t\int_0^s\|D_{-x}e_h(\mu)\|_{h,+}^2d\mu ds\\&+\frac{\|c\|^2_{L^\infty(W^{1,\infty}(0,1))}}{2\epsilon^2\min\{1,2(a_0-8\epsilon^2)\}}\int_0^t\|e_h(s)\|_h^2ds\end{aligned} \tag{37}$$

when ϵ is fixed by

$$a_0-8\epsilon^2>0. \tag{38}$$

From (37) we conclude that there exist positive constants C_1 and C_2 depending on the coefficients functions a and d and on the kernel function k_{er} such that

$$\begin{aligned}\|e_h(t)\|_h^2\ &+\int_0^t\|D_{-x}e_h(s)\|_{h,+}^2ds\le C_2h_{max}^4\int_0^t T(s)\,ds\\&+C_1(1+\|c\|^2_{L^\infty(W^{1,\infty}(0,1))})\int_0^t\big(\|e_h(s)\|_h^2+\int_0^s\|D_{-x}e_h(\mu)\|_{h,+}^2d\mu\big)ds.\end{aligned} \tag{39}$$

Finally the application of Gronwall lemma leads to (22).

■

In the upper bound (22), we have an amplification factor $e^{\Theta t}$ with $\Theta=C_1(1+\|c\|^2_{L^\infty(W^{1,\infty}(0,1))})$. In certain situations this amplification factor can be reduced to the unity by considering more strict conditions on the coefficients.

with $g(\xi) = c(x_{i-1} + \xi h_i, t)$. Applying Bramble-Hilbert lemma to estimate $\lambda(g)$ we obtain

$$|\lambda(g)| \leq C_{Z_{2,2}} h_i |\frac{\partial^2 c}{\partial x^2}(t)|_{L^1(x_{i-1},x_i)},$$

where $C_{Z_{2,2}}$ is a positive constant. Then

$$|Z_{2,2}| \leq a_b' C_{Z_{2,2}} h_{max}^2 \|D_{-x} R_h c(t)\|_{h,+} |c(t)|^2_{H^2(0,1)} \|D_{-x} e_h(t)\|_{h,+}, \tag{32}$$

which implies

$$|Z_{2,2}| \leq \frac{(a_b')^2 C_{Z_{2,2}}^2}{4\epsilon_4^2} h_{max}^4 \|c(t)\|^2_{W^{1,\infty}(0,1)} |c(t)|^2_{H^2(0,1)} + \epsilon_4^2 \|D_{-x} e_h(t)\|^2_{h,+}, \tag{33}$$

where $|a'| \leq a_b'$ in $\mathbb{R}$ and $\epsilon_4 \neq 0$ is an arbitrary constant.

(5) *Estimate for Z_3*:

Following the steps used to estimate Z_2 it can be shown the following

$$\begin{aligned} |Z_3| \ &\leq \int_0^t k_{er}(t-s) d_b C_{Z_{3,1}} h_{max}^2 |c(s)|_{H^3(0,1)} ds \|D_{-x} e_h(t)\|_{h,+} \\ &+ \int_0^t k_{er}(t-s) d_b' C_{Z_{3,2}} h_{max}^2 |c(s)|_{H^2(0,1)} \|D_{-x} R_h c(s)\|_{h,+} ds \|D_{-x} e_h(t)\|_{h,+} \end{aligned} \tag{34}$$

where $|d| \leq d_b$ and $|d'| \leq d_b'$ in $\mathbb{R}$.

From (34) we get

$$\begin{aligned} |Z_3| \ &\leq h_{max}^4 \frac{1}{4\epsilon_5^2} k\Big(d_b^2 C_{Z_{3,1}}^2 + (d_b')^2 C_{Z_{3,2}}^2 \|c\|^2_{L^\infty(W^{1,\infty}(0,1))} \Big) \int_0^t \|c(s)\|^2_{H^3(0,1)} \, ds \\ &+ 2\epsilon_5^2 \|D_{-x} e_h(t)\|^2_{h,+}, \end{aligned} \tag{35}$$

where $\epsilon_5 \neq 0$ is an arbitrary constant.

Considering in (27)-(35) $\epsilon_i = \epsilon$, $i = 0, \ldots, 5$, and taking in (25) these upper bounds we obtain

$$\begin{aligned} \tfrac{d}{dt}\|e_h(t)\|_h^2 \ &+ 2(a_0 - 8\epsilon^2) \|D_{-x} e_h(t)\|^2_{h,+} \leq \frac{1}{2\epsilon^2} \|c(t)\|^2_{W^{1,\infty}(0,1)} \|e_h(t)\|_h^2 \\ &+ \frac{1}{2\epsilon^2} k\big(d_b^2 + (d_b')^2 \|c\|^2_{L^\infty W^{1,\infty}(0,1))} \big) \int_0^t \|D_{-x} e_h(t)\|^2_{h,+} \, ds \\ &+ h_{max}^4 \frac{1}{2\epsilon^2} C_T T(t), \end{aligned} \tag{36}$$

Proof: From (15), it follows that $e_h(t)$ satisfies

$$\begin{aligned} (\frac{de_h}{dt}(t), w_h)_h \ &= \ (R_h \frac{\partial c}{\partial t}(t), w_h)_h + (a(M_h c_h(t)) D_{-x} c_h(t), D_{-x} w_h)_{h,+} \\ &+ \int_0^t k_{er}(t-s) (d(M_h c_h(s)) D_{-x} c_h(s), D_{-x} w_h)_{h,+} \, ds \\ &- (f_h(t), w_h)_h \ , \ w_h \in \mathbb{W}_{h,0}. \end{aligned} \tag{24}$$

Fixing in (24) $w_h = e_h(t)$ and considering that

$$\begin{aligned} (f_h(t), e_h(t))_h = \ &(\left(\frac{\partial c}{\partial t}\right)_h, e_h(t))_h + (a(\hat{M}_h c(t)) \hat{M}_h \frac{\partial c}{\partial x}(t), D_{-x} e_h(t))_{h,+} \\ &+ (\int_0^t k_{er}(t-s) d(\hat{M}_h c(s)) \hat{M}_h \frac{\partial c}{\partial x}(s) \, ds, D_{-x} e_h(t))_{h,+}, \end{aligned}$$

where $\left(\frac{\partial c}{\partial t}\right)_h (t)$ is defined by (12) with g replaced by $\frac{\partial c}{\partial t}(t)$ and $\hat{M}_h g(x_i) = R_h g(x_{i-\frac{1}{2}})$, $i = 1, \ldots, N$, we deduce

$$\frac{1}{2} \frac{d}{dt} \|e_h(t)\|_h^2 = T_a(t) + T_{int}(t) + \sum_{p=1}^{3} Z_p, \tag{25}$$

where

$$T_a(t) = (a(M_h c_h(t)) D_{-x} c_h(t), D_{-x} e_h(t))_{h,+} - (a(M_h c(t)) D_{-x} R_h c(t), D_{-x} e_h(t))_{h,+},$$

$$T_{int}(t) = \int_0^t k_{er}(t-s) ((d(M_h c_h(s)) - d(M_h c(s))) D_{-x} R_h c(s), D_{-x} e_h(t))_{h,+} \, ds,$$

$$Z_1 = (R_h \frac{\partial c}{\partial t}(t) - \left(\frac{\partial c}{\partial t}\right)_h, e_h(t))_h,$$

$$Z_2 = (a(M_h c(t)) D_{-x} R_h c(t) - a(\hat{M}_h c(t)) \hat{M}_h \frac{\partial c}{\partial x}(t), D_{-x} e_h(t))_{h,+},$$

and

$$Z_3 = \int_0^t k_{er}(t-s) (d(M_h c(s)) D_{-x} R_h c(s) - d(\hat{M}_h c(t)) \hat{M}_h \frac{\partial c}{\partial x}(s)), D_{-x} e_h(t))_{h,+} ds \, .$$

We estimate separately the previous terms.

(1) *Estimate for $T_a(t)$*:
We have

$$\begin{aligned} T_a &= (a(M_h c_h(t))D_{-x}e_h(t), D_{-x}e_h(t))_{h,+} \\ &\quad +((a(M_h c_h(t)) - a(M_h c(t)))D_{-x}R_h c(t), D_{-x}e_h(t))_{h,+} \end{aligned}$$

consequently, as $a \geq a_0 > 0$, we obtain

$$T_a(t) \leq -a_0\|D_{-x}e_h(t)\|^2_{h,+} + \frac{(a_b')^2}{4\epsilon_0^2}\|D_{-x}R_h c\|^2_{h,+}\|e_h(t)\|^2_h + \epsilon_0^2\|D_{-x}e_h(t)\|^2_{h,+}, \tag{26}$$

where $|a'| \leq a_b'$ in $\mathbb{R}$ and $\epsilon_0 \neq 0$ is an arbitrary constant.
From (26) we conclude

$$T_a(t) \leq (-a_0 + \epsilon_0^2)\|D_{-x}e_h(t)\|^2_{h,+} + \frac{(a_b')^2}{4\epsilon_0^2}\|c(t)\|_{W^{1,\infty}(0,1)}\|e_h(t)\|^2_h. \tag{27}$$

(2) *Estimate for $T_{int}(t)$*:
As $d \in \mathcal{C}^1_B(\mathbb{R})$, following the procedure used to deduce (27), it can be shown that

$$\begin{aligned} T_{int} \leq\ & d_b\int_0^t k_{er}(t-s)\|D_{-x}e_h(s)\|_{h,+}\,ds\|D_{-x}e_h(t)\|_{h,+} \\ & +d_b'\int_0^t k_{er}(t-s)\|D_{-x}R_h c(s)\|_{h,+}\|e_h(s)\|_h ds\|D_{-x}e_h(t)\|_{h,+} \end{aligned}$$

and then, using the discrete Poincaré-Friedrichs inequality, we deduce

$$\begin{aligned} T_{int} \leq\ & \frac{1}{4\epsilon_1^2}k\big(d_b^2 + (d_b')^2\|c\|^2_{L^\infty(W^{1,\infty}(0,1))}\big)\int_0^t \|D_{-x}e_h(s)\|^2_{h,+}\,ds \\ & +2\epsilon_1^2\|D_{-x}e_h(t)\|^2_{h,+} \end{aligned} \tag{28}$$

where $|d'| \leq d_b'$ in $\mathbb{R}$ and $\epsilon_1 \neq 0$ is an arbitrary constant.

(3) *Estimate for Z_1*:
It can be shown that for Z_1 holds the following

$$|Z_1| \leq C_{Z_1}h^2_{max}\|\frac{\partial c}{\partial t}(t)\|_{H^2(0,1)}\|D_{-x}e_h(t)\|_{h,+}$$

where C_{Z_1} is a positive constant (see [3]). Consequently we have

$$|Z_1| \leq \frac{1}{4\epsilon_2^2}C^2_{Z_1}h^4_{max}\|\frac{\partial c}{\partial t}(t)\|^2_{H^2(0,1)} + \epsilon_2^2\|D_{-x}e_h(t)\|^2_{h,+} \tag{29}$$

where $\epsilon_2 \neq 0$ is an arbitrary constant.

(4) *Estimate for Z_2*:
For Z_2 holds the representation

$$Z_2 = Z_{2,1} + Z_{2,2}$$

with

$$Z_{2,1} = (a(\hat{M}_h c(t))(D_{-x}R_h c(t) - \hat{M}_h\frac{\partial c}{\partial x}(t)), D_{-x}e_h(t))_{h,+}$$

and

$$Z_{2,2} = ((a(M_h c(t)) - a(\hat{M}_h c(t)))D_{-x}R_h c(t), D_{-x}e_h(t))_{h,+}.$$

To estimate $Z_{2,1}$ we remak that

$$Z_{2,1} = (a(\hat{M}_h c(t))\lambda(g), D_{-x}e_h(t))_{h,+},$$

with $g(\xi) = c(x_{i-1} + \xi\frac{h_i}{2})$ and

$$\lambda(g) = \frac{1}{h_i}(g(1) - g(0) - g'(\frac{1}{2})).$$

Applying Bramble-Hilbert lemma ([5]) to estimate $\lambda(g)$ we obtain

$$|\lambda(g)| \leq C_{Z_{2,1}}h_i|\frac{\partial^3 c}{\partial x^3}(t)|_{L^1(x_{i-1},x_i)},$$

where $C_{Z_{2,1}}$ is a positive constant. The last estimate leads to

$$|Z_{2,1}| \leq a_b C_{Z_{2,1}}h^2_{max}|c(t)|_{H^3(0,1)}\|D_{-x}e_h(t)\|_{h,+}, \tag{30}$$

which implies

$$|Z_{2,1}| \leq \frac{a_b^2 C^2_{Z_{2,1}}}{4\epsilon_3^2}h^4_{max}|c(t)|^2_{H^3(0,1)} + \epsilon_3^2\|D_{-x}e_h(t)\|^2_{h,+}, \tag{31}$$

where $a \leq a_b$ in $\mathbb{R}$ and $\epsilon_3 \neq 0$ is an arbitrary constant.
To estimate $Z_{2,2}$ we consider

$$\lambda(g) = \frac{1}{2}(g(1) + g(0)) - g(\frac{1}{2}),$$