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Fully explicit nonlinear optics model in a particle-in-cell framework

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ABSTRACT

A numerical technique which incorporates the nonlinear optics of anisotropic crystals into a particle-in-cell framework is described. The model is useful for simulating interactions between crystals, ultra-short laser pulses, intense relativistic electron bunches, plasmas, or any combination thereof. The frequency content of the incident and scattered radiation is limited only by the resolution of the spatial and temporal grid. A numerical stability analysis indicates that the Courant condition is more stringent than in the vacuum case. Numerical experiments are carried out illustrating the electro-optic effect, soliton propagation, and the generation of fields in a crystal by a relativistic electron bunch.

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1. Introduction

Nonlinear optics is often described in the frequency domain so that dispersive effects can be treated in a simple way. The convolution integrals associated with nonlinear effects are simplified by assuming that the radiation spectrum takes the form of a discrete set of narrow peaks. In the case of few cycle pulses, the convolution integrals cannot be reduced, and a time domain model becomes attractive. The finite-difference-time-domain (FDTD) technique is a well established method for solving the exact Maxwell equations in a bounded or periodic domain [1]. It may be used in connection with the particle-in-cell (PIC) technique to self-consistently solve for the motions of a large number of charged particles in an electromagnetic field [2]. This approach is often used to model fully nonlinear laser-plasma interactions and beam-plasma interactions. In this work, it is extended to account for nonlinear laser-crystal and beam-crystal interactions. This is accomplished by incorporating a model for bound particles into the PIC code turboWAVE [3]. The model is fully parallelized, and runs in up to three dimensions.

The PIC aspect of turboWAVE has much in common with a number of other codes designed to model laser-plasma interactions [4–10]. The nonlinear optics aspect is related to a number of other codes designed to model ultrashort pulse propagation in a nonlinear medium [11–16]. Both types of codes can be divided into those that describe the radiation by means of a complex envelope, and those that are fully explicit, i.e., those that resolve the optical time scale. TurboWAVE supports both models, but in this work only the fully explicit model is used. As a result, there is no assumption about the frequency content of the radiation, and given the right model for the dielectric response, all nonlinear and dispersive effects are accounted for.

Our model for the dielectric response generalizes the auxiliary equation technique described in Refs. [13,15]. In particular, bound charges in the dielectric are represented by effective particles, whose contribution to the four-current is computed using PIC techniques. The effective particles are subjected to forces arising from a superposition of macroscopic and microscopic fields. The macroscopic field is the usual electromagnetic field that is computed in any FDTD code, while the

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microscopic field is a three dimensional electrostatic potential representing, e.g., an atomic binding potential. The resulting equation of motion is expanded as an anharmonic oscillator equation. By using multiple species of effective particles, each satisfying a different oscillator equation, the material response can be tailored to match that of real materials over a broad range of frequencies. Free charges are self-consistently incorporated into the model by linear superposition of the free and bound sources in the FDTD field solver.[1] The resulting model is capable of modeling interactions among laser pulses, particle beams, plasmas, and dielectric crystals, in a fully dispersive, nonlinear, anisotropic, and kinetic way. To our knowledge, no other model has been implemented which simultaneously accounts for all these effects. One can argue that the auxiliary equation technique could be similarly extended, since, after all, one can recover any physics with the right "auxiliary equations." The effective particle model described here has the advantage that all of the required physics falls out of a single unifying physical principle.

In Ref. [17], the turboWAVE extensions described in this paper were introduced for the first time. In Ref. [18], the model was applied to a novel electro-optic diagnostic technique. In the present paper, the model is described in more detail, and a formal analysis of numerical stability is given. The model is extended to include third order nonlinearities, and the implementation is demonstrated via three numerical experiments.

2. Description of the model

The numerical model described here solves the exact Maxwell equations:

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \tag{1a}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1b}$$

$$\nabla \cdot \mathbf{D} = \rho \tag{1c}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{1d}$$

Here, $\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{M}$ and $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$, where $\mathbf{P}$ is the polarization and $\mathbf{M}$ is the magnetization. In the present work, we take $\mathbf{M} = 0$. The polarization can be expressed in terms of a spatially smoothed four-current due to bound charges, denoted by $(\langle \eta \rangle, \langle \mathbf{j} \rangle)$. This results in [19]

$$\nabla \times \mathbf{B} = \mu_0 (\mathbf{J} + \langle \mathbf{j} \rangle) + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} \tag{2a}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{2b}$$

$$\nabla \cdot \mathbf{E} = (\rho + \langle \eta \rangle)/\epsilon_0 \tag{2c}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{2d}$$

With this formulation, any field solver designed to account for free charges can be easily adapted to account for bound charges by making the substitution

$$(\rho, \mathbf{J}) \rightarrow (\rho + \langle \eta \rangle, \mathbf{J} + \langle \mathbf{j} \rangle) \tag{3}$$

Our model for $(\langle \eta \rangle, \langle \mathbf{j} \rangle)$ is based on calculating the motions of effective particles that respond to the superposition of a microscopic binding potential and a macroscopic electric field $\mathbf{E}$. Denoting the displacement of an effective particle from its equilibrium position by $\mathbf{r}$, and expanding the microscopic potential in a Taylor series, results in the effective particle equation of motion

$$\frac{d^2 r_i}{dt^2} + \sum_{jk} \left[2\Gamma_{ij} \frac{dr_j}{dt} + (\Omega^2)_{ij} r_j + a_{ijk} r_j r_k - b r_i r_j r_j \right] = \frac{q}{m} E_i \tag{4}$$

where the subscripts vary over Cartesian coordinates, q/m is the charge to mass ratio, and the $\mathbf{v} \times \mathbf{B}$ force is neglected. The anisotropy of the medium is represented by the tensors Γ, Ω^2, and a. These are, respectively, the damping rate, the square of the resonant frequency, and the first anharmonic coefficient. At present, the second anharmonic coefficient, b, is assumed scalar. By means of a coordinate transformation, Ω^2 can always be made diagonal. The basis vectors which induce this transformation will be denoted by $(\mathbf{e}_u, \mathbf{e}_v, \mathbf{e}_w)$. The basis vectors used for the general calculation will be denoted $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$. The crystallographic basis vectors, which generally coincide with $(\mathbf{e}_u, \mathbf{e}_v, \mathbf{e}_w)$, are denoted $(\langle 100 \rangle, \langle 010 \rangle, \langle 001 \rangle)$.

In general, the parameters in Eq. (4) depend not only on tensor indices, but also on an index p that identifies a particular particle. In other words, each particle may move in a unique potential well, and may therefore satisfy a unique equation of motion. The system of the particle together with its equation of motion is called an oscillator. In practical implementations, it is convenient to group all particles that satisfy the same equation of motion into an oscillator species with index s. Then the

[1] The coupling of free and bound charges is through the macroscopic field only, i.e., collisions are neglected. As a result, the model is most useful when the free charges do not impinge on the dielectric.