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A NEW TECHNIQUE FOR NONLINEAR OPTICAL PROBLEMS

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ABSTRACT

The propagation of high intensity or high power laser pulses presents a variety of nonlinear optical problems requiring self-consistent study. Our method treats arbitrary three-dimensional problems with unlimited phase distortion and is similar to the particle-in-cell (PIC) methods of hydrodynamics and electromagnetic plasma simulation. Our numerical algorithm is based on Maxwell's equations and is applied to laser-fusion reactor and laser amplifier problems.

I. INTRODUCTION

The propagation of high intensity or high power laser pulses presents a variety of nonlinear optical problems requiring self-consistent study. The common element of these problems is that the optical properties of the medium are changed on a time scale comparable to the length of the pulse. These medium changes may be due to the pulse intensity, such as the nonlinear refractive index leading to self-focusing; to the history of the pulse intensity, such as ionization; or they may be initiated by the pulse, such as photochemistry. Previous methods¹ have allowed computer simulations of two-dimensional (typically axisymmetric) problems involving limited phase distortion. The present (new) method allows arbitrary three-dimensional problems with unlimited distortion. The price paid for the generality (within the framework of state-of-the-art computers) is a limited capability for diffraction or interference phenomena so that the present method complements rather than replaces the others.

Our method may be viewed as a wedding of particle-in-cell (PIC) methods of hydrodynamics² and electromagnetic plasma simulation³ with ray tracing techniques. We represent the optical field by discrete entities which for lack of a better term we refer to as corpuscles, these being analogous to the

particles of the PIC method. Each of these corpuscles moves in a trajectory which is also analogous to a ray of the ray tracing technique. The ray tracing analogy breaks down, however, because corpuscle trajectories are not streamlines; trajectories which are traced out by early corpuscles in the pulse do not serve as trajectories for the later ones.

We will refer to our new method as the corpuscle-in-media (CIM) treatment. Like the methods upon which CIM is based, CIM involves ideas which are easily motivated. Following an intuitive presentation we derive the relevant equations from Maxwell's equations. We then discuss two different applications. The first of these requires the unlimited phase distortions and the second requires full three-dimensional geometry.

II. CIM METHOD

The basic idea is quite simple. The light pulse is considered as a swarm of finite corpuscles, finite in number. Each corpuscle has a position, a velocity, and an energy. It also has a phase (proper time) and polarization, if required. The medium through which the corpuscles move is similarly thought of as being broken into a collection of

finite volumes or cells. By summing the energy of corpuscles within a given cell we compute the intensity, by means of which the light pulse acts on the medium.

The computer code follows the problem in two-part, finite time steps. First the swarm of corpuscles are advanced from their old to new positions according to their velocities. Simultaneously their velocities are advanced (with changes mostly due to refraction) according to the (time-fixed) grid of medium properties. Also the corpuscle energies are advanced according to the medium's gain and/or absorption. During the second part of a time step the medium properties are updated according to the (time-fixed) optical intensities computed from the corpuscle positions and energies.

The differencing of the equations depends on the application. Generally it is best to difference the equations for the position and velocity of the corpuscles to second-order accuracy in the time step, an explicit half-step/full-step Runge-Kutta method being one way to do this. When linear or saturable gain (or absorption) is strong compared to the non-linear refractive index effects, closed exponential forms for the corpuscle weight or energy allow larger time steps. In assigning intensities onto the medium grid in computing medium forces back to the corpuscles we use the area- or volume-weighting ideas of hydrodynamics or plasma simulation³ PIC. Unlike the fluid problems, the swarm of corpuscles is finite in extent with easily described overall motions. This feature allows use of a "moving window" concept so that only part of the medium needs to be represented in computer memory at any one time. The physical scale may also be contracted or expanded between time steps in order to maintain resolution and numerical significance as the pulse moves toward or away from a focus.

Unlike most PIC problems, the very small relative motions between corpuscles cause the corpuscles to stay pretty much as originally ordered. This characteristic makes useful differently weighted corpuscles in different (original) locations and gives an important gain in the numerical significance possible with a given number of particles representing a nonuniform pulse.

Because we are following the motion of finite corpuscles, there is some temptation to describe our technique as "ray-tracing." As already discussed, this is a poor description because a "ray" is now generally thought of as a streamline, along which a stream of corpuscles flow. In unsteady cases, however, corpuscle trajectories are not streamlines and the steady ray trajectory does not exist.⁴

III. VERIFICATION

We begin with the Fourier decomposed wave equation at frequency ω , neglecting variations of the magnetic susceptibility which we take to be unity

$$\nabla^2 \underline{E} - \underline{\nabla} \underline{\nabla} \cdot \underline{E} = -\epsilon k_0^2 \underline{E}. \quad (1)$$

Here ϵ is the dielectric constant, k_0 is the free space wave number ω/c , and the full electric field associated with this frequency component is

$$\underline{E}_{full} = \text{Re} \left\{ \underline{E} \exp(i\omega t) \right\}. \quad (2)$$

This harmonic decomposition is valid even when non-linear interactions are important providing that during the time step in which we propagate the pulse, the local linearization is justified. Indeed it is this requirement which serves to determine the time step we use.

Using $\underline{\nabla} \cdot \epsilon \underline{E} = 0$ we may write Eq. (1) as

$$\nabla^2 \underline{E} + \underline{\nabla} \left[\underline{E} \cdot \underline{\nabla} \ln \epsilon \right] = -\epsilon k_0^2 \underline{E}. \quad (3)$$

Using the phase amplitude representation of $\underline{E}$,

$$\underline{E}(\underline{x}, t) = \underline{e}(\underline{x}) \exp \left[i k_0 L(\underline{x}) \right], \quad (4)$$

where $\underline{e}$ is the real vector amplitude and $L(\underline{x})$ is the optical path length, we may take advantage of the small parameters $|\underline{\nabla} E_1|/(k_0 E_1)$ and $|\underline{\nabla} \epsilon|/(k_0 \epsilon)$ (where E_1 is any component of $\underline{E}$), by expanding Eq. (3) to first order in k_0^{-1} . We get the geometrical optics equation⁵

$$(\epsilon_R + i\epsilon_I - (\underline{\nabla} L)^2) \underline{e} + (ik_0)^{-1} \left[-\nabla^2 L \underline{e} + \underline{e} \cdot \underline{\nabla} \ln(\epsilon_R + i\epsilon_I) \underline{\nabla} L - 2\underline{\nabla} L \cdot \underline{\nabla} \underline{e} \right] = 0. \quad (5)$$

In problems of interest to us, we may simplify Eq. (5) by taking further advantage of several small parameters. First, the imaginary part of the dielectric constant $\epsilon_I \sim 10^{-4}$ to 10^{-6} is small compared to the real part $\epsilon_R \sim 1$. Secondly, as noted above $\nabla \ln \epsilon_R$ is small compared to k_0 . We incorporate these approximations in the real and imaginary parts of Eq. (5) as follows

$$(\nabla L)^2 = \sqrt{\epsilon_R} \quad (6)$$

and

$$(k_0 \epsilon_I + \nabla^2 L) \underline{e} + \underline{e} \cdot \nabla \ln \sqrt{\epsilon_R} \nabla L + 2 \nabla L \cdot \nabla \underline{e} = 0 \quad (7)$$

The imaginary part, Eq. (7), may be simplified by the definition

$$g = \epsilon_I k_0 / \sqrt{\epsilon_R} \quad (8)$$

and substitution of Eq. (6) to give

$$(g |\nabla L| - \nabla^2 L) \underline{e} - \underline{e} \cdot \nabla \ln \epsilon_R \nabla L - 2 \nabla L \cdot \nabla \underline{e} = 0. \quad (9)$$

By taking the scalar product of Eq. (9) with $\underline{e}$ and noting $\underline{e} \cdot \nabla L = 0$

$$\underline{v} \cdot (e^2 \nabla L) = g e^2 |\nabla L|. \quad (10)$$

That g introduced in Eq. (8) is the intensity gain coefficient follows from Eq. (18) below.

The phase speed v in our medium is simply

$$\begin{aligned} v &= \omega/k = c k_0 / (|\nabla L| k_0) \\ &= c / |\nabla L| = c / \sqrt{\epsilon_R}. \end{aligned} \quad (11)$$

The characteristics have this speed and are in the direction of ∇L :

$$\underline{v} = (\nabla L / \sqrt{\epsilon_R}) \underline{v}. \quad (12)$$

In order to find the acceleration of the characteristics we need only operate on $\underline{v}$ with the convective derivative $d/d\tau = \underline{v} \cdot \nabla$,

$$\begin{aligned} \underline{a}(\underline{v}, \underline{x}) &= d\underline{v}/d\tau = (\underline{v} \cdot \nabla) \underline{v} \\ &= (c \epsilon_R^{-1} \nabla L \cdot \nabla) (c \epsilon_R^{-1} \nabla L) \\ &= (1/2 \nabla^2 \underline{L} - \underline{v} \nabla) \cdot \nabla \ln \epsilon_R. \end{aligned} \quad (13)$$

Equation (13) is the equation to be solved for refraction of the characteristic direction. The propagation of the optical length L is simply

$$dL/d\tau = (\underline{v} \cdot \nabla) L = c. \quad (14)$$

To find the equation of motion for e^2 , and to verify our concept of "corpuscle energy," we eliminate ∇L in Eq. (13) by substitution of Eq. (12) to obtain

$$\underline{v} \cdot \underline{v} + \underline{v} \cdot \nabla \ln (e^2 \epsilon_R) = g \underline{v}. \quad (15)$$

Again using the derivative $d/d\tau = (\underline{v} \cdot \nabla)$ and also the divergence theorem for a small volume V ,

$$\nabla^2 dV/d\tau = \underline{v} \cdot \underline{v}. \quad (16)$$

we obtain

$$d \ln(e^2 \epsilon_R V)/d\tau = g \underline{v}. \quad (17)$$

By defining the trajectory length $s = \int_0^\tau \underline{v} \cdot d\tau$ this equation may be put into the familiar form

$$e^2 \epsilon_R V = (e^2 \epsilon_R V)_{s=0} \exp \int_0^s g \, ds. \quad (18)$$

The quantity $e = e^2 \epsilon_R V$ is proportional to the energy contained in the small volume V . As expected, this quantity increases according to the intensity gain coefficient g , verifying the assignment in Eq. (8) and justifying our concept of corpuscle energy or "weight" e .

We must now reassemble our frequency components in order to describe the time dependent pulse. In the monochromatic pulse described above we determined the optical length $L(s, \omega)$ so that the time-dependent field is described by

$$\underline{E}(s, t) = \int \underline{e}(s, \omega) \cos[k_0 L(s, \omega) - \omega t] \, d\omega. \quad (19)$$

Here $\underline{e}(s, \omega)$ is centered on frequency ω_0 and has bandwidth $\Delta\omega$. All of the frequencies within the bandwidth produce nearly the same value of $L(s, \omega)$ so that we may use a linear approximation

$$L(s, \omega) = L_0(s) + \omega L_1(s), \quad (20)$$

where

$$L_1(s) = (\partial L / \partial \omega)_{\omega = \omega_0},$$

and thus

$$E(s,t) = \text{Re} \left\{ \exp \left[i k_0 L_0(s) \right] \int \underline{e}(s,\omega) \times \exp \left[i \omega \left[k_0 L_1(s) - t \right] \right] d\omega \right\}. \quad (21)$$

Now assuming that the gain $G(s) = \int_0^s g ds$ is independent of ω over the pulse bandwidth we have from Eq. (18)

$$\begin{aligned} e(s,\omega) &= e(0,\omega) \left[V(0,\omega) \epsilon_R(0,\omega) / V(s,\omega) \epsilon_R(s,\omega) \right]^{1/2} \\ &\times \left[\exp G(s)/2 \right]. \end{aligned} \quad (22)$$

where we have exhibited the explicit dependence of V and ϵ_R on path length and frequency. The major ω dependence of the right-hand side is in $e(0,\omega)$; over its bandwidth, the expression in the square root is essentially constant and may be replaced by its value at ω_0 . Hence by defining the remaining integral to be P we have

$$\begin{aligned} E(s,t) &= \text{Re} \left\{ \exp \left[i k_0 L_0(s) + G(s)/2 \right] P(k_0 L_1(s) - t) \right. \\ &\times \left. \left[v(0,\omega_0) \epsilon(0,\omega_0) / (v(s,\omega_0) \epsilon(s,\omega_0)) \right]^{1/2} \right\}. \end{aligned} \quad (23)$$

This is a pulse whose portion at $s=0$, $t=0$ arrives at s at time t given by

$$k_0 L_1(s) = t. \quad (24)$$

The group velocity v_g is ds/dt , and using Eq. (24), it is given simply by

$$\begin{aligned} v_g &= ds/dt = \left[\partial^2 k_0 L / \partial \omega \partial s \right]^{-1} \\ &= \left[\partial (k_0 |V_L|) / \partial \omega \right]^{-1} = \left[\partial k / \partial \omega \right]^{-1} \\ &= v \left[1 + 1/2 \omega \epsilon_R^{-1} \partial \epsilon_R / \partial \omega \right]. \end{aligned} \quad (25)$$

The significance of this result is that the corpuscles must be advanced with the group velocity rather than the phase velocity. When there is no dispersion, Eq. (13) represents the acceleration of the corpuscles. When dispersion is present, we may use Eqs. (25) and (13) to find the corpuscle speed from the phase speed.

IV. FIRST APPLICATION

Our first application concerns the nonlinear propagation of an intense pulse through an ionizable medium.⁶ The medium is ionized inside and behind the pulse, but not ahead or to the side of it. In consequence the medium refracts the pulse in the unfocusing sense, as if a number of negative lenses were traveling with the pulse. The total refraction may be significant, even if the change in refractive index is small because the "lens" is steady in the pulse frame. The problem is nonlinear because the fractional ionization is the time integral of a rate which depends upon the pulse intensity.

The motivation for this problem was the transport of pulses through the lithium vapor base pressure in a laser-fusion power reactor.⁷ The results show that the allowed base pressure is much less than previously thought.⁸ The problem is easily visualized from the coordinates indicated in Fig. 1.

Fig. 1. Coordinate system indicating the problem.

A plot of corpuscle weights (the tiny numbers on a relative scale of 0 to 9),⁹ locations (at the tiny numbers), and directions (small vectors pointing ahead) is shown in Fig. 2. The *a priori* (vacuum) focus of the pulse is indicated by the arrow. The vectors in this low density case may be seen to point toward it. A similar plot in Fig. 3 for a higher density shows that many of the corpuscles are now "focused" further down stream, giving an aberration which cannot be corrected by any element which a function of radius alone.

Fig. 2. Corpuscle plot for low density case.

Fig. 4. Corpuscle plot for more severe case.

Fig. 3. Corpuscle plot for moderate density case.

A more severe case, corresponding to the conditions originally chosen for the fusion-reactor,⁷ is shown to be extremely "unfocused" in Fig. 4. The extreme effect (large refraction of some corpuscles) required use of our new method rather than existing ones.

V. SECOND APPLICATION

Our second application was the propagation of light through the 1 kJ Los Alamos Nd: glass laser system.¹⁰ We were particularly concerned about the pulse's behavior in and beyond a disk amplifier. From the sketch in Fig. 5, we see this problem to be three-dimensional and to require the generality of the CIM method.

Fig. 5. Diagrammatic representation of a module consisting of two disks and the modular amplifier consisting of six modules.

The large scale effects to be studied include: (1) wandering of the beam relative to the nominal axis and wandering or altering of parts of the beam relative to each other as functions of the intensity and specified manufacturing tolerances, (2) gross self-focusing of the whole beam or parts of the beam, (3) nonuniform amplifier gain pumping and gain saturation, (4) self-consistent combinations of effects. While the CIM method lacks sufficient resolution to study small scale self-focusing, the results from stability treatment^{11,12} can be parameterized and included as a prescription on intensity, gain, and disk thickness and spacing. By use of this code, amplifier design may consider self-focusing, aperture filling fractions, alignment difficulties, and costs.

The computation following a swarm of corpuscles proceeds as outlined above. In the air spaces the propagation is linear and computer time is saved by crossing these gaps in one step. Refraction at the surface is discontinuous and is accomplished with a Snell's law subroutine including the nonlinear index.

For propagation in a nonlinear medium pulse, information is stored on a series of planes whose separation is sufficiently small to permit a linearization of the problem between planes. The intensity between planes depends on the corpuscle's direction and position as given by

$$I(x,y,z,t) = I_g(x',y',t-s/v - t_b(x',y')) ,$$

where $I_g(x,y,t)$ is the intensity on the surface of the previous plane in terms of the two transverse coordinates x and y and the time t . Also x' and y' are the locations on the surface of the projection of x,y,z back along the trajectory which is a distance s to the surface, and t_b is a function introduced for convenience.

Separate computer subroutines which correspond to many experimental device elements such as apertures, lenses, telescopes and also to the many diagnostic apparatus such as calorimeters, or time or space resolved detectors of beam intensity. There are other computer diagnostics which have no direct experimental analogue as yet such as a "time resolved burn pattern" giving a spacially and tempo-

rally resolved intensity distribution. There is also a subroutine to rotate the beam relative to the Cartesian mesh in order to test to see if a sufficient number of corpuscles per cell have been set up initially. Figure 6 shows the illuminance of the pulse as a function of the two transverse coordinates, as originally set up.

Fig. 6. Pulse illuminance (J/cm^2) is the height and the coordinates perpendicular to the propagation direction form the plane of the base. This is a test pulse with one particle per cell.

Figure 7 shows the same pulse rotated 45° when each cell contains but one corpuscle. Figures 8 and 9 show that this intolerable pulse noise is substantially reduced by using 4 and 16 corpuscles per cell, respectively.

A large number of data-card commands, each with arguments to control the propagation of the pulse, are available. Five commands are utilized for setting up the pulse. A SURFACE command advances the pulse from one surface to the next. A MEDIUM command changes the media by application of Snell's law. Other commands give the diagnostics described above. This method of using serial commands to control the propagation gives the method added flexibility and simplicity and allows preprocessing of the commands to check for errors which would ordinarily cause a computation to abort in the middle.

Fig. 7. Same as Fig. 6 but the pulse has been rotated 45° which introduces numerical noise.

Fig. 8. Same as Fig. 7 but with four particles per cell.

Fig. 9. Same as Fig. 8 but with 16 particles per cell.

The data card commands, themselves, are produced by input preprocessing which inserts specified manufacturing tolerances at random into the data card arguments.

Propagation of a 10 J, 400 ps (full width at half maximum) pulse through a 12-disk amplifier is shown in Figs. 10 ~ 15. The original spacial dependence (Airy-profile) of the pulse is that shown in Fig. 10, the clear aperture being 3.6 cm.

The original gaussian time dependence is shown in Fig. 11. Manufacturing tolerances of ± 40 min were assumed (abnormally large) for the parallelism of faces of a disk and the disks were assumed to be aligned ± 40 min relative to the nominal axis. Since random tolerances are used, the errors tend to cancel one another so that the worst amplitude distortion of the pulse may come anywhere in the amplifier. Figure 12 shows the distortion of this pulse when exiting the last disk, at 20 ps before the peak intensity of the pulse has arrived (the peak has shifted forward 50 ps due to saturation). Upon exiting the amplifier the pulse has 63 J.

The pulse illuminance as it exits the amplifier is shown in Figs. 13 and 14 as a function of the transverse coordinates and this shows relatively

little distortion compared to the distortion seen in Fig. 15 in which the pulse has run out beyond the amplifier 18.8 m in air.

Fig. 10. Pulse illuminance (J/cm^2) of a 10 J Airy-profile pulse in a square aperture of 3.6 cm x 3.6 cm.

Fig. 11. Gaussian time dependence of a 10 J Airy-profile pulse. The line segments are indicative of the numerical approximation.

Fig. 12. A contour plot of pulse intensity 20 ps before the peak intensity as the pulse exits the last disk. The contours A,B,C,D, and E are 10%, 30%, 50%, 70%, and 90% of peak, respectively. The lack of true parallelism of the disk faces accounts for the position of the peak of the pulse.

Fig. 13. A contour plot of the pulse illuminance (J/cm^2) as the pulse exits the last disk. The contours A,B,C,D, and E are 10%, 30%, 50%, 70%, and 90% of peak.

Fig. 14. A 3-D projection showing the same pulse as in Fig. 13.

Fig. 15. A contour plot of the pulse illuminance in which the pulse has run out 18.8 m beyond the amplifier in air. Note the decrease in diameter of the pulse. Same convention as in Fig. 12.

At 18.8 m run-out the distortion of the pulse is most severe at its peak intensity as is shown in Figs. 16 and 17. By comparing Figs. 14, 16, and 17 we can see that the central portion of the pulse is converging while the beginning and end of the pulse converge much more weakly. Thus, a different lens is required to focus the most intense part of the pulse than is required for the rest. Finally, the time dependence of the pulse at 18.8 m run-out is shown in Fig. 18; this is quite close to what one would expect without spatial distortion.

Fig. 16. A 3-D projection showing the pulse intensity at the peak intensity 18.8 m beyond the amplifier.

Fig. 17. A 3-D projection showing the pulse intensity near the beginning of the pulse 18.8 m beyond the amplifier end.

Fig. 18. The time dependence of the pulse at 18.8 m beyond the amplifier end. There is a slight forward shift of the peak due to saturation as one would expect.

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