Second order approximations for kinetic and potential energies in Maxwell's wave equations

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March 14, 2017

Abstract

In this paper we propose a numerical scheme for wave type equations with damping and space variable coefficients. Relevant equations of this kind arise for instance in the context of Maxwell's equations, namely, the electric potential equation and the electric field equation. The main motivation to study such class of equations is the crucial role played by the electric potential or the electric field in enhanced drug delivery applications. Our numerical method is based on piecewise linear finite element approximation and it can be regarded as a finite difference method based on non-uniform partitions of the spatial domain. We show that the proposed method leads to second order convergence, in time and space, for the kinetic and potential energies with respect to a discrete L^2-norm.

keywords: enhanced drug delivery, Maxwell's equations, finite element method, finite difference method, supercloseness, supraconvergence.

1 Introduction

We study in what follows a discretization in time and space of the following wave equation

$$a\frac{\partial^2 u}{\partial t^2} + b\frac{\partial u}{\partial t} = \nabla \cdot (D\nabla u) + f \text{ in } \Omega \times (0,T], \tag{1}$$

with the initial conditions

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,y,0) = \phi_1(x,y) \\ \\ u(x,y,0) = \phi_0(x,y), \ (x,y) \in \Omega, \end{cases} \tag{2}$$

and homogeneous Dirichlet boundary condition

$$u = 0 \text{ in } \partial\Omega \times (0,T]. \tag{3}$$

By simplicity we assume that $\Omega = (0,1) \times (0,1)$ and $u : \overline{\Omega} \times [0,T] \to \mathbb{R}$. In equation (1), the coefficient functions are x and y dependent and $a \geq a_0 > 0$ and $b \geq b_0 \geq 0$ in $\overline{\Omega}$, and D represents a diagonal matrix with positive diagonal entries d_i, $i = 1,2$, that have in $\overline{\Omega}$ a positive lower bound d_0.

Equation (1), a wave equation with a damping factor, has as a particular case the potential equation that arises from the following wave equation

$$\mu\epsilon\sigma\frac{\partial^2 V}{\partial t^2} + \mu\sigma^2\frac{\partial V}{\partial t} = \nabla\cdot(\sigma\nabla V) - \frac{\partial \rho}{\partial t}, \tag{4}$$

where V denotes the scalar potential, ϵ the electric permittivity, μ the magnetic permeability, σ the conductivity of the medium, and ρ the charge density of the current (see for instance [25]).

We remark that the results that we present in this paper can be easily extended to the initial boundary value problem (IBVP) (1)-(3) when $u : \overline{\Omega}\times[0,T]\to \mathbb{R}^n$. In this case, for $n = 3$, equation (1) has as a particular case the electric field equation

$$\mu\epsilon\frac{\partial^2 E}{\partial t^2} + \mu\sigma\frac{\partial E}{\partial t} = \Delta E - \nabla\left(\frac{\rho}{\epsilon}\right), \tag{5}$$

where E represents the electric field, ΔE the vector with components ΔE_i and $\nabla\left(\frac{\rho}{\epsilon}\right)$ the gradient of $\dfrac{\rho}{\epsilon}$ (see for instance [25]).

Our main motivation for this paper is the coupling between drug transport and electric current, which is used in several medical applications like transdermal drug delivery ([21, 22, 28, 35]), cancer treatment ([10, 38]) or ophthalmic applications ([32]). In all these applications, the drug transport is enhanced by the applied electric current. The drug mass flux is described by the Nernst-Planck equation and it is given by three main contributions: passive transport due to drug diffusion, electric enhanced drug transport that depends on the electric potential gradient or electric field, and electroosmotic transport due to fluid flow ([21, 33, 35]).

In the mathematical description of the drug time-space evolution, the authors usually assume that the potential is described by a Poisson equation when iontophoretic or electroporation protocols are applied. Without being exhaustive we refer to [6, 14, 20]. However, to obtain an accurate description of the drug evolution in a more general setting, it is necessary to construct an accurate approximation for the electric potential V defined by (4) or electric field defined by (5). It is desirable to compute a second order approximation for the gradient of the potential with respect to a discrete L^2-norm, that is, a second order approximation for the potential with respect to a discrete H^1-norm. In what concerns the electric field, the corresponding scheme leads to a second order approximation with respect to a $[H^1]^3$-discrete norm.

The method that we propose is obtained considering the well known MOL approach ([36]): a spatial discretization that leads to a semi-discrete approximation (continuous in time) followed by a time integration. The spatial discretization is defined considering a piecewise linear finite element method combined with particular integration rules that lead to a fully discrete in space scheme. It should be remarked that the constructed fully discrete scheme can be seen as a finite difference method.

The classical convergence analysis of the semi-discrete approximation using the finite difference language is based on the concept of truncation error. Although the truncation error is only of first order with respect to the norm $\|.\|_\infty$, when general non-uniform grids are considered, using our approach we prove that the finite difference approximation for the solution of the IBVP (1)-(3) is second order convergent with respect to a discrete H^1-norm provided that $u'(t)$, $u(t)\in C^4(\overline{\Omega})$, $t\in(0,T]$. This means that the corresponding numerical gradient is second order convergent with respect to a discrete L^2-norm.

Furthermore, to reduce the smoothness assumptions on the solution of the IBVP (1)-(3), we consider the approach introduced in [4] for one dimensional problems and in [16] for two dimensional elliptic equations and consider later in different contexts: in [5, 17, 19] for non-Fickian diffusion problems, and in [18] for diffusion problems in porous media. Avoiding the analytical difficulties that arise from the application of this technique we prove the same convergence result provided that $u'(t)$, $u(t) \in H^3(\Omega)$, $t \in (0,T]$.

As observed before, the semi-discrete finite difference approximation is also a fully discrete in space piecewise linear finite element approximation. In this context the obtained result is unexpected and is usually referred as a superclose result ([37]). There exist many papers about numerical methods for wave type equations, including finite differences ([1, 12]), finite elements ([3, 15]), mixed finite elements ([11, 13, 23]), and discontinuous Galerkin ([24, 30, 34]). On the other hand, only a few works have been dedicated to superclose (or superconvergent) estimates, some examples are [2, 9, 26, 27, 29, 31].

The paper is organized as follows. In Section 2 we introduce the definitions and notations used in this work and formulate our fully discrete in space method. The convergence analysis of the semi-discrete approximation for the solution of the IBVP (1)-(3) when the solution u is smooth, that is, $u'(t)$, $u(t) \in C^4(\overline{\Omega})$, is presented in Section 3. Section 4 is focused on the extension of this analysis to the non-smooth case, that is, when $u'(t)$, $u(t) \in H^3(\Omega)$. The fully discrete in time and space method is studied in Section 5 and numerical results illustrating the theoretical results established in the previous sections are presented in Section 6. Finally, in Section 7, we draw some conclusions and future work directions.

2 Fully discrete approximation in space

By $L^2(\Omega)$, $H^1_0(\Omega)$ we denote the usual Sobolev spaces equipped with the norms $\|.\|_0$, $\|.\|_1$ induced by the corresponding inner products $(.,.)$ and $(.,.)_1$. The usual inner product in $(L^2(\Omega))^2$ is represented by $((.,.))$. If $v : \overline{\Omega} \times [0,T] \to \mathbb{R}$, then $v(t) : \overline{\Omega} \to \mathbb{R}$ with $v(t)(x) = v(x,t)$, $x \in \overline{\Omega}$.

Let us consider the following variational problem: find $u(t) \in H^1_0(\Omega)$ such that

$$(au''(t), w) + (bu'(t), w) = -((D\nabla u, \nabla w)) + (f(t), w),\ t \in (0,T],$$

for $w \in H^1_0(\Omega)$, and

$$\begin{cases} u'(0) = \phi_1 \\ u(0) = \phi_0. \end{cases}$$

In $\overline{\Omega}$ we introduce a non-uniform rectangular grid defined by $H = (h,k)$ with $h = (h_1, \dots, h_N)$, $h_i > 0$, $i = 1, \dots, N$, $\sum_{i=1}^{N} h_i = 1$, and $k = (k_1, \dots, k_M)$, $k_j > 0$, $j = 1, \dots, M$, $\sum_{j=1}^{M} k_j = 1$. Let $\{x_i\}$ and $\{y_j\}$ be the non-uniform grids induced by h and k in $[0,1]$ with $x_i - x_{i-1} = h_i$, $y_j - y_{j-1} = k_j$. By $\overline{\Omega}_H$ we represent the rectangular grid introduced in $\overline{\Omega}$ that depends on H and let Ω_H and $\partial\Omega_H$ be defined by $\Omega_H = \Omega \cap \overline{\Omega}_H, \partial\Omega_H = \partial\Omega \cap \overline{\Omega}_H$.

Let $H_{max} = \max\{h_i, k_j;\ i = 1, \cdots N;\ j = 1, \cdots, M\}$. By Λ we denote a sequence of vectors $H = (h,k)$ such that $H_{max} \to 0$. Let W_H be the space of grid functions defined in $\overline{\Omega}_H$ and by $W_{H,0}$ we denote the subspace of W_H of grid functions null on $\partial\Omega_H$. Let $\mathcal{T}_H$ be a triangulation of $\overline{\Omega}$ using the set $\overline{\Omega}_H$ as vertices. We denote by diamΔ the diameter of the triangle $\Delta \in \mathcal{T}_H$. By $P_H v_H$ we denote the continuous piecewise linear interpolant of v_H with respect to $\mathcal{T}_H$.

We consider now the following piecewise linear finite element problem: find $u_H(t) \in W_{H,0}$ such that

$$(aP_H u''_H(t), P_H w_H) + (bP_H u'_H(t), P_H w_H) = -((D\nabla P_H u_H(t), \nabla P_H w_H)) + (f(t), P_H w_H), \quad (6)$$

for $t \in (0,T]$ and

$$\begin{cases} (P_H u'_H(0), P_H w_H) = (P_H R_H \phi_1, P_H w_H) \\ (P_H u_H(0), P_H w_H) = (P_H R_H \phi_0, P_H w_H), \end{cases} \tag{7}$$

for $w_H \in W_{H,0}$. In (7), $R_H : C(\overline{\Omega}) \to W_H$ denotes the restriction operator, where $C(\overline{\Omega})$ represents the space of continuous functions in $\overline{\Omega}$.

A fully discrete in space approximation is introduced now. In $W_{H,0}$ we define the inner product

$$(v_H, w_H)_H = \sum_{(x_i,y_j)\in\overline{\Omega}_H} |\square_{i,j}| v_H(x_i,y_j) w_H(x_i,y_j),\ w_H, v_H \in W_{H,0},$$

where $\square_{i,j} = (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2}) \cap \Omega$, $|\square_{i,j}|$ denotes the area of $\square_{i,j}$, and $x_{i+1/2} = x_i + \dfrac{h_{i+1}}{2}$, $x_{i-1/2} = x_i - \dfrac{h_i}{2}$, $h_{i+1/2} = x_{i+1/2} - x_{i-1/2}$ being $y_{j\pm 1/2}$ and $k_{j+1/2}$ defined analogously. Let $\|.\|_H$ be the corresponding norm.

For $v_H = (v_{1,H}, v_{2,H})$, $w_H = (w_{1,H}, w_{2,H})$, and $v_{\ell,H}, w_{\ell,H} \in W_H$, for $\ell = 1,2$, we use the notation

$$((v_H, w_H))_H = (v_{1,H}, w_{1,H})_{H,x} + (v_{2,H}, w_{2,H})_{H,y},$$

where

$$(v_{1,H}, w_{1,H})_{H,x} = \sum_{i=1}^{N}\sum_{j=1}^{M-1} h_i k_{j+1/2} v_{1,H}(x_i,y_j) w_{1,H}(x_i,y_j),$$

being $(v_{2,H}, w_{2,H})_{H,y}$ defined analogously.

Let D_{-x} and D_{-y} be the first order backward finite difference operators with respect to the variables x and y, respectively, and let ∇_H be the discrete version of the gradient operator ∇ defined by $\nabla_H u_H = (D_{-x}u_H, D_{-y}u_H)$. By D_H we denote the diagonal matrix with $d_{1,H}(x_i,y_j) = d_1(x_{i-1/2}, y_j)$ and $d_{2,H}(x_i,y_j) = d_2(x_i, y_{j-1/2})$, for $(x_i,y_j) \in \Omega_H$.

The initial value problem (6), (7) is replaced by the following fully discrete in space finite element problem: find $u_H(t) \in W_{H,0}$ such that

$$(a_H u''_H(t), w_H)_H + (b_H u'_H(t), w_H)_H = -((D_H \nabla_H u_H(t), \nabla_H w_H))_H + (f_H(t), w_H)_H, \tag{8}$$

for $t \in (0,T]$, $w_H \in W_{H,0}$, and

$$\begin{cases} u'_H(0) = R_H \phi_1 \\ u_H(0) = R_H \phi_0. \end{cases} \tag{9}$$

In (8), $a_H = R_H a$, $b_H = R_H b$, and

$$f_H(t)(x_i,y_j) = \frac{1}{|\square_{i,j}|}\int_{\square_{i,j}} f(x,y,t)\,dxdy. \tag{10}$$

We observe that the fully discrete in space finite element problem can be rewritten as a finite difference problem. In order to define such finite difference problem, we introduce the finite difference operator $\nabla^*_H = (D^*_x, D^*_y)$ where

$$D^*_x v_H(x_i,y_j) = \frac{v_H(x_{i+1},y_j) - v_H(x_i,y_j)}{h_{i+1/2}},$$

and D^*_y is defined analogously.
Then, from (8) we obtain

$$a_H u''_H(t) + b_H u'_H(t) = \nabla^*_H \cdot (D_H \nabla_H u_H(t)) + f_H(t) \text{ in } \Omega_H,\ t \in (0,T], \tag{11}$$

which is coupled with the boundary condition

$$u_H(t) = 0 \text{ on } \partial\Omega_H, \tag{12}$$

and the initial conditions (9).

In the next section we study the convergence properties of the fully discrete approximation $u_H(t)$ defined by (11), (9), and (12) or equivalently by (8), (9), and (12). The analysis technique depends on the smoothness of the solution u of the corresponding IBVP (1)-(3).

3 Convergence analysis: smooth case

Traditionally, the convergence analysis of a semi-discrete approximation $u_H(t)$ is based on the truncation error $T_H(t)$ associated with the spatial discretization. Assume for simplicity, but without loss of generality, that $d_i = 1$, $i = 1, 2$. Under this assumption, we have

$$\begin{aligned} T_H(t) = &-\big(h_{i+1} - h_i\big)\Big(\frac{1}{3}R_H\frac{\partial^3 u}{\partial x^3}(t) + \frac{1}{4}R_H\frac{\partial f}{\partial x}(t)\Big) \\ &- \big(k_{j+1} - k_j\big)\Big(\frac{1}{3}R_H\frac{\partial^3 u}{\partial y^3}(t) + \frac{1}{4}R_H\frac{\partial f}{\partial y}(t)\Big) + O(H_{max}^2), \end{aligned}$$

provided that $u(t) \in C^4(\overline{\Omega})$, $f \in C^2(\overline{\Omega})$. In $T_H(t)$, the term $O(H^2_{max})$ represents a term such that there exists a positive constant C_T satisfying

$$|O(H^2_{max})| \le C_T H^2_{max}\Big(\|u(t)\|_{C^4} + \|f(t)\|_{C^2}\Big),$$

where $\|.\|_{C^m}$ denotes the usual norm in $C^m(\overline{\Omega})$, $m \in \mathbb{N}_0$.

Let $e_H(t) = R_H u(t) - u_H(t)$ be the spatial discretization error induced by the numerical scheme. The spatial and the correspondent truncation errors satisfy the following equation

$$(a_H e''_H(t), w_H)_H + (b_H e'_H(t), w_H)_H = -((D_H \nabla_H e_H(t), \nabla_H w_H))_H + (T_H(t), w_H)_H, \tag{13}$$

for $t \in (0, T]$, $w_H \in W_{H,0}$, and

$$\begin{cases} e'_H(0) = 0 \\ e_H(0) = 0. \end{cases}$$

In the next result we establish an upper bound for the kinetic and potential energies of $e_H(t)$ where the potential energy is defined by considering the semi-norm

$$\|\nabla_H w_H\|_H = \Big(((\nabla_H w_H, \nabla_H w_H))_H\Big)^{1/2},\ w_H \in W_H.$$

Here, we denote by $\|.\|_{C^m(C^p)}$ the usual norm in $C^m(0, T, C^p(\overline{\Omega}))$, $m, p \in \mathbb{N}_0$. We observe that this result is established under too restrictive smoothness assumptions that will be weakened later. We also remark that weaker conditions were considered for first order hyperbolic problems in [39].

Theorem 1. *If the solution u of the IBVP (1)-(3) is in $C^1(0, T, C^4(\overline{\Omega})) \cap C^2(0, T, C(\overline{\Omega}))$ and $f \in C^1(0, T, C^2(\overline{\Omega}))$, then there exist positive constants C_1, C_2, independent of u, f, H, and T, such that for $H \in \Lambda$ with H_{max} small enough*

$$\begin{aligned} &\|e'_H(t)\|^2_H + \int_0^t \|e'_H(s)\|^2_H ds + \|e_H(t)\|^2_H + \|\nabla_H e_H(t)\|^2_H \\ &\qquad \le C_1 H^4_{max} e^{C_2 t}\Big(\|u\|^2_{C^1(C^4)} + \|f\|^2_{C^1(C^2)}\Big),\ t \in [0, T]. \end{aligned} \tag{14}$$

Proof: From (13) we get

$$(a_H e_H''(t), e_H'(t))_H + b_0\|e_H'(t)\|_H^2 \le -((D_H\nabla_H e_H(t), \nabla_H e_H'(t)))_H + (T_H(t), e_H'(t))_H,\ t\in(0,T]$$

that leads to

$$\frac{d}{dt}\Big(\|\sqrt{a_H}e_H'(t)\|_H^2 + 2b_0\int_0^t \|e_H'(s)\|_H^2 ds + \|\sqrt{D_H}\nabla_H e_H(t)\|_H^2\Big) \le 2(T_H(t), e_H'(t))_H, \qquad (15)$$

for $t\in(0,T]$. In (15), $\sqrt{D_H}$ is the diagonal matrix whose entries are given by $\sqrt{d_i}$, $i=1,2$. The main difficulty in the construction of a convenient upper bound for $\|\sqrt{a_H}e_H'(t)\|_H^2 + 2b_0\int_0^t \|e_H'(s)\|_H^2 ds + \|\sqrt{D_H}\nabla_H e_H(t)\|^2$ is related with the term $(T_H(t), e_H'(t))_H$. We observe that

$$(T_H(t), e_H'(t))_H = \frac{d}{dt}(T_H(t), e_H(t))_H - (T_H'(t), e_H(t))_H, \qquad (16)$$

where

$$\begin{aligned} T_H'(t) = &-\big(h_{i+1}-h_i\big)\Big(\frac{1}{3}R_H\frac{\partial^4 u}{\partial t\partial x^3}(t) + \frac{1}{4}R_H\frac{\partial^2 f}{\partial t\partial x}(t)\Big)\\ &- \big(k_{j+1}-k_j\big)\Big(\frac{1}{3}R_H\frac{\partial^4 u}{\partial t\partial y^3}(t) + \frac{1}{4}R_H\frac{\partial^2 f}{\partial t\partial y}(t)\Big) + O(H_{max}^2),\end{aligned}$$

with $|O(H_{max}^2)| \le C_T H_{max}^2\Big(\|u'(t)\|_{C^4} + \|f'(t)\|_{C^2}\Big)$.
From (15) and (16) we get

$$\begin{aligned}\|\sqrt{a_H}e_H'(t)\|_H^2 + 2b_0\int_0^t \|e_H'(s)\|_H^2 ds + \|\sqrt{D_H}\nabla_H e_H(t)\|_H^2 &\le 2(T_H(t), e_H(t))_H\\ &\quad - 2\int_0^t (T_H'(s), e_H(s))_H ds,\ t\in(0,T]. \qquad (17)\end{aligned}$$

To obtain upper bounds for the terms $(T_H(t), e_H(t))_H$, $(T_H'(s), e_H(s))_H$ we consider the generic term

$$T_{G,x}(t) = \sum_{i=1}^{N-1}\sum_{j=1}^{M-1} h_{i+1/2}k_{j+1/2}(h_{i+1}-h_i)v(x_i,y_j,t)e_H(x_i,y_j,t).$$

We have successively

$$\begin{aligned} T_{G,x}(t) &= \frac{1}{2}\sum_{i=1}^{N-1}\sum_{j=1}^{M-1} k_{j+1/2}\big(h_{i+1}^2 - h_i^2\big)\Big(v(x_i,y_j,t)e_H(x_i,y_j,t)\Big)\\ &= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i^2\Big(v(x_i,y_j,t)e_H(x_i,y_j,t) - v(x_{i-1},y_j,t)e_H(x_{i-1},y_j,t)\Big)\\ &= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i^2\int_{x_{i-1}}^{x_i}\frac{\partial v}{\partial x}(x,y_j,t)dx e_H(x_i,y_j,t)\\ &\quad -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i^3 v(x_{i-1},y_j,t)D_{-x}e_H(x_i,y_j,t)\\ &:= T_{G,x}^{(1)}(t) + T_{G,x}^{(2)}(t).\end{aligned}$$

From this, we can establish the following upper bounds

$$|T^{(1)}_{G,x}(t)| \leq \frac{1}{4\eta_1^2} H^4_{max}\|v(t)\|^2_{C^1} + \eta_1^2\|e_H(t)\|^2_H$$

and

$$|T^{(2)}_{G,x}(t)| \leq \frac{1}{4\eta_2^2} H^4_{max}\|v(t)\|^2_{C^0} + \eta_2^2\|D_{-x}e_H(t)\|^2_{H,x},$$

where η_i, $i = 1, 2$, are non-zero constants, and consequently

$$|T_{G,x}(t)| \leq \frac{1}{4\eta_1^2} H^4_{max}\|v(t)\|^2_{C^1} + \eta_1^2\|e_H(t)\|^2_H + \frac{1}{4\eta_2^2} H^4_{max}\|v(t)\|^2_{C^0} + \eta_2^2\|D_{-x}e_H(t)\|^2_{H,x}.$$

For the correspondent y term

$$T_{G,y}(t) = \sum_{i=1}^{N-1}\sum_{j=1}^{M-1} h_{i+1/2}k_{j+1/2}(k_{j+1} - k_j)v(x_i, y_j, t)e_H(x_i, y_j, t)$$

it can be shown that holds the following

$$|T_{G,y}(t)| \leq \frac{1}{4\eta_3^2} H^4_{max}\|v(t)\|^2_{C^1} + \eta_3^2\|e_H(t)\|^2_H + \frac{1}{4\eta_4^2} H^4_{max}\|v(t)\|^2_{C^0} + \eta_4^2\|D_{-y}e_H(t)\|^2_{H,y},$$

where η_i, $i = 3, 4$, are non-zero constants.

Taking $\eta_1 = \eta_3$ and $\eta_2 = \eta_4$, we deduce

$$|T_{G,x}(t)| + |T_{G,y}(t)| \leq \Big(\frac{1}{2\eta_1^2} + \frac{1}{2\eta_2^2}\Big) H^4_{max}\|v(t)\|^2_{C^1} + 2\eta_1^2\|e_H(t)\|^2_H + \eta_2^2\|\nabla_H e_H(t)\|^2_H. \tag{18}$$

From (18) we conclude for $(T_H(t), e_H(t))$ the upper bound

$$\begin{aligned}|(T_H(t), e_H(t))_H| \leq{}& \Big(\frac{1}{2\xi_1^2} + \frac{1}{2\xi_2^2}\Big) H^4_{max}\Big(\frac{1}{3}\|u(t)\|_{C^4} + \frac{1}{4}\|f(t)\|_{C^2}\Big)^2 + 3\xi_1^2\|e_H(t)\|^2_H \\ &+ \xi_2^2\|\nabla_H e_H(t)\|^2_H + \frac{1}{4\xi_1^2}C_T^2 H^4_{max}\Big(\|u(t)\|_{C^4} + \|f(t)\|_{C^2}\Big)^2,\end{aligned} \tag{19}$$

where $\xi_i, i = 1, 2$, are non-zero constants, and for $(T'_H(s), e_H(s))$ we get the upper bound

$$\begin{aligned}|(T'_H(s), e_H(s))_H| \leq{}& \Big(\frac{1}{2\xi_3^2} + \frac{1}{2\xi_4^2}\Big) H^4_{max}\Big(\frac{1}{3}\|u'(s)\|_{C^4} + \frac{1}{3}\|f'(s)\|_{C^2}\Big)^2 + 3\xi_3^2\|e_H(s)\|^2_H \\ &+ \xi_4^2\|\nabla_H e_H(s)\|^2_H + \frac{1}{4\xi_3^2}C_T^2 H^4_{max}\Big(\|u'(t)\|_{C^4} + \|f'(t)\|_{C^2}\Big)^2,\end{aligned} \tag{20}$$

where ξ_i, $i = 3, 4$, are non-zero constants.

Considering (19) and (20) in (17) and using the Poincaré-Friedrichs's inequality

$$\|w_H\|^2_H \leq \frac{1}{2}\|\nabla_H w_H\|^2_H,\ w_H \in W_{H,0},$$

we obtain

$$\begin{aligned}&a_0\|e'_H(t)\|^2_H + 2b_0\int_0^t \|e'_H(s)\|^2_H ds + \Big(\frac{d_0}{2} - 6\xi_1^2\Big)\|e_H(t)\|^2_H + \Big(\frac{d_0}{2} - 2\xi_2^2\Big)\|\nabla_H e_H(t)\|^2 \\ &\quad\leq \int_0^t 2\Big(\xi_4^2\|\nabla_H e_H(s)\|^2_H + 3\xi_3^2\|e_H(s)\|^2_H\Big)ds + CH^4_{max}\Big(R(t) + \int_0^t R(s)ds\Big),\ t \in (0, T],\end{aligned}$$

where C depends on the previous constants $\xi_i, i = 1, 2, 3, 4$, and C_T and $R(\mu) = \|u(\mu)\|^2_{C^4} + \|u'(\mu)\|^2_{C^4} + \|f(\mu)\|^2_{C^2} + \|f'(\mu)\|^2_{C^2}$.
Fixing ξ_1 and ξ_2 such that $\dfrac{d_0}{2} - 6\xi_1^2 > 0$, $\dfrac{d_0}{2} - 6\xi_2^2 > 0$, it follows that there exist positive constants C_i, $i = 1, 2$, such that

$$\begin{aligned} &\|e'_H(t)\|^2_H + \int_0^t \|e'_H(s)\|^2_H ds + \|e_H(t)\|^2_H + \|\nabla_H e_H(t)\|^2_H \\ &\quad \leq C_1 H^4_{max}\Big(R(t) + \int_0^t R(s)ds\Big) + C_2 \int_0^t \Big(\|\nabla_H e_H(s)\|^2_H + \|e_H(s)\|^2_H\Big) ds,\ t \in (0, T]. \end{aligned} \tag{21}$$

Applying Gronwall's Lemma to (21) we arrive at (14).

■

Theorem 1 enables us to conclude that

$$\|e'_H(t)\|^2_H + \int_0^t \|e'_H(s)\|^2_H ds + \|e_H(t)\|^2_H + \|\nabla_H e_H(t)\|^2_H \leq C H^4_{max},$$

and consequently

$$\|e'_H(t)\|^2_H + \|\nabla_H e_H(t)\|^2_H \leq C H^4_{max}.$$

We conclude that the IBVP defined by (11), (9), and (12) or equivalently by (8), (9), and (12) leads to a semi-discrete approximation $u_H(t)$ whose kinetic and potential energy are second order approximations for the correspondent quantities of the solution of the IBVP (1)-(3). We remark that the proof of Theorem 1 requires that $u(t), u'(t) \in C^4(\overline{\Omega})$ and $f(t), f'(t) \in C^2(\overline{\Omega})$.

4 Convergence analysis: non-smooth case

In this section we establish an upper bound analogous to (14) but under weaker assumptions than those used in the proof of Theorem 1, namely $u \in C^1(0, T, C^4(\overline{\Omega})) \cap C^2(0, T, C(\overline{\Omega}))$ and $f \in C^1(0, T, C^2(\overline{\Omega}))$. The main ingredient in the proof of the next result is the Bramble-Hilbert Lemma ([7]). Let us assume that

$$u \in \mathcal{V}_0 = \{v \in H^3(0, T, H^2(\Omega)) \cap H^1(0, T, H^3(\Omega)) : v = 0 \text{ on } \partial\Omega\}.$$

We remark that if $u \in H^m(0, T, H^p(\Omega))$ then $u \in C^{m-1}(0, T, H^p(\Omega))$, $m \in \mathbb{N}$, $p \in \mathbb{N}_0$. In the following we denote by $\|.\|_{H^m(H^p)}$ the usual norm in $H^m(0, T, H^p(\Omega))$, m, $p \in \mathbb{N}_0$.

Theorem 2. *If the solution u of the IBVP (1)-(3) is in $\mathcal{V}_0$ then there exist positive constants $C_i, i = 1, 2,$ independent of u, H, and T such that for $H \in \Lambda$ with H_{max} small enough*

$$\begin{aligned} &\|e'_H(t)\|^2_H + \int_0^t \|e'_H(s)\|^2_H ds + \|\nabla_H e_H(t)\|^2_H \\ &\quad \leq C_1 e^{C_2 t} \sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \Big(\|u\|^2_{C(H^3)} + \|u\|^2_{C^2(H^2)} + \|u\|^2_{H^1(H^3)} + \|u\|^2_{H^3(H^2)}\Big),\ t \in [0, T]. \end{aligned}$$

Proof: It can be shown that the semi-discrete error $e_H(t)$ satisfies

$$\begin{aligned} (a_H e''_H(t), w_H)_H + (b_H e'_H(t), w_H)_H = &-((D_H \nabla_H e_H(t), \nabla_H w_H))_H \\ &+ T_1(u(t), w_H) + T_2(u(t), w_H),\ t \in (0, T],\ \forall w_H \in W_{H,0}, \end{aligned} \tag{22}$$

where

$$T_1(u(t), w_H) = ((D_H \nabla_H (R_H u(t)), \nabla_H w_H))_H - (-(\nabla \cdot (D \nabla u(t)))_H, w_H)_H$$

and

$$T_2(u(t), w_H) = ((au''(t) + bu'(t))_H - R_H(au''(t) + bu'(t)), w_H)_H.$$

In the definitions of $T_1(w_H)$ and $T_2(w_H)$, $(g)_H$ is given by (10) with f replaced by $g = au''(t) + bu'(t)$ or $g = \nabla \cdot (D\nabla u(t))$.

Lemma 5.1 of [16] allows us to conclude the following estimate

$$|T_1(u(t), w_H)| \leq C\Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \|u(t)\|^2_{H^3(\Delta)}\Big)^{1/2} \|\nabla_H w_H\|_H, \; w_H \in W_{H,0}. \tag{23}$$

Moreover, Lemma 5.7 leads to

$$|T_2(u(t), w_H)| \leq C\Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \big(\|u''(t)\|^2_{H^2(\Delta)} + \|u'(t)\|^2_{H^2(\Delta)}\big)\Big)^{1/2} \|\nabla_H w_H\|_H, \tag{24}$$

for $w_H \in W_{H,0}$, and where C denotes a positive constant which is not necessarily the same one in each appearance.

If we take in (22) $w_H = e'_H(t)$ then we obtain

$$\begin{aligned}(a_H e''_H(t), e'_H(t))_H + (b_H e'_H(t), e'_H(t))_H = &-((D_H \nabla_H e_H(t), \nabla_H e'_H(t)))_H \\ &+ T_1(u(t), e'_H(t)) + T_2(u(t), e'_H(t)).\end{aligned} \tag{25}$$

As we have

$$T_i(u(t), e'_H(t)) = \frac{d}{dt} T_i(u(t), e_H(t)) - T_i(u'(t), e_H(t)), \; i = 1, 2,$$

from (25) we deduce

$$\begin{aligned}\|\sqrt{a_H} e'_H(t)\|^2_H + 2b_0 \int_0^t \|e'_H(s)\|^2_H ds + d_0 \|\nabla_H e_H(t)\|^2_H \leq 2T_1(u(t), e_H(t)) \\ + 2T_2(u(t), e_H(t)) - 2\int_0^t \Big(T_1(u'(s), e_H(s)) + T_2(u'(s), e_H(s))\Big) ds.\end{aligned} \tag{26}$$

Taking in (26) the upper bounds (23) and (24) we get

$$\begin{aligned}a_0 \|e'_H(t)\|^2_H &+ 2b_0 \int_0^t \|e'_H(s)\|^2_H ds + (d_0 - 4\xi_1^2) \|\nabla_H e_H(t)\|^2_H \\ &\leq \frac{1}{2\xi_1^2} C \sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \Big(\|u(t)\|^2_{H^3(\Delta)} + \sum_{\ell=1}^{2} \|u^{(\ell)}(t)\|^2_{H^2(\Delta)}\Big) \\ &\quad + \frac{1}{2\xi_2^2} C \sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \int_0^t \Big(\|u'(s)\|^2_{H^3(\Delta)} + \sum_{\ell=2}^{3} \|u^{(\ell)}(s)\|^2_{H^2(\Delta)}\Big) ds \\ &\quad + 4\xi_2^2 \int_0^t \|\nabla_H e_H(s)\|^2_H ds,\end{aligned}$$

where $\xi_i, i = 1, 2$, are non-zero constants. We finish the proof fixing ξ_1 such that $d_0 - 4\xi_1^2 > 0$, and applying Gronwall's Lemma.

■

Theorem 2 allows us to conclude that

$$\|e'_H(t)\|^2_H + \|\nabla_H e_H(t)\|^2_H \leq C H^4_{max} \Big(\|u\|^2_{C(H^3)} + \|u\|^2_{C^2(H^2)} + \|u\|^2_{H^1(H^3)} + \|u\|^2_{H^3(H^2)}\Big), \; t \in [0, T],$$

under weaker conditions than those imposed in Theorem 1.

5 Fully discrete approximation in time and space

Let us introduce in $[0, T]$ the time grid $\{t_n = n\Delta t, n = 0, \dots, M_t\}$ with $t_{M_t} = T$ and where Δt is the uniform time step. Let also $D_{2,t}$ be the second order centered finite difference operator in time and let D_{-t} be the first order backward finite difference operator in time. The fully discrete in time and space approximation for the solution of the IBVP (1)-(3) is defined by

$$
\begin{aligned}
(a_H D_{2,t} u_H^n, w_H)_H + (b_H D_{-t} u_H^{n+1}, w_H)_H = &-((D_H \nabla_H u_H^{n+1}, \nabla_H w_H))_H \\
&+ (f_H(t_{n+1}), w_H)_H,\ n = 1, \dots, M_t - 1, \qquad (27)
\end{aligned}
$$

for $w_H \in W_{H,0}$, with the initial conditions

$$
\begin{cases} D_{-t} u_H^1 = R_H \phi_1 \\ u_H^0 = R_H \phi_0, \end{cases} \qquad (28)
$$

and the boundary condition

$$
u_H^n = 0 \text{ on } \partial\Omega_H,\ n = 0, \dots, M_t.
$$

Equivalently, equation (27) can be written as

$$
a_H D_{2,t} u_H^n + b_H D_{-t} u_H^{n+1} = \nabla_H^* \cdot (D_H \nabla_H u_H^{n+1}) + f_H(t_{n+1}) \text{ in } \Omega_H,\ n = 1, \dots, M_t - 1. \qquad (29)
$$

The main theorem of this section is stated next.

Theorem 3. *If the solution of the IBVP (1)-(3) is in*

$$
H^1(0, T, H^3(\Omega) \cap H_0^1(\Omega)) \cap H^3(0, T, H^2(\Omega)) \cap C^3(0, T, C(\overline{\Omega})) \cap C^2(0, T, C^1(\overline{\Omega})),
$$

then, for $H \in \Lambda$ with H_{max} small enough, there exists a positive constant C, independent of u and H, such that for the error $e_H^n = R_H u(t_n) - u_H^n, n = 1, \dots, M_t$, holds the following

$$
\begin{aligned}
&\|D_{-t} e_H^n\|_H^2 + \Delta t \sum_{j=1}^n \|D_{-t} e_H^j\|_H^2 + \|\nabla_H e_H^n\|_H^2 \\
&\quad \le C\Big(\Delta t^2\Big(\|u\|_{C^4(C)}^2 + \Delta t^2 \|u\|_{C^2(C^1)}^2 + H_{max}^2 \|u\|_{C^1(C^2)}^2\Big) \\
&\qquad + \sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \Big(\|u\|_{C(H^3)}^2 + \|u\|_{C^2(H^2)}^2\Big) \\
&\qquad + \Delta t \sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \Big(\|u\|_{H^1(H^3)}^2 + \|u\|_{H^3(H^2)}^2\Big)\Big). \qquad (30)
\end{aligned}
$$

Proof: It can be shown that the error e_H^n satisfies the following equation

$$
\begin{aligned}
(a_H D_{2,t} e_H^n, D_{-t} e_H^{n+1})_H + (b_H D_{-t} e_H^{n+1}, D_{-t} e_H^{n+1})_H = &-((D_H \nabla_H e_H^{n+1}, \nabla_H D_{-t} e_H^{n+1}))_H \\
&+ \sum_{\ell=1}^3 T_\ell(u(t_{n+1}), D_{-t} e_H^{n+1}),
\end{aligned}
$$

where

$$
T_1(u(t_{n+1}), w_H) = -((D_H \nabla_H (R_H u(t_{n+1})), \nabla_H w_H)_H + (-(\nabla \cdot (D \nabla u(t_{n+1}))))_H, w_H)_H
$$

$$T_2(u(t_{n+1}), w_H) = ((au''(t_{n+1}) + bu'(t_{n+1}))_H - R_H(au''(t_{n+1}) + bu'(t_{n+1})), w_H)_H,$$

and

$$T_3(u(t_{n+1}), w_H) = (a_H(D_{2,t}R_Hu(t_{n+1}) - R_Hu''(t_{n+1})) + b_H(D_{-t}R_Hu(t_{n+1}) - R_Hu'(t_{n+1})), w_H)_H,$$

for $w_H \in W_{H,0}$.
As we have

$$(a_H D_{2,t}e_H^n, D_{-t}e_H^{n+1})_H \geq \frac{1}{2\Delta t}\Big(\|\sqrt{a}_H D_{-t}e_H^{n+1}\|_H^2 - \|\sqrt{a}_H D_{-t}e_H^n\|_H^2\Big)$$

$$(D_H\nabla_H e_H^{n+1}, \nabla_H D_{-t}e_H^{n+1})_H \geq \frac{1}{2\Delta t}\Big(\|\sqrt{D_H}\nabla_H e_H^{n+1}\|_H^2 - \|\sqrt{D_H}\nabla_H e_H^n\|_H^2\Big)$$

(see [8]), and

$$T_\ell(u(t_{n+1}), D_{-t}e_H^{n+1}) = D_{-t}T_\ell(u(t_{n+1}), e_H^{n+1}) - T_\ell(D_{-t}u(t_{n+1}), e_H^n),\ \ell = 1, 2,$$

we get

$$\begin{aligned}
&\|\sqrt{a_H}D_{-t}e_H^{n+1}\|_H^2 + 2\Delta t b_0\|D_{-t}e_H^{n+1}\|_H^2 - 2\sum_{\ell=1}^{2}T_\ell(u(t_{n+1}), e_H^{n+1}) + \|\sqrt{D_H}\nabla_H e_H^{n+1}\|_H^2\\
&\quad\leq \|\sqrt{a_H}D_{-t}e_H^n\|_H^2 + \|\sqrt{D_H}\nabla_H e_H^n\|_H^2 - 2\sum_{\ell=1}^{2}T_\ell(u(t_n), e_H^n)\\
&\quad\quad - 2\Delta t\sum_{\ell=1}^{2}T_\ell(D_{-t}u(t_{n+1}), e_H^n) + 2\Delta t T_3(u(t_{n+1}), D_{-t}e_H^{n+1}),
\end{aligned}\tag{31}$$

for $n = 1, \ldots, M - 1$.
Inequality (31) leads to

$$\begin{aligned}
&\|\sqrt{a_H}D_{-t}e_H^{n+1}\|_H^2 + 2\Delta t b_0\sum_{j=1}^{n+1}\|D_{-t}e_H^j\|_H^2 - 2\sum_{\ell=1}^{2}T_\ell(u(t_{n+1}), e_H^{n+1}) + \|\sqrt{D_H}\nabla_H e_H^{n+1}\|_H^2\\
&\quad\leq \|\sqrt{a_H}D_t e_H^1\|_H^2 + 2\Delta t\|D_{-t}e_H^1\|_H^2 + \|\sqrt{D_H}\nabla_H e_H^1\|_H^2 - 2\sum_{\ell=1}^{2}T_\ell(u(t_1), e_H^1)\\
&\quad\quad - 2\Delta t\sum_{j=1}^{n}\Big(\sum_{\ell=1}^{2}T_\ell(D_{-t}u(t_{j+1}), e_H^j) + T_3(u(t_{j+1}, D_{-t}e_H^{j+1}))\Big),
\end{aligned}$$

for $n = 1, \ldots, M_t - 1$. The terms $T_\ell(u(t_{n+1}), e_H^{n+1})$, $\ell = 1, 2$, satisfy (23) and (24), respectively, with $w_H = e_H^{n+1}$, and for $T_\ell(D_{-t}u(t_{n+1}), e_H^n)$, $\ell = 1, 2$, we have

$$|T_1(D_{-t}u(t_{n+1}), e_H^n)| \leq C\frac{1}{\sqrt{\Delta t}}\Big(\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\|u\|_{H^1(t_n,t_{n+1},H^3(\Delta))}^2\Big)^{1/2}\|\nabla_H e_H^n\|_H \tag{32}$$

and

$$|T_2(D_{-t}u(t_{n+1}), e_H^n)| \leq C\frac{1}{\sqrt{\Delta t}}\Big(\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\|u\|_{H^3(t_n,t_{n+1},H^2(\Delta))}^2\Big)^{1/2}\|\nabla_H e_H^n\|_H. \tag{33}$$

For the term $T_3(u(t_{n+1}), D_{-t}e_H^{n+1})$ it is easy to show the following

$$|T_3(u(t_{n+1}), D_{-t}e_H^{n+1})| \leq C\Delta t\|u\|_{C^3(C)}\|D_{-t}e_H^{n+1}\|_H. \tag{34}$$

Considering in (31) the upper bounds (23), (24) for $|T_\ell(u(t_{n+1}), e_H^{n+1})|$, $\ell = 1, 2$, and (32), (33) for $|T_\ell(D_{-t}u(t_{n+1}), e_H^n)|$, $\ell = 1, 2$, and (34) for $|T_3(u(t_{n+1}), D_{-t}e_H^{n+1})|$, we find

$$\begin{aligned}
&a_0\|D_{-t}e_H^{n+1}\|_H^2 + 2\Delta t(b_0 - \xi_3^2)\sum_{j=1}^{n+1}\|D_{-t}e_H^j\|_H^2 + \big(d_0 - 4\xi_1^2\big)\|\nabla_H e_H^{n+1}\|_H^2 \\
&\quad\leq \|\sqrt{a_H}D_{-t}e_H^1\|_H^2 + 2\Delta t b_0\|D_{-t}e_H^1\|_H^2 + \|\sqrt{D_H}\nabla_H e_H^1\|_H^2 + T_{n+1}(u) + \Delta t\sum_{j=1}^{n} 4\xi_2^2\|\nabla_H e_H^j\|_H^2
\end{aligned}$$

for $n = 1, \ldots, M_t - 1$, and where

$$\begin{aligned}
T_{n+1}(u) = C\Big(&\frac{1}{2\xi_1^2}\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\Big(\|u(t_{n+1})\|_{H^3(\Delta)}^2 + \sum_{\ell=1}^{2}\|u^{(\ell)}(t_{n+1})\|_{H^2(\Delta)}^2\Big) \\
&+ C\Delta t\sum_{j=0}^{n}\Big(\frac{1}{2\xi_2^2}\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\Big(\|u\|_{H^1(t_j,t_{j+1},H^3(\Delta))}^2 + \|u\|_{H^3(t_j,t_{j+1},H^2(\Delta))}^2\Big) \\
&+ \frac{1}{2\xi_3^2}\Delta t^2\|u\|_{C^3(t_j,t_{j+1},C(\overline{\Omega}))}^2\Big)
\end{aligned}$$

with $\xi_i, i = 1, 2, 3$, non-zero constants.
Fixing ξ_1 and ξ_3 such that $d_0 - 4\xi_1^2 > 0$, $b_0 - \xi_3^2 > 0$, and considering the discrete Gronwall's Lemma we conclude that there exist positive constant C_1, C_2 such that

$$\begin{aligned}
&\|D_{-t}e_H^{n+1}\|_H^2 + \Delta t\sum_{j=1}^{n+1}\|D_{-t}e_H^j\|_H^2 + \|\nabla_H e_H^{n+1}\|_H^2 \\
&\qquad\leq C_1\Big(\|D_{-t}e_H^1\|_H^2 + \|\nabla_H e_H^1\|_H^2 + \max_{j=2,\ldots,n+1} T_j(u)\Big)\Big(1 + Te^{C_2 n\Delta t}\Big),
\end{aligned} \tag{35}$$

for $n = 1, \ldots, M_t - 1$. To obtain the final error estimate we need to compute an upper bound for $\|D_{-t}e_H^1\|_H^2$ and $\|\nabla_H e_H^1\|_H^2$. From the first relation of (28) and as the initial velocity is defined by ϕ_1, we have

$$D_{-t}e_H^1 = D_{-t}R_H u(t_1) - R_H u'(t_0)$$

and then

$$\|D_{-t}e_H^1\|_H^2 \leq \frac{1}{2}\Delta t^2\|u\|_{C^2(C)}^2. \tag{36}$$

We also have

$$\nabla_H D_{-t}e_H^1 = \nabla_H D_{-t}R_H u(t_1) - R_H\nabla u'(t) + O(H_{max}),$$

where $|O(H_{max})| \leq CH_{max}\|u\|_{C^1(C^2)}$. Since $\nabla_H D_{-t}R_H u(t_1) - R_H\nabla u'(t) = O(\Delta t + H_{max})$, where $|O(\Delta t + H_{max})| \leq C\Big(H_{max}\|u\|_{C^1(C^2)} + \Delta t\|u\|_{C^2(C^1)}\Big)$, then

$$((\nabla_H D_{-t}e_H^1, \nabla_H e_H^1))_H = ((T(u(t_1)), \nabla_H e_H^1))_H, \tag{37}$$

with

$$|T(u(t_1))| \leq C\Big(\Delta t\|u\|_{C^2(C^1)} + H_{max}\|u\|_{C^1(C^2)}\Big).$$

From (37) we obtain

$$(1-2\xi^2)\|\nabla_H e_H^1\|_H^2 \le \|\nabla_H e_H^0\|_H^2 + \frac{\Delta t^2}{2\xi^2}\|T(u(t_1))\|_H^2,$$

where $\xi \neq 0$. As $e_H^0 = 0$, then, there exists a positive constant C such that

$$\|\nabla_H e_H^1\|_H^2 \le C\Delta t^2\Big(\Delta t^2\|u\|_{C^2(C^1)} + H_{max}^2\|u\|_{C^1(C^2)}\Big). \tag{38}$$

To conclude (30) we observe that combining (36), (38) with (35) we obtain

$$\begin{aligned}&\|D_{-t}e_H^{n+1}\|_H^2 + 2\Delta t\sum_{j=1}^{n+1}\|D_{-t}e_H^j\|_H^2 + \|\nabla_H e_H^{n+1}\|_H^2 + \|e_H^{n+1}\|_H^2\\ &\quad\le C\Big(\Delta t^2\Big(\|u\|_{C^3(C)}^2 + \Delta t^2\|u\|_{C^2(C^1)}^2 + H_{max}^2\|u\|_{C^1(C^2)}^2\Big) + \max_{\ell=2,\ldots,n+1} T_\ell(u)\Big),\end{aligned}$$

for $n = 1,\ldots,M_t-1$, and some positive constant C.

■

Theorem 3 allows us to conclude that the numerical scheme defined by (27) or (29), together with the initial conditions (28) and homogeneous Dirichlet boundary conditions, satisfies

$$\|D_{-t}e_H^n\|_H^2 + \|\nabla_H e_H^n\|_H^2 \le C\big(\Delta t^2 + H_{max}^4\big).$$

The first order term in the previous upper bound is due to the discretization of the first order time derivatives in the wave equation and in the initial condition using a first order operator. To increase the time convergence order we should increase the order of the time discretization. We rewrite the IBVP (1), (2) and (3) with $f=0$ in the equivalent form

$$\begin{cases} a\dfrac{\partial u}{\partial t} = w - bu \\ \dfrac{\partial w}{\partial t} = \nabla.(D\nabla u) \qquad \text{in } \Omega\times(0,T]\end{cases} \tag{39}$$

with the initial conditions

$$\begin{cases} w(x,y,0) = a\phi_1(x,y) + b\phi_0(x,y) \\ u(x,y,0) = \phi_0(x,y), \qquad (x,y)\in\Omega,\end{cases} \tag{40}$$

and the boundary conditions

$$\begin{cases} w(x,y,t) = 0 \\ u(x,y,t) = 0 \qquad (x,t)\in\partial\Omega\times(0,T].\end{cases} \tag{41}$$

To get a second order approximation for u and w we use a standard procedure used in first order time derivative problems: we consider the Crank-Nicolson approach. Let u_H^n and w_H^n be the corresponding approximations defined by the finite difference scheme: for $n = 0,\ldots,M_t-1$,

$$\begin{cases} a_H D_{-t}u_H^{n+1} = \dfrac{w_H^{n+1}+w_H^n}{2} - b_H\dfrac{u_H^{n+1}+u_H^n}{2} \\ D_{-t}w_H^{n+1} = \nabla.\Big(D_H\nabla_H\Big(\dfrac{u_H^{n+1}+u_H^n}{2}\Big)\Big) \qquad \text{in } \Omega_H,\end{cases} \tag{42}$$

$$\begin{cases} w_H^0 = a_H R_H \phi_1 + b_H R_H \phi_0 \\ \\ u_H^0 = R_H \phi_0 \qquad\qquad \text{in } \Omega_H \end{cases} \tag{43}$$

and

$$\begin{cases} w_H^n = 0 \\ \\ u_H^n = 0 \qquad \text{on } \partial\Omega \times \{1, \ldots, M_t\}. \end{cases} \tag{44}$$

We observe that the previous solutions u_H^n and w_H^n satisfy

$$\begin{cases} (a_H D_{-t} u_H^{n+1}, v_H)_H = (\dfrac{w_H^{n+1} + w_H^n}{2}, v_H)_H - (b_H \dfrac{u_H^{n+1} + u_H^n}{2}, v_H)_H \\ (D_{-t} w_H^{n+1}, v_H)_H = -((D_H \nabla_H \Big(\dfrac{u_H^{n+1} + u_H^n}{2}\Big), \nabla_H v_H))_H \qquad\qquad \forall v_H \in W_{H,0}. \end{cases} \tag{45}$$

We remark that we also have

$$\begin{aligned} ((a_H D_{-t} \nabla_H u_H^{n+1}, \nabla_H v_H))_H \quad &= ((\nabla_H (\Big(\frac{w_H^{n+1} + w_H^n}{2}\Big), \nabla_H v_H))_H \\ &-((b_H \nabla_H \Big(\frac{u_H^{n+1} + u_H^n}{2}\Big), \nabla_H v_H))_H, \end{aligned} \tag{46}$$

for all $v_H \in W_{H,0}$.

By e_u^n and e_w^n we represent the global errors in u_H^n and w_H^n, respectively. It can be shown that

$$(D_{-t} e_w^{n+1}, v_h)_H = -((D_H \nabla_H \Big(\frac{e_u^{n+1} + e_u^n}{2}\Big), \nabla_H v_H))_H + (T_{1,H}^n(u), v_H)_H, \tag{47}$$

for all $v_H \in W_{H,0}$, where

$$\begin{aligned} \|T_{1,H}^n(u)\|_H \le C \quad &\Big(\Delta t^4 \|u\|_{C^4(C)} + \Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \big(\|u(t_{n+1})\|^2_{H^3(\Delta)} + \|u(t_n)\|^2_{H^3(\Delta)}\big)\Big)^{1/2} \\ &+\Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \big(\|\frac{\partial w}{\partial t}(t_{n+1})\|^2_{H^2(\Delta)} + \|\frac{\partial w}{\partial t}(t_n)\|^2_{H^2(\Delta)}\big)\Big)^{1/2}\Big) \\ \le C \quad &\Big(\Delta t^4 \|u\|_{C^4(C)} + \Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \|u\|^2_{C(H^3)}\Big)^{1/2} \\ &+\Big(\sum_{\Delta \in \mathcal{T}_H} (diam\Delta)^4 \|u\|^2_{C^2(H^2)}\Big)^{1/2}\Big). \end{aligned} \tag{48}$$

Taking $v_H = e_w^{n+1} + e_w^n$ we obtain

$$\|e_w^{n+1}\|_H^2 = \|e_w^n\|_H^2 - \Delta t((D_H \nabla_H \Big(\frac{e_u^{n+1} + e_u^n}{2}\Big), \nabla_H (e_w^{n+1} + e_w^n)))_H + \Delta t(T_1^n(u), e_w^{n+1} + e_w^n)_H. \tag{49}$$

From (46) we can deduce the following

$$\begin{aligned} ((D_H \nabla_H \Big(\frac{e_w^{n+1} + e_w^n}{2}\Big), \nabla_H \Big(e_u^{n+1} + e_u^n\Big)))_H \quad &= ((a_H D_H D_{-t} \nabla_H e_u^{n+1}, \nabla_H \Big(e_u^{n+1} + e_u^n\Big)))_H \\ &+((b_H D_H \nabla_H \Big(\frac{e_u^{n+1} + e_u^n}{2}\Big), \nabla_H (e_u^{n+1} + e_u^n)))_H \\ &+((T_{2,H}^n(u), \nabla_H \Big(e_u^{n+1} + e_u^n\Big)))_H, \end{aligned} \tag{50}$$

where

$$\begin{aligned}\|T^n_{2,H}(u)\|_H &\leq C\Delta t^{3/2}\Big(\Big(\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}\int_{t_n}^{t_{n+1}}\int_{x_{i-1}}^{x_i}\big(\frac{\partial^4 u}{\partial t^3\partial x}(x,y_j,t)\big)^2 dxdt\Big)^{1/2}\\ &\qquad +\Big(\sum_{i=1}^{N-1}\sum_{j=1}^{M} h_{i+1/2}\int_{t_n}^{t_{n+1}}\int_{y_{j-1}}^{y_j}\big(\frac{\partial^4 u}{\partial t^3\partial y}(x_i,y,t)\big)^2 dydt\Big)^{1/2}\Big) \qquad (51)\\ &\leq C\Delta t^2\|u\|_{C^3(C^1)}.\end{aligned}$$

Inserting (50) in (49) we get

$$\begin{aligned}\|e_w^{n+1}\|_H^2 + \|\sqrt{a_H D_H}\nabla_H e_u^{n+1}\|_H^2 &= \|e_w^n\|_H^2 + \|\sqrt{a_H D_H}\nabla_H e_u^n\|_H^2\\ &+\Delta t(T^n_{1,H}(u), e_w^{n+1}+e_w^n)_H \qquad (52)\\ &-\Delta t((T^n_{2,H}(u), \nabla_H(e_u^{n+1}+e_u^n)))_H.\end{aligned}$$

Equality (52) leads to

$$\begin{aligned}\|e_w^{n+1}\|_H^2 + \|\sqrt{a_H D_H}\nabla_H e_u^{n+1}\|_H^2 &\leq \frac{1+2\epsilon^2\Delta t}{1-2\epsilon^2\Delta t}\Big(\|e_w^n\|_H^2 + \|\sqrt{a_H D_H}\nabla_H e_u^n\|_H^2\Big)\\ &+\frac{\Delta t}{2\epsilon^2(1-2\epsilon^2\Delta t)}\Big(\|T^n_{1,H}(u)\|_H^2 + \|\frac{\sqrt{D_H^{-1}}}{a_H}T^n_{2,H}(u)\|_H^2\Big).\end{aligned} \qquad (53)$$

where $\epsilon \neq 0$, and provided that $1-2\epsilon^2\Delta t > 0$.
As $e_w^0 = e_u^0 = 0$, from (53) we finally obtain

$$\|e_w^{n+1}\|_H^2 + \|\sqrt{a_H D_H}\nabla_H e_u^{n+1}\|_H^2 \leq Ce^{\frac{4\epsilon^2 n\Delta t}{1-2\epsilon^2\Delta t}} \max_{j=0,\ldots,n}\Big(\|T^j_{1,H}(u)\|_H^2 + \|T^j_{2,H}(u)\|_H^2\Big). \qquad (54)$$

where $C > 0$ denotes a constant independent of Δt and H.
Finally, using the Poincaré-Friedrichs's inequality we conclude that

$$\|e_w^{n+1}\|_H^2 + \|\nabla_H e_u^{n+1}\|_H^2 + \|e_u^{n+1}\|_H^2 \leq C\Big(\Delta t^4 + H_{max}^4\Big), \qquad (55)$$

provided that

$$u \in C^4(0,T,C(\overline{\Omega}) \cap C^3(0,T,C^1(\overline{\Omega}) \cap C^2(0,T,H^2(\Omega)) \cap C(0,T,H^3(\Omega)\cap H^1_0(\Omega)).$$

6 Numerical results

In the following we present some numerical tests that illustrate the theoretical results obtained in previous sections. In accordance with the discussion in Sections 4 and 5 we consider two problems of type (1)-(3), one with a smooth solution (Example 1) and the other with a non-smooth solution (Example 2). In both cases we take $T = 0.05$ and use the uniform time step $\Delta t = 10^{-5}$. Moreover, the coefficient functions of the wave equation (1) are given by: $a(x,y) = x^2$, $b(x,y) = 1+x+y$, $d_1(x,y) = 2+y^2$, and $d_2(x,y) = 1+x$. These functions satisfy the restrictions formerly imposed.

Example 1 To illustrate the smooth case convergence rate we define the initial conditions (2) and the function f in (1), such that, the exact solution of problem (1)-(3) is given by

$$u(x, y, t) = e^t(1 - x)(1 - \cos(4\pi y))\sin(xy).$$

Note that u fulfills the assumptions of Theorem 1, namely, $u \in C^1(0, T, C^4(\overline{\Omega})) \cap C^2(0, T, C(\overline{\Omega}))$. It can also be verified that $f \in C^1(0, T, C^2(\overline{\Omega}))$.

Example 2 For the non-smooth case we consider the exact solution of problem (1)-(3) given by

$$u(x, y, t) = e^t \sin(xy)(2x - 2)(y - 1)|2y - 1|^{1+\alpha}, \quad \alpha \in \mathbb{R}.$$

The initial conditions and the function f are defined in accordance with (2) and (1), respectively. In this example, u is under the conditions of Theorem 2, when $\alpha > 2$. On the other hand, e.g., for $\alpha = 1.1$, we have that $u(t) \in H^2(\Omega)$ and those conditions are not meet.

The two previous examples are successively solved on grids H_k $(k = 1, \ldots, 6)$ of increasing size. We start with an initial random mesh H_1 and the grid H_{k+1} is obtained from the grid H_k by inserting new grid points at the midpoints of the grid H_k. To calculate the numerical rate of convergence we define the error

$$E_H = \max_{n=1,\ldots,M_t} \|D_{-t}e_H^n\|_H^2 + \|\nabla_H e_H^n\|_H^2$$

and use the relation

$$\text{rate} = \frac{\log E_{H_k} - \log E_{H_{k+1}}}{\log 2},$$

where E_{H_k} denotes the error E_H on the grid H_k.

The results obtained for Example 1 are shown in Table 1 and they confirm the theoretical $O(H_{max}^2)$ convergence rate of Theorem 1. The data in Table 1 for Example 2 with $\alpha = 2.1$ also verifies the second order convergence rate of the non-smooth case, as proven in Theorem 2. Again in Table 1, we display the results obtained for Example 2, but now using $\alpha = 1.1$, that is, when the solution $u(t)$ belongs to $H^2(\Omega)$. The numerical rate of convergence of order $O(H_{max})$

Example 1			Example 2 ($\alpha = 2.1$)			Example 2 ($\alpha = 1.1$)		
H_{max}	E_H	rate	H_{max}	E_H	rate	H_{max}	E_H	rate
1.301e-1	4.578e-1	-	1.577e-1	3.272e-2	-	1.713e-1	4.228e-2	-
6.505e-2	1.182e-1	1.953	7.885e-2	8.697e-3	1.912	8.566e-2	2.005e-2	1.076
3.252e-2	2.973e-2	1.991	3.943e-2	2.200e-3	1.983	4.283e-2	9.440e-3	1.087
1.626e-2	7.441e-3	1.998	1.971e-2	5.513e-4	1.997	2.141e-2	4.466e-3	1.080
8.131e-3	1.860e-3	2.000	9.857e-3	1.378e-4	2.001	1.071e-2	1.978e-3	1.175
4.065e-3	4.649e-4	2.001	4.928e-3	3.443e-5	2.000	5.354e-3	9.152e-4	1.112

Table 1: Results of the numerical convergence tests.

suggests that at least the restriction $u(t) \in H^3(\Omega)$ of Theorem 2 is optimal, in the sense that cannot be weakness without losing the second order rate. We remark that, using the results established in [16] and following the steps of Theorem 2, it can be proved that the rate of convergence is in fact $O(H_{max})$ when $u(t) \in H^2(\Omega)$. For illustration, we present in Figure 1 the numerical solution and square of the error e_H^n for each of the examples considered.

In the next experiment we examine the rate of convergence in time. For that we solve Example 3 for successively smaller time steps Δt and using a fixed spatial grid with $H_{max} =$ 3.913e-3.

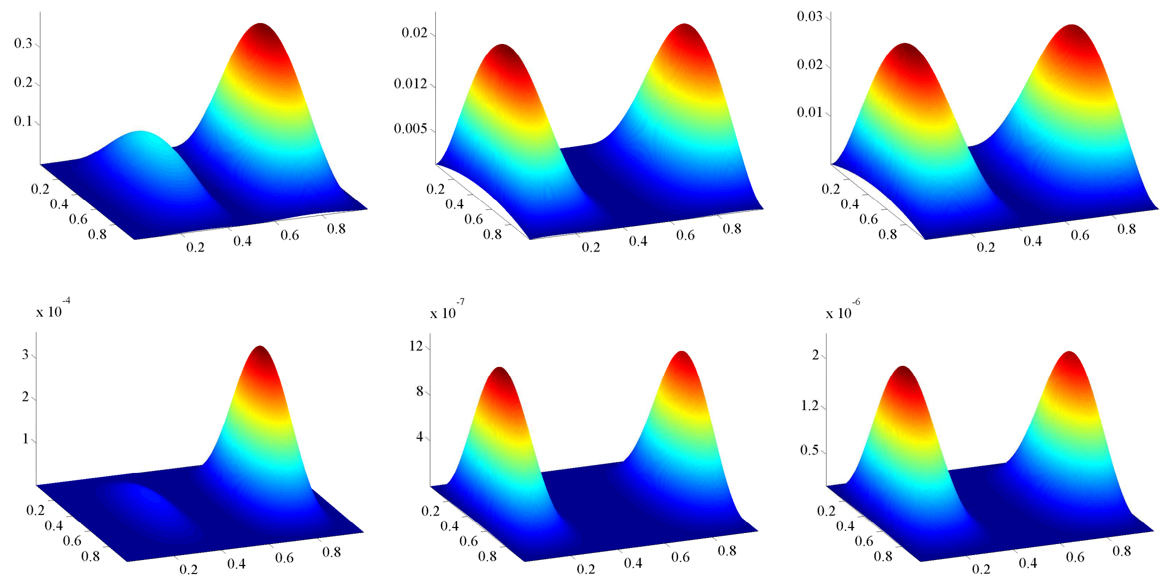

Figure 1: From left to right: numerical solution u_H^n (first row) and square of the error e_H^n (second row) on the grid H_6 at $T = 0.05$; for Example 1 and Example 2 with $\alpha = 2.1$ and $\alpha = 1.1$.

In this example we use a larger value of T, namely, $T = 3$. The results of our simulation are presented in Table 2 and they confirm the theoretical $O(\Delta t)$ convergence rate of Theorem 3 as well as the $O(\Delta t^2)$ convergence rate of the second order in time scheme (42)–(44). Some representative figures are shown in Figure 2. Note that in accordance with estimate (55) we define the following error expression for the second order scheme

$$E_{H,2} = \max_{n=1,\dots,M_t} \|e_w^n\|_H^2 + \|\nabla_H e_u^n\|_H^2 + \|e_u^n\|_H^2.$$

Example 3 Let us consider problem (1)-(3) with coefficient functions $a(x, y) = 5(1 + x)$, $b(x, y) = xy$, $d_1(x, y) = 1 + x$, and $d_2(x, y) = y$, exact solution given by

$$u(x, y, t) = e^t (x - 1) \sin(\pi x)(y - 1) \sin(\pi y),$$

and properly defined initial conditions and function f.

Example 3 (2nd order scheme)			Example 3 (1st order scheme)		
Δt	$E_{H,2}$	rate	Δt	E_H	rate
5.000e-1	3.950e-1	-	5.000e-1	24.89e-1	-
2.500e-1	9.949e-2	1.989	2.500e-1	13.78e-1	0.853
1.250e-1	2.486e-2	2.001	1.250e-1	7.285e-1	0.920
6.250e-2	6.151e-3	2.015	6.250e-2	3.754e-1	0.956
3.125e-2	1.478e-3	2.057	3.125e-2	1.907e-1	0.977

Table 2: Numerical convergence rate in time.

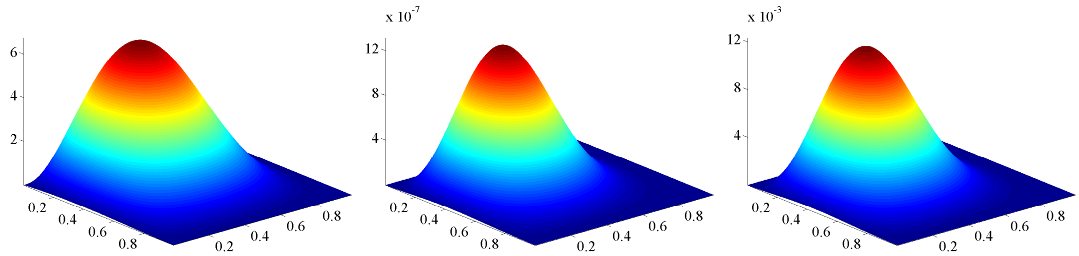

Figure 2: From left to right: numerical solution u_H^n obtained with the second order in time scheme and square of the error e_u^n for the second order in time scheme and the first order in time scheme; results for Example 3 using $\Delta t = 0.0625$.

7 Conclusions

In this work a numerical scheme for the discretization of a wave type equation was proposed and studied. The main goal was to establish conditions that allow to obtain second order approximations, in space and time, for the kinetic and potential energies with respect to a discrete L^2-norm.

The main results of this paper are Theorem 1 and Theorem 2. In these theorems convergence properties of the semi-discrete solution defined by the fully discrete in space piecewise linear finite element method (8), (9), and (12), which is equivalent to the finite difference method (11), (9), and (12), were analyzed. Two cases corresponding to smooth and non-smooth assumptions for the solution of the correspondent continuous IBVP were considered. For each case, two complete different techniques of analysis were followed to derive second order approximations for the kinetic and potential energies. Theorem 1 establishes the second order convergence for the smooth case, while Theorem 2 deals with the non-smooth case. The discrete in time version of Theorem 2 was studied in Section 5.

Numerical experiments illustrating the obtained theoretical results were also included. In particular, Example 2 with $\alpha = 1.1$, illustrates that the convergence rate established in Theorem 2 is optimal in the sense that if $u(t) \in H^2(\Omega)$ then the rate of convergence is only $O(H_{max})$. The proof of this fact can be done following the proof of Theorem 2 and the results presented in [16].

The main motivation for this work is the coupling between the electric potential, or electric field, and diffusion of a drug in a target tissue. In fact, in iontophoresis or electroporation applications, electric fields are used to enhance drug diffusion and absorption by the target tissue. The wave equations governing the electric potential and the electric field, equations (4) and (5), respectively, are particular cases of the general equation (1). In future work we intent to address this more complex problem which is obtained coupling a equation of type (1) with a properly defined parabolic equation for the drug concentration.

8 Acknowledgments

This work was partially supported by the Centre for Mathematics of the University of Coimbra – UID/MAT/00324/2013, funded by the Portuguese Government through FCT/MCTES and co-funded by the European Regional Development Fund through the Partnership Agreement PT2020. D. Jordão was supported by FCT PhD scholarships PD/BI/128068/2016 and L. Pinto was also supported by FCT scholarship SFRH/BPD/112687/2015.

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