Noniterative second harmonic ultrasound field simulations: an axisymmetric approach

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Abstract

Nonlinear numerical modeling of finite amplitude acoustic beams has a key role in understanding the effects of nonlinearities and in the design of state-of-art ultrasonic systems. The Khokhlov–Zabolotskaya–Kuznetsov (KZK) equation is the most accurate model describing the combined effects of diffraction, absorption and nonlinearity in ultrasound wave propagation.

KZK solutions usually follow two different approaches: the spectral method and the time domain method; the first one is well suited for periodic ultrasound excitation, while the second is more efficient in propagation of short pulses. As finite difference methods and stepping techniques are usually employed in most realizations, prediction accuracy and computational burden of arbitrary depth ultrasound field simulations are strongly related to the depth itself.

The work described in this report points to develop a model for simulating second harmonic ultrasound fields while featuring equations that can be solved without the use of iterative techniques. By using a proper domain change and dealing with the integration in the axial direction with a proper approximation, robust estimations of nonlinear sound fields are produced for both focused and unfocused axisymmetrical sources.

Predicted fields profiles for nonlinear propagation in water from real transducers will be presented and compared with measurements from water tank experiments.

Introduction

In the early years of clinical application of ultrasound (US) it was believed that non-linear behaviors could be observed only at very high signal power. However, as it was lately discovered while studying contrast agents, the excitation of higher frequencies due to tissues nonlinearities is commonly occurring, even at the signal powers involved in clinical applications.

The principle which leads to the generation of these additional frequency tones is simple. A traveling US beam causes local compression and rarefaction in the material which is traversing in. These slight alterations in density imping the US beam propagation speed, causing the compression part of the pulse to travel relatively faster with respect to the rarefaction part. The distortion of the signal waveform grows over traveling distance and generates the additional harmonics.

Interestingly, these overtones behave a differently than the fundamental: while the latter monothonically decays with depth due to attenuation, the formers start by building with depth up to a peak of maximal intensity before decaying. By using such tones, better axial resolution due to shorter wavelength, better lateral resolution due to improved focusing, and less reverberation artifacts are obtained, usually leading to much cleaner images.

The most widely used equation for describing the combined effect of diffraction, nonlinearity and absorption in directional sound beams is the Khokhlov–Zabolotskaya–Kuznetsov (KZK) equation [1]

$$\frac{\partial^2 p}{\partial z\, \partial \tau} = \frac{c_0}{2}\nabla_\perp^2 p + \frac{\delta}{2c_0^3}\frac{\partial^3 p}{\partial \tau^3} + \frac{\beta}{2\rho_0 c_0^3}\frac{\partial^2 p^2}{\partial \tau^2} \qquad (1)$$

where p is the local overpressure, z the axial distance from the probe, τ the retarded time frame; regarding the parameters, c_0 is the sound speed, δ its diffusivity, β the non-linearity coefficient, and ρ_0 the density, all referred to the material in which propagation occurs.

Two different approaches are usually followed to address this simulation problem: the spectral method [2] and the time domain method [3]. The first describes the US source by means of its Fourier expansion, thus generating a set of coupled equations that can be efficiently solved using a finite difference algorithm. This method is most suited when periodic US excitation is involved as Fourier expansion well captures the information of the signal in a small number of coefficients.

On the contrary, the second involves a technique called operator-splitting which tackle the overall solution by solving adsorption, diffraction and nonlinear propagation independently in the time-domain. This method is usually more efficient in simulating short pulses propagation as long as a high number of Fourier coefficients is required to accurately represent the US pulse.

Both these approaches exploit a discretization scheme to solve the propagation problem along the depth direction. This yield a prediction accuracy and computational burden strongly related to the depth itself for US field simulations at arbitrary depth. Moreover, numerical solutions usually suffer from artifact occurrence in the very near field because of the limited depth step sizes and limited time duration or frequency resolution retained.

Although care must be exercised while simulating near fields because of the parabolic approximation [1] leading to (1), we deem possible to alleviate both these problems by analytically addressing the integration along the depth direction within an appropriate framework.

Model equations

The need of numerical methods first arose to face the difficulties in analytically solving the nonlinear model equation describing US propagation of plane waves. Next, as interest turned toward directional sound beams, it was promptly observed that the presence of an analytical solution is not always granted due to the effect of diffraction in (1).

Following the fact that, when periodic excitations in time domain are to be addressed, the time dependence in KZK equations can be dropped by employing a Fourier series representation, a combined Fourier–Hankel approach can be used to address both the time and radial dependence [4]. In fact, as hinted by the derivation of the Green's function for (1) [5], the Hankel Transform (HT) can be used along with the Fourier Transform (FT) to remove partial differentiations.

In particular, the pressure p can be expressed through its transform q in the Fourier–Hankel domain as

$$p(z, r, \tau) = \mathbb{H}^{-1}_{k,r}\mathbb{F}^{-1}_{\omega,\tau} q(z, k, \omega) \quad (2)$$

where $\mathbb{H}^{-1}_{k,r}$ and $\mathbb{F}^{-1}_{\omega,\tau}$ are operators representing respectively the inverse HT and FT. Then, by exploiting the properties of both operator kernels, it is possible to express each term in (1) as

$$\frac{\partial^2 p}{\partial\tau\partial z} = \mathbb{H}^{-1}_{k,r}\mathbb{F}^{-1}_{\omega,\tau}(j\omega)\frac{\partial q}{\partial z} \quad (3)$$

$$\nabla^2_\perp p = \mathbb{H}^{-1}_{k,r}\mathbb{F}^{-1}_{\omega,\tau}(-k^2)q \quad (4)$$

$$\frac{\partial^3 p}{\partial\tau^3} = \mathbb{H}^{-1}_{k,r}\mathbb{F}^{-1}_{\omega,\tau}(-j\omega^3)q \quad (5)$$

$$\frac{\partial^2 p^2}{\partial\tau^2} = \mathbb{H}^{-1}_{k,r}\mathbb{F}^{-1}_{\omega,\tau}(-\omega^2)f \quad (6)$$

where the dependencies of p, q and f have been dropped for the sake of readability and the auxiliary function f is defined as

$$f = \iiint_D q(z, x, \bar\omega)\, q(z, y, \omega - \bar\omega)\, \mathbb{K}(x, y, k)\, dx\, dy\, d\bar\omega \quad (7)$$

with the integral being calculated on the rectangular domain $D = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}$; finally, according to [6], the term $\mathbb{K}(x, y, k)$ can be evaluated exactly to

$$\mathbb{K}(x, y, k) = \frac{xy}{(2\pi)^{3/2}\Delta_{x,y,k}} \quad (8)$$

if x, y and k are the sides of a triangle of area Δ; otherwise $\mathbb{K}(x, y, k)$ is set to 0.

Plugging back (3) - (6) into (1), the resulting right and left hand side terms are equal for arbitrary r and τ iff

$$\frac{\partial q}{\partial z} = -\frac{\delta\omega^2}{2c_0^3}q - \frac{c_0 k^2}{2j\omega}q + \frac{j\omega\beta}{2\rho_0 c_0^3}f \quad (9)$$

and $q(z, k, 0) = 0$.

In order to solve (9) we propose to start from the solution of the associated homogeneous ODE: by setting $f = 0$ and using the source boundary condition at $z = 0$, the following solution is obtained

$$\begin{aligned} q(z, k, \omega) &= \exp\left(-\left(\frac{\delta\omega^2}{2c_0^3} + \frac{c_0 k^2}{2j\omega}\right) z\right) q(0, k, \omega) \\ &= \mathbb{Q}(z, k, \omega)p_s(k, \omega) \end{aligned} \quad (10)$$

where $p_s(k, \omega)$ is the Hankel-Fourier Transform of the US pulse at the source and, in agreement with [4], $\mathbb{Q}(z, k, \omega)$ is the transform of the Green's function of prescribed ODE problem. The term $p_s(k, \omega)$ can be factorized when dealing with planar, unfocused transducers, as it is possible to separate the pulse frequency content $p_s^{(u)}(\omega)$ from the Hankel transform $t_s(k)$ of the amplitude radial profile of the transducer.

In order to extend these results to the non-linear case we propose to follow a perturbative approach by introducing a local perturbation $\phi(z, k, \omega)$ superimposed to $p_s(k, \omega)$ and redefine $q(z, k, \omega)$ as

$$\tilde q(z, k, \omega) = \mathbb{Q}(z, k, \omega)\big(\phi(z, k, \omega) + p_s(k, \omega)\big) \quad (11)$$

Then, by plugging (11) back into (9) and solving with respect to ϕ, the following result is obtained:

$$\phi(z, k, \omega) = \frac{j\omega\beta}{2\rho_0 c_0^3}\int_0^z \frac{f(\zeta, k, \omega)}{\mathbb{Q}(\zeta, k, \omega)}d\zeta \quad (12)$$

As a consequence, if the perturbation is faint enough, the following approximation of the integral in (12) holds

$$\iiint_D \mathbb{P}_s \int_0^z \frac{\mathbb{Q}(\zeta, x, \bar\omega)\mathbb{Q}(\zeta, y, \omega - \bar\omega)}{\mathbb{Q}(\zeta, k, \omega)} d\zeta\, dx\, dy\, d\bar\omega \quad (13)$$

with

$$\mathbb{P}_s = p_s(x, \bar\omega)\mathbb{K}(x, y, k)p_s(y, \omega - \bar\omega)$$

where the integral in ζ can be evaluated exactly due to the fact that its argument is a combination of exponential functions. Then, by plugging into (11) both (12) and (13), the final result is obtained

$$\tilde q = \mathbb{Q}(z, k, \omega)[p_s(k, \omega) + q_h(0, k, \omega)] - q_h(z, k, \omega) \quad (14)$$

where the function $q_h(z, k, \omega)$ is defined according to (15) with $\alpha(k, \omega)$ being the argument of the exponential function in $\mathbb{Q}$. The function q_h represents the contribute to the US field due to the second harmonic when the source pulse is a pure sinusoidal tone; otherwise, in case of multitone pulses, it describes all the possible contributes due to sum- and difference- frequency generation.

In order to reduce the computational cost required by the numerical evaluation of q_h, some approximation can be applied to (15): first we perform a variable change in order to obtain an integration domain D where $\mathbb{K}(x, y, k)$ evaluates always non-null

$$x \leftarrow \frac{u - v}{2},\ y \leftarrow \frac{u + v}{2} \Rightarrow D \leftarrow [k, +\infty) \times [-k, k] \times \mathbb{R}$$

Also including the variable change Jacobian into $\mathbb{K}$, into the transformed domain this function evaluates to

$$\bar{\mathbb{K}}(u, v, k) = \frac{1}{2}\frac{(2\pi)^{-3/2}(u^2 - v^2)}{\sqrt{u^2 - k^2}\sqrt{k^2 - v^2}} \quad (16)$$

$$q_h(z,k,\omega) = \frac{j\omega\beta}{2\rho_0 c_0^3} \iiint_D \frac{q(z,x,\bar{\omega})\mathbb{K}(x,y,k)q(z,y,\omega-\bar{\omega})}{\alpha(x,\bar{\omega})+\alpha(y,\omega-\bar{\omega})-\alpha(k,\omega)} dx\,dy\,d\bar{\omega} \qquad \alpha(k,\omega) = \frac{\delta\omega^2}{2c_0^3} + \frac{c_0 k^2}{2j\omega} \tag{15}$$

so q_h can be conveniently rewritten as

$$q_h = \frac{1}{2(2\pi)^{3/2}} \int_k^\infty \int_{-k}^k \frac{(u^2-v^2)\Gamma_h(u,v,k,\omega)}{\sqrt{u^2-k^2}\sqrt{k^2-v^2}}\, du\, dv \tag{17}$$

where the function Γ_h collects the terms in q_h other than $\mathbb{K}$. Then, by accepting a certain degree of approximation on the complex argument of Γ_h, one can apply the first mean value theorem for integration to eliminate the integration in v, thus obtaining

$$q_h \simeq \frac{1}{4\sqrt{2\pi}} \int_k^\infty \frac{u^2-v_0^2}{\sqrt{u^2-k^2}}\, \Gamma_h(u,v_0,k,\omega)\, du \tag{18}$$

where v_0 is a properly chosen value in the range $[-k,k]$. Although leading to a slight overestimation, the choice $v_0 = k$ is very useful as it allows, after some algebraic manipulations, to write q_h as the following bidimensional weighted convolution on $\mathbb{R}^2$

$$q_h \simeq \iint q(z,\bar{k},\bar{\omega})\ \mathbb{W}\ q(z,k-\bar{k},\omega-\bar{\omega})\ d\bar{k}\ d\bar{\omega} \tag{19}$$

$$\mathbb{W} = \frac{1}{\sqrt{2\pi}}\ \frac{j\omega\beta}{\rho_0 c_0^3}\ \frac{\sqrt{|\bar{k}|}\sqrt{|k-\bar{k}|}[1-H(\bar{k})H(k-\bar{k})]}{\alpha(\bar{k},\bar{\omega})+\alpha(k-\bar{k},\omega-\bar{\omega})-\alpha(k,\omega)}$$

where $H(x)$ is the Heaviside step function. The weight function $\mathbb{W}$ does not depend on z and can thus be precomputed. Other approximations can be performed on $\mathbb{W}$ in order to further reduce the computational cost at the price of less accuracy on the estimation of q_h.

Propagation algorithm

The algorithm descending from the model equation discussed so far can be summarized in the following steps:

1. Setup radial and temporal sampling grid
2. Precalculate $\alpha(k,\omega)$ and $\mathbb{W}$
3. Compute $p_s(k,\omega)$ using FT and HT
4. Precalculate $q_h(0,k,\omega)$
5. For every desired depth z_i
   (a) Compute $q(z_i,k,\omega)$ using (10)
   (b) Compute $q_h(z_i,k,\omega)$ using (19)
   (c) Compute $\tilde{q}(z_i,k,\omega)$ using (14)
   (d) Compute $p(z_i,r,t)$ using IFT and IHT

The use of fast FT (FFT) and quasi-discrete HT [7] allows to contain the computational cost of steps 3 and 5d while preserving a good accuracy. As a consequence of (19), the total computational cost for a simulation consisting of N_z depth planes and based on a grid of cardinality $N_k \times N_\omega$ is of the order of $N_z N_k^2 N_\omega^2$. Moreover, if a proper factorization of $\mathbb{W}$ can be estimated off-line, equation (19) can be computed by means of bidimensional FFT, thus further improving computational efficiency.

Running this algorithm on a 4 GB, 2.53 GHz Intel® Core™ 2 Duo machine running Matlab™ 7.7.0, took 25.2 s to perform a simulation of a radial focused transducer on a grid consisting of $N_z = 21$ depth steps, $N_k = 201$ radial steps and $N_\omega = 401$ time steps. Remarkably, steps 3 and 5d took only 0.05 s and 0.17 s respectively, while the largest part of computation time is consumed by non-linear effects, which amounts to almost 70% of the total. As a comparison, a KZKTexas run with the same setup on the same machine required 69.3 s.

Experimental validation

In order to validate experimentally the proposed non-linear algorithm some experiments have been conducted in a fresh water tank.

The experimental setup for these measurements consisted of an Agilent 33250A arbitrary function generator driving an EMV 150A250 150 W amplifier powering an Panametrics A392S flat immersion NDT transducer, a Precision Acousitc HPM1/1 1 mm needle hydrophone mounted on a tri-axial positioning system built using two Newport M-IMS600CC and two Newport M-IMS400CC axial drives coordinated by a Newport XPS Motion Controller Unit, and a Dell Pentium® 4 workstation mounting an Acquiris DP308 signal acquisition board and running Matlab™.

Transducer reported diameter is 38.1 mm with a central frequency of 1.0 MHz. For simulation purposes, we described its radial profile by means of the function $(1-(r/r_0)^m)^2$ in the interval $[0, r_0]$, 0 outside, already discussed in [8] with $r_0 = 19.05$ mm and $m = 16$, while water parameters were estimated according to [9] from temperature.

In each experiment the positioning system was setup for scanning a box roughly centered around the transducer axis, with a constant depth step of from slice to slice, comprising large part of the near field. After acquisition, the actual position for the transducer axis inside the scanned region was estimated; then data in each slice were realigned in order to compensate for relative tilting between the transducer and the acquisition system; finally the recorded data were converted to cylindrical coordinates by means of interpolation techniques. Recorded data are then plotted against the results of 3 different US field simulators: the proposed algorithm, the same using (15) in place of (19) and KZKTexas [3].

The function generator was programmed to output a 5 cycle, 1 MHz sinusoidal burst; by adjusting signal amplitude, we set the pressure at the source first at $p_0 \simeq 108$ kPa then at $p_0 \simeq 330$ kPa. During each experiment, 22 slices were acquired, from 1 to 22 cm away from the transducer surface, with a step of 1 cm, roughly covering respectively 1/4 of the Rayleigh distance.

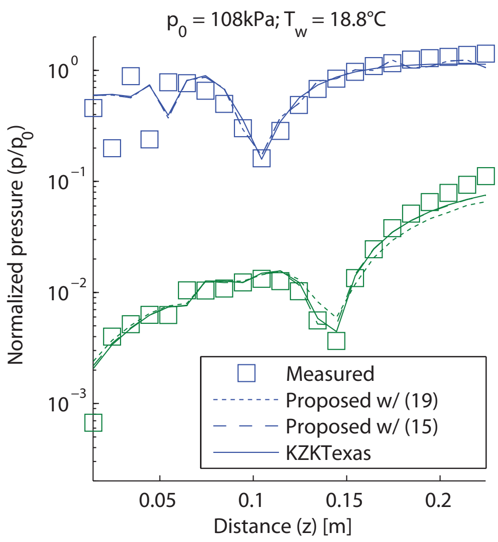

Figure 1: Comparison of recorded and simulated fundamental (top) and second harmonic (bottom) for a 5 cycle, 1 MHz sinusoidal burst during a propagation experiment at 108 kPa as a function of depth.

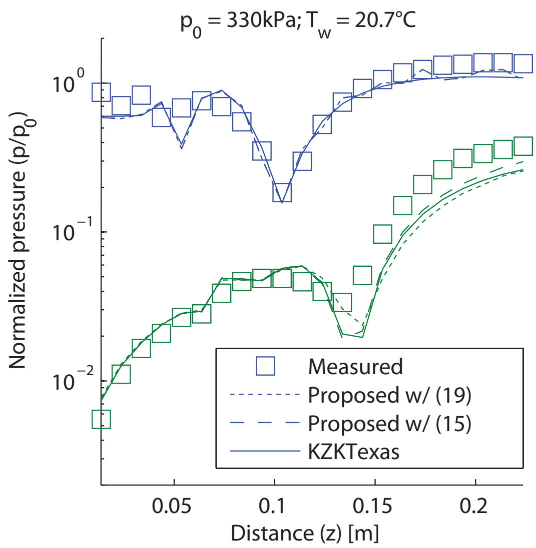

Figure 2: Comparison of recorded and simulated fundamental (top) and second harmonic (bottom) for a 5 cycle, 1 MHz sinusoidal burst during a propagation experiment at 330 kPa as a function of depth.

Results shown in Figure 1 and Figure 2 confirm that the fundamental tone is well reconstructed by each algorithm, producing almost indistinguable results over large part of the inspected field. Moreover, when relying on the exact formula (15), simulations of the harmonic term performed with the proposed algorithm yield a slightly better agreement with measurements. In the case of KZKTexas, improvements are due to the fact that our solution addresses the propagation in the axial direction in an exact way rather then relying on stepping techniques, thus avoiding error accumulation. Conversely, with respect to (19), adherence to the measured curves is better as a full 3D integration is performed instead of a 2D approximation. Finally, it is relavant to observe the computational time required by each algorithm to simulate these experimental setup: KZKTexas simulation lasted over 17.3 min, the exact algorithm required 15.2 min, while the proposed approximation only 1.4 min, yielding a noticeable speed improvement without a significative loss of accuracy.

Conclusions

In this work we presented a non-iterative algorithm, suitable for the simulation of ultrasonic sound fields, based on an approach accurate up to the computation of all first order sum- and difference-frequency components. Robust estimations of the non-linear sound field emitted by axisymmetrical sources were obtained by introducing a perturbative term into the homogeneous solution of the KZK equation in the Fourier–Hankel domain. Simulation obtained with both the exact and a faster, although approximate version of our algorithm were compared with measurements performed in a water tank as well as with another well established algorithm in literature. Comparisons under different source pressures highlight that the proposed equations are capable to produce results in excellent agreement with the measurements without the use of any stepping technique.

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