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

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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.

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

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

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 $\frac{\rho}{\epsilon}$ (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 $L^2(\Omega)$, $H_0^1(\Omega)$ 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 $u(t)\in H_0^1(\Omega)$ such that

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