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Extending the utility of the parabolic approximation in medical ultrasound using wide-angle diffraction modeling

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Abstract

Wide-angle parabolic models are commonly used in geophysics and underwater acoustics but have seen little application in medical ultrasound. Here a wide-angle model for continuous-wave high-intensity ultrasound beams is derived which approximates the diffraction process more accurately than the commonly-used Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation without increasing implementation complexity or computing time. A method for preventing the high spatial frequencies often present in source boundary conditions from corrupting the solution is presented. Simulations of shallowly focused axisymmetric beams using both the wide-angle and standard parabolic models are compared to assess the accuracy with which they model diffraction effects. The wide-angle model proposed here offers improved focusing accuracy and less error throughout the computational domain than the standard parabolic model, offering a facile method for extending the utility of existing KZK codes.

I. Introduction

As high-intensity focused ultrasound (HIFU) continues to find new medical applications and sees increasing clinical use, the ability to characterize HIFU devices becomes more important. Due to the limitations of measurement methods, modeling is an essential adjunct to bench testing [1], and is often used for treatment planning [2], [3]. The KZK equation is the most popular model for HIFU beam simulation due to its balance of tractability and utility. It is fairly easy to implement, soluble via efficient numerical methods, and includes the relevant physical processes over a broad regime of validity. However, KZK is limited in its ability to capture diffraction physics at angles greater than about 20° from the propagation axis [4], [5], [6], [7]. This limitation is due to the low-order approximation of the diffraction operator in the Westervelt equation from which KZK is derived [8]. Simulation of shallow-focus continuous-wave HIFU beams is typically performed using the more complicated Westervelt equation [9], [10].

The so-called wide angle parabolic equation (WAPE) was first developed as an intermediate between standard parabolic models and the more general Helmholtz equation in geophysics [11], [12] and underwater acoustics [13], [14]. The equation has also been applied to therapeutic ultrasound to model hyperthermia using a linear array [15], was compared against other models in the context of time-domain analysis of shock propagation in heterogeneous media [16], and was used to model nonlinear ultrasound fields in air [17]. WAPE models employ high-order approximations of the diffraction operator by retaining

more terms in its Taylor expansion [13], approximation by rational function [11], [12], [14], [15], or more advanced methods [18]. In this paper the frequency-domain representation of the Westervelt equation is simplified to account for forward-wave propagation only, and the resulting pseudo-differential operator is approximated using rational functions (Padé approximations) to model continuous-wave finite-amplitude beams when backscatter and reflection are negligible. A family of numerical schemes for approximating the solution of the one-way Westervelt equation is presented, with particular attention paid to addressing oscillatory artifacts resulting from source boundary conditions with steep spatial gradients. A scheme which prevents these oscillations from corrupting the solution is also presented. The wide-angle and KZK models share the same attenuation and nonlinear terms, but differ in their account of diffraction. Thus a linearized and lossless WAPE model is compared with the narrow-angle parabolic model in the context of a focused axisymmetric source.

The proposed wide-angle parabolic model is so similar in its implementation to finite-difference and finite-element methods commonly used to compute solutions to the KZK equation, it represents a facile improvement of existing codes. Another method for improving the utility of the KZK model is to employ an *equivalent source*, wherein the geometry of the planar source boundary condition is modified to correct for errors incurred in narrow-angle propagation modeling [19]. Indeed the equivalent source method is applicable to wide-angle models and could provide further improvements in the quality of the solution, particularly in a neighborhood about the focus. However, the purpose of the present manuscript is to detail a propagation model that more accurately captures diffraction of the acoustic field.

II. Methods

In this section a system of equations for modeling high-intensity continuous wave ultrasound beams in homogenous media is derived from a generalized Westervelt equation. Once obtained, the diffraction term is approximated using Padé forms which result in a family of WAPEs suitable for efficient code implementation and numerical computation. It is shown that the nonlinear and attenuation terms in these WAPE models are identical to those in the corresponding frequency-domain KZK system; the two approaches differ only in their account of diffraction. While it is certain that different diffraction results have a consequent effect on the nonlinear interaction of the field, isolating the diffraction modeling capability is a necessary first step to characterize the models.

A. The one-way generalized Westervelt equation

Directional sound beams produced by therapeutic ultra-sound devices are accurately modeled by a generalized West-ervelt equation

$$\nabla^2 p - \frac{1}{c_0^2} \frac{\partial^2 p}{\partial t^2} - \frac{2}{c_0} \frac{\partial}{\partial t} [(\alpha(\omega) * p(\omega))] = - \frac{\beta}{\rho_0 c_0^4} \frac{\partial^2 p^2}{\partial t^2}, \quad (1)$$

where p is the time-dependent pressure field and $p(\omega)$ is its frequency-domain analog. The medium is characterized by its small-signal sound speed c_0 , mass density ρ_0 , nonlinear parameter β , and attenuation and phase velocity dispersion rates given by the respective real and imaginary parts of α . The frequency-dependence of these rates is taken into account by convolution with the pressure field

$$\alpha(\omega) * p(\omega) = \int_{-\infty}^{\infty} \alpha(t - t') p(t') dt' . \quad (2)$$

If attenuation is quadratic with frequency then it may be written as $\alpha(\omega) = \delta \omega^2 / 2c_0^3$, where δ is the diffusion of sound [20], and in this special case the medium is dispersionless [21]. Then the convolution $\alpha * p = -(\delta / 2c_0^3)(\partial^2 p / \partial t^2)$ and Equation (1) reduces to the Westervelt equation [22].

When the duration of transducer operation is long compared to the acoustical period, a time-harmonic ansatz is valid and the field may be factored as

$$p(\mathbf{r}, t) = p_0 \sum_{n=1}^{\infty} \left[A_n(\mathbf{r}) e^{in(k_0 z - \omega_0 t)} + A_n^*(\mathbf{r}) e^{-in(k_0 z - \omega_0 t)} \right], \quad (3)$$

where p_0 is the source pressure amplitude, $\mathbf{r}$ is the position vector, the complex amplitude functions A_n are independent of time t , and the superscript asterisk indicates complex conjugation. This form may be viewed as a correction to plane wave propagation in the positive z -direction with fundamental wavenumber k_0 and angular frequency ω_0 . Although typical testing and treatment procedures involve transducers operating at one frequency, the sum accounts for higher harmonic generation due to the nonlinear response of the medium. The harmonics are indexed using the positive integers n . Scaling the spatial dimensions by a characteristic length a associated with the source transducer (for example, $\zeta = z/a$) results in a dimensionless frequency-domain system of equations

$$\begin{aligned} & \frac{\partial^2 A_n}{\partial \zeta^2} + 2ik_0 a n \frac{\partial A_n}{\partial \zeta} + (k_0 a n)^2 X_n A_n + 2ik_0 a^2 n \alpha_n A_n \\ & = \frac{\beta p_0 (k_0 a n)^2}{p_0 c_0^2} \sum_{m=1}^{\infty} A_m (A_{n-m} + 2A_{m-n}^*), n = 1, 2, \dots \end{aligned} \quad (4)$$

with

$$X_n = \frac{1}{(k_0 a n)^2} \nabla_{\perp}^2 . \quad (5)$$

Here $\alpha_n = \alpha(n\omega_0)$ and $\nabla_{\perp}^2$ is the transverse Laplacian, acting perpendicular to the propagation direction.

The frequency-domain representation facilitates modeling media for which the attenuation is not simply quadratic with frequency, as phase velocity dispersion is calculated from attenuation using the Kramers-Krönig relations and generalized function theory [23].

In cases where backscatter and reflection are negligible, Equation (4) may be simplified by neglecting the part of the linear operator which accounts for backward propagation. To do this, the first three terms of the operator on the left-hand side are factored into

$$\left[\partial_{\zeta} + ik_0 a n (1 + \sqrt{1 + X_n}) \right] \times \left[\partial_{\zeta} + ik_0 a n (1 - \sqrt{1 + X_n}) \right]. \quad (6)$$

It is not yet clear which factor governs forward propagation, but applying the Hankel transform permits a cylindrical mode analysis from which propagation direction can be determined. In Hankel space, Expression (6) becomes

$$\left[\partial_{\zeta} + ik_0 a n (1 + \sqrt{1 - \bar{s}^2/n^2}) \right] \times \left[\partial_{\zeta} + ik_0 a n (1 - \sqrt{1 - \bar{s}^2/n^2}) \right]. \quad (7)$$

Here $\bar{s} = s/k_0 a$ is the scaled, continuous index of cylindrical modes, with $\bar{s} < n$ representing propagating modes and $\bar{s} > n$ evanescent modes. The boundary condition $A(\zeta \rightarrow \infty) = 0$ requires evanescent modes to decay with increasing ζ , a property of only the second factor. Thus it is the second factor that describes forward propagation. In most applications of the wide-angle parabolic approximation, the governing equation is linear and homogenous, so the first factor is simply dropped. Equation (4) has a nonzero right hand side, so simply dropping one factor results in a dimensional imbalance when transforming back to the original unscaled variables. To maintain the proper dimensionality, the first factor is approximated by separating orders of the large parameter $k_0 a$ (ranging from roughly 40 to 500 in typical therapeutic ultrasound applications). Writing $\partial_{\zeta} + ik_0 a n (1 + \sqrt{1 + X_n}) = ik_0 a n [2i + \mathcal{O}(1/k_0 a)]$ and neglecting higher-order terms, the one-way frequency-domain generalized Westervelt equation is obtained:

$$\begin{aligned} \left[\partial_{\zeta} + ik_0 a n (1 - \sqrt{1 + X_n}) + \alpha_n \right] A_n &= - \frac{i\beta p_0 k_0 a n}{2\rho_0 c_0^2} \quad (8) \\ &\times \sum_{m=1}^{\infty} A_m (A_{n-m} + 2A_{m-n}^*), n = 1, 2, \dots \end{aligned}$$

This system reduces to the familiar KZK system by expanding the pseudo-differential operator $\sqrt{1 + X_n} = 1 + \frac{1}{2}X_n + \mathcal{O}(1/k_0^4 a^4)$ and neglecting the higher-order terms. Like KZK, this system is closed with boundary conditions at the source and the transverse extent of the solution domain.

B. Numerical schemes for wide-angle parabolic equations

The one-way Westervelt equation (8) may be solved numerically using operator splitting [24], in which different specialized methods are applied to the diffraction, attenuation, and nonlinear terms of the equation independently [7], [25]. As the attenuation and nonlinear terms are the same as that in the KZK equation, the focus of this subsection, and indeed the rest of this paper, is on approximation and efficient numerical solution of the linear equation

$$\frac{\partial A}{\partial \zeta} + ik_0 a (\sqrt{1 + \bar{X}} - 1)A, \quad (9)$$

which accounts only for field diffraction. Here the subscript n is omitted as it suffices to study only the fundamental field. The stepwise solution of this equation is

$$A(\boldsymbol{\rho}, \zeta + \Delta\zeta) = e^{ik_0 a \Delta\zeta (\sqrt{1 + \bar{X}} - 1)} A(\boldsymbol{\rho}, \zeta), \quad (10)$$

where $\boldsymbol{\rho} = \mathbf{r}/a$ is the transverse coordinate vector. The solution is advanced to the position $\zeta + \Delta\zeta$ by applying the exponential term, known as the propagator, to the solution at ζ . Wide-angle parabolic models are obtained by replacing the propagator with the Padé(M, N) approximation [26]

$$e^{ik_0 a \Delta\zeta (\sqrt{1 + \bar{X}} - 1)} \simeq \frac{\prod_{m=1}^M (1 + a_m X)}{\prod_{n=1}^N (1 + b_n X)}. \quad (11)$$

The coefficients a_m and b_n are determined by equating the Taylor series expansion of the propagator with the Padé approximation, collecting the orders of X , and solving for the coefficients. This approach results in Crank-Nicolson type integration schemes:

$$\prod_{n=1}^N (\mathbf{I} + b_n \mathbf{X}) \mathbf{A}^{(q+1)} = \prod_{m=1}^M (\mathbf{I} + a_m \mathbf{X}) \mathbf{A}^{(q)}, \quad (12)$$

where $\mathbf{A}^{(q)}$ is the matrix of discrete complex pressure amplitude values at the q th integration step. This system requires M complex matrix-vector multiplications and N complex matrix inversions to advance the field one step. Using finite-difference or finite-element discretization results in sparse matrices for which these operations are efficiently performed. Moreover, with these discretizations the perfectly matched layer (PML) absorbing boundary condition [27], [28] may be applied in the same manner as the standard narrow-angle parabolic approximation. The details of the PML implementation used in this work are described in Appendix A.

The simplest Padé approximation which offers more accurate diffraction modeling than the standard narrow-angle parabolic equation is Padé(1,1), the coefficients of which are

$$a_1 = \frac{1 + i\mu}{4}, b_1 = \frac{1 - i\mu}{4}, \quad (13)$$

where $\mu = k_0 a \zeta$. Upon discretization of the transverse coordinates, this results in a numerical scheme of the form

$$\left(\mathbf{I} + \frac{1 - i\mu}{4} \mathbf{X}\right) \mathbf{A}^{(q+1)} = \left(\mathbf{I} + \frac{1 + i\mu}{4} \mathbf{X}\right) \mathbf{A}^{(q)}. \quad (14)$$

Comparing this to the Crank-Nicolson technique commonly applied to the narrow-angle parabolic equation

$$\left(\mathbf{I} - \frac{i\mu}{4} \mathbf{X}\right) \mathbf{A}^{(q+1)} = \left(\mathbf{I} + \frac{i\mu}{4} \mathbf{X}\right) \mathbf{A}^{(q)} \quad (15)$$

shows that there is no additional computational work required to obtain the diffraction modeling advantage of this WAPE. Both methods require one matrix-vector multiplication and one solution of a sparse linear system to advance the field one step, and the memory requirements for both methods are identical.

The stability properties of Padé methods can be determined by analyzing their approximants in the spatial frequency domain. In the absence of attenuation, the Padé(1,1) scheme is

$$\hat{A}^{(q+1)} = \Phi_{1,1}(\bar{s}) \hat{A}^{(q)}, \quad (16)$$

with the evolution operator

$$\Phi_{1,1}(\bar{s}) = \frac{4 - (1 + i\mu)\bar{s}^2}{4 - (1 - i\mu)\bar{s}^2}. \quad (17)$$

Here $\bar{s} \equiv s/k_0 a$. Since $|\Phi_{1,1}| = 1$ for all values of $\bar{s}$ and μ , it is a unitary transformation. Hence the amplitude of each cylindrical mode s remains constant as the evolution occurs. This contrasts with the evolution operator of the original equation

$$\Phi_{exact}(\bar{s}) = \exp \left[i\mu \left(\sqrt{1 - \bar{s}^2} - 1 \right) \right]. \quad (18)$$

where the amplitude of modes for which $\bar{s} \ll 1$ is constant but modes above this cutoff are attenuated. Therefore this scheme is only appropriate when the spatial frequency spectrum of the source boundary condition is limited. Otherwise unattenuated high frequency modes can corrupt the solution.

When using any parabolic model, there are two different ways to approach this problem. The first is to use a boundary condition which is devoid of high frequency content. In practice, however, boundary conditions with sharp discontinuities (and resulting broad spectra) are commonly used to represent the source. Thus a focus of this section is the second approach: to employ an integration scheme with appropriate numerical damping near the source. Then any high frequencies present in the boundary condition are sufficiently filtered. In simulations of the KZK equation, it is common to use the implicit Euler [29], [30] or analogous method [7] near the boundary and then switch to Crank-Nicolson for the rest of the simulation (the damping characteristics are quantified in the following paragraph). The transition distance is where the integration method is changed is typically found for a given system geometry by increasing its value in linear simulations until oscillatory artifacts are no longer present in the solution.

In the context of wide-angle methods, the Padé(1,2) approximation is well-suited for use near a discontinuous boundary condition. Its evolution operator is asymptotically similar to $\Phi_{\text{exact}}(\bar{s})$, as they both tend to zero as $\bar{s} \rightarrow \infty$. However, equating the approximation with a Taylor expansion and matching terms to third-order results in a scheme in which the numerical damping depends on μ . In high-resolution solutions, which are ultimately necessary to resolve small spatial scales when nonlinear effects are included, oscillatory artifacts can occur. To achieve a scheme which damps high frequency modes regardless of the grid resolution, Padé(1,2) is equated with the Taylor series to second-order accuracy in the diffraction operator, and the third parameter is left free to tune the algorithm. This results in an evolution operator of the form

$$\Phi_{1,2}(\bar{s}; \nu) = \frac{1 - \nu \bar{s}^2}{1 - (\nu - i\frac{\mu}{2})\bar{s}^2 - \frac{\mu}{8}(\mu - i + 4i\nu)\bar{s}^4}, \quad (19)$$

where the tuning parameter $\nu = \nu(\mu)$. It can be shown that $\text{Im}(\nu) = \mu^{1/2} - \text{Re}(\nu)$ results in $|\Phi_{1,2}(\bar{s}; \nu)| \leq 1$, a necessary condition for stability of the numerical scheme. The evolution operators of $\Phi_{1,2}(\bar{s}; \nu)$, $\Phi_{\text{exact}}(\bar{s})$, and $\Phi_{\text{Euler}}(\bar{s}) = (1 + i\mu \bar{s}^2)^{-1}$ are shown in Figure 1. The sharp transition from propagating to decaying modes is visible with the inflection point in the exact curve at $s = k_0 a$. While not shown in the figure, note that the evolution operator corresponding to the Padé(1,1) scheme has constant unit amplitude. The curve representing the implicit Euler scheme quickly falls below unit amplitude, indicating its strong damping quality. However it damps some modes for which $s < k_0 a$ which results in reduction of detail in the solution. The shape of the curve for the Padé(1,2) scheme varies according the choice of ν . The curve shown corresponds to $\nu = 0.05 + 0.45i\mu$, and was chosen as a compromise between preserving the energy in the propagating modes and damping modes higher in the spectrum, however no effort was made to quantitatively optimize the parameter. Solutions using this value of ν show no loss of detail nor spurious oscillations, and this value was used to produce the simulation results reported in the Results Section. Other choices are certainly possible and result in different characteristics of the evolution operator. As the value of ν tends toward a smaller (more negative) imaginary part, the transition in the evolution operator between propagating and decaying modes becomes less sharp. Constraining ν to the

line $\text{Im}(\nu) = \mu[1/2 - \text{Re}(\nu)]$ still allows for tuning the characteristics of the scheme. Decreasing the real part of ν improves high frequency damping but the damping can extend into $\bar{s} < 1$. Increasing the real part of ν results in less damping of high frequencies but preserves the propagating modes, and small changes in the value of ν result in increasingly large changes in the evolution operator.

Implementing this scheme requires factorization of the denominator in Equation (19) so that standard methods for solving sparse linear systems may be employed. This results in the coefficients

$$a_1 = \nu \quad (20)$$

$$b_1 = \frac{1}{2} \left[\nu - i\frac{\mu}{2} - \sqrt{\nu(\nu + i\mu) + \frac{\mu}{4}(\mu - 2i)} \right] \quad (21)$$

$$b_2 = \frac{1}{2} \left[\nu - i\frac{\mu}{2} - \sqrt{\nu(\nu + i\mu) + \frac{\mu}{4}(\mu - 2i)} \right] \quad (22)$$

and the discretized scheme

$$(\mathbf{I} + b_1 \mathbf{X})(\mathbf{I} + b_2 \mathbf{X}) \mathbf{A}^{(q+1)} = (\mathbf{I} + a_1 \mathbf{X}) \mathbf{A}^{(q)}, \quad (23)$$

which requires one matrix-vector multiplication and the solution of two sparse linear systems. The additional matrix inversion required over the Padé(1,1) method represents the computational cost of achieving the proper damping properties while maintaining second-order accuracy in the approximation of the diffraction operator and hence wide-angle performance. This additional computational effort is typical of all methods used to damp the spurious modes intrinsic to parabolic approximations. The implicit Euler method is only accurate to $\mathcal{O}(\zeta)$, so a much smaller ζ must be used to maintain accuracy which requires many more solutions of the linear system. Similarly, more advanced techniques such as the Radau-collocated implicit Runge-Kutta methods [31], which extend the favorable damping properties of implicit Euler to $\mathcal{O}(\zeta^2)$ or better accuracy, require the solution of two or more linear systems. In this respect the wide-angle model proposed here requires no additional computational overhead compared to the numerical methods used for narrow angle parabolic models. Moreover, it represents a facile way to obtain greater simulation utility for practitioners already familiar with traditional numerical methods for the KZK model.

III. Results

The accuracy of the proposed WAPE model is compared with the standard narrow-angle model by examining both the error distribution in the entire computational domain as well as

the focusing accuracy, that is, the ability of the models to predict the characteristics of the focal lobe. In order to assess the error incurred by these models, solutions of Equation (9) supplemented with a suitable boundary condition must be obtained. Since no closed-form analytic solution of this pseudo-differential equation exists, a very accurate numerical method which admits errors much smaller than those incurred by the two parabolic models is a sufficient comparator. The required accuracy is achieved by numerically evaluating the corresponding Green's function solution, given by

$$A(\rho, \zeta) = 2\pi \int_0^1 G(\rho, \zeta; \rho') A(0, p') p' dp', \quad (24)$$

$$G(\rho, \zeta; \rho') = \frac{e^{-ik_0 a \zeta}}{2\pi} \int_0^\infty e^{i\zeta \sqrt{k_0^2 a^2 - s^2}} J_0(\rho' s) J_0(\rho s) s ds. \quad (25)$$

This is an exact solution of Equation (9) subject to the boundary condition $A(\rho, 0)$, a planar source located at $\zeta = 0$ radiating in the positive ζ -direction with an active radius a such that $A(\rho > 1, 0) = 0$, with $\rho = r/a$. To achieve focusing, the phase of the source is that of a spherical wave converging at the focal depth $z = d$:

$$A(\rho, 0) = e^{-ik_0 \sqrt{a^2 \rho^2 + d^2}} U(1 - \rho), \quad (26)$$

where U is the unit step (Heaviside) function. The maximum off-axis propagation angle with this geometry is given by $\theta = \tan^{-1}(a/d)$.

The integral appearing in the Green's function is evaluated over the range of propagating modes $s < k_0 a$. The transformation $s = k_0 a \sin \psi$ is used to regularize the frequency of oscillations present in the integrand and facilitates determining the sampling rate required to resolve its features accurately for all values of the parameters $k_0 a$, ζ , ρ' and ρ . A 6th-order endpoint-corrected trapezoid rule [32] is used to evaluate both integrals in Equations (24) and (25) to high precision.

Solutions of the standard narrow-angle parabolic model

$$\frac{\partial A}{\partial \zeta} = \frac{ik_0 a}{2} X A \quad (27)$$

are obtained using the aforementioned second-order Radau collocated implicit Runge-Kutta method for $z < 0.1d$ and the Crank-Nicolson scheme thereafter. The same transition distance between methods was used for the WAPE model, consisting of parameterized Padé(1,2) and Padé(1,1). The boundary condition (26) is used in all simulations and only lossless, linear media are considered to isolate the diffraction modeling capability of these approaches.

In the following analyses, all the solutions, narrow- and wide-angle parabolic as well as the comparator, were checked to ensure convergence and minimize discretization error. Thus, the results presented here allow an accurate assessment of the ability of the two parabolic models to approximate solutions of the original equation.

A. Focusing accuracy

To assess the ability of each of the narrow- and wide-angle models to produce an accurate focal lobe, several quantities of interest which characterize the focal lobe are measured against the comparator. These include the peak pressure, the axial location at which the peak occurs, the axial location of the focal lobe center, focal lobe length, and focal lobe width.

The latter three quantities are determined by comparing the contours of the pressure amplitude distributions of both the approximate and comparator solutions at -6 dB from the pressure peak of the comparator solution. The axial lobe location is determined by averaging the minimum and maximum axial values of the contour. The metric used to evaluate the accuracy of each quantity of interest Q is

$$E_Q = 100 \times \frac{Q_{approx} - Q_{comp}}{Q_{comp}}. \quad (28)$$

This metric is similar to the percent relative error but absolute values are not taken. Thus the sign of the error is retained which indicates whether the quantity of interest generated by the approximation is greater or less than that generated by the comparator. For example, the focal lobe length produced by the narrow-angle parabolic equation is shown with a dashed line in the lower left position of Figure 2. For $\theta < 42.5^\circ$, the error E_Q is negative, indicating the quantity is underpredicted by the narrow-angle model. This figure also shows the error in the quantities of interest as determined for $\theta \in [15^\circ, 60^\circ]$ at $k_0 a = 105$. The narrow-angle model fails to produce a defined focal lobe at $\theta > 45^\circ$, so those results are suppressed. The error curves show that if the practitioner is willing to accept at most 5% error in any of these quantities of interest, the narrow-angle model is useable up to $\theta = 25^\circ$, while the wide-angle model is good to $\theta = 48^\circ$. In terms of the F -number $F = (2 \sin \theta)^{-1}$, which characterizes the geometry of spherical bowl transducers, these angles correspond to $F/1.18$ and $F/0.67$, respectively. Also presented in Figure 2 is a comparison of the run times needed to complete these simulations. All simulations were conducted using the same discretization of 100 points per wavelength in both dimensions. The curves show that the WAPE model requires the same amount of computational work as the narrow-angle model.

Figure 3 shows the same analysis but at triple the source frequency, which corresponds to $k_0 a = 314$. Here the narrow-angle model failed to produce measureable focal lobes for $\theta > 37.5^\circ$ and the wide-angle model failed at $\theta > 55^\circ$. The 5% error tolerance in these quantities occurs at 24° and 46° for the narrow- and wide-angle models, respectively. This similarity to the tolerance at 1 MHz indicates the error is only weakly dependent on frequency. Again the computational work required by the models is almost identical.

B. Error distribution

The spatial distribution of the error committed by each of the narrow- and wide-angle models over the entire computational domain (not including the PML) is measured against the comparator using the metric

$$E(r, z) = 20 \log_{10} \frac{|A_{approx}(r, z) - A_{comp}(r, z)|}{|A(0, 0)|}, \quad (29)$$

which gives the result in dB relative to the source pressure amplitude. The error incurred by both the narrow- and wide-angle models are presented in Figure 4 at two different focusing depths corresponding to maximum off-axis propagation angles of $\theta = 18.4^\circ$ and $\theta = 33.7^\circ$. An examination of the error of both parabolic approximations shows that much of the error originates from the edge of the boundary condition where the source pressure distribution is discontinuous. For the case of deep focusing $d = 3a$, the largest error committed by the narrow-angle model occurs on axis in the prefocal region near the focus. The error in the results of the wide-angle model also peaks prefocally but much further from the focal lobe. In the shallow focused $d = 1.5a$ case, the location of the maximum error follows a similar trend. The value of both the maximum error is shown in Table I, where the subscripts of E indicate the model: n for narrow-, w for wide-angle. Interestingly, the wide-angle model incurs less error at $\theta = 33.7^\circ$ than the narrow-angle model at $\theta = 18.4^\circ$, the latter of which is generally regarded as within the regime of applicability for the narrow-angle model.

To quantify the error over the entire computational domain, the mean values of E are also shown in Table I.

IV. Conclusion

In this paper a one-way, finite-amplitude, frequency-domain wave equation was derived and a family of approximation schemes introduced to facilitate efficient numerical solution and code implementation of the diffraction term, the only part of the model which differs from the commonly-used KZK model. Thus the equation is simplified to isolate its diffraction modeling capability. The problem of high spatial frequency components corrupting the solution is addressed in the context of this wide-angle model and a method with appropriate numerical damping characteristics is presented for use near a discontinuous source boundary condition. The solutions of the model are measured against those of a suitable comparator: the corresponding Green's function solution. The focusing accuracy of both the wide- and commonly-employed narrow-angle models are compared in the context of five metrics characterizing the focal lobe. The analysis shows the proposed wide angle model performs acceptably at off-axis propagation angles approximately twice as large as the capability of the narrow-angle model, allowing accurate modeling of the focal lobe at focusing depths less than half of that achievable by the narrow-angle model given the same source boundary condition. In 3D simulations, steering angles should also improve twofold using the wide-angle model. Computation times are also compared and no penalty in using the wide angle model is observed. The spatial distribution of error over the entire computational domain is

also compared with the wide-angle model showing at least 5 dB improvement in accuracy over the narrow-angle model.

While axisymmetric beams were used in this comparison, the wide-angle models can accomodate full 3D simulations, as well as spatially-varying medium characteristics as long as backscatter and reflection are negligible effects. Since there is no computational or code implementation overhead, these methods effectively extend the utility of the KZK model to the shallow focus and steered-beam scenarios.

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Appendix A: The perfectly matched layer

This discussion of the PML absorbing boundary condition follows [28] and extends its application to the cylindrical coordinate system. Consider the diffraction equation

$$\frac{\partial A}{\partial z} = \frac{i}{2k_0} \frac{\partial^2 A}{\partial \xi^2} \quad (30)$$

and apply the ansatz $A = \exp(ik\zeta + \sigma z)$ to obtain the dispersion relation

$$\sigma(k) = \frac{-ik^2}{2k_0}. \quad (31)$$

Since σ is purely imaginary, this equation supports propagating modes of all spatial frequencies k . Now introduce the coordinate transformation

$$x = \int_0^\xi \frac{d\xi'}{u(\xi')} \quad (32)$$

to obtain the transformed equation

$$\frac{\partial A}{\partial z} = \frac{i}{2k_0} u \frac{\partial}{\partial x} \left(u \frac{\partial A}{\partial x} \right) \quad (33)$$

and corresponding dispersion relation

$$\sigma(k) = \frac{-i}{2k_0} (k^2 u^2 - ikuu'). \quad (34)$$

The function u is unity within the physical domain of the problem, thereby preserving the characteristics of the original equation there, but undergoes a rotation to $\sqrt{-i}$ in the PML so that waves in this region are gradually converted from propagating to decaying. In this work the form of u was chosen as

$$u(x) = \exp \left[-i \frac{\pi}{4} \phi(x) \right] \quad (35)$$

with

$$\phi(x) = \begin{cases} 0 & x < w \\ 2(x - w)/T & w < x < w + T/2 \\ 1 & w + T/2 < x < w + T \end{cases} \quad (36)$$

Here the PML has thickness τ and begins at $x = w$, which designates the width (distance from $x = 0$) of the region of interest. The transition from propagating to decaying modes occurs in the first half of the PML, where ϕ is linearly increasing, while the second half is purely absorptive with ϕ constant. While x is real valued, the rotation of u from 1 to $\sqrt{-i}$ requires that ξ become complex valued in the PML. This kind of absorbing boundary is sometimes called *complex grid stretching* [33]. The region of interest $w = 1.05a$ and PML thickness $\tau = \lambda$ effectively suppressed reflection artifacts in the solutions analyzed in this work.

While this PML is developed in the context of the narrow-angle parabolic equation, it performs well for the wide-angle generalization, as it is not necessary to model waves accurately in the PML but rather simply prevent them corrupting the solution in the domain of interest.

In three dimensional cartesian space, Equation (33) may be written as

$$\frac{\partial A}{\partial z} = \frac{i}{2k_0} u(x, y) \nabla_{\perp} \cdot [u(x, y) \nabla_{\perp} A]. \quad (37)$$

A transformation to axisymmetric cylindrical coordinates, so that $A = A(r, z)$ and $u = u(r)$ results in the PML-modified diffraction equation

$$\frac{\partial A}{\partial z} = \frac{i}{2k_0} \left[u^2 \frac{\partial^2 A}{\partial r^2} + \left(\frac{u^2}{r} + uu' \right) \frac{\partial A}{\partial r} \right]. \quad (38)$$

This modified form of the transverse Laplacian operator is employed in both the narrow- and wide-angle models used to obtain the results reported here.

Biography

Joshua E. Soneson studied physics at California State University, Fullerton, and completed a B.Sc. degree there in 2000. He earned M.Sc. and Ph.D. degrees in applied mathematics at the University of Arizona in 2002 and 2005, respectively, where he studied ultra-short optical pulse dynamics in nanocomposite media. After completing a postdoctoral appointment at the U.S. Food and Drug Administration, he continued at the FDA and is now a Staff Mathematician in the Division of Applied Mechanics. His research interests include algorithm development, nonlinear dynamics, and modeling and simulation of medical devices and bioeffects.

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Fig. 1.

Evolution operators plotted in absolute value as a function of the scaled index of cylindrical modes. The solid line is the parameterized Padé(1,2) approximation with $\text{Re}(\nu) = 0.05$, the dashed line is exact, and the dotted line indicates the implicit Euler method for comparison. These curves correspond to a discretization of 30 points per wavelength.

Fig. 2.

Percent error committed by the narrow- (dashed lines) and wide-angle (solid lines) parabolic models for five quantities of interest that characterize the focal lobe as a function of the maximum off-axis propagation angle θ at $k_0 a = 105$. The plot in the lower right position compares the simulation run times.

Fig. 3.

Percent error committed by the narrow- (dashed lines) and wide-angle (solid lines) parabolic models for five quantities of interest that characterize the focal lobe as a function of the maximum off-axis propagation angle θ at $k_0 a = 314$. The error metric is Equation (28). The plot in the lower right position compares the simulation run times.

Fig. 4.

Error committed by the narrow- (left) and wide-angle (right) parabolic models at different focusing depths, indicated by black crosshairs. The top row results from focusing at $d = 3a$ and the bottom row from $d = 1.5a$, corresponding to maximum off-axis propagation angles of $\theta = 18.4$ and $\theta = 33.7^\circ$, respectively. The error is displayed in dB relative to the source pressure amplitude and is computed using Equation (29). In these simulations $k_0 a = 105$.

TABLE I

Maximum and mean error (DB)

Focus	$\max(E_n)$	$\max(E_w)$	$\langle E_n \rangle$	$\langle E_w \rangle$
Deep	12.3	6.4	-9.6	-23.0
Shallow	28.0	11.2	-15.2	-26.6

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