NUMERICAL ALGORITHMS FOR DISPERSIVE, ACTIVE, AND NONLINEAR MEDIA WITH APPLICATIONS TO THE PASER*

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Abstract

The PASER [1] is one of the first advanced accelerator modeling applications that requires a more sophisticated treatment of dielectric and paramagnetic media properties than simply assuming a constant permittivity or permeability. So far the PASER medium has been described by a linear, frequency-dependent, single-frequency, scalar dielectric function. We have been developing algorithms to model the high frequency response of dispersive, active, and nonlinear media with an emphasis on areas most useful for PASER simulations. The work described also has applications for modeling of other electromagnetic problems involving realistic dielectric and magnetic media. Results to be reported include treatment of multiple Lorentz resonances based on auxiliary differential equation, Fourier, and hybrid approaches.

INTRODUCTION

While L-band superconducting rf will be the technology base for the International Linear Collider, there is still a need for the development of new acceleration methods. Smaller research linacs, next generation light sources and heavy ion accelerators would benefit from a new compact and inexpensive accelerating device. While work in the area of accelerating structures loaded with dielectric media [2, 3] has been pioneered at Argonne, so far this effort has focused on the use of dielectric slow-wave structures in which the dielectric plays an entirely passive role. Primarily computational work on a class of dielectric laser-driven microstructures co-developed by the ANL group has also resulted in advances in the understanding of laser-based acceleration [4].

There has been a considerable amount of interest and effort in acceleration methods that involve transfer of energy directly from a gain medium (one in which a population inversion has been generated) to a charged particle beam. Accelerators based on this idea have the potential to provide accelerating gradients in excess of 1 GeV/m. The effect is similar to the action of a maser or laser with the stimulated emission of radiation being produced by the interaction of the electromagnetic field of the beam with the medium. While the PASER effect has been studied theoretically there has so far been only one experiment in this area and no numerical simulations that take the detailed properties of the medium into account. This proposal will lead to both an improved conceptual understanding of the PASER through the development of

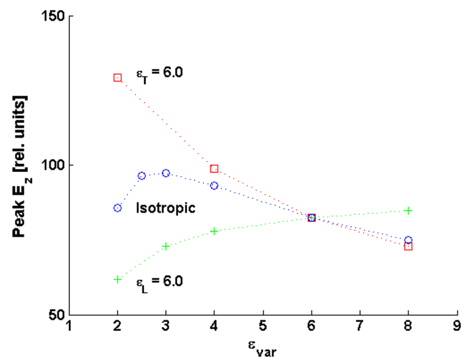

Figure 1: Effect of media anisotropy on wakefields in a dielectric structure. Red: constant transverse component of permittivity = 6.0, axial component varying. Green: constant axial component, transverse component varying. Blue: isotropic case, both axial and transverse components varied.

sophisticated and physically realistic numerical models of the effect and also to new experimental demonstrations of particle acceleration by an active medium.

There are a number of possible implementations of active media devices for particle acceleration. The first involves acceleration of a single bunch by the bulk active medium (the basic PASER concept) without the use of a resonant structure. A second related technique would load the active medium in a resonant structure, similar to the dielectric wakefield accelerator [2], with the fundamental resonant frequency of the structure adjusted to correspond to the frequency of the lasing transition. The device could then be used to amplify the wakefield of a drive beam for acceleration of a trailing witness beam. Yet another approach is to use the active medium, loaded into a resonant cavity of the appropriate frequency and with appropriate optical pumping as an rf power source to drive a conventional iris-loaded or dielectric structure directly.

ANISOTROPY AND NONLINEARITY

We have used the FDTD code Arrakis [6] to investigate electromagnetic fields in anisotropic and nonlinear dielectric structures. The Lax-Wendroff algorithm is specially suited for handling nonlinear problems.

We first consider the case of a simple nondispersive anisotropy in a dielectric wakefield structure. Since we are considering a 2D system only, the permittivity tensor has the form $\overleftrightarrow{\varepsilon} = \begin{bmatrix} \varepsilon_T & 0 \\ 0 & \varepsilon_L \end{bmatrix}$. The dimensions of the device are a=1cm, b=.5 cm. The fundamental TM_{01} frequency for

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an isotropic ε=6 is 7.1 GHz. Fig.1 shows a comparison of the peak axial electric field for a fixed bunch length for three cases (ε_T = const., ε_L = const., $\varepsilon_T = \varepsilon_L$). A significant difference (enhancement of the accelerating field by ~30%) is observed between the isotropic and anisotropic cases.

Arrakis has also been used to model nonlinear media. In ref. [12] the case of a weak quadratic nonlinearity of the form $D(E) = \varepsilon_1 (1 - \frac{tE^2}{2E_{max}{}^2})E$ with t = 0.1 the fractional change in the permittivity at $E = E_{max}$. We modeled a beam-excited cylindrical resonator loaded with this material. The the nonlinearity produced a phase shift and amplitude enhancement in the wake potential over what would be expected in the linear case, and the creation of higher frequency Fourier components.

DISPERSIVE AND ACTIVE MEDIA

In the context of our work on developing a microwave PASER [7], we have been investigating algorithms for modeling a medium with a complex frequency dependent permeability in a finite difference time domain (FDTD) framework using the auxiliary differential equation (ADE) method [5]. (The approach for a dielectric medium is completely analogous.) An active medium is one in which the imaginary part of the susceptibility χ'' is negative.

The paramagnetic medium is assumed to be optically pumped to create a population inversion. The relationship between the magnetic susceptibility χ'' and the spin density Δn achieved in the population inversion is given by $\chi'' = \frac{1}{8}[J(J+1) - M(M+1)]\hbar\gamma^2 \Delta n g(f - f_0)$ [8].

In the case of an active medium Δn and hence χ'' are negative; consequently an electromagnetic wave traversing the medium gains energy. We assume that J=1, M=0 (corresponding to an M=1→0 transition). $g(f - f_0)$ is the line shape function.

Depletion of the energy in the inversion by stimulated or spontaneous emission is not accounted for in this model; Δn is assumed to remain constant.

We begin by assuming the following Lorentz form for the complex permeability of an active paramagnetic medium [9]:

$$\mu(\omega) = 1 + \frac{4\pi\kappa}{\omega_0^2 - \omega^2 + 2i\sigma_0\omega} \equiv 1 + \frac{4\pi\kappa}{D(\omega, \omega_0, \sigma_0)} \quad (1)$$

with $\kappa \equiv \frac{\Delta n}{2}\hbar\gamma^2$, γ is the gyromagnetic ratio. ω_0 is the frequency of the maser transition line and σ is a quantity related to the width of the line.

We want to be able to apply this relation between B and H in a time domain finite difference code. We write $B(\omega) = \mu(\omega)H(\omega)$ and following Taflove [5], convert this to a time domain ordinary differential equation by applying the Fourier transform relation $-i\omega \rightarrow \frac{d}{dt}$ to Eq. (1).

Usually only the imaginary part of the ε or μ is modeled in this approach to provide an effective frequency dependent conductivity for the medium. We have treated both the real and imaginary parts of the permittivity simultaneously to compute dispersion effects as well.

After clearing the denominators, the auxiliary differential equation (ADE) for the constitutive relation then becomes

$$\frac{d^2B}{dt^2} + \sigma\frac{dB}{dt} + \omega_0{}^2\ B(t) = \frac{d^2H}{dt^2} + \sigma\frac{dH}{dt} + (\omega_0{}^2 + 4\pi\kappa)\ H(t) \quad (2)$$

In the following analysis we suppress the spatial indices for the B and H fields. Δt is the time step size. We need to solve for H(t) in terms of the B and H fields at previous time steps and B at the present time. Expanding the fields in a Taylor series around t-Δt and requiring that H satisfies the ADE (2) to second order in time we obtain

$$H(t) = \sum_{k=1}^{2} a_k\ H(t-k\Delta t) + \sum_{k=0}^{2} b_k\ B(t-k\Delta t) + O(\Delta t^3) \quad (3)$$

The coefficients a_k and b_k that make the expression correct to second order are

$$\begin{aligned} b_0 &= (\omega_0^2 + \frac{1}{\Delta t^2} - \frac{3}{2}\frac{\sigma}{\Delta t})D \\ b_1 &= 2(\frac{\sigma}{\Delta t} - \frac{1}{\Delta t^2})D \\ b_2 &= (-\frac{\sigma}{2\Delta t} + \frac{1}{\Delta t^2})D \\ a_1 &= -b_1 \\ a_2 &= -b_2 \end{aligned} \quad (4)$$

with

$$D \equiv \frac{1}{(\omega_0^2 + 4\pi\kappa + \frac{1}{\Delta t^2} - \frac{3}{2}\frac{\sigma}{\Delta t})} \quad (5)$$

Implementation of this algorithm requires additional memory for backstorage of the H and B fields at previous timesteps. By reuse and overwriting of arrays only four additional arrays of size(H) are required. The algorithm was debugged by first implementing it in a 1D Matlab code.

The algorithm was then implemented in the FDTD code Arrakis [6]. The algorithm used for the field advance in Arrakis is actually a two-step Lax-Wendroff rather than the more usual Yee algorithm. The only additional complication is the need to apply our algorithm twice on each time step, once for the predictor step and once for the corrector. After the B field is advanced in time according to Faraday's law, the H field is needed to advance E through Ampere's law. Eq. (3), a discretized version of Eq. (2) is used in each mesh cell containing the active medium to obtain H(B).

We are also interested in media with multiple resonances. The presence of two close transition lines (one absorbing and one emitting) inferred from this spectrum are common to all the optically pumped active paramagnetic media that are being used in the Euclid experiments [10]. This suggests the use of a phenomenological two resonance Lorentz model,

$$\chi''(\omega) = 4\pi \,\mathrm{Im}\left[\frac{\kappa_1}{D(\omega,\omega_1,\sigma_1)} + \frac{\kappa_2}{D(\omega,\omega_2,\sigma_2)}\right] \quad (6)$$

where $\chi'' = \mathrm{Im}\,\mu$ to provide a more accurate description of the susceptibility. Results of a least squares fit to this model are also plotted. The model provides a reasonable approximation to the data in this case; some of the deviations are due to additional resonances caused by the fullerene component alone.

As before, we apply the transformation $i\omega \to -\frac{d}{dt}$ to the expression for the complex permittivity. Adapting the ADE technique to the two pole model is straightforward. For each mesh cell *jkl* containing the active medium we obtain the 4th order ordinary differential equation $D_1 D_2 B_{jkl}(t) = (D_1 D_2 + 4\pi\kappa_1 D_2 + 4\pi\kappa_2 D_1) H_{jkl}(t)$, where

$$D_m \equiv (\omega_m^2 + \frac{d^2}{dt^2} - \sigma_m \frac{d}{dt}).$$

This is then discretized to obtain an expression for H_n in terms of H_{n-1}, H_{n-2}, B_n, B_{n-1}, B_{n-2} that is correct to second order in time (n is the discrete time index). The algorithm requires an extra 6 words of storage for each cell although it may be possible to reduce this further.

Adding an additional resonance term to Eq. (6) increases the order of the auxiliary differential equation from 4 to 6, problematic both in terms of backstorage and stability of the algorithm. One possible approach is to find a different parameterization of the susceptibility that exhibits good agreement with the measurements but leads to a lower order ADE.

A less computationally and memory intensive approximate algorithm can be obtained by ignoring the cross terms in the expansion of (6), i.e. by treating the medium as consisting of two independent Lorentz components. The discretized ADE (3) is applied to the medium-containing mesh cells in a "checkerboard" pattern, alternating the coefficients corresponding to the parameters of the two resonances.

An alternative to the ADE algorithm is based on the use of the Fast Fourier Transform. In rough outline the Fourier algorithm is as follows: Consider the frequency domain constitutive relation $D(\omega) = \varepsilon(\omega) E(\omega)$, where the functional form of the permittivity is known. Using a time domain algorithm, we can obtain the needed Fourier components of E at timestep t_n by storing a time history of the field in each dielectric mesh cell and computing $FFT[E(t_n)] = E(\omega_j)$. Then

$$D(t_n) = FFT^{-1}[\sum_j \varepsilon(\omega_j)\tilde{E}(\omega_j)].$$

This approach requires more backstorage than the ADE method, but unlike the ADE approach (where the order of the ODE to be solved increases with each added resonance) the required memory does not increase with the number of resonances.

An equivalent approach [5] is to notice that the constitutive relation can be written as a convolution $D(t) = \int_{\tau=0}^{t} \varepsilon(\tau) E(t-\tau) d\tau$. Here $\varepsilon(t)$ is the inverse Fourier transform of the frequency dependent permittivity. For certain functional forms of the permittivity and permeability (including Lorentz) the convolution can be reduced to a simple running summation in each media-containing mesh cell.

SUMMARY

The primary goal of this research is the development of algorithms for modeling the high frequency and optical properties of dielectric and paramagnetic materials with an emphasis on problems relevant to the PASER. The applicability of this work however is not limited to PASER related problems. One example is the expanding research area of metamaterials [11]. Numerical modeling of systems involving bulk metamaterials requires the accurate handling of dispersive permittivities and permeabilities.

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