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Energy stable discontinuous Galerkin methods for Maxwell's equations in nonlinear optical media

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ABSTRACT

The propagation of electromagnetic waves in general media is modeled by the time-dependent Maxwell's partial differential equations (PDEs), coupled with constitutive laws that describe the response of the media. In this work, we focus on nonlinear optical media whose response is modeled by a system of first order nonlinear ordinary differential equations (ODEs), which include a single resonance linear Lorentz dispersion, and the nonlinearity comes from the instantaneous electronic Kerr response and the residual Raman molecular vibrational response. To design efficient, accurate, and stable computational methods, we apply high order discontinuous Galerkin discretizations in space to the hybrid PDE-ODE Maxwell system with several choices of numerical fluxes, and the resulting semi-discrete methods are shown to be energy stable. Under some restrictions on the strength of the nonlinearity, error estimates are also established. When we turn to fully discrete methods, the challenge to achieve provable stability lies in the temporal discretizations of the nonlinear terms. To overcome this, novel strategies are proposed to treat the nonlinearity in our model within the framework of the second-order leap-frog and implicit trapezoidal time integrators. The performance of the overall algorithms are demonstrated through numerical simulations of kink and antikink waves, and third-harmonic generation in soliton propagation.

1. Introduction

Nonlinear optics is the study of the behavior of light in nonlinear media. This field has developed into a significant branch of physics since the introduction of intense lasers with high peak powers. In nonlinear media, the material response depends nonlinearly on the optical field, and many interesting physical phenomena, such as frequency mixing and second/third-harmonic generation have been observed and harnessed for practical applications. We refer to classical textbooks [4,6,38] for a more detailed review of the field of nonlinear optics.

Our interest here is in the development of novel numerical schemes for the Maxwell's equations in nonlinear optical media. Relative to the widely used asymptotic and paraxial wave models derived from Maxwell's equations, such as nonlinear Schrödinger equation (NLS) and beam propagation method (BPM) [4,6], simulations of the nonlinear Maxwell's system in

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the time domain are more computationally intensive. However, these simulations have the advantage of being substantially more robust because they directly solve for fundamental quantities, the electromagnetic fields in space and time. These simulations also avoid the simplifying assumptions that lead to conventional asymptotic and paraxial propagation analyses, and are able to treat interacting waves at different frequencies directly [29]. Recent optics and photonics research has focused on phenomena at smaller and smaller length scales or multiple spatial scales. For such phenomena simulating the full Maxwell PDE models is important in adequately capturing useful optical effects [21,29,42].

When Maxwell's equations are considered to model the electromagnetic (EM) waves propagating through a nonlinear optical medium, the medium response is described by constitutive laws that relate the electric field **E** and the electric flux density **D** through the polarization **P** of the medium. In this work, we focus on a macroscopic phenomenological description of the polarization, which comprises both linear and nonlinear responses. Specifically, the linear response is modeled by a single resonance Lorentz dispersion, while the nonlinear response is cubic and incorporates the instantaneous *Kerr* effect and the delayed nonlinear Lorentz dispersion called *Raman scattering*. Within this description, we will follow the *auxiliary differential equation* (ADE) approach, where the linear and nonlinear Lorentz dispersion is represented through a set of ODEs, describing the time evolution of **P** (hence of **D**) forced by **E**, appended to Maxwell's equations. An alternative representation is via a *recursive convolution method*, where **D** is computed from **E** through a time convolution integral [41].

In the literature, finite difference time domain (FDTD) based, finite element (FEM) based, pseudospectral based methods, finite volume (FV) based, among others, are available for the integration of the full Maxwell's equations in nonlinear media, along with appended ODEs for the material response. The Yee scheme [44] is an FDTD method for Maxwell's equations that has long been one of the gold standards for numerical simulation of Maxwell's equations in the time domain, especially for linear problems [41]. Maxwell's equations in a linear Lorentz medium with a nonlinear Kerr response are investigated in [26,40], while in [20], additional effects due to Raman scattering are studied through a 1D FDTD analysis. More references for linear and nonlinear Lorentz dispersion, can be found in [5,23,39] for the 1D case, and in [18,30,45] for 2D and 3D cases. Yee based FDTD approaches result in second order schemes which accumulate significant errors over long time modeling of wave propagation [13,14]. While higher order FDTD methods can alleviate this issue, they can be cumbersome in modeling complex geometries. On the other hand, though the FEMs are well suited for modeling complex geometries, they have not been well developed for nonlinear Maxwell models. FEM analysis for some nonlinear models can be found in [17]. In [43] a pseudospectral spatial domain (PSSD) approach is presented for linear Lorentz dispersion and nonlinear Kerr response, and in [31] optical carrier wave shock is studied using the PSSD technique. FV based methods for nonlinear Kerr media are addressed in [2,15] in which the Maxwell–Kerr model is approached as a hyperbolic system and approximated by a Godunov scheme, and a third order Roe solver, respectively, in one and two spatial dimensions.

In this work, we use high order discontinuous Galerkin (DG) methods for the spatial discretization of our nonlinear Maxwell models. This is motivated by various properties of DG methods, including high order accuracy, excellent dispersive and dissipative properties in standard wave simulations, flexibility in adaptive implementation and high parallelization, and suitability for complicated geometry (e.g., [11,25]). DG methods differ from classical finite element methods in their use of piecewise smooth approximate functions, while inter-element communication is achieved through the use of numerical fluxes, which are consistent with the physical fluxes and play a vital role in accuracy, stability, energy conservation, and computational efficiency. For the nonlinear Maxwell models that we consider, with the numerical fluxes chosen to be either central or alternating, the solutions to the semi-discrete DG methods satisfy an energy equation just as the exact solutions do, hence the methods are energy stable, even in the presence of both the Kerr and Raman nonlinear effects. Another dissipative flux, inspired by the upwind flux for Maxwell's equations in a linear nondispersive dielectric [24], called "upwind flux" in this paper, is also considered with the respective energy stability established. For the semi-discrete methods with all three types of numerical fluxes, error estimates are carried out under some additional assumptions on the strength of the nonlinearity in the underlying model.

In addition to the error estimates, the nonlinearity in the model poses challenges to the design of fully discrete schemes with provable energy stability. As one major contribution, we propose in this work a novel strategy to discretize the nonlinear terms within the commonly used second-order leap-frog and implicit trapezoidal temporal discretizations. The resulting fully discrete methods are proved to be stable. More specifically, the method with the modified leap-frog time discretization is conditionally stable under a CFL condition, which is the *same* as the one for Maxwell's equations without Kerr, linear and nonlinear Lorentz dispersion; while the fully implicit method with the modified trapezoidal temporal discretization is unconditionally stable. In both cases, we find it important, at least from the theoretical point of view, to discretize the ODE part of the system *implicitly*. To our best knowledge, the temporal discretizations that are adapted to nonlinear models and with *provable stability* are not yet available. In the present work, the methods and numerical verification are presented for the model in one dimension, and their extension to higher dimension will be explored in a separate paper.

DG methods have grown to be broadly adopted for EM simulations in the past two decades. They have been developed and analyzed for time dependent linear models, including Maxwell's equations in free space (e.g., [9,12,24]), dispersive media (e.g., [19,28,33,37]), as well as metamaterials (e.g., [8,34–36]). However, there exists only limited study for DG methods for nonlinear Maxwell models. For example, in [3,16], Kerr nonlinearity is investigated, where the entire Maxwell PDE-ODE system is cast as a nonlinear hyperbolic conservation law, for which DG methods have long been known for their success. A relaxed version of the Kerr model, called the Kerr–Debye model, was examined in [27], where a second-order asymptotic-preserving and positivity-preserving DG scheme is designed and analyzed.