Higher Order Variational Time Discretizations for Nonlinear Dispersive Wave Equations

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Abstract

We investigate the numerical simulation of complex nonlinear optical processes in dispersive media. A mathematical model and numerical discretization techniques are developed. In particular we study higher order variational time discretizations and the implementation of a perfectly matched layer within this framework. We use a scheme which combines finite element techniques with the concepts of collocation methods yielding discrete continuously differentiable in time solutions. We verify our techniques with convergence tests. As a practical example we investigate the generation of THz frequency radiation in periodically poled crystals.

Keywords: nonlinear optics, absorbing boundary conditions, variational time discretization

1 Introduction

Nonlinear optical phenomena form the basis of a wide range of applications such as novel optical sources and measurements or diagnostic techniques. With growing technical complexity, the reliability of models and algorithms, optimal numerical performance and minization of costs and time in computer simulations remain key demands for investigations of nonlinear optical phenomena. We develop efficient and accurate methods for modelling complex phenomena in nonlinear optics. For the discretization we use variational space time methods. Within this framework we focus on higher order variational time discretizations. For these higher order time discretizations we implement absorbing boundary conditions based on perfectly matched layers.

2 Physical Model

Our model is motivated by the generation of THz radiation in periodically poled nonlinear crystals. THz radiation has a wide range of applications, e. g. medical imaging, biochemistry or free electron lasers. We address the arising physical problem with a dispersive and nonlinear model for the propagation of electromagnetic waves in the time domain. We transform the equations and quantites by applying a time transformation $\tilde{t} = c_0 t$ and omit the $\tilde{\cdot}$ from now on. We use a Lorentz model for the dispersion and include a second order instantaneous nonlinearity. In the Lorentz model the electric permittivity and refractive index can be modeled by the equation

$$n(\nu)^2 = n_\omega^2 + \frac{(n_\Omega^2 - n_\omega^2)\nu_t^2}{\nu_t^2 - \nu^2 + \mathrm{i}\Gamma_0 \nu}\,, \tag{1}$$

where Γ_0 is the damping coefficient and ν_t the phonon frequency. From this we derive the auxiliary differential equation (ADE) for Lorentz materials in the time domain (2a). We couple (2a) with the electromagnetic wave equation which leads to

$$\begin{aligned} &\partial_{tt} P + \Gamma_0 \partial_t P + \nu_t^2 P \\ &\qquad - (n_\Omega^2 - n_\omega^2)\nu_t^2 E = 0\,, \quad \text{(2a)} \\ &- \Delta E + n_\omega^2 \partial_{tt} E + (n_\Omega^2 - n_\omega^2)\nu_t^2 E - \nu_t^2 P \\ &\qquad - \Gamma_0 \partial_t P + \chi^{(2)} \partial_{tt}(|E|\,E) = 0. \quad \text{(2b)} \end{aligned}$$

In numerical simulations, wave propagation has to be truncated to bounded regions. To this end we apply the complex frequency shifted PML which allows us to derive ADEs similar to the Lorentz dispersion. This leads to a high level of flexibility regarding the applications of discretization techniques. We approximate (2) by a finite element method in space and time, along the lines of [3]. We employ a higher order time discretization by extending [1] to (2). The method in [1] has shown to be superior over standard continuous and discontinuous methods. It establishes a direct connection between the Galerkin method for the time discretization and the classical collocation methods, thereby achieving the

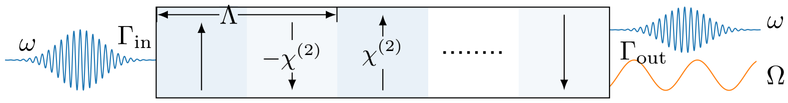

Figure 1: Example of a peridically poled crystal with period Λ. The pump pulse $g(t)$ at frequencies $\omega_{1,2}$ enters the crystal on Γ_{in}. In the subsequent layers THz radiation is generated.

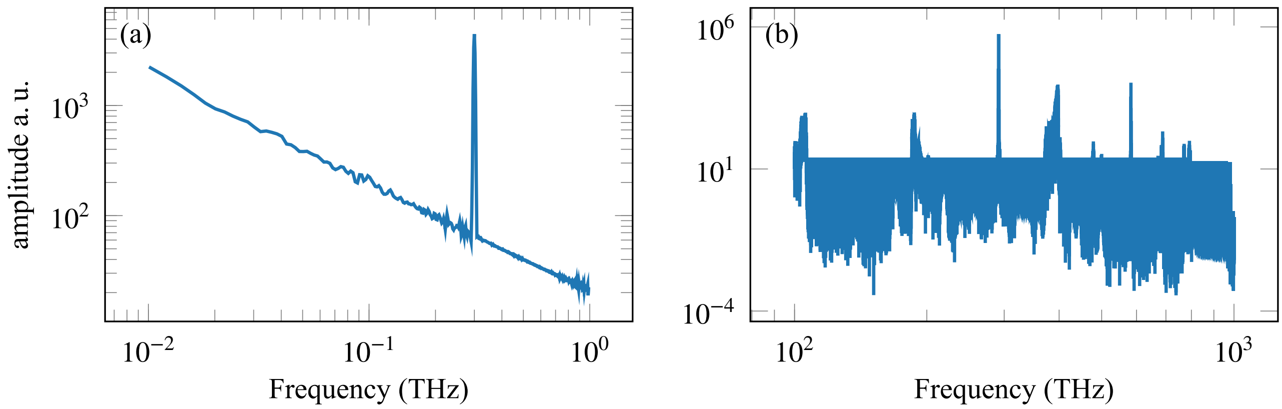

Figure 2: Frequency spectrum of the pulse $g(t)$ after it has passed 25 periods of the crystal (a) in the 0.1 THz to 1 THz region and (b) in the optical region from 100 THz to 1000 THz.

accuracy of the former with the reduced computational costs of the latter. The time discrete solutions are continuously differentiable by construction. The linearization is done by a damped version of Newton's method, and the arising linear systems are solved by a preconditioned GMRES method.

3 Numerical investigations

We simulate THz generation in a periodically poled crystal by two Gaussian shaped pump pulses $g(t) = \exp\left(-2\log 2\left(\frac{t}{\tau}\right)^2\right)(\cos(2\pi\omega_1 t)+\cos(2\pi\omega_2 t))$ separated in center frequency by the THz frequency. We use a full width half maximum $\tau = 200\,\text{ns}$ and frequencies $\omega_1 = 291.56\,\text{THz}$, $\omega_2 = 291.26\,\text{THz}$. The pulse is applied at the left-hand side of the crystal by a Dirichlet boundary condition and then propagates through the domain until the PML is hit on the right-hand side. The problem setting is sketched in Fig. 1. For the implementation we use the finite element toolbox deal.II [2] along with the Trilinos library. The simulated results are presented in Fig. 2. We see, besides the THz radiation generated by difference frequency mixing in Fig 2(a), the harmonics in the optical domain in Fig. 2(b) simultaneously generated by second harmonic and sum-frequency generation.

4 Conclusion

We presented a mathematical model and finite element time domain framework for accurate and efficient simulation of phenomena in nonlinear optics. The approach employed has the advantage of a high flexibility with respect to physical models, simulation domains and order of approximation and accuracy. Although our implementation is highly efficient and the results are promising, a further reduction of computational costs is still needed.

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