

## ENERGY STABLE TIME DOMAIN FINITE ELEMENT METHODS FOR NONLINEAR MODELS IN OPTICS AND PHOTONICS

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**Abstract.** Novel time domain finite element methods are proposed to numerically solve the system of Maxwell's equations with a cubic nonlinearity in the spatial 3D case. The effects of linear and nonlinear electric polarization are precisely modeled in this approach. In order to achieve an energy stable discretization at the semi-discrete and the fully discrete levels, a novel technique is developed to handle the discrete nonlinearity, with spatial discretization either using edge and face elements (Nédélec-Raviart-Thomas) or discontinuous spaces and edge elements (Lee-Madsen). In particular, the proposed time discretization scheme is unconditionally stable with respect to the electromagnetic energy and is free of any Courant-Friedrichs-Lewy-type condition. Optimal error estimates are presented at semi-discrete and fully discrete levels for the nonlinear problem. The methods are robust and allow for discretization of complicated geometries and nonlinearities of spatially 3D problems that can be directly derived from the full system of nonlinear Maxwell's equations.

**Key words.** Finite element analysis, nonlinear Maxwell's equations, energy stability, convergence analysis, error estimate, time domain analysis.

### 1. Introduction

In nonlinear Optics and Photonics, the presence, behaviour and application of light or photons in nonlinear media, in which the polarization density  $\mathbf{P}$  depends nonlinearly on the electric field  $\mathbf{E}$ , are investigated. Nonlinear effects are observed and used in many real-world applications, e.g., in lasers because of their high light intensities. Nonlinear optical phenomena, in which the optical fields are not considered to be too large, e.g., parametric and instantaneous nonlinear optical phenomena (i.e., lossless and dispersion-free materials) are often described mathematically by means of a power series expansion of the dielectric polarization density  $\mathbf{P}$  with respect to the electric field  $\mathbf{E}$ . Frequently, the behaviour of light waves in a material is modeled by means of a third-order polarization response, that is the polarization  $\mathbf{P} = \mathbf{P}(\mathbf{E})$  is a cubic polynomial in the electric field intensity  $\mathbf{E}$ . The fundamental concepts of nonlinear Optics can be found in details in [11, 8, 38, 2]. Due to the wide range of the nonlinear Optics applications, numerous numerical techniques for approximating the solutions of the mathematical models are employed, for instance slowly-varying envelope approximations (SVEA), beam propagation (BP), finite difference time domain (FDTD), time domain finite element (TDFE), time domain discontinuous Galerkin (TDDG) methods, – among them pseudo-spectral–, finite volume (FV) methods, and many more. The development of efficient and accurate productive numerical techniques plays an essential role for many real-world applications.

The method of SVEA is normally used for the approximate solution of nonlinear problems that are close to linear ones, and oscillations that are close to harmonic

ones [11]. Since it is based on the assumption that the amplitude of the wave changes slowly in time and space compared to the wave period, it is thus quite restrictive for many applications. The BP method with second-order indices of refraction was employed for modeling of nonlinear optical devices exhibiting on-axis behaviour [17]. Classical FDTD methods are considered as robust numerical schemes for linear and nonlinear models in Optics and Photonics [48, 26, 50, 27, 46, 16, 21, 13, 34, 24]. However, they exhibit considerable limitations in their application, for example with regard to their applicability to complex geometries, less smooth data (e.g., due to material interfaces), etc. In particular, the spatial domain is discretized by regular, structured (quadrilateral or hexahedral) and staggered grids. The difference scheme presented in [48] served as the basis for one of the most frequently used methods for solving the linear Maxwell's equations. This scheme is of second order in time and shows a significant numerical spread over long time intervals of the simulation of wave propagation [13]. FDTD simulations for the full system of nonlinear Maxwell's equations have been presented in [27, 50]. Among other things, interacting waves of different frequencies could be treated directly [27]. The auxiliary differential equation (ADE) method along with finite difference time domain (FDTD) schemes has been originally employed for linear dispersive materials [26], and for the coupling between the polarization vector and the electric field intensity [20, 50]. This scheme was applied to second- and third-order nonlinear phenomena including spatial soliton propagation [20, 25], linear and nonlinear interface scattering [49], and pulse propagation through nonlinear wave guides [51]. In the paper [9], a higher-order discontinuous Galerkin method for spatial 1D discretization in conjunction with the ADE approach for the treatment of nonlinearity was investigated, where the energy stability of the proposed methods could be proven. In the latter respect, this work is very closely related to our results.

A lot of interesting modeling and simulation results for linear and nonlinear Lorentz dispersion with nonlinear Kerr response in case of 1D, 2D and 3D can be found in [19, 23, 10, 43, 25, 41, 36]. Among nonstandard difference methods, pseudospectral spatial domain schemes have been employed for optical carrier shock [28] and linear Lorentz dispersion with nonlinear response [47] simulation.

In this paper, based on the semi-discrete mixed finite element method [3], [4] and the fully discrete finite element method [5], [6], we provide the detailed proofs of our results to the fully time-dependent Maxwell's equations with cubic nonlinearities as a supplement to [7].

Let  $\Omega$  be a simply connected domain in  $\mathbb{R}^3$  with Lipschitz boundary  $\Gamma$  and unit outward normal  $\mathbf{n}$  on  $\Gamma$ . Let  $\mathbf{D} = \mathbf{D}(\mathbf{x}, t)$ ,  $\mathbf{B} = \mathbf{B}(\mathbf{x}, t)$ ,  $\mathbf{E} = \mathbf{E}(\mathbf{x}, t)$  and  $\mathbf{H} = \mathbf{H}(\mathbf{x}, t)$  represent the electric displacement field, magnetic induction, electric and magnetic field intensities, respectively, where  $\mathbf{x} \in \Omega$  and the time variable  $t$  ranges in some interval  $(0, T)$ ,  $T > 0$ . Given an electric current density  $\mathbf{J} = \mathbf{J}(\mathbf{x}, t)$ , Maxwell's curl-equations in SI units read as

$$(1) \quad \begin{aligned} \partial_t \mathbf{D} - \nabla \times \mathbf{H} &= \mathbf{J} & \text{in } \Omega \times (0, T), \\ \partial_t \mathbf{B} + \nabla \times \mathbf{E} &= 0 & \text{in } \Omega \times (0, T). \end{aligned}$$

The electric displacement  $\mathbf{D}$  and magnetic induction  $\mathbf{B}$  are related to the electric and magnetic fields, respectively, through the following constitutive laws:

$$(2) \quad \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}(\mathbf{E}), \quad \mathbf{B} = \mu_0 \mathbf{H}.$$

The vacuum permittivity and permeability are denoted by the constants  $\varepsilon_0 > 0$  and  $\mu_0 > 0$ , respectively. Often the polarization  $\mathbf{P} = \mathbf{P}(\mathbf{E})$  is approximated by a