Mathematics of Nonlinear Acoustics: Modeling - Analysis - Numerics - Inverse Problems

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Abstract

High intensity (focused) ultrasound HIFU is used in numerous medical and industrial applications ranging from litotripsy and thermotherapy via ultrasound cleaning and welding to sonochemistry. We will highlight some mathematical and computational aspects related to the relevant nonlinear acoustic phenomena, namely

- modeling of high intensity ultrasound phenomena as second and higher order wave equations
- some parameter asymptotics
- absorbing boundary conditions for the treatment of open domain problems
- optimal shape design
- imaging with nonlinear waves

The contents is based on joint work with Vanja Nikolić, Gunther Peichl, William Rundell, Igor Shevchenko, and Mechthild Thalhammer.

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1 Models of nonlinear acoustics

Our work on partial differential equations (PDEs) modeling nonlinear acoustic wave propagation is motivated by numerous applications of high intensity focused ultrasound ranging from lithotripsy and thermotherapy via welding and sonochemistry to ultrasound cleaning.

The following brief derivation of the fundamental acoustic equations closely follows the review [14]. More details can be found, e.g, in [9, 10].

The main physical quantities involved in the description of sound propagation are

- the acoustic particle velocity $\vec{v}$;
- the acoustic pressure p;
- the mass density ϱ;

that can be decomposed into their constant mean and a fluctuating part

$$\vec{v} = \vec{v}_0 + \vec{v}_\sim\,, \quad p = p_0 + p_\sim\,, \quad \varrho = \varrho_0 + \varrho_\sim,$$

where $\vec{v}_0 = 0$ in the absence of a flow.

These quantities are interrelated to each other by the following physical balance and material laws:

- the Navier Stokes equation (balance of momentum) which under the assumption $\nabla\times\vec{v} = 0$ reads
$$\varrho\Big(\vec{v}_t + \nabla|\vec{v}|^2\Big) + \nabla p = \Big(\frac{4\mu_V}{3} + \zeta_V\Big)\triangle\vec{v}\,, \tag{1}$$
where ζ_V is the bulk viscosity and μ_V the shear viscosity;
- the equation of continuity (balance of mass)
$$\nabla\cdot(\varrho\vec{v}) = -\varrho_t\,; \tag{2}$$
- the equation of state relating the acoustic pressure and density fluctuations $p_\sim$ and $\varrho_\sim$:
$$\varrho_\sim = \frac{p_\sim}{c^2} - \frac{1}{\varrho_0 c^4}\frac{B}{2A}p_\sim^2 - \frac{\varkappa}{\varrho_0 c^4}\Big(\frac{1}{c_V} - \frac{1}{c_p}\Big)p_{\sim t}\,, \tag{3}$$
where B/A is the parameter of nonlinearity, $\varkappa$ the adiabatic exponent, and c_p, c_V the specific heat capacitance at constant pressure and constant volume, respectively.

Analogously to the derivation of the linear wave equation from the linearized versions of these equations, we proceed by subtracting the divergence of (1) from the time derivative of (2) to eliminate the linear velocity term, and inserting the state equation to eliminate the mass density. In the resulting second order in time PDE, we may neglect higher order terms, according to a certain hierarchy, which in nonlinear acoustics is known as Blackstock's scheme [2, 27] and distinguishes between the following categories:

- *First order.* These are linear with respect to the fluctuating quantities and are not related to any dissipative effect;
- *Second order.* Terms of this order are obtained as the union of quadratic and dissipative linear terms (that is, those terms that contain the viscosities as pre-factors);
- *Higher order.* All remaining terms.

Blackstock's scheme therefore prescribes that one should retain only first and second order terms. Additionally, a result called the *substitution corollary* allows us to replace any quantity in a second or higher order term by its first order approximation.

This yields Kuznetsov's equation [25, 26]

$$\begin{aligned} &p_{\sim tt} - c^2\triangle p_\sim - b\triangle p_{\sim t} \\ &= \left(\frac{1}{\varrho_0 c^2}\frac{B}{2A}p_\sim^2 + \varrho_0|\vec{v}|^2\right)_{tt} \end{aligned} \tag{4}$$

where b is the diffusivity of sound, $b = \frac{1}{\varrho_0}\left(\frac{4\mu_V}{3} + \zeta_V\right) + \frac{\varkappa}{\varrho_0}\left(\frac{1}{c_V} - \frac{1}{c_p}\right)$ and we have related the velocity to the pressure via the linearization of (1),

$$\varrho_0\vec{v}_t = -\nabla p_\sim\,, \tag{5}$$

which together with the substitution corollary allowed us to replace $c^2\nabla\cdot\triangle\vec{v} = \nabla\cdot\vec{v}_{tt} = -\frac{1}{\varrho_0}\triangle p_{\sim t}$; moreover, again using the substitution corollary we set $\rho_0 c^2\triangle|\vec{v}|^2 = \rho_0|\vec{v}|^2_{tt}$, $\frac{\varkappa}{\varrho_0 c^2}p_{\sim ttt} = \frac{\varkappa}{\varrho_0}\triangle p_{\sim t}$.

If we ignore local nonlinear effects modeled by the quadratic velocity term, thus approximating $\rho_0|\vec{v}|^2_{tt} \approx \frac{1}{\rho_0^2 c^2}p^2_{tt}$, we arrive at the Westervelt equation

$$p_{\sim tt} - c^2\triangle p_\sim - b\triangle p_{\sim t} = \frac{\beta_a}{\varrho_0 c^2}p^2_{\sim tt} \tag{6}$$

with $\beta_a = 1 + B/(2A)$, cf., [33]. Under the already made assumption $\nabla\times\vec{v} = 0$ on a simply connected domain there exists an acoustic velocity potential ψ with $\vec{v} = -\nabla\psi$, whose constant part by (5) can be chosen such that

$$\varrho_0\psi_t = p\,. \tag{7}$$

Hence both equations (4) and (6) can as well be written in terms of the acoustic velocity potential ψ

$$\begin{aligned} &\psi_{tt} - c^2\triangle\psi - b\triangle\psi_t \\ &= \frac{1}{c^2}\Big(\beta_a(\psi_t)^2 + s_{\mathrm{WK}}\left[c^2|\nabla\psi|^2 - (\psi_t)^2\right]\Big)_t \end{aligned} \tag{8}$$

with $s_{\mathrm{WK}} = 0$ for (6) and $s_{\mathrm{WK}} = 1$ for (4).

Further simplifications of the model lead to the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation [35]

$$2cp_{\sim xt} - c^2\triangle_{yz}p_\sim - \frac{b}{c^2}p_{\sim ttt} = -\frac{\beta_a}{\varrho_0 c^2}p^2_{\sim tt} \tag{9}$$

(with the coordiate system possibly rotated so that x is the direction of sound propagation and Δ_{yz} the Laplace operator with respect to the coordinates orthogonal to the propagation direction) and the well-known Burgers' equation in one space dimension, [5].

On the other hand, taking into account interdependenc of further quantities such as entropy, heat flux and temperature, we arrive at higher order models of nonlinear acoustics, such as the Blackstock-Crighton equation [2, 4, 9]

$$\begin{aligned} &(\partial_t - a\Delta)\left(\psi_{tt} - c^2\Delta\psi - b\Delta\psi_t\right) - r\Delta\psi_t \\ &= -\left(\frac{B}{2Ac^2}(\psi_t^2) + |\nabla\psi|^2\right)_{tt} \end{aligned} \tag{10}$$

where $a = \frac{\nu}{\mathrm{Pr}}$ is the thermal conductivity or the Jordan-Moore-Gibson-Thompson equation JMGT [8, 12, 13, 31]

$$\begin{aligned} &\tau\psi_{ttt} + \psi_{tt} - c^2\Delta\psi - b\Delta\psi_t \\ &= -\left(\frac{B}{2Ac^2}(\psi_t)^2 + |\nabla\psi|^2\right)_t \end{aligned} \tag{11}$$

where τ is the relaxation time, that allows to counteract the infinite speed of propagation paradoxon arising in (4) and (6). Also replacement of the strong damping term $b\Delta\psi_t$ by fractional order derivatives leads to refinements of the model, such as, e.g., the fractional JMGT equation

$$\begin{aligned} &\tau^\alpha D_t^{2+\alpha}\psi + \psi_{tt} - c^2\Delta\psi - (\delta + \tau^\alpha c^2)\Delta D_t^\alpha\psi \\ &= \left(\frac{B}{2Ac^2}(\psi_t)^2 + |\nabla\psi|^2\right)_t \end{aligned} \tag{12}$$

or Kuznetsov's equation with Caputo-Wismer Kelvin damping

$$\begin{aligned} &\psi_{tt} - c^2\Delta\psi - \delta\Delta D_t^\alpha\psi \\ &= \left(\frac{B}{2Ac^2}(\psi_t)^2 + |\nabla\psi|^2\right)_t \end{aligned}$$

taking into account power law frequency dependence of the attenuation.

Challenges in the analysis of these models arise from the fact that they exhibit potential degeneracy or equivalently nonlinear state dependence of the wave speed. Let us illustrate this by means of the Westervelt equation (with u denoting the pressure)

$$u_{tt}-c^2\Delta u-b\Delta u_t = -\tfrac{k}{2}(u^2)_{tt} = -ku\, u_{tt}-k(u_t)^2$$

that is,

$$(1+ku)u_{tt} - c^2\Delta u - b\Delta u_t = -k(u_t)^2$$

This reveals the fact that degeneracy occurs for $u \leq -\frac{1}{k}$ and similar considerations hold for the other equations mentioned above (Kuznetsov, JMGT, Blackstock-Crighton). The equation above also illustrates state dependence of the effective wave speed, since we can rewrite it as

$$u_{tt} - \tilde{c}^2\Delta u - \tilde{b}(u)\Delta u_t = f(u)$$

with $\tilde{c}(u) = \frac{c}{\sqrt{1+ku}}$, $\tilde{b}(u) = \frac{b}{1+ku}$, $f(u) = \frac{k(u_t)^2}{1+ku}$ as long as $1+ku > 0$ – otherwise the model loses its validity.

2 Singular limits

We are interested in the question whether some of the above models can be recovered as limits of others as certain parameters tend to zero. Examples of such singular limits are vanishing thermal conductivity $a \searrow 0$ in the Blackstock-Crighton equation (10) or vanishing relaxation time $\tau \searrow 0$ in the JMGT equation (11). In both cases the formal limit is obviously Kuznetsov's equation (4). Mathematically, this leads to the question in which function spaces the limits of ψ^a and ψ^τ exist and at which rate convergence occurs. Interestingly, but also intuitively, this requires a compatibility condition on the initial data in case of (10), while this is not needed for (11), where the highest order time derivative term vanishes as in the limiting case, which is not the case for (10). Further examples are the limit as $\alpha \nearrow 1$ in (12) with limit equation (11), where the leading derivative order in the PDE changes with α; the limit as $\delta \searrow 0$ in (6) or (4), which leads to a change of the qualitative behaviour from global in time well-posedness to potential blow up in finite time.

Details on this can be found, e.g., in [3, 15–19, 24]

3 Absorbing boundary conditions

Whenever a physical acoustic domain is truncated for computational purposes, appropriate

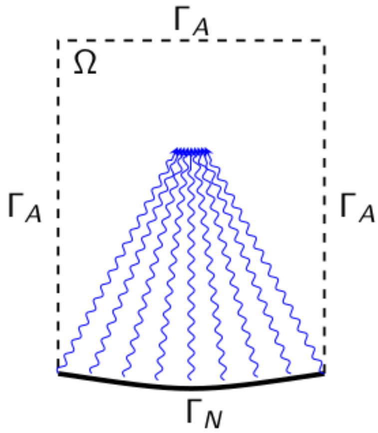

Figure 1: Computational setup with absorbing boundary Γ_A

boundary conditions have to be imposed in order to avoid spurious reflections at the artificial boundary, see, e.g., Fig. 1 for a typical computational setup in the simulation of ultrasound waves focused by an array of piezoelectric transducers. The vast majority of approaches for this purpose fall under one of the two categories of perfactly matched layers PML or absorbing boundary conditions ABC. We here focus on the latter paradigm. The derivation of ABCs is based on (formal) pseudodifferential calculus to approximately factorize the wave differential operator, which for this purpose has to be linearized for any of the above models. In case of the Westervelt equation in two space dimensions, this leads to the following zero and first order conditions

$$\begin{aligned} u_n &= -\tfrac{1}{c}\sqrt{1+ku}\, u_t \\ u_{n\,tt} &= -\tfrac{1}{c}\sqrt{1+ku}\, u_{ttt} + \tfrac{1}{2c}\sqrt{1+ku}u_{\vartheta\vartheta t} \\ &\quad + \tfrac{kc}{4\sqrt{1+ku}}\big(u_t - \tfrac{1}{\frac{1}{c}\sqrt{1+ku}}u_n\big)u_{tt} \\ &\quad - \tfrac{kc}{4\sqrt{1+ku}^3}\big((\tfrac{1}{2}u_t + \tfrac{c}{\sqrt{1+ku}}u_n\big)u_{\vartheta\vartheta} \end{aligned}$$

on $\partial\Omega$, where n is the normal and θ the tangential direction. An analysis of the damping properties of the resulting boundary conditions can be carried out by means of energy estimates. Details and computational results can be found in [23, 30].

4 Optimization problems related to ultrasound focusing

The task of focusing the nonlinearly propagating waves in HIFU leads to PDEe constrained optimization problems. As an example, consider

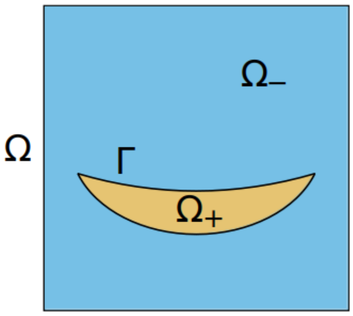

Figure 2: Schematic of an acoustic lens

shape optimization of an acoustic lens, see Fig. 2 Taking into account acoustic-acoustic coupling between lens and fluid domain, as well as power law damping $D(\nabla u_t) = b(1+\delta|\nabla u_t|^{q-1})\nabla u_t$, this leads to the problem

$$\min_{\substack{\Omega_+\in\mathcal{O}_{\rm ad}\\ u\in L^2(\Omega\times[0,T])}} \int_0^T \int_\Omega (u-u_{\rm d})^2\,dx\,ds$$

subject to

$$\begin{cases} \frac{1+ku}{\lambda}u_{tt} - \mathrm{div}(\frac{1}{\varrho}\nabla u) - \mathrm{div}(D(\nabla u_t)) \\ \qquad\qquad = -\frac{k}{\lambda}(u_t)^2 \quad \text{in } \Omega_+\cup\Omega_- \\ [[u]] = 0 \quad \text{on } \Gamma = \partial\Omega_+ \\ \left[\left[\frac{1}{\varrho}\frac{\partial u}{\partial n_+} + D(\nabla u_t)\cdot n_+\right]\right] = 0 \quad \text{on } \Gamma = \partial\Omega_+ \\ u = 0 \quad \text{on } \partial\Omega \\ (u,u_t)|_{t=0} = (u_0,u_1) \end{cases}$$

where $[[\cdot]]$ denotes the jump over the interface, $\mathcal{O}_{\rm ad}$ is a set of admissible domains and the coefficients λ, ϱ, b, k take different values in the two subdomains, that is, $\lambda = \begin{cases}\lambda_+ \text{ in } \Omega_+ \\ \lambda_- \text{ in } \Omega_-\end{cases}$, etc. Using the method of mappings, one can define domain deformations that allow to compute a shape derivative in (a) strong and (b) weak form, respectively; that is, as a functional (a) concentrated on the interface Γ, or (b) distributed over the domain Ω. Based on this, gradient descent methods for computing improved shapes can be derived. For details we point to [20, 28].

5 Imaging with nonlinear ultrasound waves

We finally dwell on recent work on nonlinearity parameter imaging [1,6,7,11,29,32,36,37], which leads to the inverse problem of identifying the space-dependent coefficient $k(x)$ in Westervelt equation

$$\begin{aligned} &\left(u+k(x)u^2\right)_{tt} - c_0^2\Delta u - \delta\Delta D_t^\alpha u = r \\ &\qquad\qquad\qquad \text{in } \Omega\times(0,T) \\ &u = 0 \text{ on } \partial\Omega\times(0,T), \\ &u(0)=0, \quad u_t(0)=0 \quad \text{in } \Omega \end{aligned}$$

(with excitation r) from boundary observations

$$g = u \quad \text{on } \Sigma\times(0,T),$$

where $\Sigma\subset\overline{\Omega}$ represents the receiving transducer array. Challenges in this problem result form the fact that the model equation is nonlinear, with the nonlinearity occuring in the highest order term. The unknown coefficient $k(x)$ actually appears in this nonlinear term. Moreover, $k(x)$ is spatially varying whereas the data $g(t)$ is in the "orthogonal" time direction. This is well known to lead to severe ill-conditioning of the inverse problem. In [21, 22], we carry out investigations on the degree of this ill-posedeness as well as its dependence on the fractional order $\alpha\in[0,1]$ of attenuation. Moreover, a uniqueness result for the linearized problem (see also [34]) as well as some preliminary reconstruction results based on Newton's method are provided.

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