Modeling of Wave Propagation for Medical Ultrasound: A Review

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***Abstract*—Numerical modeling of medical ultrasound has advanced tremendously in the past two decades. This opens up a great number of opportunities for medical ultrasound and associated technologies. Numerous new governing equations and algorithms have emerged and been applied to studying various medical ultrasound applications, including ultrasound imaging, photo-acoustic imaging, and therapeutic ultrasound. In addition, thanks to the rapid development of computers, modeling acoustic wave propagation in three-dimensional, large-scale domains has become a reality. This article will provide an indepth literature and technical review of recent progress on numerical modeling of medical ultrasound. Future challenges will also be discussed.**

I. Introduction

In the last two decades, we have witnessed a tremendous amount of development of medical ultrasound in both the imaging and therapy communities. The technologies and equipment associated with medical ultrasound are noninvasive, portable, and relatively inexpensive (particularly for imaging) compared with competing technologies. Consequently they are increasingly widely used in clinical applications, such as B-mode and tissue harmonic imaging of parts of the human body, and treatment of uterine fibroids [1] and brain tumors [2]. To improve these applications, it is vital to have a fast, accurate, and versatile ultrasound propagation model. For example, numerical simulations can be utilized to shed light on why tissue harmonic imaging (THI) and super-harmonic imaging (SHI) are superior to conventional B-mode imaging under realistic medical diagnostic conditions. Relevant features of these imaging methods, including the lateral beam shape and axial pulse shape, can conveniently be compared by means of numerical simulations [3]. Results from simulations (such as the optimal transmission frequency) can in turn guide the design of phased arrays so as to achieve optimal imaging performance.

This paper intends to offer an overview on recent developments on numerical modeling of medical ultrasound. A variety of model equations will be first reviewed, including the Westervelt equation and the Khokhlov–Zabolotskaya–Kuznetsov (KZK) equation. The solution methods for these equations will then be discussed. We will first review methods for solving the linear wave equation, followed by methods for solving the nonlinear wave equation. The applications of numerical modeling in transducer design and characterization, ultrasound imaging, and treatment planning will be presented. Finally, we will address future challenges of medical ultrasound modeling. Because the majority of ultrasound approaches only involve longitudinal waves, this review will not include shear wave modeling. The readers are referred to [4]–[6] for information on some existing methods for shear wave modeling.

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II. Model Equations

A. Westervelt Equation

The Westervelt equation recently emerged as a very popular model equation for ultrasound modeling because of its high accuracy. The generalized Westervelt equation reads [7], [8]

$$\rho\nabla\cdot\left(\frac{1}{\rho}\nabla p\right)-\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2}+\frac{\delta}{c^4}\frac{\partial^3 p}{\partial t^3}+\frac{\beta}{\rho c^4}\frac{\partial^2 p^2}{\partial t^2}=0, \quad (1)$$

where p is the sound pressure, c is the speed of sound, δ is the sound diffusivity, β is the coefficient of nonlinearity, and ρ is the ambient density. All parameters can be spatially varying functions. Note that (1) is different from the original Westervelt equation used to study parametric arrays [9], which does not take the medium heterogeneity into account. In (1), the first term takes diffraction into account. The third term accounts for attenuation. The last term introduces the quadratic nonlinearity. Several simplified versions can be derived from (1). For instance, the one-way Westervelt equation with retarded time can be found in [10]. By using constants for all acoustic parameters, the Westervelt equation for homogeneous media can be recovered [11]

$$\nabla^2 p-\frac{1}{{c_0}^2}\frac{\partial^2 p}{\partial t^2}+\frac{\delta_0}{{c_0}^4}\frac{\partial^3 p}{\partial t^3}+\frac{\beta_0}{\rho_0 {c_0}^4}\frac{\partial^2 p^2}{\partial t^2}=0, \quad (2)$$

where c_0, ρ_0, δ_0, and β_0 are the acoustic parameters for the background medium. For axis-symmetrical problems, the Laplace operator can be written in cylindrical coordinates [12]. The linear acoustic wave equation can be derived by setting β_0 to 0, so that

$$\nabla^2 p-\frac{1}{{c_0}^2}\frac{\partial^2 p}{\partial t^2}+\frac{\delta_0}{{c_0}^4}\frac{\partial^3 p}{\partial t^3}=0. \quad (3)$$

We do not intend to devote a separate section to the linear wave equation model [13]. It will be discussed within the Westervelt equation section. Eqs. (2) and (3) are useful for studies on characterizing acoustic fields of transducers and comparing them with experimental data obtained from underwater measurement [14]. They are sometimes also used for approximately estimating the acoustic field in biological tissues [15] which are sometimes considered weakly heterogeneous. Eq. (1) is used when medium heterogeneity must be considered, e.g., studying the propagation of ultrasound beams through the skull [7], [16]. On the other hand, nonlinear equations (1) and (2) must be used when high-pressure ultrasound is present, e.g., lithotripsy [17], histotripsy [18], and tissue harmonic imaging (THI) [19]. Some studies have suggested that using the linear acoustic approximation could underestimate the temperature elevation in tissue [15]. Soneson and Myers examined the problem of determining the thresholds at which nonlinear effects become important [20]. The choice of using the nonlinear or linear wave equation also depends on the available computational resources. In general, solving the nonlinear wave equation calls for considerably more refined spatial and temporal resolutions because the presence of higher harmonics, especially when high-pressure wave fields are simulated, as in the context of high-intensity focused ultrasound (HIFU).

The Westervelt equation can be considered as a simplification of the Kuznetsov equation (see Section II-C) [21]. It is considered an appropriate approximation when local effects can be ignored, which is generally true when the propagation distance is much greater than a wavelength or sound beams are highly directional (e.g., quasi-plane waves) [22]. A recent study suggested that the Westervelt equation is accurate even for highly focused transducers (aperture angle at 80°) [23]. All in all, there seems to be a general consensus that the Westervelt equation is not only suitable for numerical modeling but could also provide very accurate solutions to acoustic wave propagation for problems of interest in the medical ultrasound community. The suitability of the Westervelt equation for numerical modeling, however, still depends on the available computational and implementation resources.

One variation of (1)–(3) occurs when considering arbitrary frequency-dependent absorption laws and dispersion. Although it is straightforward to consider these two phenomena in the frequency domain, it is intrinsically difficult in the time domain. Eqs. (1) and (2) only consider the thermoviscous absorption, in which $\delta_0 = 2\alpha_0 {c_0}^3/\omega^2$ (α_0 is the absorption coefficient and ω is the angular frequency) and therefore the absorption is proportional to frequency squared. Dispersion is also not accounted for. To consider absorption following arbitrary power laws and dispersion due to thermal relaxation in tissue, a variety of approaches have been proposed [8], [24]–[29]. For example, Szabo derived a causal convolution operator that accounts for both power law absorption and dispersion [26]. This approach was later verified numerically [30] and modified by Chen and Holm [25]. Ochmann and Makarov used fractional derivative to account for the power law absorption [31]. Kelly and McGough proposed a hierarchical fractal network model to describe the power law absorption [28]. Treeby and Cox used a fractional Laplacian to model power law absorption and dispersion [24]. An alternative wave equation for homogeneous media was derived and reads

$$\nabla^2 p - \frac{1}{{c_0}^2}\frac{\partial^2 p}{\partial t^2} + \left\{\tau_0 \frac{\partial}{\partial t}(-\nabla^2)^{y/2} + \eta_0(-\nabla^2)^{(y+1)/2}\right\} p + \frac{\beta_0}{\rho_0 {c_0}^4}\frac{\partial^2 p^2}{\partial t^2} = 0, \tag{4}$$

where τ_0 and μ_0 are two proportionality coefficients and y is the power law exponent. This term yields a dispersion relation of the form

$$\tilde{k}^2 = \frac{\omega^2}{c_0^2} + \frac{2i\alpha_0\omega^{y+1}}{c_0} + \frac{2\alpha_0 \tan(\pi y/2)\omega^{y+1}}{c_0}, \tag{5}$$

where $\tilde{k}$ is the complex wave number. Note that (4) is slightly different from [24, Eq. (28)], where the nonlinearity is not considered. For a more detailed summary of time-domain approaches for absorption modeling, readers are referred to [24].

B. Khokhlov–Zabolotskaya–Kuznetsov (KZK) Equation

Although the numerical ultrasound community has gradually gravitated toward the Westervelt equation in recent years, the KZK equation has been the most widely used equation because it is the simplest model which includes diffraction, absorption, and nonlinear effects. The KZK equation accounting for energy losses was first published in 1971 [32] and there has been a tremendous amount of numerical investigation since then. The KZK equation can be viewed as the parabolic approximation of the Westervelt equation, and therefore it is less accurate in the near field and at a position off the main axis. In other words, wide-angled or steered beams [33] cannot be accurately modeled by the KZK equation. For a focused transducer, the KZK equation is in theory valid for waves traveling within 15° to 16° of the nominal axis of the beam (typically is the z-axis) [34], [35]. This is roughly equivalent to an f-number >1.5. In practice, however, it was found that the KZK equation can be relatively accurate in the frequency domain for f-number at 1.0 (about 25° off the nominal axis) [36]. The parabolic form of the wave equation can be solved with efficient numerical techniques, which is the main advantage of the KZK equation. The KZK equation is an equation of evolution type and has the first-order derivative with respect to the propagation main axis, and it therefore inherently describes one-way wave propagation.

The KZK equation for homogeneous, thermoviscous media can be written as [22]

$$\frac{\partial^2 p}{\partial z \partial t'} - \frac{c_0}{2}\nabla_\perp^2 p - \frac{\delta_0}{2{c_0}^3}\frac{\partial^3 p}{\partial t'^3} - \frac{\beta_0}{2\rho_0 {c_0}^3}\frac{\partial^2 p^2}{\partial t'^2} = 0, \quad (6)$$

where t' is the retarded time ($t' = t - z/c_0$), and $\nabla_\perp^2 = (\partial^2/\partial x^2) + (\partial^2/\partial y^2)$ is the transverse Laplacian. In cylindrical coordinates, the transverse Laplacian is $\nabla_\perp^2 = (\partial^2/\partial r^2) + (1/r)(\partial/\partial r)$ [37]. By dropping $\nabla_\perp^2$ (i.e., diffraction), the KZK equation reduces to the Burgers equation. Eq. (6), however, is rarely directly solved. Other forms of the KZK equation exist. For instance, by integrating both sides of (6) with regard to time and taking arbitrary absorption and dispersion into account, we arrive at an extended KZK equation [38]

$$\begin{aligned}\frac{\partial p}{\partial z} &= \frac{c_0}{2}\int_{-\infty}^{t'} \nabla_\perp^2 p \,\mathrm{d}t'' + \frac{\delta_0}{2{c_0}^3}\frac{\partial^2 p}{\partial \tau^2} + \frac{\beta_0 p}{\rho_0 {c_0}^3}\frac{\partial^2 p}{\partial t'} \\ &\quad + \sum_v \frac{c_v'}{c_0^2}\int_{-\infty}^{t'} \frac{\partial^2 p}{\partial t''^2} e^{-(t'-t'')/t_v} \mathrm{d}t'',\end{aligned} \quad (7)$$

where t_v is the relaxation time and c_v is the small-signal speed of sound increment for each relaxation process v ($v = 1, 2, \ldots$). Eq. (6) can be transformed into nondimensional form for simplification. For example, in Cartesian coordinates, (7) can be transformed into

$$\begin{aligned}\frac{\partial P}{\partial \sigma} &= \frac{1}{4}\int_{-\infty}^{\tau}\left(\frac{1}{G_x}\frac{\partial^2 P}{\partial X^2} + \frac{1}{G_y}\frac{\partial^2 P}{\partial Y^2}\right)\mathrm{d}\tau' + A\frac{\partial^2 P}{\partial \tau^2} + NP\frac{\partial P}{\partial \tau} \\ &\quad + \sum_v D_v \int_{-\infty}^{\tau} \frac{\partial^2 p}{\partial \tau'^2} e^{-(\tau-\tau')/\theta_v} \mathrm{d}\tau',\end{aligned} \quad (8)$$

for rectangular transducers [38], where

$$\begin{aligned}&P = p/p_0, \quad \tau = \omega_0 t', \quad X = x/a, \quad Y = y/b, \quad \sigma = z/d, \\ &G_x = k_0 a^2/2d, \quad G_y = k_0 b^2/2d, \quad N = d/\overline{z}, \\ &A = \alpha_0 d, \quad D_v = k_0 d c_v'/c_0, \quad \theta_v = \omega_0 t_v.\end{aligned}$$

p_0 is a characteristic pressure, ω_0 is a characteristic angular frequency, a and b are the characteristic lengths in the x- and y-directions, d is a characteristic length in the propagation direction, $k_0 = \omega_0/c_0$, $\overline{z}$ is the plane wave shock formation distance [$= 1/(\beta\varepsilon k)$, where ε is the peak particle velocity Mach number], and α_0 is the thermoviscous absorption coefficient at the characteristic frequency. The dimensionless KZK equation in cylindrical coordinates can be found in [37] and [39], which is useful for axis-symmetrical problems, e.g., acoustic fields of circular apertures. Augmented KZK equations for heterogeneous media were derived by Jing and Cleveland [40] and Varslot and Taraldsen [41]. The KZK equation was validated by comparing it to the Westervelt equation both numerically and experimentally [12]. The error introduced by the parabolic approximation was examined in [34], [42], and [43]. It was found that, for small f-numbers (f-number = 1.5), the lateral beam-plot could exhibit 2 to 3 dB errors.

C. Other Equations

Although the Westervelt and KZK equation are the two most widely used equations for medical ultrasound modeling, other model equations also exist and will be briefly reviewed here. The Kuznetsov equation, which is considered to be a more accurate equation than the Westervelt equation for nondirectional beams and in the near field, can be written as [32]

$$\begin{aligned}&\frac{\partial^2 \phi}{\partial t^2} - {c_0}^2 \nabla^2 \phi \\ &\quad = \frac{\partial}{\partial t}\left[\frac{1}{\rho_0}\left(\mu_\mathrm{B} + \frac{4}{3}\mu\right)\nabla^2\phi + (\nabla\phi)^2 + \frac{\beta - 1}{{c_0}^2}\left(\frac{\partial \phi}{\partial t}\right)^2\right],\end{aligned} \quad (9)$$

where ϕ is the velocity potential, μ_B is the coefficient of bulk viscosity, and μ is the coefficient of shear viscosity. There is a direct relation between the diffusivity and the two coefficients [22]. Roughly on the same order of accuracy, an equation in terms of the acoustic pressure yields

$$\begin{aligned}&\nabla^2 p - \frac{1}{{c_0}^2}\frac{\partial^2 p}{\partial t^2} + \frac{\delta_0}{{c_0}^4}\frac{\partial^3 p}{\partial t^3} + \frac{\beta_0}{\rho_0 {c_0}^4}\frac{\partial^2 p^2}{\partial t^2} \\ &\quad + \left(\nabla^2 + \frac{1}{c_0^2}\frac{\partial^2}{\partial t^2}\right)L = 0,\end{aligned} \quad (10)$$

where L is the Lagrangian density of acoustical energy [22], [23]. By dropping L, (10) reduces to the Westervelt equation. Note that for plane progressive waves, L is exactly equal to zero. Directly solving (9) or (10) is extremely challenging and they have not been shown to be considerably more accurate than the Westervelt equation for medical ultrasound problems; therefore, they are rarely used in the medical ultrasound community. However, under the weakly nonlinear assumption, numerical studies using (9) and (10) were carried out. For example, the lossless, perturbed Kuznetsov's equations were solved by the finite element method and the solutions were compared with those of the KZK equation [42]. Eq. (10) under the weakly nonlinear assumption was solved by the angular spectrum approach and was compared with the Westervelt equation for focused transducers [23]. It was found that the Westervelt equation is accurate even for highly focused transducers (aperture angle at 80°).

Another model equation is the spheroidal beam equation (SBE) [44]–[46]. Similar to the KZK equation, SBE is also a parabolic equation. It is, however, more suitable for focused transducers because of the use of the oblate spheroidal coordinates. In addition, linear and nonlinear acoustic simulations showed that the SBE equation is more accurate than the KZK equation for focused transducers and is valid for an aperture half-angle up to 40° [44]. It should be pointed out that the SBE contains two different equations: one for the spherical wave region and the other for the focus region.

Furthermore, Kamakura *et al.* derived a wide-angle one-way wave equation using the split-step Padé approximation [47]. It was shown to be valid for an aperture half-angle up to 40°. Treeby *et al.* [48] and Tabei *et al.* [49] studied first-order wave equations and solved them using the k-space method. One advantage of using first-order wave equations is that a perfectly matched layer (PML) can be more easily incorporated [49], [50]. A PML is an artificial absorbing layer that is commonly used to minimize reflection from artificial boundaries of the computational domain. The first-order wave equations are particularly suited to being solved by time-domain methods, such as the finite-difference time-domain (FDTD) method [51]. The nonlinear first-order wave equations read

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} &= -\frac{1}{\rho}\nabla p, \\ \frac{\partial \rho'}{\partial t} &= -(2\rho' + \rho)\nabla \cdot \mathbf{u}, \\ p &= c^2\left(\rho' + \frac{B}{2A}\frac{\rho'^2}{\rho} - \hat{\mathbf{L}}\rho'\right), \end{aligned} \tag{11}$$

where $\mathbf{u}$ is the velocity vector, ρ' is the acoustic density, B/A is the nonlinearity parameter, and $\hat{\mathbf{L}}$ is a power-law absorption operator. For linear acoustics, it is sufficient to only consider two coupled equations (pressure-velocity formulation) [50]. An asymptotic model that extends parabolic approximation for acoustic fields of strongly focusing transducers was developed in [52].

Finally, although it is typically sufficient to consider only the quadratic nonlinearity term, it was argued that for some applications (e.g., extra-corporeal shock wave lithotripsy) for which the pressure is extremely high (>100 MPa), cubic nonlinearity should also be taken into account. Wave equations with higher orders can be found in [53]–[56].

III. Solution Methods

This section will review solution methods for solving the aforementioned linear wave equations, Westervelt equation, and KZK equation. Because analytical solutions only exist for few circumstances [42], [57]–[59], the focus of this section is purely numerical methods for two- and three-dimensional wave propagation. We will emphasize the methods used in the medical ultrasound community. There are some different developments in other areas, such as room acoustics and geophysics, but they will not be discussed in this paper. A recent review of this topic (solution methods) can be also found in [60].

A. Linear Wave Equation

Among the three equations, the linear wave equation [e.g., (3)] is the easiest to solve because the nonlinearity term vanishes. For the linear wave equation in homogeneous media, several approaches are available for time-harmonic solutions, including the Rayleigh–Sommerfeld integral [59], [61], fast near-field method (FNM) [62]–[64], and angular spectrum approach (ASA) [65]–[68]. Although the first approach is rather time consuming, particularly in the near field, the second approach specifically addresses this problem by using one-dimensional integrals. In particular, FNM removes the singularity in the integrand, resulting in a smooth integral which is evaluated using quadrature methods with spectral accuracy. The ASA is emerging as a widely used approach in medical ultrasound modeling because of its high accuracy and efficiency because it utilizes the 2-D fast Fourier transform (FFT). In this approach, computing the acoustic field on a desired plane from a known plane requires only a single operation. For circularly symmetrical problems, the 2-D Fourier transform can be reduced to the Hankel transform [69], although it is still not as efficient as the 1-D FFT. The errors of ASA resulting from discrete Fourier transform (DFT) and discretization as well as spatial aliasing are discussed in [70] and [71]. The spatial aliasing can be overcome by using the so-called "spatial propagator" as opposed to the "spectral propagator." Alternatively, this error can be reduced by using an absorption layer [72]. Attenuation can be conveniently accounted for by considering a complex wave number [73]. Most recently, Koskela *et al.* [74] introduced a novel stochastic ray-tracing method to predict the HIFU fields. They verified the model using experiments on *ex vivo* tissue.

For transient solutions, the spatial impulse response approach [75], [76] and ASA [69], [77] have been used. Although the spatial impulse response approach excels in computing the acoustic field at an arbitrary point, the ASA is more suited when the acoustic field on a certain plane is desired. The ASA is also capable of backward propagating the acoustic field: if the field on a plane away from the source is known, the field on another plane closer to the source can be extrapolated [65], [78]. Although the Rayleigh–Sommerfeld integral and spatial impulse response approaches can be applied to nonplanar/focused transducers, the ASA is more often used for planar transducers and the focusing can be achieved assuming phased arrays. Nevertheless, there have been some recent developments that extend the ASA to curved transducers [79], [80]. For example, in a hybrid method, the Rayleigh–Sommerfeld integral can be used first to calculate the acoustic field on a certain plane (an acoustic hologram), and then the ASA method can be used to calculate the field on any plane parallel to that initial plane. The inclusion of attenuation and dispersion in these two approaches was discussed in [11], [81]. Because ASA employs a frequency-domain formulation, it allows straightforward implementations of general dispersions [11].

For heterogeneous media, different approaches are typically required for solving the wave equation [e.g., (1) without the nonlinearity term]. One exception is layered structures with weak contrast, where the ASA method can still be conveniently used [68], [82] with reasonable accuracy. A very recent paper developed a new, hybrid ASA method to deal with linear, heterogeneous media, although only up to the first-order reflections were considered [83]. The three most commonly used approaches for solving the heterogeneous media wave equation in the medical ultrasound community are the FDTD method [84]–[87], pseudo-spectral time-domain method (PSTD) [88]–[95], and k-space time-domain (KSTD) method [49], [96]–[102], although they can also be used to study wave propagation in homogenous media [51]. Although FDTD uses finite difference to approximate the spatial derivative in the wave equation, the other two spectral approaches use the Fourier transform to compute the spatial derivative and are considerably more accurate with low numerical dispersion errors (not to be confused with the true physical dispersion caused by the acoustic media). It must be emphasized that this is only the case when spectral methods are used to approximate smooth functions. When used to approximate fields with steep gradients or discontinuities (such as shocked fields as well as some source functions), they could be less efficient than low-order methods. In general, the most commonly used FDTD scheme (fourth order in space and second order in time) requires 8 to 10 grid points per wavelength to achieve reasonably accurate results, whereas the other two approaches theoretically only need 2 grid points per wavelength for smooth fields [100]. The k-space method is considered more accurate or efficient than the pseudo-spectral method because it uses a semi-analytical time-stepping scheme [96], whereas the pseudo-spectral method uses finite-difference approximation. Consequently, the k-space method allows for a larger time step and is less time-consuming [100]. Both of these two spectral methods have the so-called wrap-around problem, because the use of FFT implies that the acoustic field is periodic. The PML or absorption layer can be used to minimize this artifact [7], [49]. One drawback of the spectral methods is that their errors grow as the contrast (heterogeneity) becomes greater [100]. This is, however, not a significant concern for problems encountered in medical ultrasound because the contrast is in general relatively small.

All three approaches can be applied to either the second-order wave equation or the first-order wave equations. When applied to the first-order wave equations, it is common to use staggered grids [49] for better accuracy. When applied to the second-order wave equation and when heterogeneity of the density exists, it is common to define a normalized wave field $f = p/\sqrt{\rho}$ to remove the first-order derivative term in the wave equation [100]. For instance, (1), without the nonlinearity term, can be transformed into

$$\nabla^2 f - \frac{1}{{c_0}^2}\frac{\partial^2 f}{\partial t^2} = f\sqrt{\rho}\nabla^2\frac{1}{\sqrt{\rho}} + \frac{1}{c_0^2}\left(\frac{c_0^2}{c^2} - 1\right)\frac{\partial^2 f}{\partial t^2} - \frac{\delta}{c^4}\frac{\partial^3 f}{\partial t^3}. \tag{12}$$

The transformed equation with the nonlinearity term can be found in [7]. In some problems, a hybrid approach seems to be more efficient. For instance, Qiao *et al.* [103] used the Rayleigh–Sommerfeld integral first to compute the field on the posterior surface of the rib cage. The k-space was then used to estimate the field through the rib cage. In the last step, the ASA was used to simulate the field behind the rib. Finally, finite-difference frequency-domain methods and finite element methods (FEM) also exist [104], [105] but are not frequently used for medical ultrasound modeling.

B. Westervelt and KZK Equations

For homogeneous media, currently existing approaches for solving the nonlinear wave equation often use an operator-splitting scheme. In this scheme, the effects of diffraction, nonlinearity, and attenuation are computed separately using specialized numerical algorithms. Because these three effects are in fact interdependent, the operator-splitting scheme will inevitably introduce errors. However, these errors are reasonably small as long as small steps are taken [106]. Cleveland *et al.* [39, Appendix B] showed that as the step size approaches zero, the splitting scheme exactly solves the original equation. Christopher and Parker used a scheme equivalent to a first-order operator-splitting scheme for nonlinear wave modeling [107]. Tavakkoli *et al.* applied a second-order operator-splitting (Strang splitting) scheme which allows for a larger step size [108] and has been widely used thereafter. Some mixed time-domain/frequency-domain methods use the operator splitting and FFT to take advantage of frequency-domain linear methods and superior time-domain nonlinear methods [106]. This section intends to focus on methods for solving the diffraction and nonlinearity. For the absorption, briefly, it can be solved either in the frequency domain [109] or the time domain [37].

For the diffraction part, the solution methods used for solving the linear acoustic wave equation can be used. For instance, Tavakkoli *et al.* [108] and Khokhlova *et al.* [109] used the Rayleigh integral for solving the full diffraction field. Christopher and Parker used an exact formulation based on the Kirchhoff–Helmholtz integral to model full diffraction from axisymmetric transducers [107]. Zemp *et al.* used the ASA and addressed the sampling and aliasing issues [106]. It was found to be more computationally efficient than the Rayleigh integral. Similarly, Yuldashev and Khokhlova made use of the ASA for solving the diffraction term in the Westervelt equation [10]. Spatial filtering and artificial absorption were used to minimize numerical errors. They studied the acoustic field from a multi-element high-intensity focused ultrasound (HIFU) transducer. Berntsen, Lee, and Hamilton used an implicit backward difference method in the near field and the Crank-Nicolson method beyond the near field for solving the diffraction term in the KZK equation [37], [110]. Their algorithm targets axisymmetric problems. This finite-difference approach was later adopted in [111], [112] for studying focused transducers and was improved by using the alternating direction implicit method and extended to non-axisymmetric problems [38], [113]. Very recently, Hasani *et al.* further improved the accuracy of this finite-difference method using a five-point scheme [114].

For the nonlinearity part, solution methods can be divided into two groups: time-domain methods and frequency-domain methods. In general, frequency-domain methods are more suited to problems with weak nonlinearity, whereas time-domain methods are advantageous for strongly nonlinear waves. This is because the computation time approximately increases as M^2 (where M is the number of harmonics) for the frequency-domain methods. On the other hand, the computation time is proportional to M for time-domain methods [37].

The first exclusively frequency-domain method was developed by Aanonsen *et al.* [115]. This method and its modified version were popular in the 1980s [116], [117] and 1990s [118]. In this approach, a Fourier series expansion of the pressure is substituted into the KZK equation and the resulting system of equations is solved using an implicit backward difference scheme. Later, Christopher and Parker used the frequency-domain solution to the Burgers' equation to account for nonlinearity [107]. Khokhlova *et al.* developed a frequency-domain method that uses the fourth-order Runge–Kutta method [109]. To reduce the computational burden, the number of harmonics included in the solution gradually grew as the propagation distance increased. In their paper, the frequency-domain method was also compared with a time-domain method for its accuracy. An asymptotic spectral algorithm that enables modeling strongly nonlinear waves with shock fronts using a few number of harmonics (~30) was developed and used to study both plane wave propagation [119] and enhanced thermal effects in focused beams [120].

Time-domain methods were first introduced by Lee and Hamilton [37]. Implicit analytical solution (the Poisson solution) was used to solve for the nonlinear term [108], [121]. Varslot and Taraldsen used the method of characteristics to solve the nonlinearity term [41]. To achieve good results, 10 to 15 samples per wavelength at the highest harmonic frequency were needed. To model highly nonlinear shock waves in the time domain, Pinton and Trahey investigated the validity of Godunov's method and the monotonic up wind scheme [17]. It was found that they are significantly more efficient than the implicit solution-based method. Yuldashev and Khokhlova used a hybrid method to model nonlinearity [10]. The frequency-domain method was used in the near field and the Godunov-type method [122] was used when the steepness of the wave profile exceeded a certain quantity.

Other approaches not using the splitting scheme are also reviewed here for completeness. Hallaj and his coworkers performed FDTD on the Westervelt equation using cylindrical coordinates [15], [123]. Doinikov *et al.* implemented three-dimensional FDTD and compared numerical results with experimental data from a phased array [124]. Other demonstrations of FDTD for solving the full nonlinear wave equation can be found in [12], [125], and [126]. A modified ASA was introduced by Jing *et al.* to solve the Westervelt equation [11]. Similar to the ASA for solving the linear wave equation, this approach is capable of backward projection, which could extrapolate fields very close to the source plane (i.e., transient nonlinear acoustical holography) [127]. A recent paper proposed two improved stepping schemes for the modified ASA, which were shown to be considerably more efficient and accurate [128]. Under weakly nonlinear conditions, the modified ASA can be simplified to allow an arbitrary step size for rapid field estimation [129]. Huijssen and Verweij developed an iterative nonlinear contrast source (INCS) method for solving the Westervelt equation [130]. They treated the nonlinear term as a contrast source and used a filtered convolution method to minimize the computation [131]. When strong contrast sources are present (e.g., strong and inhomogeneous attenuation), the nonlinear contrast source can be linearized to resolve the convergence problem [132]. This approach relies on the four-dimensional Fourier transform and therefore could require a large memory size for large-scale problems. Unlike many other approaches which assume the main nonlinear distortion is in the direction normal to the transducer surface [41], [106], both methods (modified ASA and INCS methods) are free of any assumed wave-field directionality [11], [130]. This is considered more accurate, particularly for highly focused transducers and steered beams. Other researchers have used FEMs, although they are in general computationally less efficient [42], [133], [134].

Several numerical methods have been used to solve the nonlinear wave equation for heterogeneous media. For example, Pinton *et al.* implemented a FDTD algorithm that accounts for nonlinearity, heterogeneity, and frequency-dependent attenuation [8]. They used the algorithm to study ultrasound pulse propagating through a human abdominal wall. Jing *et al.* developed a k-space method based on the Westervelt equation [7]. They showed that the k-space method is superior to the FDTD method because it requires fewer grid points per wavelength. Only thermoviscous absorption was considered, however. Treeby *et al.* [48] developed the k-space method based on the first-order nonlinear wave equation [i.e., (11)]. Treeby later improved this k-space method for strongly nonlinear problems by using nonuniform grids [135]. One-dimensional problems were demonstrated to validate the algorithm. The INCS method is intrinsically suited to modeling heterogeneous media [131], [136]. For example, Demi *et al.* studied nonlinear wave propagation in media with spatially inhomogeneous attenuation [137]. Varray *et al.* [138] extended the ASA to modeling inhomogeneous nonlinearity coefficient and used their algorithm to generate B-mode images [139]. Jing and Cleveland derived a modified KZK equation for heterogeneous media [40]. They dealt with the spatial variation in the sound speed and nonlinearity using the Poisson solution. The term that accounts for the density fluctuations was solved using a first-order finite difference scheme. Varslot and Taraldsen used an implicit Euler scheme to find the numerical solution for both the diffraction and the scattering [41]. The methods of both

Jing and Cleveland [40] and Varslot and Taraldsen [41] assume one-way propagation, and therefore ignore the high-order scattering. Albin *et al.* [140] solved the nonlinear acoustics Navier–Stokes equations using the Fourier continuation (FC) method. An array of rigid cylinders were considered as scatterers and the FC method was found to be highly efficient.

To close this section, a table (Table I) is provided to summarize and recap a selected group of modern ultrasound modeling algorithms. Studies comparing different algorithms can be found in [141]–[143]. Although it is difficult to assess exactly the computational load of each algorithm because they are highly problem-dependent, in general, spectral, one-way models are more computationally efficient than finite-difference or finite-element-based, full-wave models.

IV. Applications

Numerical modeling of medical ultrasound has a wide range of applications for both ultrasound imaging and therapeutic ultrasound. This section discusses its applications in four main categories.

A. Transducer Design

Numerical modeling greatly facilitates transducer design. A series of iterative modeling steps can be performed to obtain the optimal transducer design and shed light on how a certain variable (e.g., frequency, focal length, etc.) affects the acoustic field. For example, Al-Bataineh *et al.* [147] used the k-space method to design transducer arrays for prostate cancer treatment. The design was validated by using MRI thermometry. Pajek and Hynynen [148] designed semi-spherical arrays for stroke treatment using numerical simulations. It was found that extremely high powers are needed to achieve inertial cavitation transcranially above 1 MHz. Zeng *et al.* [149] utilized a waveform-diversity-based approach for optimizing three-dimensional power depositions generated by ultrasound phased arrays. Heat volume within the tumor was increased with simultaneously decreased normal tissue heating. Baron *et al.* [150] used the FDTD method to study intracranial acoustic fields in clinical trials of sonothrombolysis. Their model has proven useful for transducer design for sonothrombolysis. They concluded that the hemorrhages observed in the TRUMBI study are possibly due to standing waves formed in the brain at a low frequency. Newer therapeutic applications such as histotripsy that rely on very high pressure levels and the presence of shock fronts at the focus require transducers specifically designed for these applications. Recently a method to determine parameters of transducers to achieve shock formation regimes and certain shock amplitudes at the focus was developed based on the multi-parametric modeling of the KZK equation [151]. Other studies on this topic can be found in [152]–[158].

B. Transducer Acoustic Field Characterization

Exact knowledge of the acoustic field including side lobes and focal dimensions of the field produced by a transducer is critically important in evaluating its efficacy and safety. Accurate measurement of the four-dimensional field (x, y, z, and time t) could be challenging and unrealistically time consuming particularly at high frequencies. For highly nonlinear fields, the hydrophone could also be easily damaged by cavitation. Numerical modeling has been used as an important adjunct for transducer characterization. In this case, a numerical model including both a governing wave equation and a boundary condition that corresponds to a certain ultrasound transducer will be used. Setting a realistic boundary condition to the Westervelt or KZK models is an important and nontrivial problem for obtaining a correct solution that corresponds to the experiment. Acoustic holography or back-projection method has been developed and validated for single-element transducers operating in both continuous wave (CW) [159] and transient [160] cases and for transducer arrays [14] to obtain realistic distribution of vibrational velocity or acoustic pressure at the transducer surface. Clement and Hynynen [65] used the ASA to implement forward and backward projection and to characterize phased array transducers. For nonlinear fields, Jing and coworkers [127], [128] demonstrated that a transient nonlinear acoustical holography could be used to characterize HIFU transducers. This type of approach has been recognized to be the most accurate, and the IEC standard for characterizing high-intensity fields includes a normative annex on acoustic holography (back-projection) methods [161]. Simpler methods of varying parameters of a boundary condition, typically, the aperture and acoustic pressure of a single-element source, to match experimentally measured beam scans on the axis and in the focal plane, can be also used. It has been shown that the KZK equation with the boundary condition set in this way provides accurate results for nonlinear pressure fields in the focal region of the beam for transducers with up 80° focusing angle [36]. Similar approaches were adopted by Bessonova and Wilkens [162] and Chen *et al.* [163] to examine focused transducers. Chen *et al.*, however, chose the SBE as the governing equation. A method of setting a boundary condition by direct measurement of acoustic field close to the source has been used to characterize the field of a clinical shockwave therapy device [164].

KZK equation for wave propagation in water written in dimensionless form contains only two parameters that are combinations of the transducer and propagation medium parameters. For practical applications, besides developing new codes, already existing data of multi-parametric modeling of the KZK equation for a focused piston source can be useful for evaluation of the degree of nonlinear effects and corresponding outputs for quasilinear propagation condition, shock formation, and saturation regimes in water [145]. Again, the parameters of the equivalent sin-

TABLE I. A Summary of Modern Ultrasound Modeling Algorithms.

Authors	Governing equation	Solution method	Remarks
Christopher and Parker [68]	Linear wave equation, axisymmetric	ASA	Hankel transform was used. Valid for homogeneous/layered media with frequency dependent attenuation.
Christopher and Parker [107]*	Equivalent to the Westervelt equation, axisymmetric	Operator-splitting	A follow-up paper to [68]. Used ASA for the diffraction and solved the nonlinear part in the frequency domain.
Lee and Hamilton [37]*	KZK equation, axisymmetric	Operator-splitting	Solved the diffraction using finite-difference schemes and nonlinear part in the time domain. Valid for thermoviscous, homogenous media.
Cleveland *et al.* [39]*	KZK equation, axisymmetric	Operator-splitting	A follow-up paper to [37]. A time-domain relaxation algorithm was demonstrated.
Tavakkoli *et al.* [108]*	KZK equation, axisymmetric	Operator-splitting	First paper that used a second-order operator-splitting scheme in nonlinear wave modeling. Valid for homogeneous media with frequency-dependent absorption and dispersion.
Liu [89]+	Linearized, coupled first-order acoustic equations	PSTD	Valid for linear, heterogeneous, dispersionless media.
Hallaj and Cleveland [15]*	Westervelt equation	FDTD	Valid for thermoviscous, homogeneous media.
Yuan *et al.* [51]†	Linearized, coupled first-order acoustic equations	FDTD	Valid for linear, heterogeneous media with relaxation dominated attenuation.
Kamakura *et al.* [44]*	SBE	Frequency-domain, finite difference	Valid for thermoviscous, homogeneous media. Considered geometrically focused transducers.
Mast *et al.* [100]†	Linear wave equation	KSTD	Valid for heterogeneous media. Nonlinearity and absorption were not considered.
Khokhlova *et al.* [109], Filonenko and Khokhlova [144]*	KZK equation, axisymmetric	Operator-splitting	Solves both diffraction and nonlinear part in the frequency domain, variable number of harmonics and spatial windows to optimize modeling shock wave propagation; power law of absorption with dispersion in [144].
Tabei *et al.* [49]†	Linearized, coupled first-order acoustic equations	KSTD	Valid for heterogeneous media with relaxation absorption. Nonlinearity was not considered.
Clement and Hynynen [82]	Linear wave equation	ASA	Valid for homogeneous/layered media with frequency-dependent attenuation and dispersion.
Zemp *et al.* [106]*	Equivalent to the Westervelt equation	Operator-splitting	An extension of [107]. Solved the diffraction using ASA and nonlinear part in the frequency domain. Attenuation is combined with the nonlinear substep. Valid for homogeneous media with frequency-dependent attenuation.
Varslot and Taraldsen [41]*	Modified KZK and Westervelt equations	Operator-splitting	Solved the diffraction using either a finite difference scheme or a pseudo-differential model. The nonlinear part was solved using the method of characteristics. Power-law absorption was considered. Heterogeneities were considered but multiple scatterings were not taken into account.
Khokhlova *et al.* [113]*	KZK equation, 3-D	Operator-splitting	Solves nonlinear part in the time domain; diffraction, absorption, and dispersion part in the frequency domain; power law of absorption with dispersion for short pulses.
Canney *et al.* [36], Bessonova *et al.* [145]*	KZK equation, axisymmetric	Operator-splitting	Combined frequency and time domain for the nonlinear term, Godunov-type algorithm is used for modeling shock wave propagation; boundary condition set based on measurement in [36].
Huijssen and Verweij [130]*†	Westervelt equation	INCS	Valid for heterogeneous media with frequency-dependent absorption and dispersion.
Yuldashev and Khokhlova [10], Kreider *et al.* [14]*	Westervelt equation	Operator-splitting	Diffraction in k-space and frequency domain; nonlinear term both in frequency and time domains; Godunov-type algorithm for modeling shock wave propagation; boundary condition obtained from acoustic holography measurements in [14].
Jing *et al.* [128], [146]*	Westervelt equation	Modified ASA	Valid for homogeneous media with arbitrary absorption and dispersion.
Treeby *et al.* [48] and Jing *et al.* [7]*†	Westervelt equation [7] or coupled nonlinear wave equations [48]	KSTD	Both valid for heterogeneous media. Jing *et al.* [7] only considered thermoviscous media, whereas Treeby *et al.* [48] considered power law absorption.

*The corresponding method models nonlinear wave propagation.
†The corresponding method is a full-wave method: no parabolic approximation; considers multiple scattering.

gle-element source for the KZK model can be determined by matching beam scans measured at low power level to the linear solution of the KZK equation. More relevant literature on transducer characterization can be found in [10], [14], [160], [165], and [166].

C. Ultrasound Imaging

Numerical modeling helps researchers better understand the limitation of ultrasound imaging and validate or improve methodologies [167]–[175]. It also facilitates

TABLE II. A Summary of Currently Existing Open-Source Software for Ultrasound Modeling.

Software	Nonlinearity	Heterogeneity	GPU support
Field II [211]	No	No	No
FOCUS [62]	KZK-based	Layered structures	No
Abersim [212]	Westervelt/KZK-based	Random phase layer	No
KZK Texas/Bergen code [37], [110]	KZK-based	No	No
K-WAVE [199]	Westervelt-based	Arbitrary heterogeneity	Yes
HIFU simulator [213]	KZK-based	Layered structures	No
CREANUIS [139]	Westervelt-based	Inhomogeneous nonlinearity coefficients	Yes

imaging approaches such as full waveform tomography (FWT) and photo-acoustic tomography (PAT). For example, Li and Zagzebski [176], Treeby *et al.* [177] investigated B-mode and tissue harmonic imaging using numerically acquired pulse echoes. Pinton *et al.* [19] used an FDTD algorithm to study sources of image degradation in fundamental and harmonic ultrasound imaging. Van Neer *et al.* [3] numerically studied and compared fundamental, second-harmonic, and super-harmonic echocardiography at their optimal transmission frequencies. Several paper studied the phase aberration in tissue and discussed its effect on imaging [86], [178], [179]. In FWT, ultrasound modeling plays an indispensable role. FWT is an iterative approach for generating quantitative images of sound speed and attenuation. Each iteration involves at least two full wave propagation problems (forward and backward propagation). FWT is emerging as a powerful imaging approach and has been recently applied to breast imaging [180]–[182]. Another area that heavily utilizes ultrasound modeling is PAT, particularly when the time-reversal approach is adopted. Treeby *et al.* [183] used the k-space method and demonstrated how received photo-acoustic signals can be numerically back-propagated to generate PAT images in absorptive media. Treeby and other researchers have followed along this line and applied PAT to areas such as brain imaging [184]–[186]. In PAT, linear acoustics is typically assumed because of the low pressure involved.

D. Treatment Planning

High-intensity therapeutic ultrasound (HITU) treatment planning relies on numerical modeling to predict the pressure distribution and temperature elevation in a patient's body. In return, it provides guidance on the needed phase delays and "dose" for the treatment and optimizes the outcome of the therapy. In general, a patient's CT or MRI images are used as input for the numerical modeling. Treatment planning is especially important for brain therapy (e.g., treating essential tremor, stoke, brain tumor, etc.), because the phase distortion caused by the skull must be compensated. Clement and Hynynen [187] used a modified ASA to estimate the required phased delay on each element to focus ultrasound beams through skulls. CT images of the skulls are used as the input to provide the density and speed of sound. This approach has been successfully applied to clinical studies [2]. Aubry *et al.* [188] and Jing *et al.* [189] used time-domain, full scattering methods to estimate the phase delay. Although more time consuming than the ASA method, their approaches could be more accurate in the megahertz range. A similar topic is transcostal beam focusing and relevant studies can be found in [103], [190]. Solovchuk *et al.* [191] studied the importance of nonlinear wave propagation on treatment planning. They found that the temperature rise can be strongly enhanced by nonlinear waves. Wu *et al.* [192] developed an integrated tool for HIFU treatment planning that includes ultrasound simulation and interactive visualization. For other research on this topic, the readers are referred to [16], [193]–[196]. It is worth mentioning that, ultrasound modeling models will only perform as well as they are trusted to produce reliable outcomes. This trust should be understood by evaluating uncertainties that could affect the algorithms. Sinden and ter Haar discussed three types of uncertainties in treatment planning and their impact [197]: errors in segmentation of images and acoustic and thermal parameters of tissue, image registration errors, and artifacts due to organ motion and deformation. Vaughan and Hynynen specifically looked at the effects of parameter errors (speed of sound and CT data errors) in the simulation of transcranial focused ultrasound [198]. It was found that the predicted pressure can change by a few percent because of the parameter errors they considered.

V. Discussion and Conclusion

There has been a tremendous amount of development in medical ultrasound modeling over the past twenty years. In addition, there is a trend of making ultrasound modeling algorithms freely available by the developers. Seven types of popular open-source software on medical ultrasound modeling are listed in Table II, although in fact there are more than seven types of software packages available in the public domain. The open-source software packages have generated a strong, positive impact and moved medical ultrasound forward. For instance, the K-WAVE software [199] (based on the k-space method), released in 2010, was quickly adopted by the medical ultrasound community and used widely to study PAT and ultrasound imaging [184]–[186], [200]. While being optimistic overall, we must point out that several challenges still exist for ultrasound modeling. Computational speed is still a concern even though current computers are much more powerful than twenty years ago and modeling algorithms have been improved. This is particularly a problem for shock wave modeling (e.g., histotripsy and boiling histotripsy), which calls for both extremely fine spatial and temporal resolutions. There are some methods that could help reduce the temporal resolution, such as the Godunov's method [10], Gagenbauer reconstructions [201], and a modified spectral method [119]. Nevertheless, there are no efficient ways to deal with the discontinuity in the spatial domain caused by shock waves. Even for linear wave modeling, a dramatic speed-up could be beneficial. For example, real-time or quasi-real-time treatment planning could reduce both the waiting time for the patients and the cost [189]. The most efficient approaches (ASA or k-space) used in medical ultrasound still require at least 2 grid points per smallest wavelength simulated. An algorithm that breaks this limit while remaining accurate could be a breakthrough. The ultra-weak variational formulation (UWVF) seems to meet this requirement [202]. This approach, however, could have stability problems and has not been widely used. Other than further improving modeling algorithms, researchers have also investigated the use of parallel computing [101], [104] and graphic processing units (GPUs) [7], [177], [199], [203]–[206] for faster modeling. For example, almost one order of magnitude speed-up using a single GPUs was reported in [7]. As a final remark, realistic modeling of ultrasound interacting with biological tissue is always desired, but may be quite challenging because of the complex nature of the *in vivo* environment. In addition, when cavitation and/or boiling occurs, the widely varying stochastic nature of cavitation strongly limits the applicability of existing computer models to treatment planning scenarios. Articles addressing these problems are scarce [207]–[209], and clearly more extensive studies are warranted. For example, the wave equation could be coupled with the acoustic streaming hydrodynamic equations or bubble dynamics equations to study their effects on tissue heating [210].

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