4aPA1. Experimental verification of a wave-vector-frequency-domain nonlinear acoustic model

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In this paper, a recently developed wave-vector-frequency-domain method for nonlinear wave propagation is modified and verified by underwater experiments. An improved numeric scheme is proposed that increases the accuracy from first-order to second-order, thereby allowing for a larger step-size and reduced computation time. A specially designed focused transducer was used to generate short high intensity pulses. 2D scans were conducted at a pre-focal plane, which were later used as the input to the numerical model to predict the acoustic field at other planes including the focal plane. Good agreement was observed between the simulation and experiment.
INTRODUCTION

Accurate and efficient numerical simulations for nonlinear/shock wave propagation are critical for understanding many interesting nonlinear acoustic behaviors and could assist the design of therapeutic and imaging ultrasound arrays. While the KZK equation [1] has been used for decades for nonlinear wave simulations [2, 3], new methods have been emerging that are based on the Westervelt equation [4, 5, 6, 7, 8, 9, 10, 11, 12, 13], which is more accurate especially in the near-field and for highly focused transducers. Different types of approaches have been proposed for solving the Westervelt equation. For example, the Westervelt equation can be decomposed into three equations, each representing the diffraction, absorption and nonlinearity [13, 14, 15]. The equation for diffraction can be solved by the angular spectrum approach, and the equation for nonlinearity can be either solved in the frequency-domain or time-domain (e.g., Godunov-type scheme if shock waves are present). The total solution is acquired by a splitting scheme. These approaches typically assume the nonlinearity builds up mainly in the z-direction (the direction normal to the transducer surface), thus are less accurate for highly focused transducers. The Westervelt equation can be also solved entirely in the time-domain by using the FDTD method or k-space methods [11, 7, 8]. These methods require more computational resource, but are considered advantageous if the medium under study is heterogeneous. This is because the medium properties (speed, density, and absorption) can be functions of the position, which is generally not possible in angular spectrum methods. Other approaches include an iterative scheme for solving the Westervelt equation [10], in which the nonlinearity and absorption are modeled as contrast source terms. This approach needs the complete time history of the acoustic field (a 4D matrix) to be stored, which could potentially be a limitation in terms of memory requirement when large-scale problems are modeled.

This paper is based on a recently proposed wave-vector-frequency-domain approach [5, 6], which has been proven valid for both weakly nonlinear and strongly nonlinear/shock waves through numerical simulations. This approach is designed for homogenous media, and accounts for nonlinearity in arbitrary direction. In addition, as this approach operates in the frequency-domain, dispersion and frequency-dependent absorption can be naturally taken into account. In this paper, the accuracy of the wave-vector-frequency-domain algorithm is significantly improved using a new numerical scheme based on the trapezoidal rule integration. The validity is verified by comparing with underwater experimental data.

THEORY

We start with the time-domain Westervelt equation in a homogeneous medium [5].

\[ \nabla^2 p(\mathbf{r}, t) - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} p(\mathbf{r}, t) + \delta \frac{\partial^3}{\partial t^3} p(\mathbf{r}, t) + \frac{\beta}{\rho_0 c_0^4} \frac{\partial^2}{\partial t^2} p^2(\mathbf{r}, t) = 0 \]

(1)

where \( p \) is the sound pressure, \( c_0 \) is the sound speed, \( \delta \) is the sound diffusivity, \( \beta \) is the nonlinearity coefficient, \( \rho_0 \) is the ambient density. Although the Westervelt equation intrinsically assumes quasi-plane waves, it was recently proven accurate for even highly focused transducers [4].

By Fourier solution of the temporal dimension, as well as the Cartesian x- and y- dimensions, Eq. (1) is transformed to,

\[ \frac{\partial^2}{\partial z^2} P(k_x, k_y, z, \omega) + K^2 P(k_x, k_y, z, \omega) - \frac{\beta \omega^2}{\rho_0 c_0^4} P(k_x, k_y, z, \omega) \otimes P(k_x, k_y, z, \omega) = 0 , \]

(2)

where

\[ P(k_x, k_y, z, \omega) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(\mathbf{r}, t) e^{-i(k_x x + k_y y - \omega t)} \, dx \, dy \, dt , \]

\[ P(k_x, k_y, z, \omega) \otimes P(k_x, k_y, z, \omega) \]

\[ = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(k_x', k_y', z, \omega') P(k_x - k_x', k_y - k_y', z, \omega - \omega') \, dk_x' \, dk_y' \, d\omega' , \]

(3)

\[ K^2 = \frac{\omega^2}{c_0^2} - k_x^2 - k_y^2 - i \frac{\delta \omega^3}{c_0^4} , \]

(4)

\[ \frac{\partial^2}{\partial z^2} k \]

(5)
and \( \omega \) is the angular frequency, \( k_x \) and \( k_y \) are the wave numbers. The convolution resulting from the nonlinear term in Eq. (1) transfers energy between spatial frequencies. This is important as it guarantees that the interaction between wave propagation in different directions is accounted. The convolution can be conveniently and efficiently implemented using the fast Fourier transforms.

For one-directional forward propagation, the solution to Eq. (2) is shown to be [5, 16]

\[
P(z) = P(0)e^{iKz} + \frac{Me^{iKz}}{2iK} \int_0^z e^{-iKz'} F\left(P(z')\right)dz',
\]

where \( M = \frac{\beta \omega^2}{\rho_0 c_0^4} \) and \( F\left(P(z')\right) = P(k_x, k_y, z', \omega) \otimes P(k_x, k_y, z', \omega) \).

In a previous paper, the integral equation (6) was solved by the left-hand Riemann sum, such that

\[
P(z + \Delta z) = P(z)e^{iKz} + \frac{Me^{iKz}}{2iK} F\left(P(z)\right)\times \Delta z.
\]

By projecting the planar acoustic field at the initial/source plane in the forward direction in increments of \( \Delta z \), the acoustic field at any plane can be predicted. While this Riemann sum based scheme is robust for weakly and moderately nonlinear wave modeling, it suffers from an intrinsically low accuracy when strongly nonlinear/shock waves are to be modeled. In these cases, because a large number of harmonics are modeled, an extremely small step-size \( \Delta z \) is required for reasonable accuracy and stability, which leads to intolerably long computation time. To this end, a modified scheme is presented below

\[
P^0(z + \Delta z) = P(z)e^{iKz} + \frac{Me^{iKz}}{2iK} F\left(P(z)\right)\times \Delta z,
\]

\[
P^1(z + \Delta z) = P(z)e^{iKz} + \frac{Me^{iKz}}{2iK} \left[ F\left(P(z)\right) + F\left(P^0(z + \Delta z)\right)e^{-iKz}\right] \times \frac{\Delta z}{2}.
\]

The above numerical scheme is based on the Trapezoidal rule integration. To acquire the acoustic field \( P^1 \) (superscript denotes step number) at \( z + \Delta z \), two steps are required. In the first step, an approximate acoustic field \( P^0 \) at \( z + \Delta z \) is estimated using the left-hand Riemann sum, i.e., Eq. (7). This essentially provides the right-end point value (with a certain error) for the Trapezoidal integration, which is carried out in the second step. Note that the acoustic field at \( z \) \( (P(z)) \) readily provides the left-end point value. The computation time for this scheme is roughly doubled compare to the previous one, as two steps are needed for projecting the field by \( \Delta z \). Nevertheless, as shown below, the significantly higher accuracy gained from this new scheme compensates for its longer computation time for a fixed \( \Delta z \). This modified scheme can be potentially further improved by calculating the middle and right-end point using the Trapezoidal integration, and the carrying out the Simpsons integration. This will be detailed in a forthcoming paper.

**RESULTS**

**Error study**

It is well known that the left-hand Riemann sum has first-order accuracy while the Trapezoidal integration has third-order accuracy. However, since the right-end point value is only an approximation in this case, the accuracy of this modified scheme is expected to be between first- and third-order. To verify this hypothesis, Eq. (8) was implemented to compare numerical results with the Fubini solution. Accordingly, one-dimensional wave propagation was simulated, where a sinusoidal burst of ten circles was used as the excitation signal. The frequency was 5 MHz, the initial pressure amplitude was 5 MPa. For the medium, the nonlinearity coefficient was 3.5 and the speed of sound was 1500m/s. Two sets of simulations were implemented: the first one propagated the wave for a distance of 0.39\( \sigma \) (\( \sigma \) is the shock formation distance), and the second one is 0.49\( \sigma \). In each case, 40 harmonics were considered in the simulation, and the step-size \( \Delta z \) was varied with regard to the wavelength \( \lambda \) (or \( \sigma \)) to generate different results for comparison with the analytic solution. The errors were quantified by
\[ E = \frac{\| P_{num}(t) - P_{exact}(t) \|}{\| P_{exact}(t) \|}, \]  

where \( \| p(t) \| \) is the L2 norm of \( p(t) \). Table I and II list the results.

### TABLE 1. Least square errors for the distance of 0.39σ.

<table>
<thead>
<tr>
<th>( \Delta z )</th>
<th>Riemann sum Error</th>
<th>Trapezoidal integration Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>8( \lambda )(0.39σ)</td>
<td>0.060</td>
<td>0.016</td>
</tr>
<tr>
<td>4( \lambda )(0.195σ)</td>
<td>0.032</td>
<td>0.004</td>
</tr>
<tr>
<td>2( \lambda )(0.098σ)</td>
<td>0.0165</td>
<td>0.0012</td>
</tr>
<tr>
<td>( \lambda )(0.049σ)</td>
<td>0.008</td>
<td>0.00051</td>
</tr>
<tr>
<td>( \lambda / 2 )(0.024σ)</td>
<td>0.0041</td>
<td>0.00043</td>
</tr>
</tbody>
</table>

### TABLE 2. Least square errors for the distance of 0.49σ.

<table>
<thead>
<tr>
<th>( \Delta z )</th>
<th>Riemann sum Error</th>
<th>Trapezoidal integration Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10( \lambda )(0.49σ)</td>
<td>0.093</td>
<td>0.0325</td>
</tr>
<tr>
<td>5( \lambda )(0.24σ)</td>
<td>0.053</td>
<td>0.0091</td>
</tr>
<tr>
<td>2.5( \lambda )(0.12σ)</td>
<td>0.027</td>
<td>0.0024</td>
</tr>
<tr>
<td>1.25(0.061σ)</td>
<td>0.014</td>
<td>0.00086</td>
</tr>
<tr>
<td>0.625( \lambda )(0.03σ)</td>
<td>0.0068</td>
<td>0.00066</td>
</tr>
</tbody>
</table>

We have several observations.

1. The Riemann sum error is proportional to the step-size, so that as the step-size is reduced by a half, the error is also approximately reduced by a half. Therefore the Riemann sum has first-order accuracy.

2. From the first three rows in each table, it can be seen that the Trapezoidal integration error is proportional to the step-size square. In other words, as the step-size is reduced by a half, the error is reduced to roughly a quarter. Therefore this new numerical scheme approximately has second-order accuracy. It is noted that the Trapezoidal integration error converges starting from the fourth row; this is possibly due to other numerical errors that are independent on the step-size, e.g., Fourier transform and convolution.

### Experimental verification

We used a custom made 100 μm diameter fiber optic hydrophone for acoustic field mapping. This hydrophone was calibrated with a reference hydrophone (Onda HGL-0085, SN:1258) from 0.25 MHz to 40 MHz following IEC 62127-2: Calibration for ultrasonic fields up to 40 MHz. A therapy transducer was placed in a distilled water bath degassed to a dissolved oxygen level of 60% or less and maintained at a temperature of 23.5 to 24 degrees centigrade. The excitation signal was a 2-cycle pulse with a center frequency of 700 kHz. The transducer focus, as defined by the maximum peak-to-peak pressure, was located using the fiber optic hydrophone and a custom-build 3-axis computer controlled positioning system. The hydrophone was then repositioned to automatically acquire a 2D XY 30mm pre-focal plane of data. The scanning area was 60 mm × 60 mm with a resolution of 0.5 mm. The fiber optic hydrophone DC voltage was monitored and recorded during data acquisition. This voltage was used to compensate the voltage-to-pressure waveform deconvolution program written in Matlab for the quality of the optical fiber cleaved. The average of 100 voltage waveforms obtained by the hydrophone at each point in space was deconvolved to produce a 3D (x,y and time) pressure dataset. The sampling frequency was increased form 100 MHz to 160 MHz during the deconvolution process. One line scan was then obtained crossing the focal point along the z-axis to obtain a benchmark for comparison. Un-averaged pressure waveforms were obtained in this scan to limit error due to occasional cavitation on the hydrophone tip. The 30 mm pre-focal plane was the 2D XY source plane, whose acoustic field was used as the input to the nonlinear wave propagation program.

The numerical simulation was broken down into three parts in order to reduce required memory. In the first step, the propagation distance was 15 mm, and the data was interpolated to have a spatial resolution of 0.25 mm. The temporal resolution was 6.24 ns, \( \Delta z \) was 0.11 mm. In the second step, the propagation distance was 10 mm; the
spatial resolution was 0.125 mm; the temporal resolution was 3.12 ns; Δz was 0.021 mm. An artificial diffusivity $7.5 \times 10^{-5} \text{m}^2 \text{s}^{-1}$ was added. In the last step, the propagation distance was 5 mm; the spatial resolution was 0.125 mm; the temporal resolution was 1.04 ns; Δz was 0.012 mm. An artificial diffusivity $17.5 \times 10^{-5} \text{m}^2 \text{s}^{-1}$ was added. The step-size Δz is relatively small as the temporal resolution was small, i.e., a large number of harmonics were considered. Nevertheless, an even smaller step-size is required if the previous Riemann sum based numerical scheme was used due to its large error, leading to longer computation times. For the medium property, the speed of sound in the water was 1493 m/s; the nonlinearity coefficient was 3.5; the attenuation coefficient $\alpha/f^2$ was $25 \times 10^{-15} \text{Np/m/Hz}^2$.

Figure 1(left) shows the pressure at the center of the 5mm pre-focal plane. As the nonlinearity involved in this case was very strong, shock waves can be observed in both simulation and experiment even on this pre-focal plane. Figure 1(right) presents the pressure at the focal point. It is noted that experimental result shows a lower pressure especially for the third peak. This is because the hydrophone is band-limited, thus “filtering out” the high frequency component. Nevertheless, in overall, excellent agreement is obtained.

**Figure 1.** (Left) Pressure at the center of the 5mm pre-focal plane. (Right) Pressure at the focal point.

### Conclusions

A wave-vector-frequency-domain nonlinear wave propagation model is studied in this paper. Compared with a previous study, an improved numerical scheme which utilizes the trapezoidal integration is proposed and it yields a significantly higher accuracy. Experimental studies for a therapeutic transducer were carried out which successfully validate the numerical model. Good agreement was found on both pre-focal plane and focal plane.

### REFERENCES


